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A hydrological model for root zone water storage simulation on a global scale

Ganquan Mao[1] and Junguo Liu[1]

[1]School of Environmental Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, China

Correspondence: Junguo Liu (junguo.liu@gmail.com, liujg@sustc.edu.cn)

Abstract. The soil water stored in the root zone is a critical variable for many applications as it plays a key role in several hydrological and atmospheric processes. Many studies have been done to obtain reliable soil water information in the root zone layer. However, most of them are mainly focused on the soil moisture in a certain depth rather than the water stored in the entire rooting system. In this work, a hydrological model is developed to simulate the root zone water storage (RZWS) on a global scale. The model is based on a well validated lumped model and has been extended now to a distribution model. To reflect the natural spatial heterogeneity of the plant rooting system across the world, a key variable that influencing the RZWS, i.e. root zone storage capacity (RZSC), is integrated into the model. The newly developed model is evaluated on runoff and RZWS simulation across ten major basins. The evaluation of runoff indicates the strong capacity of the model for monthly simulation with a good performance on time series and distribution depiction. Results also show the ability of the model for RZWS dynamics mimicing in most of the regions. This model may offer benefits for many applications due to its ability for RZWS simulation. However, attentions need to also be paid for application as the high latitude regions are not investigated by this work due to the incomplete latitudinal coverage of the RZSC. Therefore, the performance of the model in such regions is not justified.

1 Introduction

Soil moisture is one of the critical variables in earth system dynamics (Sheffield and Wood, 2008) and is claimed an Essential Climate Variable by the World Meteorological Organization due to its key role played in several hydrologic and atmospheric processes (Legates et al., 2011). The soil water stored in the plant root zone is of great importance in some fields of application, e.g. agriculture, as it represents the reservoir of the plant available water and mediates numerous sub-surface processes (Sabater et al., 2007; Wang et al., 2015; Cleverly et al., 2016). A fundamental limiting factor that constrains crop yields is the water resources in root zone (Tobin et al., 2017). The water stored in root zone is also directly linked with one of the importance water resources for ecosystems, i.e. green water resources, as the green water is defined as the water originates from precipitation that stored in the unsaturated soil and eventually consumed by plants through evapotranspiration (Falkenmark and Rockström, 2006; Liu and Yang, 2010).

There are several methods for soil moisture estimation including situ measurements, satellite-based approaches and model simulation (Paulik et al., 2014; Dumedah et al., 2015; Colliander et al., 2017; Zhang et al., 2017; Berg et al., 2017). Especially in recent years, a variety of specific sensors and systems have been built for soil moisture measuring globally, e.g. the Advanced Microwave Sounding Radiometer for Earth Observation System (AMSR-E) and the AMSR-2 (Njoku et al., 2003), the Soil Moisture Ocean Salinity (SMOS) (Kerr et al., 2010), Soil Moisture Active Passive (SMAP) mission (Entekhabi et al., 2010). These sensors are able to provide continuous estimations of soil moisture worldwide.

Obtaining reliable root zone water storage is still challenging, as it cannot be directly observed (González-Zamora et al., 2016). Satellite remote sensing itself can only detect the soil water at surface layer (in most of cases with a depth of 5 cm) and has the shortcoming to look into the deep soil profile (Petropoulos et al., 2015). A lot of effort has been done recently by researchers to retrieve root zone soil moisture (RZSM), a variable that is very close to the RZWS. Tobin et al. (2017) developed an exponential filter to leverage the remote sensed surface soil moisture to produce RZSM. Faridani et al. (2017) and Baldwin et al. (2017) applied a soil moisture analytical relationship (SMAR) model to generate RZSM where the surface soil moisture is the input. Apart from remote sensing based approaches, hydrological models and land surface models are important tools for moisture simulation as they work both in the past and future (Xia et al., 2014; Sheikh et al., 2009; Albergel et al., 2018; Samaniego et al., 2018). Additionally, many studies estimate the RZSM by combining remotely sensed soil moisture with different models using data assimilation techniques (Rebel et al., 2012; Renzullo et al., 2014a, b). However, all these studies estimated the root zone soil moisture until a certain depth, e.g. 100 cm, thus still hold the drawbacks to accurately calculate the water stored in the entire root zone layer. Since the rooting depth is location dependent and could reach an depth of more than 30 meters (Fan et al., 2017).

Alternatively, RZSM can also be obtained by investigating and applying the relationship between RZSM and different vegetation indices derived from MODIS or Landsat satellites, e.g. the Normalized Difference Vegetation Index (NDVI) and the Enhanced Vegetation Index (EVI) (Santos et al., 2014; Wang et al., 2007; Schnur et al., 2010; Liu et al., 2012). Nevertheless, their work either stick at a certain soil depth assuming the consistent rooting depth or estimates only the water content ratio assuming the homogeneous soil profile rather than the water amount covering the entire spatial heterogeneous rooting system (Fan et al., 2017). So far, studies that directly focus on the root zone water storage are still rare.

Recently, Sriwongsitanon et al. (2016) investigated the relation between root zone water storage and Normalized Difference Infrared Index and found a promising correspondence between them, especially in the dry seasons, where water stress exists. However, the NDII is an index value that reflects only the dynamics of RZWS rather than the absolute value. Moreover, remote sensing based approaches only allow us for the historical analysis. While the ability for predicting the RZWS, usually hold by models, is still missing, which is crucial for impact studies, e.g. agricultural drought analysis (Keyantash and Dracup, 2002). But the work of Sriwongsitanon et al. (2016) provided enlightenments for future RZWS related studies, as their findings support NDII to be a potential proxy for RZWS. This is critical for mitigating the major challenge, i.e. there is no direct observation of root zone water storage for evaluation, in the field of hydrological modelling.

In this study, a global hydrological model is developed to simulate root zone water storage, a key variable for eco-hydrological studies. Though many of global hydrological models (GHMs) have already been developed and most of the them are similar in

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general hydrological components simulation (Sood and Smakhtin, 2015), the developed model has its unique scheme for root zone processes depiction, thus it allows for RZWS simulation with the ability for considering the global spatial heterogeneous rooting system. The model has the similar input requirements to most of the existing GHMs and can also generate general hydrological variables in addition to the RZWS. Since it simulates the RZWS which is of great importance for both hydrology and ecology, and will be further developed in the future for water and ecosystem related applications. The newly developed model is named as Water And ecosYstem Simulator (WAYS). The ultimate goal of this study is to test the feasibility of WAYS for RZWS simulation on a global scale, an added-value feature useful for many applications.

2 Model Description

2.1 General Overview

WAYS is a hydrological model implementation in Python. It is a process-based model that assums water balance at grid cell level. The development of WAYS is based on a lumped conceptual model with an HBV-like model structure, called the FLEX model (Fenicia et al., 2011; Gao et al., 2014a). The FLEX model has been widely used and validated at the basin scale to simulate the soil moisture content and root zone water storage (Gao et al., 2014b; Nijzink et al., 2016; de Boer-Euser et al., 2016; Sriwongsitanon et al., 2016). Benefit from its flexible modelling framework, we have now extended it to a spatially distributed global hydrological model. In addition, some improvements are made to increase the model capacity at global scale, e.g. more sophisticated soil water storage capacity strategy and supports of more land cover.

WAYS is a raster-based model that calculates the water balance and simulates the hydrological processes in a fully distributed way. It works on a daily time step and the model structure consists of five conceptual reservoirs: the snow reservoir S_w (mm) representing the surface snow storage, the interception reservoir S_i (mm) expressing the intercepted water in canopy, the root zone reservoir S_r (mm) describing the root zone water storage in the unsaturated soil, the fast response reservoir S_f (mm), and the slow response reservoir S_s (mm). Two lag functions are applied to describe the lag time from storm to peak flow (T_{lagF}) and the lag time of recharge from the root zone to the groundwater (T_{lagS}). In addition to the water balance equation, each reservoir has also process functions to connect the fluxes entering or leaving the storage compartment (so-called constitutive functions). Fig. 1 provides a schematic representation of how the vertical water balance is modelled in WAYS and the basic equations are shown in Table 1. The parameters that regulates the different simulation steps are described below, and the changes we made to the original FLEX model are highlighted. The original lumped model FLEX has 28 parameters in total that considers four land use types in the basin (Gao et al., 2014a). In order to reduce the computation cost of calibration and avoid the over-fitting issues at global scale, some calibrated parameters are replaced by the empirical values from literatures, e.g. the snow melt ratio F_{DD}, the capacity of interception reservoir $S_{i,max}$, the groundwater recharge factor f_s and the maximum value for groundwater recharge $R_{s,max}$.

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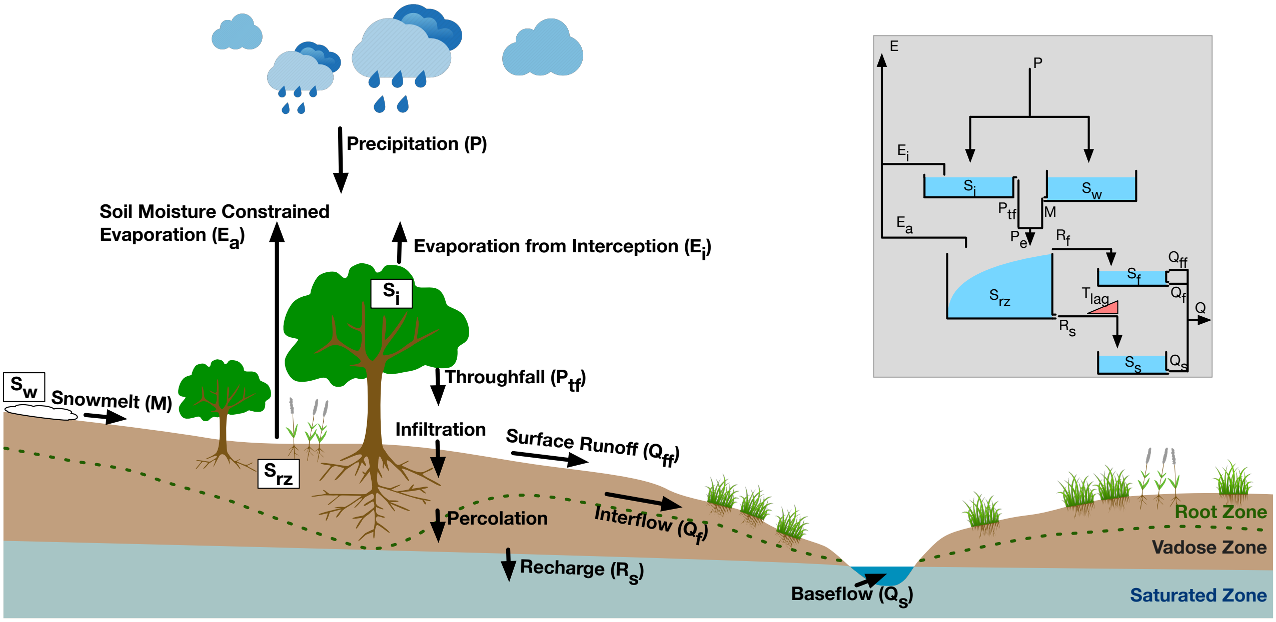

Figure 1. Model structure of the WAYS

2.2 Interception and Snow Routine

In WAYS model, the precipitation is allowed to be intercepted by canopy or stored as snow before enter into the root zone reservoir.

Interception happens during the rain days when the temperature above the threshold temperature T_t. Interception reservoir stores the intercepted precipitation by canopy before it reaches the soil and will directly evaporated back into the atmosphere. The canopy water balance equation is shown in Eq. (1). Where the precipitation P (mm/day) is the inflow and the precipitation throughfall P_{tf} (mm/day) and the interception evaporation E_i (mm/day) are the outflows. The calculation of precipitation throughfall P_{tf} is simply based on comparing the rainfall P_r (mm/day) to the water already stored in the interception reservoir S_i (mm) and the capacity of interception reservoir $S_{i,max}$ (mm) (Eq. (2)). In FLEX model, the interception evaporation E_i is assumed to be the potential evaporation and the interception capacity is a calibrated parameter. In WAYS, the interception evaporation E_i is calculated based on potential evaporation E_0 (mm/d), the storage of the interception reservoir S_i (mm) and the interception reservoir storage capacity $S_{i,max}$ (Eq. (3)) by following Deardorff (1978). The interception capacity $E_{i,max}$ is calculated by using the equation Eq. (4), where m_c is 0.3 mm and L is the leaf area index which is calculated based on a modified phenology model in Jolly et al. (2005) by replacing the original vapour pressure stress function with soil moisture in the model (Wang-Erlandsson et al., 2014).

The snow simulation is based on a simple degree-day algorithm (Rango and Martinec, 1995) which is successfully applied in hydrological models in many studies (Comola et al., 2015; Bair et al., 2016; Krysanova and Hattermann, 2017). The water

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balance in snow reservoir is described in Eq. (5) and the constitutive equations is shown in Eq. (6) in Table 1. Below the threshold temperature T_t (°C), precipitation P (mm/day) falls as snow P_s (mm/day) and is added to snow storage S_w (mm). Above the threshold temperature T_t, snow melts if it is available with a certain ratio per degree (F_{DD}). Both the threshold temperature T_t and the snow melt ratio F_{DD} are parameters that calibrated in FLEX model. Following Müller Schmied et al. (2014), T_t is set to 0 °C and F_{DD} is set for different land cover classifications ranging from 1.5 mm/d per degree to 6 mm/d per degree in WAYS. It is also important to be aware that the snow melt water is conceptualized in the model to directly infiltrate into the soil in the model, thus effectively bypassing the interception reservoir.

2.3 Root Zone Routine

The effective root zone routine is the core of the WAYS model. It controls both the evapotranspiration and the runoff generation by precipitation partitioning. Similar to the interception and snow routine, the change of root zone water storage S_{rz} (mm) over time t (day) is described in Eq. (7) with effective precipitation P_e (mm/day) as inflow and soil moisture constrained evaporation E_a (mm/day) and runoff R (mm/day) as outflows. In FLEX model, the runoff generation is calculated based on the widely used beta function of the Xinanjiang model (Zhao, 1992) that is a function of the relative soil moisture in the unsaturated soil layer. The beta function for calculation of runoff in WAYS is replaced by a modified version from the work of Sriwongsitanon et al. (2016) to link the function to the water storage in the root zone layer. Depending on the root zone water storage S_{rz}, a part of effective precipitation turns into runoff and the rest are infiltrated into soil and recharges the root zone layer. The runoff coefficient is determined by both the relative soil water content $S_{rz}/S_{rz,max}$ in root zone and the shape parameter β that describing the spatial process heterogeneity over pixels at global scale. The root zone storage capacity used in WAYS is derived by applying the method in Wang-Erlandsson et al. (2016) which calculates the soil moisture deficit based on satellite-based evaporation and precipitation, while it is a calibrated parameter in FLEX.

The soil moisture constrained evaporation, sometime also known as actual evapotranspiration, is calculated as a function of potential evaporation left-over $E_0 - E_i$ (mm/day), relative soil water content $S_{rz}/S_{rz,max}$, shape parameter β and scale parameter C_e that indicates the fraction of $S_{rz,max}$ above which the transpiration is no longer limited by soil moisture stress. Since the root zone routine connects both the runoff and evapotranspiration and the runoff generation function is modified, the actual evapotranspiration function in WAYS is also revised accordingly from the original one in FLEX model (Sriwongsitanon et al., 2016). The scale parameter C_e was set to 0.5 in FLEX model when applying at basin scale and it becomes a calibrated parameter in WAYS at global scale.

2.4 Slow Response Routine

The water balance in slow response reservoir S_s (mm) is simple with the groundwater recharge R_s (mm/day) as inflow and baseflow Q_s (mm/day) as outflow (Eq. (11)). The groundwater recharge R_s is depicted in WAYS by applying a splitter function that is described in Eq. (12). It separates the runoff into preferential flow and groundwater recharge based on the groundwater recharge factor f_s that is ranging between 0 and 1. In WAYS, the amount of groundwater recharge is also limited by a maximum groundwater recharge $R_{s,max}$ (mm/day) for each grid cells which is specified by soil texture, while there is no constrain of

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maximum value for groundwater recharge in FLEX model. The values of $R_{s,max}$ used in this study are 7, 4.5 and 2.5 for sandy soil, loamy soil and clayey soil by following Döll and Fiedler (2008).

The groundwater recharge factor f_s is a calibrated parameter in FLEX model while in WAYS, it is now determined by applying the approach developed by Döll and Fiedler (2008) which is a function of global digital maps of slope, soil texture, geology, and permafrost. The method is simple and computationally inexpensive and it has been validated at global scale in many subsequent publications, e.g. Döll et al. (2012) and Döll et al. (2014). All the related parameters are provided by look-up tables in the work of Döll and Fiedler (2008) and the only changes we made is that the input data of groundwater recharge method, e.g. the global relief data and the global soil texture map, has been updated accordingly based on the newly available data (Hanasaki et al., 2018). The outflow of the slow response reservoir, i.e. baseflow, is modelled with the function described in Eq. 13, where the baseflow coefficient K_s is set to 100 globally followed by the work of Döll et al. (2003).

2.5 Fast Response Routine

The preferential flow R_f (mm/day) is routed directly into the fast response reservoir S_f (mm) and it is divided into surface runoff Q_{ff} (mm/day) and interflow Q_f (mm/day). The water balance in the fast response reservoir is shown in Eq. (14). In FLEX model, it is assumed that the preferential flow is routed into the fast response reservoir based on a lag-function that represents the time lag between storm and fast runoff generation. In WAYS, we have assumed that the preferential flow will route into the fast response reservoir directly without any delay globally as it is run at the daily time scale.

Similar to the slow response reservoir, the fast response reservoir is also set as a linear-response reservoir, representing a linear relationship between water storage and water release. The surface runoff generation only active when the storage of the fast response reservoir exceeds the specified threshold S_{ftr} with a generation ratio K_{ff} (Eq. (16)), while the interflow Q_f is simply calculated in proportion to the already stored water in the fast response reservoir with the fraction of $1/K_f$ (Eq. (17)).

2.6 Additional Model Adaptation

In addition to above-mentioned model description, some modifications and assumptions are necessary to adapt the model to global scale. In WAYS, the actual evaporation from open water bodies is assumed to be the potential evapotranspiration and the freezing of open water bodies is not considered in the model. Potential evapotranspiration is derived by Hamon equation (Hamon, 1961) in FLEX model, and it is now replaced by the using the Penman-Monteith FAO 56 PM method (Allen et al., 1998). In the FLEX model, capillary rise from groundwater is also considered. However in WAYS, the feature for capillary rise simulation is removed as it cannot be taken into account when no information is available at the global scale. The WAYS model is written in Python version 3.6. In order to benefit from supercomputer, the model is designed with full support for parallel computation.

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Table 1. Water balance and constitutive equations used in WAYS

Reservoirs	Water balance equations	Constitutive equations
Interception reservoir	$$\frac{dS_i}{dt} = P_r - E_i - P_{tf} \quad (1)$$	$$P_{tf} = P_r - (S_{i,max} - S_i) \quad (2)$$ $$E_i = E_p\left(\frac{S_i}{S_{i,max}}\right)^{2/3} \quad (3)$$ $$S_{i,max} = m_c L \quad (4)$$
Snow reservoir	$$\frac{dS_w}{dt} = \begin{cases} -M & \text{if } T > T_t \\ P_s & \text{if } T \leq T_t \end{cases} \quad (5)$$	$$M = \begin{cases} min(S_w, F_{DD}(T - T_t)) & \text{if } T > T_t \\ 0 & \text{if } T \leq T_t \end{cases} \quad (6)$$
Root zone reservoir	$$\frac{dS_{rz}}{dt} = P_e - R - E_a \quad (7)$$	$$P_e = P_{tf} + M \quad (8)$$ $$\frac{R}{P_e} = 1 - \left(1 - \frac{S_{rz}}{(1+\beta)S_{rz,max}}\right)^{\beta} \quad (9)$$ $$E_a = (E_0 - E_i) \cdot min\left(1, \frac{S_{rz}}{C_e S_{rz,max}(1+\beta)}\right) \quad (10)$$
Slow response reservoir	$$\frac{dS_s}{dt} = R_s - Q_s \quad (11)$$	$$R_s = min(f_s R, R_{s,max}) \quad (12)$$ $$Q_s = S_s/K_s \quad (13)$$
Fast response reservoir	$$\frac{dS_f}{dt} = R_f - Q_{ff} - Q_f \quad (14)$$	$$R_f = R - R_s \quad (15)$$ $$Q_{ff} = max(0, S_f - S_{ftr})/K_{ff} \quad (16)$$ $$Q_f = S_f/K_f \quad (17)$$

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3 Model Setups

For the assessment of model performance, the WAYS model is applied at global scale with the spatial resolution of 0.5 degree for the historical period from 1971 to 2010. Two simulations are conducted based on two products of global root zone storage capacity from Wang-Erlandsson et al. (2016). The model is calibrated in the period 1986-1995 and validated in the period of 2001-2010 depends on the availability of the reference data.

3.1 Driving Data

3.1.1 Meteorological Data

The model is driving by the climate data set from the Global Soil Wetness Project 3 (Kim, 2017), GSWP3 (http://hydro.iis.u-tokyo.ac.jp/GSWP3/), for the historical period from 1971 to 2010. GSWP3 data set is generated based on the Twentieth Century Reanalysis project (Compo et al., 2011). It has been proved to be able to represent realistic sub-monthly variability over the entire 20*th* century (1901-2010) and has been used as a forcing data set in several other hydrological modelling studies (Veldkamp et al., 2017; Masaki et al., 2017; Liu et al., 2017; Tangdamrongsub et al., 2018). The climate variables used in this study includes precipitation, minimum temperature, maximum temperature, relative humidity, surface downwelling longwave radiation, surface downwelling shortwave radiation and wind speed at 10 meter. All the variables are at daily scale and 0.5 degree spatial resolution and the wind speed at 10 meter are converted to the wind speed at 2 meter based on the conversion function in Allen et al. (1998), as it is required by the Penman-Monteith FAO 56 PM method for potential evapotranspiration calculation.

3.1.2 Land Use Data

The land cover data we used is the Global Mosaics of the standard MODIS land cover type data product (MCD12Q1) with a spatial resolution of 0.5 degree in the year of 2001, which is derived from the IGBP Land Cover Type Classification (17 classes) and are reprojected into geographic coordinates of latitude and longitude on the WGS 1984 coordinate reference system (Friedl et al., 2010).

3.1.3 Root Zone Storage Capacity

The root zone storage capacity (RZSC) data is a crucial parameter in WAYS. The global root zone storage capacity data used in this study is from Wang-Erlandsson et al. (2016) that is derived by using the “Earth observation-based” method. This method determines the soil moisture deficit at global scale by using the state-of-the-art observation-based precipitation data and satellite-based evaporation data, under the assumption of vegetation optimises its root zone storage capacity to bridge critical dry periods and do not invest more in their roots than necessary. It has been well justified (de Boer-Euser et al., 2019) and overcomes the shortcomings of the traditional methods (look-up table approach; field observation based approach) at the

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global scale, such as data scarcity, location bias, risks unlikely vegetation and soil combinations due to data uncertainty (Feddes et al., 2001).

Since there are two global root zone storage capacity products ($S_{R,CHIRPS-CSM}$ and $S_{R,CRU-SM}$) presented by Wang-Erlandsson et al. (2016) based on different precipitation and evaporation data sets and there is no preference on each products. In this study, both RZSC products are used. $S_{R,CHIRPS-CSM}$ covering the latitudes from 50°N to 50°S and is derived based on the United States Geological Survey (USGS) Climate Hazards Group InfraRed Precipitation with Stations (CHIRPS) precipitation data (Funk et al., 2014) and the ensemble mean of three satellite-based global-scale evaporation data sets: the Commonwealth Scientific and Industrial Research Organisation (CSIRO) Moderate Resolution Imaging Spectroradiometer (MODIS) Reflectance Scaling EvapoTranspiration (CMRSET) data (Guerschman et al., 2009), the Operational Simplified Surface Energy Balance (SSEBop) data (Senay et al., 2013), and the MODIS evapotranspiration (MOD16) data (Mu et al., 2011). $S_{R,CRU-SM}$ covering the latitudes from 80°N to 56°S and is derived by using the Climatic Research Unit Time Series version 3.22 precipitation data (Harris et al., 2014) together with the ensemble mean of only SSEBop and MOD16 due to the reason that CMRSET overestimates evaporation at high latitudes (Wang-Erlandsson et al., 2016). Two selected global root zone storage capacity products are shown in Fig. 2 and their mean Latitudinal values are shown in Fig. 3. Similar pattern and magnitude of RZSC can be found and there is good agreement between two products at different latitudes, especially at low latitudes around the Equator which reflect the fluctuation with high consistency. The large difference are seen mainly in the northern Mid-latitude area, where the absolute difference in percentage is still less than 20%.

3.2 Calibration Data

The WAYS model is calibrated against the ISLSCP II UNH/GRDC Composite Monthly Runoff data (Fekete et al., 2011) from 1986 to 1995 at 0.5 degree resolution, which is a composite runoff data combines simulated water balance model runoff estimates and monitored river discharge. The ISLSCP II UNH/GRDC Composite Monthly Runoff data is also a standard dataset in the second phase of ISIMIP (Inter-Sectoral Impact Model Inter-comparison Project) project (ISIMIP2a) (Warszawski et al., 2014) for calibration and validation, as it assimilates discharge measurement at gauge stations and also preserves the spatial specificity of the water balance while constrained by the station observations. The data can be downloaded from The Oak Ridge National Laboratory Distributed Active Archive Center (ORNL DAAC) (https://daac.ornl.gov/cgi-bin/dsviewer.pl?ds_id=994).

3.3 Validation Data

In this study, the ERA-Interim/Land runoff data is used for the validation of runoff simulation and the Normalized Difference Infrared Index (NDII) is used for the validation of the WAYS model for root zone water storage simulation. By considering the time period of coverage of both data sets (ERA-Interim/Land: 1979-2010, NDII: 2000-present) and also the study period (1971-2010) of this work, the period 2001-2010 are select as the validation period.

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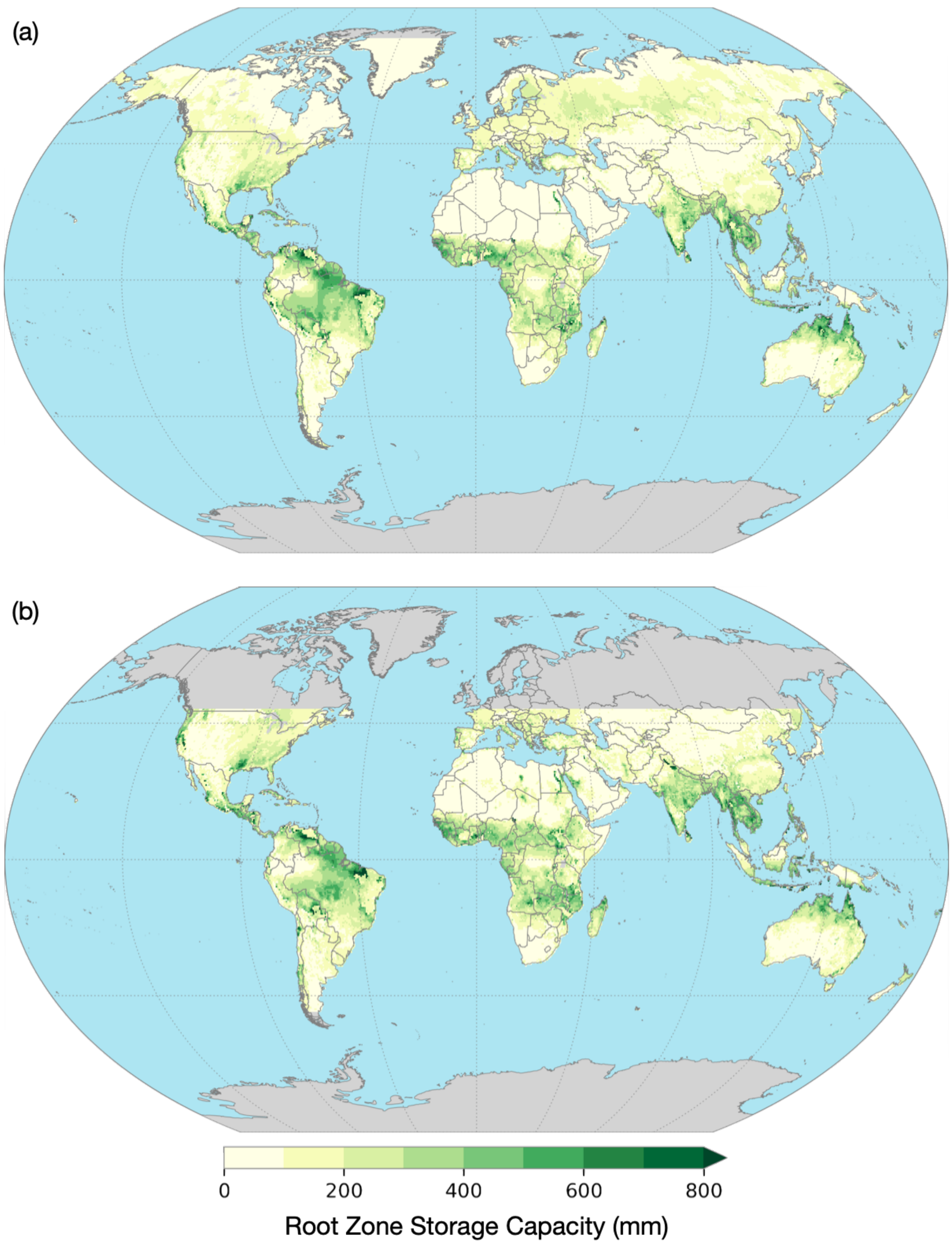

Figure 2. Two global root zone storage capacity products at 0.5 degree: (a) $S_{R,CRU-SM}$; (b) $S_{R,CHIRPS-CSM}$. Figures are produced based on the data provided by Wang-Erlandsson et al. (2016). Grey color indicates no data.

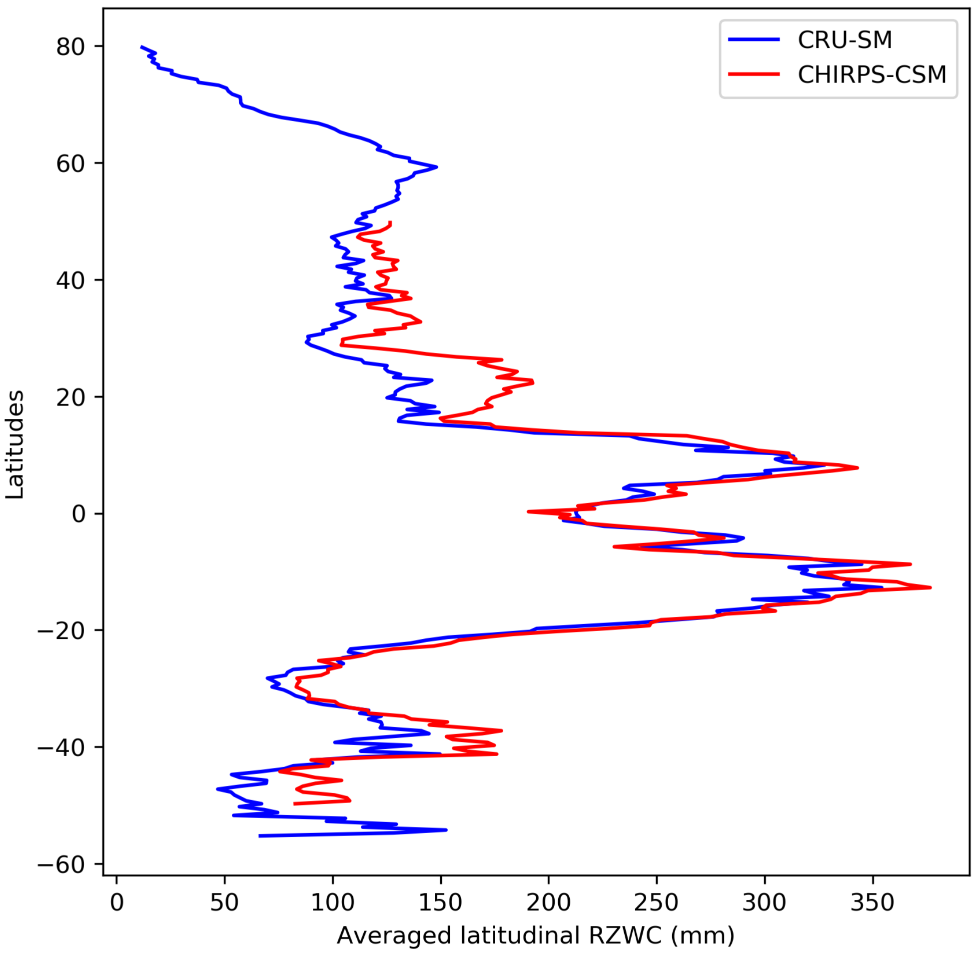

Figure 3. Mean Latitudinal root zone storage capacity of $S_{R,CRU-SM}$ and $S_{R,CHIRPS-CSM}$

3.3.1 ERA-Interim/Land Runoff Data

ERA-Interim/Land is a global land surface reanalysis data set that is produced by the European Centre for Medium-Range Weather Forecasts (ECMWF) (Balsamo et al., 2015). Since the ERA-Interim/Land is well assessed with quality check by comparing with ground-based and remote sensing observations, it has been used as reference data for many studies (Xia et al., 2014; Dorigo et al., 2017). ERA-Interim/Land runoff data is one of the variable in ERA-Interim/Land reanalysis data set and it is also widely used as benchmark data (Alfieri et al., 2013; Orth and Seneviratne, 2015; Reichle et al., 2017), due to its good agreements with Global Runoff Data Centre (GRDC) data set and the large improvement compared to the ERA-Interim runoff reanalysis data which was used to be one of the reference data (Wang-Erlandsson et al., 2014; Balsamo et al., 2015).

The ERA-Interim/Land runoff data used for this study is downloaded from ECMWF website (http://apps.ecmwf.int/datasets/) at 0.5 degree resolution and daily scale from 2001 to 2010.

3.3.2 NDII Data

NDII has been developed by Hardisky et al. (1983) for satellite imagery analysis based on infrared reflectance (NIR) and short wave infrared reflectance (SWIR) by calculating the ratios of different values between them. NDII has been found to have strong correlation with vegetation water content and canopy water thickness (Serrano et al., 2000; Jackson et al., 2004; Hunt and Yilmaz, 2007; Wilson and Norman, 2018). It can also be used to effectively determine the water stress of plants by taking the advantage of the property of shortwave infrared reflectance, which has the negative relationship with leaf water content because of the large absorption by leaves (Steele-Dunne et al., 2012; Friesen et al., 2012; van Emmerik et al., 2015). Recently, Sriwongsitanon et al. (2016) found a promising linkage between NDII and the root zone water storage. Even though the NDII reflects the dynamics of RZWS better in moisture stress periods rather than in periods of moisture stress free, the general good correspondence between NDII and RZWS offering a potential value of the NDII as a proxy for RZWS. Therefore, in this study NDII is used as the benchmark to assess the performance of the model for RZWS depiction.

NDII is calculated by applying the following equation from Hardisky et al. (1983):

$$NDII = \frac{\rho_{0.85} - \rho_{1.65}}{\rho_{0.85} + \rho_{1.65}} \tag{18}$$

where $\rho_{0.85}$ is the reflectance at $0.85\,\mu\mathrm{m}$ wavelength and $\rho_{1.65}$ is the reflectance at $1.65\,\mu\mathrm{m}$ wavelength. NDII is a normalized index that ranges between -1 and 1. A low value of NDII indicates high canopy water stress, which also reflects the less water content in the root zone (Sriwongsitanon et al., 2016).

In our work, the NDII is computed based on the satellite data MODIS level 3 surface reflectance product (MOD09A1) (Vermote, 2015), which provides an estimate of the surface spectral reflectance of Terra MODIS Bands 1 through 7 corrected for atmospheric conditions such as gasses, aerosols, and Rayleigh scattering in the Sinusoidal projection. The MOD09A1 product is available at 8-day temporal scale and 500 m spatial resolution globally from 2000-02-24 to present. Each MOD09A1 pixel contains the value that is selected from all the acquisitions within the 8-day composite on the basis of high observation coverage, low view angle, the absence of clouds or cloud shadow, and aerosol loading. The satellite image processing and NDII calculation are done by using the Google Earth Engine platform (http://earthengine.google.com). Since some of the MOD09A1 images are missing. In total, 452 NDII rasters are generated for the validation period (2001-2010).

3.4 Calibration Strategy

A global parameter optimization algorithm (Tolson and Shoemaker, 2007), dynamically dimensioned search (DDS), has been applied in this study for model parameters calibration. DDS is designed for computationally expensive optimization problems and has been used in many studies related to the distributed hydrological model calibration at global and regional scales (Moore et al., 2010; Kumar et al., 2013; Rakovec et al., 2016; Nijzink et al., 2018; Smith et al., 2018).

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Since the reference data, i.e. ISLSCP II UNH/GRDC data, is at monthly temporal scale, the simulated runoff by WAYS in the calibration period (1986-1995) is also averaged to the monthly scale for the sake of consistency. The criteria of fit for calibration is Nash-Sutcliffe efficiency coefficient (NSE) and the optimization algorithm DDS is run with 2000 iterations for each grid cells for parameter estimation.

4 Model Evaluation

To evaluate model performance, simulated runoff and root zone water storage are compared to the reference data (see Section 3.3) for the validation period (2001-2010) in ten major river basins of the world by considering the coverage of the root zone storage capacity products ($S_{R,CHIRPS-CSM}$ covers only the latitudes from 50°N to 50°S).

4.1 Runoff Evaluation

The WAYS simulated runoff are compared to the ERA-Interim/Land runoff as well as the multi-model global runoff simulations from ISIMIP2a project. ISIMIP is a community-driven global platform that supports for model inter-comparison studies at both global and regional scales, while ISIMIP2a focuses on the historical period and all the models are driven by four state-of-the-art climate forcing (Warszawski et al., 2014). Since the ISIMIP2a simulations are widely studied and discussed in many studies (Schewe et al., 2014; Müller Schmied et al., 2016; Gernaat et al., 2017; Zaherpour et al., 2018), the comparison between WAYS and ISIMIP2a models can provide added-value for evaluation in addition to examine only with reference data. To make the climate forcing consistent with WAYS model, only the GSWP3 driven simulations are used for comparison. The evaluation is done at monthly scale even though the WAYS model simulates the runoff at daily scale due to the reason that only monthly runoff are available for some of the ISIMIP2a models (Warszawski et al., 2014).

Figure 4 shows the time series of runoff from reference data and different models. WAYS_CRU in the legend indicates the runoff simulated by WAYS model with root zone storage capacity product $S_{R,CRU-SM}$ and WAYS_CHIRPS implies the simulation with RZSC product $S_{R,CHIRPS-CSM}$. First, it can be seen that two WAYS simulations with different RZSC products show extremely good correspondence in all selected basins. This is consistent with the investigation of RZSC data sets in Section 3.1.3 where there is a high consistency in two used products even RZSC itself naturally shows high variability along the latitudes (see Figure 2 and 3). This confirms the robustness of RZSC products we used in our WAYS model for runoff simulation. Results show good agreements between WAYS simulations and the reference data, i.e. ERA-Interim/Land in the selected basins, whilst ISIMIP2a models present stark differences in simulating runoff. E.g. ISIMIP2a models show a clear trend of overestimation in some of the basins (Mississippi, Ganges, Yangtze, Parana and Murray Darling), where the spread of the runoff ensembles are also large. This is partly due to the reason that some of the ISIMIP2a models are not calibrated at all (Zaherpour et al., 2018), whilst the WAYS is calibrated to a Composite Monthly Runoff data set which assimilates the monitored river discharge (Fekete et al., 2011).

In Mekong rive basin, all the models show a high consistency in monthly runoff generation with a narrow spread of the ensemble. This can be contributed by the natural characteristics of Mekong river, i.e. highly predictable timing and size of

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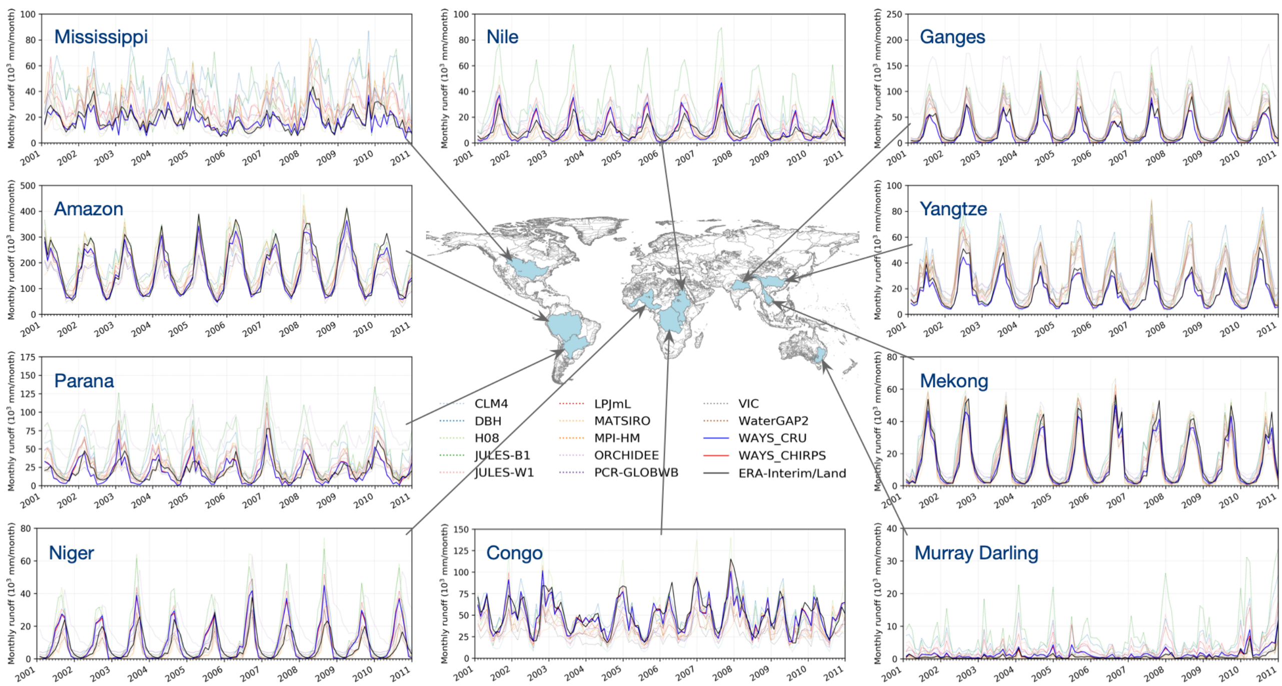

Figure 4. Time series of monthly runoff simulated by WAYS and also ISIMIP2a models as well as the reference data. The highlighted basins in the world map indicates the selected catchments for model evaluation. The solid lines in blue and red indicate the WAYS simulation with two different RZSC products. The solid line in black indicates the reference data and dash lines represents the simulation of ISIMIP2a models.

the wet-season peak. Because precipitation in this region is concentrated in an extremely regular wet-season peak under the impact of tropical monsoon (Adamson et al., 2009). The outperforming of WAYS is also observed in the northernmost (Mississippi) and southernmost (Murray Darling) catchments in our selected basins, whilst ISIMIP2a models show extremely large differences in runoff simulation with large uncertainties. The good performance is particularly highlighted in Murray Darling basin, the monthly runoff are extremely low due mainly to the anthropogenic climate impacts (Cai and Cowan, 2008; Potter and Chiew, 2011), which is extremely difficult for other models to capture it without overestimations (see Figure 4). A slight overestimation is found in WAYS model in two African basins, i.e. Nile and Niger. This can be explained by the general overestimation of precipitation value in climate forcing data GWSP3 in these regions (Muller Schmied et al., 2016). In these two regions, ISIMIP2a simulations also show dramatic overestimations. Oppositely, models show a trend of underestimation in anther African basin Congo. This might be caused by both the quality of precipitation and the complexity of natural processes here (Tshimanga and Hughes, 2014). Wang-Erlandsson et al. (2014) reported in his work that Congo precipitation and runoff estimates are particularly uncertain in general. It is worth to highlight that the WAYS model can still capture well the monthly variability of runoff in this basin.

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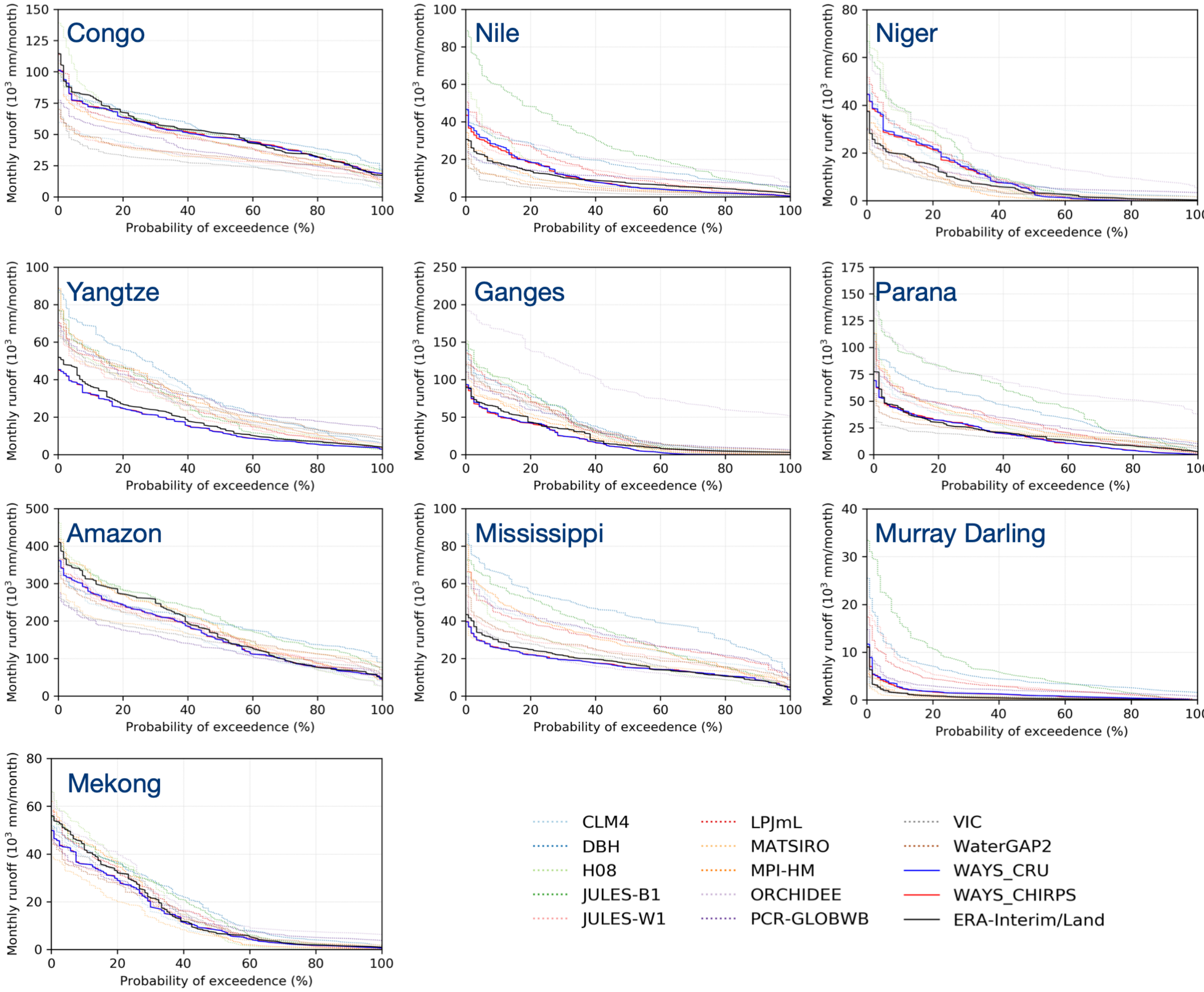

Figure 5. The probability of exceedence for monthly runoff simulated by different models as well as the reference data in ten selected basins. The solid lines in blue and red indicate the WAYS simulation with two different RZSC products. The solid line in black indicates the reference data and dash lines represents the simulation of ISIMIP2a models

To evaluate the ability of the WAYS model for distribution replication, a comparison study on he probability of exceedance is done and the result is shown in Figure 5. The probability of exceedence reveals of the model performance at different magnitudes. With a visual inspection, we can see that WAYS is able to reproduce the runoff distribution well with a good match to the ERA-Interim/Land data, especially in the basins of Congo, Parana and Mississippi, while the ISIMIP2a model simulated runoff skewed differently to the ERA-Interim/Land runoff distribution. In a few basins (Nile, Ganges, Parana and Mississippi), some of the ISIMIP2a model even show a bear-sized shift of distribution to the reference data highlight that these models struggle to simulation the monthly runoff at all different magnitudes. In Nile and Niger, WAYS also shows a slight offset for both simulations, but still lie within the uncertainty range. Results also show a large uncertainty of the runoff simulations in upper tails which reflects the larger deviation in high value producing than in middle and low value simulation for the models. Such biases in reproducing the runoff distribution in ISIMIP2a models, in turn delivers large ensemble spreads in time series.

To further assess the performance of WAYS model, three general metrics for runoff comparison are selected for the evaluation, i.e. Nash-Sutcliffe Efficiency (NSE), root mean squared error (RMSE) and percent bias (PBIAS). The estimated scores from the monthly runoff time series for WAYS and ISIMIP2a models are present in Figure 6. For better comparison, the NSE values are converted to the values of 1-NSE, thus the numbers closer to 0 indicates better performance. The model performance of WAYS is generally better compared to the ISIMIP2a models and the estimated scores based on different criteria are also close to the benchmarks. The 1-NSE comparison (Figure 6 (a)) indicates that model performance of WAYS in the selected basins except for Niger and Nile is particularly favorable when compared to the other ISIMIP2a models. In these basins, both of two WAYS simulations (WAYS_CRU and WAYS_CHIRPS) are ranked in the top five (14 model simulations in total in comparison). In six basins, both of the WAYS simulations have the 1-NSE metric scores less than 0.3 resulting a value of NSE larger than 0.7. In Yangtze, Amazon and Mekong, the WAYS mode is even ranked as the best one with both of two simulations outperformed others. The relatively low performance of WAYS in Niger and Nile is the result of the model slightly overestimating middle and high runoff values (Figure 5). The RMSE comparison (Figure 6 (b)) delivers similar information as 1-NSE comparison that WAYS shows generally better performance. In Amazon, all the model simulations show large RMSE due to the large value of monthly runoff in this catchment. By examining the percent bias (Figure 6 (c)), it is evident that WAYS model performs well in most of the basins, as the scores of the two WAYS simulations are close to the benchmark. The relatively poor performance of WAYS model on percent bias assessment is found in Murray Darling basin with the PBIAS values are round 100%, but they are still lie within the uncertainty range by checking with other models. This large value may be caused by the extremely low runoff induced low value of the benchmark, while a little difference in absolute value will cause large difference in the percentage.

Combining time series analysis, most commonly used metrics examination in hydrology as well as the probability of exceedence assessment, our results show a comprehensive assessment of the model performance on runoff simulation. Strong performance of WAYS with subtle difference between runoff simulation and reference data in all the tests indicating particularly favourable applicability of WAYS in runoff simulation across major basins. Even though, relatively poor performance are found in two African basins, but the biases are still lie within the uncertainty range by investigating other models. Such

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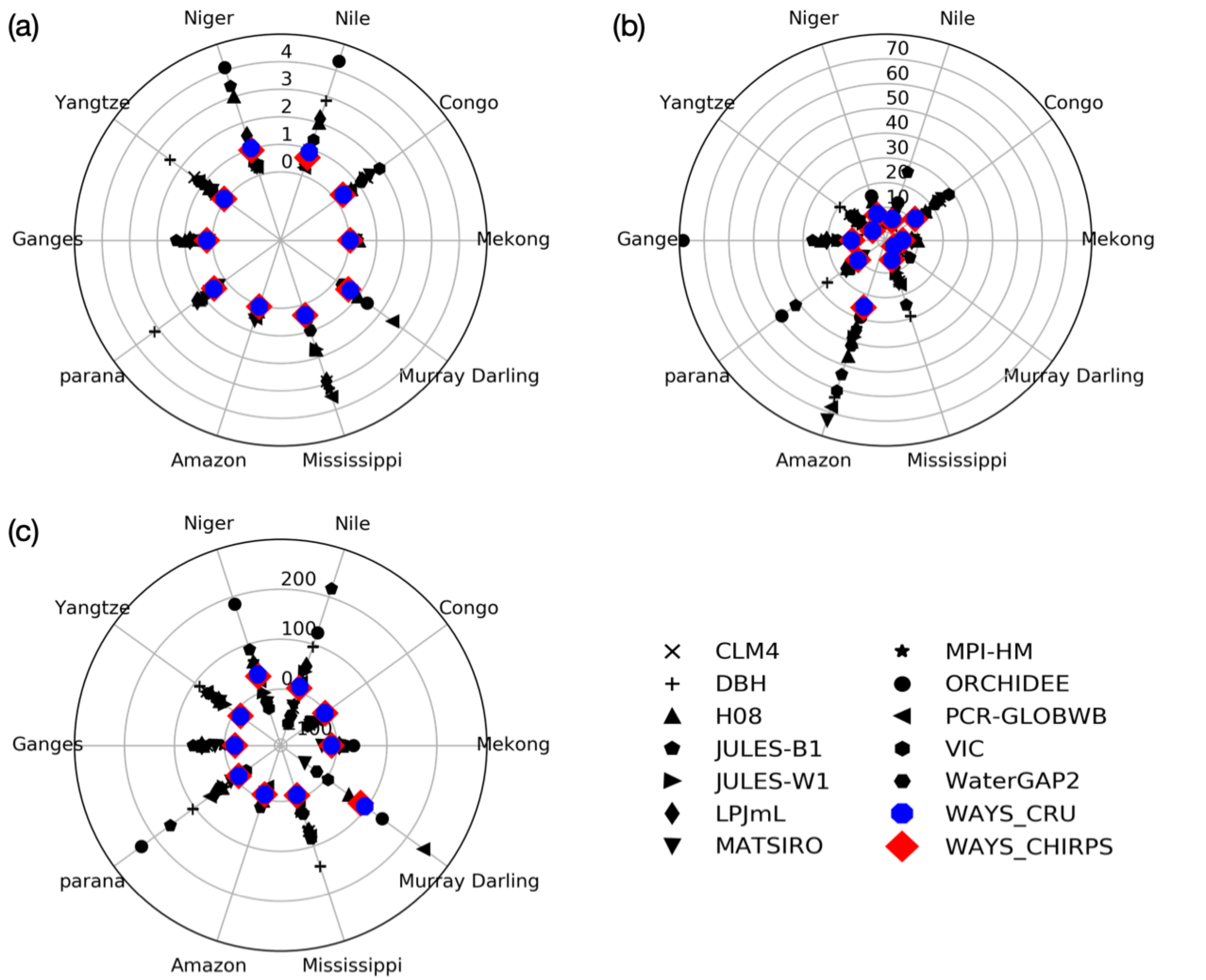

Figure 6. The catchments clockwise pole plot according to different metrics, (a) 1-NSE, (b) RMSE, (c) PBIAS. Colored makers indicate the score for WAYS model with two different simulations and black makers represent the score for ISIMIP2a models. For all the metrics, the value of 0 is the benchmark.

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trend of overestimation could also be explained by the overestimation of precipitation value in forcing data in this regions (Muller Schmied et al., 2016). In addition, it is worth acknowledging that global hydrological models show large different in runoff simulation across basins. Previous studies emphasized that large ensemble spreads from GHMs could caused by model structural uncertainties (Haddeland et al., 2011; Gudmundsson et al., 2012). Lacking of physical process representations, e.g. transmission loss, in the hydrological models can also explain some of the biases between simulated runoff and the reference data (Gosling and Arnell, 2011).

4.2 The Validation of Root Zone Water Storage

Similar to the runoff evaluation, the performance of the simulation of root zone water storage by WAYS model is also evaluated at ten major river basins in the period from 2001 to 2010. Since the NDII is a normalized index and in a 8-day temporal scale, WAYS simulated root zone water storage is firstly averaged to 8-day temporal scale and then normalized to the range between 0 and 1 before the comparison. A few time steps are missing in the NDII data set. To keep the compared data sets consistent, only pair-wised RZWS data are selected for the model evaluation.

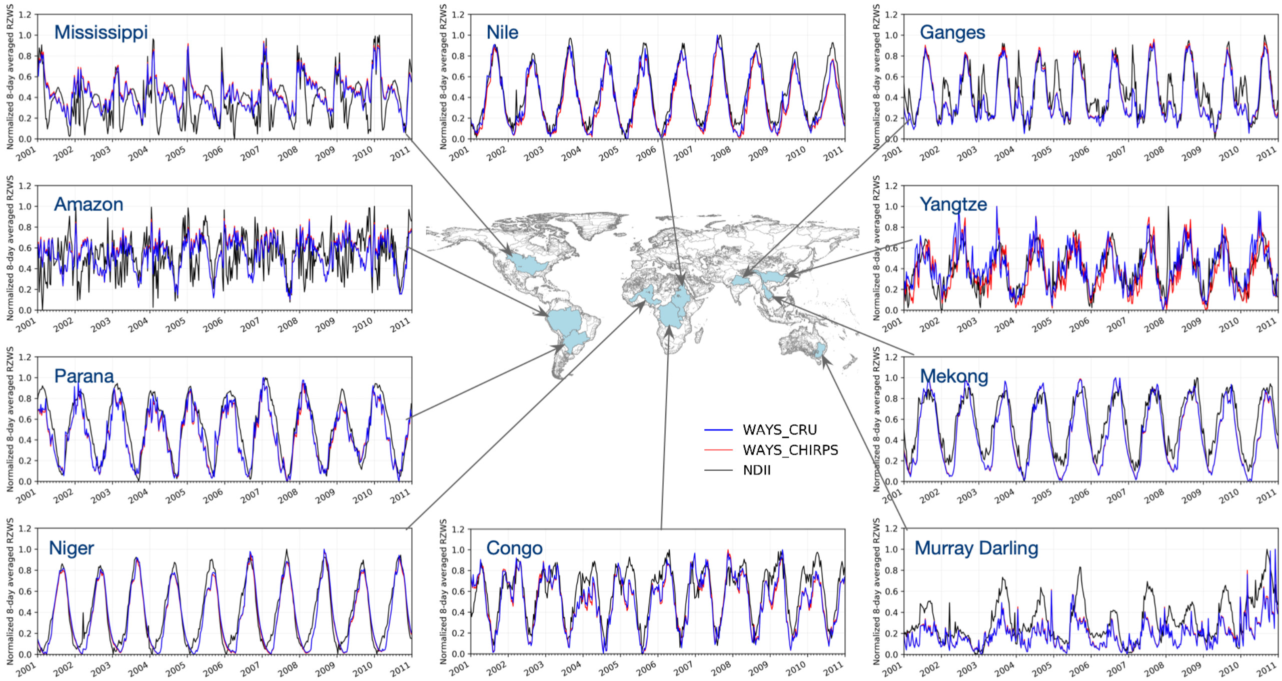

Figure 7. Time series of 8-day normalized RZWS simulated by WAYS model and NDII value.

The 8-day NDII values are compared to the 8-day averaged root zone water storage values of WAYS model and the results are shown in Figure 7 and Table 2. Figure 7 shows the comparison of time series of NDII and simulated RZWS in the selected basins and Table 2 presents the corresponding rank correlation (Spearman's rho) between NDII and RZWS. The simulated RZWS by GEPCI-hydro is not compared to other model, as the RZWS variable is not available in other GHMs. For ISIMIP2a,

Table 2. The rank correlation of NDII and WAYS simulated RZWS in ten selected basins

Selected River Basins	**Models**	
	WAYS_CRU	WAYS_CHIRPS
Congo	0.875	0.862
Nile	0.962	0.966
Niger	0.955	0.960
Yangtze	0.709	0.754
Ganges	0.802	0.807
Parana	0.932	0.938
Amazon	0.533	0.506
Mississippi	0.675	0.661
Murray Darling	0.667	0.678
Mekong	0.945	0.943

some models produced the root zone soil moisture with a fixed depth of soil profile in the model structure. However, it is still a different variable compared with root zone water storage.

First, it is clear to see that NDII shows totally different patterns in different basins. Clear seasonal cycles are shown in Nile, Mekong, Niger river basins and so on. Camel-like structures are observed in Ganges and Congo and relatively complex patterns are represented in Mississippi, Murray Darling and Amazon. The simulated RZWS shows a good agreement in time series with NDII in most of the selected basins. High values of rank correlation are also detected in these regions. Seven catchments out of ten have the rank correlation value higher than 0.7, especially in Nile, Niger, Parana and Mekong, the correlation coefficients are even higher than 0.9 indicating the strong model performance of WAYS in these basins for root zone water storage simulation, as the NDII reflects the soil water content in the root zone (Sriwongsitanon et al., 2016). Two simulated RZWS time series with different root zone storage capacity products show also identical behaviour with subtle differences between each other, except in the Yangtze river basin due to the relatively larger differences in averaged RZSC of two products ($S_{R,CRU-SM}$: 135 mm, $S_{R,CHIRPS-CSM}$: 163 mm) in this basin. In Ganges and Congo, the NDII time series show a two-humped structure while the WAYS model can still capture it, even though underestimations are detected in some years. The rank correlation coefficients in these two catchments are higher than 0.8. In Yangtze, a suddenly high value of NDII is found on the day of 25th of August in 2008. By investigating the NDII values a few days before and after and also the precipitation amount in this period, the unrealistic high value might be caused by the quality of satellite data MOD09A1 on that day, since it can be affected by many issues including clouds, shadow, view angle, aerosol loading and so on (Vermote, 2015).

The relatively larger differences between NDII and simulated RZWS are also found in some catchments. In Mississippi, WAYS shows a good performance on large values simulation while struggles to simulate low values with considerable overestimations on it. Therefore the rank correlation is also relatively low in this catchment with values around 0.67. The Mississippi river basin is the northernmost catchment in our selected basins. The NDII show totally different pattern compare to the others,

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while WAYS simulated RZWS show relatively clear seasonal variation. The possible explanation on it could be either NDII has difficulty to reflect the RZWS or the WAYS has shortcoming to simulate the RZWS in this region. Because some studies reported that spurious seasonal and inter-annual variations also exist in soil moisture in this basin (Yang et al., 2015). Oppositely, WAYS shows a trend of underestimation in Murray Darling. The possible reason behind could be the underestimated RZSC in this region as well as the intensive human activities including dam construction, water diversion system and river management, which will impact both the RZSC estimation and RZWS simulation (Reid et al., 2002; Kingsford, 2000). In Amazon, the model can only captures a few downward trough and shows difficulty to represent the complete complex dynamics of NDII, resulting the lowest value of the rank correlation (0.533 and 0.506) among all the selected basins. The primary reason of this low performance could be the inability of NDII to represent RZWS in relatively wet regions where water stress for plant is low. (Sriwongsitanon et al., 2016). In our selected basins, Amazon has the highest averaged annual precipitation amount with a number of 2201 mm/year in the validation period. In this case, the performance of WAYS on RZWS simulation in such regions cannot be justified.

Overall, these model validation results over the ten selected river basins deliver generally good evaluated values that suggesting capability of the WAYS model for RZWS simulation, especially for inter-annual variability simulation. However, attention should also be paid in some regions, e.g. the basins in high latitudes in the Northern Hemisphere as well as the regions with plenty precipitation where moisture stress might be low and NDII may not reflect correctly the RZWS dynamics (Sriwongsitanon et al., 2016).

5 Discussion and conclusion

In this study, a global hydrological model has been developed that aims to simulate the soil water volume storied in the entire root zone, a critical variable for eco-hydrology related researches, by considering the globally spatial heterogeneity of the plant rooting system. The primary motivation behind the development of WAYS is to improve the integrality of soil water simulation in hydrological models by acknowledging the key role played in many applications by RZWS as it connects the climate, hydrology and earth surface systems (Savenije and Hrachowitz, 2017). Existing models represent soil profile with different schemes (Devia et al., 2015). However they still suffering from the structure limitations of the models to reflect the soil water dynamics for entire rooting system (Bierkens, 2015; Sood and Smakhtin, 2015). A persistent weakness in the RZWS simulation in the hydrological models is the lack of direct observation for the model evaluation (Sriwongsitanon et al., 2016).

Benefiting from recent progresses made in the field of hydrology and remote sensing, the WAYS model is developed based on an advanced lumped model FLEX (Fenicia et al., 2011; Gao et al., 2014a) and evaluated with a proxy of RZWS, a remote sensing based index NDII (Hardisky et al., 1983). NDII is not new, but strong linkage between NDII and RZWS found by Sriwongsitanon et al. (2016) enlightened the work of us. The potential candidate as a proxy of RZWS bridges the gaps in the field, where RZWS cannot be directly observed at large scale. The model FLEX is widely used and validated for root zone water dynamics simulation but at basin scale (Gao et al., 2014b; Nijzink et al., 2016; de Boer-Euser et al., 2016; Sriwongsitanon et al., 2016). A variety of modifications and extensions made based on FLEX allows WAYS to simulate the hydrological cycles at global scale with an advanced schema in root zone system. Another key parameter that allows appropriate RZWS simulation in WAYS is the global RZSC produced recently by Wang-Erlandsson et al. (2016). Before that, it is usually obtained from look-up approaches with inherently large uncertainty in it. RZSC reveals the spatial heterogeneity of the plant rooting system and has direct relation with RZWS. Since the RZSC is produced under the assumption that plants do not invest more in their roots than necessary to bridge a dry period. Thus, this assumption is also hold by our work and the root zone reservoir (Section 2.3) actually defines the part of the unsaturated zone that determines the dynamics of the runoff regime (Sriwongsitanon et al., 2016; Savenije and Hrachowitz, 2017).

The major goal of this study is to test the feasibility of WAYS for reliable RZWS simulation. The newly developed model is validated on both the runoff simulation and also RZWS simulation. Strong performance are found in runoff simulation, especially its vantage performance compared to the ISIMIP2a models. In addition to the runoff depiction, the WAYS model show also a good representation of RZWS with high values of rank correlation in most of the validated regions. The evaluation results confirm the capacity of WAYS as a useful tool to simulate the hydrological elements, particularly RZWS, at global scale. However, we have to highlight that the model also shows less preference in some regions, e.g. Amazon, in RZWS simulation, where the reference data NDII may have shortcoming to reflect RZWS. It is also important to note that the high latitude regions are not covered by one of the key parameter, i.e. root water storage capacity, used by the WAYS model, only major river basins in middle and low latitudes are investigated. Thus, the performance of the model in the other regions is not justified. This is one of the limitations of this work and further investigations is needed.

It also needs to be aware that during the evaluation of RZWS, the reference data NDII is a normalized index based on surface reflectance can reflects only the dynamics of the RZWS rather than the absolute value (Sriwongsitanon et al., 2016). So, the real value based evaluation could be much more helpful for the model application. This could be another limitation of the work. But it also emphasizes the importance and necessity of this work from the following two aspects: 1) remote sensing based approach, e.g. NDII, is so far one of the best available method for root zone information retrieving (Tobin et al., 2017). However, it still limited by the real value reflection. This urges the model development as it has the ability for absolute value simulation. 2) remote sensing based approach works only on historical analysis which limits its ability for future impact studies. This also motive the model development as it work both for past and future after appropriate evaluation.

In summary, the newly developed global hydrological model WAYS improves the integrality of soil water simulation in hydrological models as it simulates the water stored in the entire root zone. This added-value feature could benefit for many applications related to the root zone processes. Moreover, this can also advances the hydrological model itself as the water storied in root zone controls the partitioning of the precipitation into evaporation, infiltration and runoff in the model (Liang et al., 1994). The precise simulation of variables in root zone could benefits the simulation of other elements in the model, thus advances the model simulation towards advanced philosophy, i.e. get the right answers for the right reasons rather than simply to get the right answers (Kirchner, 2006).

Code and data availability. The source code is availiable from the corresponding author on request. The meteorological data used in this work are available at the data center of the "Global Soil Wetness Project 3" (http://hydro.iis.u-tokyo.ac.jp/GSWP3/). The land use data is available at Global Land Cover Facility (http://www.landcover.org). The root zone storage capacity is collected from the work of Wang-Erlandsson et al. (2016). The runoff data for model calibration is available at the Oak Ridge National Laboratory Distributed Active Archive Center (ORNL DAAC) (https://daac.ornl.gov/cgi-bin/dsviewer.pl?ds_id=994). The runoff data for model evaluation is available at the European Centre for Medium-Range Weather Forecasts (ECMWF) website (http://apps.ecmwf.int/datasets/). The DNII data and simulated hydrological data are available upon request to the corresponding author.

Author contributions. GM and JL contributed equally to the paper. GM and JL designed the study, analysed data and wrote the paper. JL designed the model structure and GM wrote the model code.

Competing interests. The authors declare that they have no conflict of interest.

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