On the contribution of remote sensing-based calibration to model multiple hydrological variables

Aline Meyer Oliveira^{1,1,1}, Ayan Fleischmann^{2,2,2}, and Rodrigo Paiva^{1,1,1}

¹IPH/UFRGS

²Federal University of Rio Grande do Sul

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Abstract

The accuracy of hydrological model predictions is limited by uncertainties in model structure and parameterization, and observations used for calibration, validation and model forcing. Conventionally, calibration is performed with discharge estimates. However, the internal processes in the model might be misrepresented, i.e., the model might be getting the "right results for the wrong reasons", which compromises model reliability. An alternative is to calibrate the model parameters with remote sensing (RS) observations of the water cycle. Previous studies highlighted its potential to improve discharge estimates, but put much less effort on investigating other variables of the water cycle. In this study, we analyzed in detail the contribution of five different RS-based variables (water level (h) from Jason-2, flood extent (A) from ALOS-PALSAR, terrestrial water storage (TWS) anomalies from GRACE, evapotranspiration (ET) from MOD16 and soil moisture (W) from SMOS) to calibrate a hydrological-hydrodynamic model for a tropical study region with floodplains in the Amazon basin. Calibration with TWS, ET, W, and h+W were able to improve discharge estimates by around 16% to 48%. Water cycle representation was also improved (e.g., calibration with h improved not only h estimates but also A, TWS and ET). By analyzing differing calibration setups, a consistent selection of complementary variables for model calibration resulted in better performances than incorporating all RS variables into the calibration. By looking at multiple RS observations of the water cycle, we were able to found inconsistencies in model structure and parameterization, which would remain unknown if only discharge observations were considered.

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On the contribution of remote sensing-based calibration to model multiple hydrological variables in tropical regions

3 A. M. Oliveira^{* 1}, A. S. Fleischmann¹, and R. C. D. Paiva¹

4 ¹ Instituto de Pesquisas Hidráulicas (IPH), Universidade Federal do Rio Grande do Sul –

5 UFRGS, Av. Bento Gonçalves, 9500, Porto Alegre 90050-260, RS, Brazil.

6 Corresponding author: Aline Meyer Oliveira (alinemey@gmail.com)

7 Abstract

8 The accuracy of hydrological model predictions is limited by uncertainties in model 9 structure and parameterization, and observations used for calibration, validation and model forcing. While calibration is usually performed with discharge estimates, the 10 11 internal model processes might be misrepresented, and the model might be getting the 12 "right results for the wrong reasons", thus compromising model reliability. An 13 alternative is to calibrate model parameters with remote sensing (RS) observations of 14 the water cycle. Previous studies highlighted the potential of RS-based calibration to improve discharge estimates, focusing less on other variables of the water cycle. In this 15 16 study, we analyzed in detail the contribution of five RS-based variables (water level (h), 17 flood extent (A), terrestrial water storage (TWS), evapotranspiration (ET) and soil 18 moisture (W)) to calibrate a coupled hydrologic-hydrodynamic model for a large Amazon sub-basin with extensive floodplains. Single-variable calibration experiments 19 20 with all variables were able to improve discharge KGE from around 6.1% to 52.9% 21 when compared to a priori parameter sets. Water cycle representation was improved 22 with multi-variable calibration: KGE for all variables were improved in the evaluation period. By analyzing different calibration setups, a consistent selection of 23

complementary variables for model calibration resulted in a better performance than
incorporating all RS variables into the calibration. By looking at multiple RS
observations of the water cycle, inconsistencies in model structure and parameterization
were found, which would remain unknown if only discharge observations were
considered.

Keywords: hydrological modeling, multi-variable calibration, Amazon, hydrodynamic
modeling, large basins.

31

32 1 Introduction

33 The accurate representation of hydrologic processes in mathematical models remains a 34 key challenge in water resources research and applications (Baroni et al., 2019; Clark et al., 2015; Kirchner, 2006; Nearing et al., 2016; Semenova & Beven, 2015) due to 35 36 uncertainties in model structure (Wagener et al., 2003), parameterization (Gharari et al., 37 2014; Shafii & Tolson, 2015), and observations (Di Baldassarre & Montanari, 2009). These uncertainties might lead to inaccurate predictions of hydrological variables for 38 39 water resources and natural hazards management (Grimaldi et al., 2019; Montanari & 40 Koutsoyiannis, 2014), and for quantification of impacts of climate change and 41 anthropogenic effects on the water cycle (Haddeland et al., 2006; Teutschbein & 42 Seibert, 2012; C. Y. Xu et al., 2005). This problem has led for instance to initiatives to 43 better constrain the terrestrial water budget by fusing models and Earth Observation datasets (M. Pan & Wood, 2006; Pellet et al., 2019). 44

Traditionally, hydrological models are calibrated against gauged streamflow data, whichmight hamper predictions in ungauged sites, since it does not guarantee an accurate

47 representation of other water cycle components (e.g., soil moisture and 48 evapotranspiration), thus leading to uncertainty in hydrologic predictions (Hrachowitz et al., 2013). Moreover, many parameter sets can provide equally acceptable performances 49 for streamflow evaluation (i.e., the equifinality thesis), but they might be "right for the 50 51 wrong reasons" (Beven, 2006; Kirchner, 2006). Several solutions have been proposed to improve process representation and reduce uncertainty in model predictions, such as the 52 generalized likelihood uncertainty estimation (Beven & Binley, 1992), dynamic 53 54 identifiability analysis (Wagener et al., 2003), multiscale parameter regionalization (Samaniego et al., 2010), and multi-objective calibration (Yapo et al., 1998). However, 55 these are ongoing developments, and stand out as one of the twenty-three unsolved 56 57 problems in hydrology (Blöschl et al., 2019): "how can we disentangle and reduce model structural/parameter/input uncertainty in hydrological prediction?". 58

59 In addition to the presented solutions, an alternative is the use of complementary 60 datasets besides streamflow observations for model calibration (e.g., Crow et al., 2003; 61 Franks et al., 1998; Lo et al., 2010; López et al., 2017; Rajib et al., 2016), data assimilation (e.g., Brêda et al., 2019; Houser et al., 1998; Mitchell et al., 2004; Paiva et 62 63 al., 2013; Pathiraja et al., 2016; Reichle et al., 2002; Vrugt et al., 2005), or validation (e.g., Alkama et al., 2010; Motovilov et al., 1999; Neal et al., 2012; Siqueira et al., 64 2018). Such approaches are promising to improve representation of processes in 65 66 hydrological models (Clark et al., 2015), reduce uncertainty in hydrological predictions (Gharari et al., 2014), understand equifinality (Beven, 2006), and perform predictions in 67 68 ungauged or poorly-gauged sites (Sivapalan et al., 2003). However, distributed data of complementary hydrological variables (e.g., evapotranspiration, soil moisture) are 69 70 scarce, and in-situ measurements present poor spatial and temporal representativeness.

71 In this context, remote sensing (RS) observations have stood out in the last decade 72 because of their increasing spatial and temporal resolutions, free availability in many cases, and capability to record less monitored hydrological variables such as soil 73 74 moisture, evapotranspiration, and terrestrial water storage (Lettenmaier et al., 2015). For 75 instance, GRACE mission provided monthly estimates of changes in water storage on a 76 global coverage with an accuracy of 2 cm when uniformly estimated over land and oceans (Tapley et al., 2004). Missions such as SMOS, SMAP, AMSR-E and ASCAT 77 78 were estimated to provide soil moisture data with a median RMSE of 0.06-0.10 m³/m³ 79 for the CONUS (Karthikeyan et al., 2017). Altimeters such as Envisat, Jason-2 and 80 ICESat-1 and ICESat-2 can yield water level data with an accuracy ranging from 0.04 m 81 to 0.42 m, involving trade-offs between temporal resolution from 10 to 91 days, and 82 cross-track separation from 15 to 315 km (Jarihani et al., 2013), while the future SWOT 83 mission will provide at least one water level measurement every 21 days for global 84 rivers wider than 100 m (Biancamaria et al., 2016).

Although previous studies have analyzed the value of integrating RS data into hydrological modeling through calibration or data assimilation (see review by Xu et al., 2014 and Jiang & Wang, 2019), this topic has not been fully explored to its potential yet. Therefore, in section 1.1, we present major knowledge gaps in the context of RSbased calibration of hydrological models through an extensive literature review. In section 1.2, we describe the aims and contributions of this study.

91

92 1.1 Literature review on calibration of hydrological models with RS data

A comprehensive, yet non-exhaustive literature review of studies that used RS datasetsfor parameter estimation in hydrological models is presented in this section and

summarized in Figure 1. A total of 62 research articles was found (Supplementary 95 Material Table S1). Most publications involved large study areas (> 1000 km²), which is 96 expected because of the usual coarse resolution of RS products. Most studies used RS-97 98 derived evapotranspiration for model calibration, followed by soil moisture (Figure 1b), 99 but there were also attempts for calibration of up to eight different RS-derived variables (Nijzink et al., 2018). This indicates a still existent knowledge gap regarding which RS-100 derived variables are more useful for model calibration. Indeed, many recent studies 101 102 have investigated the added value of RS-derived information to calibrate hydrological 103 models (Figure 1d; Table S1).

104 Most of the studies (69.35%) used only one RS product for model calibration (Figure 105 1e, in black), while twelve studies (19.35%) used two products, and five (8.06%) used three products. Only few studies used more than three RS products for model 106 calibration (Demirel et al., 2019; Nijzink et al., 2018). Some studies addressed the use 107 108 of RS data to estimate discharge in ungauged basins (Kittel et al., 2018; Sun et al., 2010), while others focused on narrowing the parameter search space, and thus 109 110 equifinality reduction, by combining multiple variables for calibration (e.g., Nijzink et 111 al., 2018; Pan et al., 2018). This is confirmed by Figure 1e (in blue), which demonstrates that the vast majority of researches used two variables for calibration (in 112 general, discharge and a RS-derived variable). Within these studies, some analyzed 113 model performance in terms of discharge only, while others considered different 114 variables (Figure 1e, in red), providing a more comprehensive discussion on 115 116 inconsistencies of hydrological models (e.g., Koch et al., 2018; Li et al., 2018).

117 Regarding how RS is incorporated into the model calibration procedure (Figure 1h),118 65.6% of the articles used RS-based spatially distributed information, thus calibrating

the model with distributed objective functions (e.g., pixel-by-pixel or by sub-basin).
Within these studies, bias-insensitive functions have been recently introduced (e.g.,
Koch et al., 2018; Demirel et al., 2018; Zink et al., 2018; Dembele et al., 2020), being
important for reducing the impact of RS data uncertainty on the parameter estimation
procedure. The remaining publications (34.4%) incorporated RS data as an average for
the whole basin.

125 Finally, there is still a need for more studies in tropical regions (especially South America) (Figure 1c), which have particular hydro-climatic characteristics, and so have 126 127 different requirements than temperate regions on model process representation (e.g., snow-related processes might not be so relevant in some tropical areas, whereas an 128 129 accurate representation of floodplains might be). In the case of basin with complex river-floodplain interactions as in the Amazon, an accurate flood wave routing method 130 is required to correctly depict the water transport along the drainage network. Our 131 132 analysis shows that most studies used simple flood wave routing schemes such as kinematic wave or Muskingum (Figure 1g). Only 10.4% attempted to couple hydrologic 133 and river hydrodynamic models, highlighting the necessity of better understanding the 134 applicability of RS-based calibration in basins with major flat regions with wetlands 135 (Hodges, 2013; Neal et al., 2012; Pontes et al., 2017). 136



Figure 1. Summary of the literature review on 62 studies that incorporated RS datasets for parameter estimation in hydrological models (see Table S1 in Supplementary Material). (a) Classification of publications based on the drainage area of study sites (an average value was considered for publications that used multiple study sites); (b) distribution of studies based on the calibration variable; (c) geographical distribution of study sites; (d) number of publications

per year; (e) number of RS products involved in calibration (in black), number of independent
calibration variables (in blue), and number of model outputs evaluated (in red); (f) classification
of models based on their spatial configuration; (g) model type; and (h) use of RS data

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148 **1.2** Aims and Contributions of this paper

149 Our study addresses major knowledge gaps identified in the previous literature review 150 in the context of RS-based calibration of hydrological models. Firstly, most of the 151 studies analyzed two or less variables (Figure 1e). Here, we used RS observations of a number of variables for model calibration, 152 namely soil moisture, large evapotranspiration, terrestrial water storage, flood extent and river water levels, and thus 153 154 move beyond the contributions of RS for improving only discharge estimates. By simultaneously looking at different variables, we also move towards an improved 155 156 representation of the water cycle as a whole, enhancing our ability to identify model 157 limitations and inconsistencies. Furthermore, most studies to date focused on European, 158 temperate watersheds (Figure 1c), which largely differ from tropical basins in terms of 159 hydroclimatic characteristics and river-wetland interactions. In this context, large-scale, 160 coupled hydrologic-hydrodynamic models have faced major developments in recent years (Yamazaki et al 2011, Paiva et al 2013, Fleischmann et al 2020), but to our 161 162 knowledge the complementarity of hydrologic (soil moisture, evapotranspiration, terrestrial water storage) and hydrodynamic (flood extent and river water level) RS 163 164 observations for model calibration has not yet been addressed in the literature. Here we 165 present a study case in a tropical basin with extensive floodplains in the Amazon with a 166 state-of-the-art coupled hydrologic-hydrodynamic model, which together with the previously mentioned advances provide important contributions to the growing 167 168 literature of RS-based calibration of hydrological models. This study aims to investigate

the applicability of multiple RS observations in an accessible approach to model andrepresent the water cycle accurately.

171

172 2 Methods

173 2.1 Experimental design

A hydrologic-hydrodynamic model (MGB; (Collischonn et al., 2007)) is set up for a
case study in the Amazon (Purus River Basin) with a priori parameter sets based on
their variability as reported in literature (references in Table S2). The study is then
divided into two steps.

Firstly, a sensitivity analysis is performed to understand how different parameter sets
(river hydraulic, soil, vegetation) affect model output variables (river discharge, flood
extent, river water level, soil moisture, evapotranspiration and terrestrial water storage).

181 Then, a calibration step is performed in which the model is calibrated with the wellknown MOCOM-UA optimization algorithm (Yapo et al., (1998)) considering six 182 183 variables: (1) in-situ streamflow (one gauge at the basin outlet), and RS freely available, 184 state-of-the-art observations of (2) water level (one satellite altimetry virtual station), (3) 185 flood extent (sum of flooded areas over the Lower Purus River Basin), (4) terrestrial 186 water storage (TWS), (5) evapotranspiration, and (6) soil moisture. Variables (4), (5) 187 and (6) are averaged over the whole basin. The calibration of each variable is performed 188 individually (single-variable), and evaluated for all variables. All calibration 189 experiments are repeated three times with differing initial parameter sets to ensure that 190 convergence is not dependent on the initial parameter sets. Given limitations on the 191 availability of simultaneous RS time coverage, the model is calibrated for one time

period (2009-2011), and evaluated for: (i) the same time period of calibration; and (ii) 192 for a different period (2006–2008 for discharge, flood extent, TWS, ET and 2013–2014 193 194 for water level and soil moisture). To understand how lumped calibration can retrieve 195 the remotely sensed spatial patterns, a qualitative evaluation is provided additionally. A 196 final test is performed in which two multi-variable calibration experiments are conducted: (i) calibration with all analyzed variables, except discharge; and (ii) 197 calibration with two complementary variables (water level and soil moisture), which are 198 199 selected for simultaneous calibration for being complementary and having led to satisfactory calibration performance. 200

201

202 2.2 Study area: Purus River Basin

203 The Purus River Basin (Figure 2) in Amazon has a drainage area of approximately 204 236,000 km², and river discharge ranges from around 1,000 (June-December) to 12,000 205 m^{3}/s (January-July) at Canutama gauge. Because of its large area, it is compatible with 206 the spatial resolution of RS products (e.g., a pixel of GRACE presents spatial resolution 207 of roughly 300-400 km). Purus river has minor anthropogenic influences, which 208 simplifies the modeling process. The climate is equatorial (Figure 2d), and mean annual 209 rainfall is 2147 mm/year (according to in-situ gauges). Purus was selected because of its representativeness of tropical regions as the Amazon basin, which is the largest river in 210 211 the world (Holeman, 1968), and it is characterized by extensive floodplains (Junk, 1997). For instance, on the lower Purus, the floodplain width is in the order of 30 km, 212 213 which corresponds to approximately 30 times the main channel width (Paiva et al., 214 2011). These floodplains allow a satisfactory flood extent monitoring by RS image classification, which contributes to the suitability of Purus River Basin for this study. 215





Figure 2. Study area: Purus River Basin. (a) drainage network (in blue), location of the
discharge gauge (Canutama, triangle in red), tracks of the spatial altimetry mission Jason 2
(dashed black lines), location of the altimetry virtual station (circle, in black), and the area used
for extraction of flood extent (Lower Purus, pink polygons); (b) Hydrological Response Units
(Fan et al., 2015); (c) Bare Earth Digital Elevation Model (O'Loughlin et al., 2016); (d)
Köppen-Geiger Climatic Zones (Kottek et al., 2006).

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225 2.3 Hydrologic-hydrodynamic model: MGB

The MGB ("Modelo de Grandes Bacias", a Portuguese acronym for "Large Basin 227 Model") is a semi-distributed, hydrologic-hydrodynamic model (Collischonn et al., 228 229 2007; Pontes et al., 2017). It was chosen for this study because (1) it has been widely and successfully applied in several South American basins (e.g., Paiva et al., 2013; 230 231 Siqueira et al., 2018); (2) it is representative and similar to other conceptual hydrological models like VIC (Liang et al., 1994) and SWAT; and (3) the hydrological 232 component is tightly coupled to a hydrodynamic routing scheme, allowing the 233 234 simulation of complex flat, tropical basins. Moreover, the source code of MGB is freely available at <u>www.ufrgs.br/lsh</u>. 235

236 Within the model structure, basins are discretized into unit-catchments, which are further divided into Hydrological Response Units (HRU's) based on soil type and land 237 use. Model parameters are specific for each of the HRUs. A vertical water balance is 238 239 performed for each HRU, considering canopy interception, soil infiltration, evapotranspiration, and generation of surface, subsurface and groundwater flows. Soil is 240 241 represented as a bucket model with a single layer. Flow generated in each HRU is routed to the outlet of the unit-catchment with linear reservoirs. Outflow from each unit-242 catchment is then propagated through the stream network by using a 1D hydrodynamic 243 244 model based on the inertial approximation proposed by Bates et al. (2010). The stream 245 network is derived from Digital Elevation Model (DEM) processing. The model has 19 parameters, which are further detailed in the next section. Other model inputs are 246 247 precipitation, climate data, soil type and land use maps, which are further described in section 2.6 Model Setup. 248

249

250 2.4 A priori uncertainty of model parameters

Within MGB model, there are parameters related to vegetation cover (albedo, leaf area index, vegetation height and Penman-Monteith surface resistance), river hydraulics (Manning's roughness, and width and depth parameters related to geomorphological relationships), and conceptual parameters related to soil water budget (Wm, b, Kbas, Kint, XL, CAP, Wc, CI, CS, CB), which are further detailed in Supplementary Material (Table S2). Out of the 19 model parameters, six are fixed and 13 are calibrated.

The a priori uncertainty of MGB model parameters is estimated based on their variability as reported in literature (references in Table S2). Supplementary Material (Table S2) presents the calibration parameters, their initial values, range, and the references that support these assumptions.

262

263 2.5 Sensitivity analysis

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265 In order to understand how different parameter sets (river hydraulic, soil, vegetation) 266 affect model output variables (river discharge, flood extent, river water level, soil moisture, evapotranspiration and terrestrial water storage), multiple model runs were 267 268 conducted considering four uncalibrated model setups: (1) varying only soil parameters; 269 (2) varying only vegetation parameters; (3) varying only hydraulic parameters; (4) 270 varying all parameters together. One hundred runs were conducted in triplicate to ensure 271 that convergence is not dependent on the initial parameter sets, thus resulting in 300 runs for each setup. In this step, no RS-based calibration is performed yet. 272

Parameters were varied considering a uniform distribution, and results were analyzed in
terms of mean RMSD (root mean square deviation) of each variable, by comparing each
run with a reference one (i.e., the initial run with the initial parameter set as defined in

Supplementary Material Table S2). This was performed in order to understand the sources of model uncertainties related to different sets of parameters (e.g., are flood extent estimates sensitive to vegetation parameters, or are ET estimates sensitive to hydraulic parameters?). The dispersion of model outputs was also compared to uncertainty in the observations, as derived from literature.

281 To understand which variables are inter-related in the model, we further analyzed the results of setup "(4) varying all parameters together". This was done by firstly 282 283 computing the Kling-Gupta Efficiency metric (KGE; Gupta et al., (2009)) between the perturbed runs and a reference one (i.e., run with the initial parameter set) for each 284 285 variable, and then calculating the Pearson correlation (r) between KGE values for each 286 pair of variables (e.g., discharge and water level, discharge and flood extent, and so 287 forth). This experiment is relevant to evaluate whether two variables get improved or 288 get worsened together, or whether a variable improvement impacts on the deterioration of another. In other words, this approach allows to evaluate the correlation between the 289 290 variables.

291

292 2.6 Model setup

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The Bare Earth Digital Elevation Model (DEM; O'Loughlin et al., 2016) (Figure 2c) was used for stream network computation and basin discretization with the IPH-HydroTools GIS package (Siqueira et al., 2016). The original DEM resolution is 90 m, and it was resampled to 500 m to facilitate GIS processing. An upstream area threshold of 100 km² was adopted to delineate the drainage network, and unit-catchments were discretized by dividing the stream network into fixed reach length of 10 km, resulting in

2957 unit-catchments for the whole basin. Soil type and land cover maps were extracted 300 301 from the HRU discretization developed by Fan et al. (2015) (Figure 2b): (1) deep and (2) shallow forested areas, (3) deep and (4) shallow agricultural areas, (5) deep and (6) 302 303 shallow pasture, (7) wetlands, (8) semi-impervious areas, and (9) open water, where 304 "deep soils" refer to soils with high water storage capacity, and "shallow soils" are those with low water storage capacity. In the Purus River Basin, 57.4% of the region is 305 covered by forest with deep soils, 26.9% by forest with shallow soils, and 13.7% by 306 307 wetlands (i.e., river floodplains). Daily precipitation data were derived from TMPA 3B42 (version 7), with spatial resolution of 0.25° x 0.25° (Huffman et al., 2007; 308 309 available at: <https://gpm.nasa.gov/data-access/downloads/trmm>), and were interpolated with the nearest neighbor method for the centroid of each unit-catchment. 310 Long term climate averages for mean surface air temperature, relative humidity, 311 312 insolation, wind speed and atmospheric pressure were obtained from the Climatic 313 Research Unit database 2000; available (New et al., at: 314 <<u>http://www.cru.uea.ac.uk/data</u>>), at a spatial resolution of 10', and also interpolated 315 with the nearest neighbor method.

316

317 2.7 Model calibration

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The MOCOM-UA calibration algorithm (Yapo et al., 1998; Multi-objective global optimization for hydrologic models) was adopted due to its satisfactory performance when coupled with hydrological models (e.g., Collischonn et al., 2008; Maurer et al., 2009; Naz et al., 2014). MOCOM-UA is an evolutionary algorithm, based on SCE-UA (Duan et al., 1992), that simultaneously optimizes a model population with respect to different objective functions. The algorithm converges towards the Pareto optimum,

when all points in the population become non-dominated. The model population 325 326 consists of randomly distributed points within the parameter search space, and it reflects the a priori uncertainty of model parameters. Here, the population size was set to 100 327 individuals. The altered model parameters and their respective ranges are described in 328 Supplementary Material Table S2. All calibration experiments are repeated three times 329 (totaling 300 initial runs) with differing initial parameter sets to ensure that convergence 330 331 is not dependent on the initial parameter sets. Initial parameters are set as the mean of 332 their literature-based range (Table S2).

Objective functions to be optimized depend on the calibration setup. In the singlevariable calibration, for each variable, three objective functions (*OF*) that summarize the agreement between simulated and observed (RS) time-series are simultaneously optimized: Pearson correlation (r), ratio of averages (μ_{i}/μ_{obs}), and ratio of standard deviations (σ_{i}/σ_{obs}), which are associated to the individual terms of KGE metric. These 3 objective functions are depicted in Equations 1 to 3, where X denotes the assessed variables (Q, h, A, TWS, ET or W).

340
$$OF_1 = \left(\frac{\mu_{\iota}}{\mu_{obs}}\right)_X (1); OF_2 = \left(\frac{\sigma_{\iota}}{\sigma_{obs}}\right)_X (2); OF_3 = r_X (3)$$

For the multi-variable calibration, the objective functions are the KGE of each variable
considered: firstly, five objective functions were considered (KGE of all variables
except discharge), as depicted in Equations 4 to 8.

344
$$OF_1 = KGE_h(4); OF_2 = KGE_A(5); OF_3 = KGE_{TWS}(6); OF_4 = KGE_{ET}(7); OF_5 = KGE_W(8)$$

Secondly, two objective functions were adopted and simultaneously calibrated (KGE of
selected variables 1 (x) and 2 (y)), as depicted in Equations 9 and 10.

347
$$OF_1 = KGE_x(9); OF_2 = KGE_y(10)$$

Results are expressed in terms of a Skill Score (S) (Equation 11; Zajac et al., 2017), in order to evaluate the improvement (or deterioration) in the representation of a variable when the model is calibrated with a given variable, compared to the uncalibrated setup.

351

$$S = \frac{KGE_{calibrated} - KGE_{initial}}{1 - KGE_{initial}} (11)$$

353

354 KGE_{calibrated} is the mean KGE resulting from running the model with the 355 calibrated parameters. KGE_{initial} is the mean KGE resulting from running the model with 356 the a priori parameter sets (i.e., randomly selected parameters within an a priori range of 357 parameter values).

358

359 2.8 Calibration/Evaluation Data

360 In the next paragraphs we introduce the data used for model calibration and evaluation,

361 as well as how MGB outputs were evaluated in comparison to them.

362 -In-situ discharge measurements were obtained from the Brazilian Water Agency Hidroweb 363 database (available at: <http://www.snirh.gov.br/hidroweb/publico/apresentacao.jsf>), 364 at the gauge "Canutama" (code: 13880000; location: S ° 32' 20.04"; W 64° 23' 8.88"; drainage area: 365 366 236,000 km², period of data availability: 1973 to 2016). Uncertainty in discharge 367 observations can be estimated as ranging from 6.2% to 42.8% at the 95% confidence level, with an average of 25.6% (Di Baldassarre & Montanari, 2009). Discharge was 368 369 evaluated on a daily basis.

- Remotely sensed water level data were obtained from Jason-2 mission, which presents 370 371 an orbit cycle of approximately 10 days, and tracks separated by approximately 300 km at the equator (Lambin et al., 2010). It presents an accuracy of approximately 0.28 m 372 (Jarihani et al., 2013), and data are available since 2008. The virtual station presented in 373 Figure 1 corresponds to Track number 165. Processed data for this study were 374 downloaded from the Hydroweb/Theia database (available at: <http://hydroweb.theia-375 land.fr>). Water level was computed in MGB at the unit-catchment associated to the 376 377 altimetry virtual station, being an advantage of using the hydrodynamic scheme for flood routing instead of the Muskingum simplification. Simulated and RS water level 378 data were compared every 10 days in terms of anomaly (values subtracted from long 379 term average). 380

- Satellite flood extent data were derived from ALOS-PALSAR imagery, which 381 382 presents a ground resolution of 100 m (Rosenqvist et al., 2007). Images were 383 downloaded from Alaska Satellite Facility (available at: <https://www.asf.alaska.edu/>) 384 in processing level 1.5, which already presents geometric and radiometric corrections. A 385 3 x 3 median filter was used to remove speckle noise (Lee et al., 2014). Images were 386 classified into water (backscattering coefficient less than -14 dB), non-flooded forest 387 (between -14 dB and -6.5 dB), and flooded forest (higher than -6.5 dB) classes, 388 according to Hess et al. (2003) and Lee et al. (2014). The uncertainty of flood extent 389 estimates was estimated based on the RMSE between the resulting classification of this 390 study, and the dual-season mapping developed by Hess et al. (2003). Simulated and RS flood extent data were compared for the pink area depicted in Figure 1, in order to avoid 391 spurious flood extent data in regions that are known to be not subject to flooding. 392 393 ALOS-PALSAR presents a recurrence cycle of 46 days (from 2006 to 2011), and flood 394 extent data were available and compared to MGB for 21 dates.

- Satellite-based terrestrial water storage (TWS) anomalies were extracted from 395 GRACE mission, launched in March 2002. GRACE provides monthly TWS estimates 396 based on anomalies in gravitational potential, at a resolution of 300-400 km, with a 397 398 uniform accuracy of 2 cm over the land and ocean regions (Tapley et al., 2004). TWS anomalies were retrieved from three processing centers - GFZ (Geoforschungs Zentrum 399 Potsdam, Germany), CSR (Center for Space Research at University of Texas, USE), 400 and JPL (Jet Propulsion Laboratory, USA), available at https://grace.jpl.nasa.gov/, 401 402 and then the mean value based on the three products was averaged for the whole basin. 403 In MGB, TWS values were computed as the sum of water storage of all hydrological 404 compartments: river, floodplains, soil, groundwater and vegetation canopy. Simulated 405 and RS-based TWS were compared in terms of anomaly (values subtracted from long 406 term average) at a monthly time-scale.

- Satellite-based evapotranspiration estimates were retrieved from the MOD16 product, 407 derived by an algorithm presented by Mu et al. (2011) based on the Penman-Monteith 408 409 equation. The dataset covers the period 2000-2010 with a spatial resolution of 1 km for global vegetated land areas. Because of that, even though MGB evapotranspiration is 410 calculated for flooded areas (open water evaporation in main channel and floodplains) 411 412 and vegetation for water balance purposes, only the vegetation-ET output was compared 413 to MOD16. MOD16 products are provided in 8-days, monthly and annual intervals. Monthly intervals were used here and averaged for the whole basin. Accuracy of 414 415 MOD16 along the Amazon basin is estimated as 0.76 mm/day (Gomis-Cebolla et al., 416 2019). MOD16 is available data at: < 417 https://www.ntsg.umt.edu/project/modis/mod16.php>. In MGB, evapotranspiration is computed via Penman-Monteith equation, based on the climate input variables. 418

- Satellite-based soil moisture is derived from the SMOS mission (Kerr et al., 2001), 419 processed by the Centre Aval de Traitement des Données SMOS (CATDS), and 420 421 downloaded in processing level 4, which combines lower level products with data from 422 other sensors and modeling/data assimilation techniques. The daily L4 root zone soil 423 moisture product at 0-1 m soil depth (Al Bitar et al., 2013) were used (available at: <https://www.catds.fr/Products/Available-products-from-CEC-SM/L4-Land-research-424 425 products>), and data from ascending and descending orbits were averaged for the whole 426 basin. In MGB, soil moisture as a saturation degree was computed as the water in the 427 soil compartment divided by the maximum water capacity of the soil (Wm parameter). 428 Since MGB estimates saturation degree values for a soil bucket reservoir, SMOS values 429 were rescaled for the range 0 - 100% according to the Min/Max Correction method described by Tarpanelli et al. (2013) and applied by some studies (e.g., Rajib et al., 430 431 2016; Silvestro et al., 2015), and them compared to MGB on a daily time-scale as an 432 average for the whole basin.

433

434 **3** Results and discussion

Results are structured as follows. Firstly, the sensitivity analysis is presented with
discussions on model uncertainties (Section 3.1). Then, results for model calibration are
presented, with discussions on how RS-based model calibration can improve discharge
and the water cycle representation as a whole (Section 3.2).

440 **3.1** Sensitivity analysis

441 A sensitivity analysis was carried out to understand how different parameter types (river 442 hydraulic, soil, vegetation, and all together) affect the variation of different hydrological 443 processes in MGB (Figure 3a). This was performed by analyzing the dispersion of six 444 output variables (discharge, water level, flood extent, TWS anomalies, vegetation ET, 445 and soil moisture). These results are also compared with an estimate of the uncertainties 446 of observations (values provided in section *2.8 Calibration/Evaluation Data*), and are 447 discussed in the subsequent sections.



Figure 3. a) Sensitivity analysis of different model output variables to varying sets of
parameters (hyd=hydraulics, soil, veg=vegetation, and all together). The a priori dispersion of
the model parameters, for each output variable, is compared to the reported uncertainty for the
in-situ / RS product estimates, previously described in the Cal/Eval data section (no uncertainty

estimation is provided for the soil moisture root zone product given absence of this estimate for the Amazon region). **b**) Correlation matrix (Pearson coefficient) between performance metrics (KGE) for the six analyzed variables, by varying all parameters together. KGE values are computed by comparing multiple runs with the reference simulation (i.e., the initial run with the initial parameter set as defined in Supplementary Material Table S2). Q = discharge, h = water level, A = flood extent, TWS = total water storage anomalies, ET = vegetation evapotranspiration, W = soil moisture.

461

462 **3.1.1** How do varying model outputs relate to uncertainty in the observations?

Some variables present in-situ/RS observations that have uncertainties significantly 463 lower than the overall dispersion of the model, e.g., 25 % for discharge observations, 464 while model overall parameter dispersion is ~160%. This pattern is also found for water 465 466 level and TWS estimates, and implies that these observations might be useful to 467 constrain the model. Nonetheless, uncertainties in RS products of flood extent (~50%) and vegetation ET ($\sim 23\%$) are in the same order of magnitude of model overall 468 parameter dispersion, which might hamper their contribution for model calibration, due 469 to their high uncertainties. 470

471

472 **3.1.2** Which sets of parameters are related to which variables?

The overall model dispersions are related to different sets of parameters: discharge, water level, and TWS are more strongly related to hydraulics and soil parameters, and to a lesser extent to vegetation parameters. Flood extent estimates are strongly related to hydraulic parameters, and less to soil and vegetation. As expected, soil moisture and vegetation ET estimates relate to vertical water balance processes, being insensitive to hydraulic parameters. Soil moisture (W) is more sensitive to soil parameters, while 479 vegetation ET is more sensitive to vegetation parameters. These results are very useful 480 to understand the RS-based calibration experiments addressed in section 3.2. For 481 instance, if model calibration with ET or W is achieved through optimization of 482 hydraulic parameters, it would highlight that the model would have "gotten the right 483 results for the wrong reasons". The same would occur if flood extent calibration 484 targeted soil or vegetation parameters.

485

486 3.1.3 Which variables are inter-related?

487 By varying all parameters together, there is a high correlation (greater or equal to 0.4) between the performance of discharge and flood extent, water level and flood extent, 488 flood extent and TWS, and ET and TWS (Figure 3b). High correlations between 489 490 discharge, water level and flood extent are expected because of their strong association through river transport processes. However, correlation between discharge and water 491 492 level is not too high (0.30), and this is probably due to high uncertainties in hydraulic 493 parameters, and to the large distance separating the water level virtual station and the 494 streamflow gauge. Furthermore, high correlations between TWS and flood extent might 495 be related to surface water storage dynamics which are especially relevant in regions 496 with floodplains.

In general, a high correlation between variables in Figure 3b should be reflected in positive results when calibrating with a given variable and evaluating with the other highly correlated variable (single-variable calibration). This may also indicate that observations of these variables are redundant if used simultaneously in a multicalibration framework. However, high correlations in Figure 3b followed by deterioration after the single-variable calibration process might indicate structural errors in the model, or in the observations. We stress however that this study did not attempt to quantify structural errors. Conversely, low correlations in Figure 3b, followed by
improvement in performances with the calibration with multiple variables, might
indicate complementarity between variables.

507

508 3.2 Model calibration

509

510 3.2.1 How RS-based model calibration improves discharge estimates?

For the evaluation time period (2006-2008 for discharge, flood extent, TWS, ET and 511 512 2013–2014 for water level and soil moisture), calibration with all RS products led to 513 improvements in discharge estimates (Figure 4a). For the calibration time period (2009-514 2012), TWS, ET and soil moisture RS products also led to improvements in discharge 515 estimates, while water level and flood extent led to discharge overestimation in wet 516 periods (Figure 4a). This could be due to high uncertainties in the observations (Figure 517 3a), but if this was the case, it would also be reflected in a poor performance for water 518 level and flood extent when discharge is the target variable for calibration (Figure 4b). which does not occur. Therefore, calibration with discharge leads to reasonable 519 520 parameter sets for the performance of discharge itself, and also water level and flood 521 extent. However, it does not lead to the best hydraulic arrangement, which might be 522 achieved more successfully when calibrating with water level or flood extent.

523 Nonetheless, both water level and flood extent observations are representative of a 524 specific location in the basin (Figure 2), and calibration with these variables might lead 525 to the best parameter arrangement for these locations, but not for the whole watershed. 526 A more spatially-consistent use of these observations should improve their usability to 527 constrain models and improve discharge estimates, such as the studies of Kittel et al. (2018), that used radar altimetry measurements at 12 locations in the basin, Schneider et
al. (2017), that used data from 13 virtual stations, or Liu et al. (2015), that used water
level measurements at four virtual stations, and flood extent for stream segments at
different locations in the basin.

RS variables as TWS, ET, and soil moisture were able to improve discharge estimates 532 533 by S =13.7% (KGE_{cal}=0.36), S= 52.9% (KGE_{cal}=0.64), and S = 27.0% (KGE_{cal}=0.45) (Figure 5-I, calibration period) or S = 27.4% (KGE_{eval}=0.52), S = 6.1% (KGE_{eval}=0.37), 534 535 S = 12.3% (KGE_{eval}=0.43) (Figure 5-II, evaluation period), which is especially relevant 536 in the context of the Prediction in Ungauged Basins initiative (Hrachowitz et al., 2013; 537 Sivapalan et al., 2003). These results agree with previous studies, such as López et al. (2017) that found good performances in discharge estimates by model calibration with 538 539 GLEAM ET and ESA CCI soil moisture, or Nijzink et al. (2018), that found improvements in discharge by using soil moisture products (AMSR-E, ASCAT) and 540 541 TWS from GRACE.

542 The multi-variable calibration experiment considering all variables except discharge 543 (Figure 5b) resulted in a Skill Score of S = 17.4% (KGE_{eval}=0.45) for discharge in the evaluation period. This is relevant for estimating discharge in poorly gauged basins. 544 545 Nonetheless, for the calibration period, Skill Score had a low value (S = 1.7%, KGE_{cal}=0.25), reflecting some limitations when retrieving discharges, probably because 546 547 of potential trade-offs between variables (Koppa et al., 2019). RS uncertainties can be reduced in model calibration, for instance by using bias-insensitive metrics (e.g., 548 Demirel et al., 2018; Zink et al., 2018; Dembele et al., 2020), or explicitly including 549 them into the objective functions (Aires, 2014; Croke, 2009; Foglia et al., 2009; Peña-550 Arancibia et al., 2015). 551



a) Calibration with single variables / Evaluation with discharge

553 Figure 4. (a) Daily time series of discharge, when calibrating the model with six different 554 variables. (b) Time series of the six variables when calibrating the model with discharge 555 observations only (discharge, water level, flood extent and soil moisture are at a daily time step, 556 while TWS and ET are at a monthly time step). KGEini is the mean KGE of initial runs, 557 KGEcal is the mean KGE of calibrated runs, evaluated for the same period of calibration, 558 KGEeval is the mean KGE of calibrated runs, evaluated for a different period than calibration. 559 Time series for all variables by calibrating the model with all setups is presented in 560 Supplementary Material (Figure S1).

561



I) Evaluation for the period of calibration

563 Figure 5. Boxplots of mean KGE for the evaluation of multiple variables with different

calibration strategies. (I) Evaluation for the period of calibration (2009 – 2012); (II) Evaluation

for a different period than calibration (2006 - 2008 for Q, A, TWS, ET; 2013 - 2014 for h and

- 566 W). "Initial guess" refers to model runs with the a priori parameter sets. (a) Single-variable
- 567 (discharge, water level, flood extent, TWS, vegetation ET, soil moisture) and (b) multi-variable

calibration (all except discharge, water level + soil moisture). The spread of the values in the
boxplots stems from 300 model runs (100 for each of three calibration experiments). Numbers
next to the boxplots represent Skill Score (%). Colors refer to classes of skill score. Please note
that the KGE scales are different for each variable. Asterisks refer to cases when the evaluation
period resulted in a different performance than the calibration period (i.e., positive Skill Score in
calibration followed by negative Skill Score in evaluation, or vice-versa). Please note that Skill
Score values are computed based on mean values, while the boxplots depict median values.

575

576 **3.2.2** How does RS-based model calibration improve the water cycle

577 representation?

When performing a single-variable calibration, the performance of the variable itself 578 579 always improves, which is evidenced by the positive values in the main diagonal 580 (Figure 5-I-a, for calibration period, and Figure 5-II-a, for evaluation period). 581 Calibration with water level was also able to improve estimates of flood extent, TWS, 582 ET and soil moisture (cal period), and all variables (eval period). Calibration with flood 583 extent improved water level, TWS, ET and soil moisture. Calibration with TWS improved all variables. Calibration with ET was able to improve discharge and flood 584 585 extent. Calibration with soil moisture improved all variables but ET. Results for 586 calibration and evaluation periods agree (i.e., improvement (positive Skill Score) or deterioration (negative Skill Score) for both cal and eval) in 43 out of the 48 cases 587 (89.6%). In the five remaining cases (10.4%), results between calibration and evaluation 588 589 periods differ: three of them are in the evaluation with TWS, and two of them are in the 590 discharge evaluation (calibration with water level and flood extent).

591 In the best modeling scenario, calibration with any variable should improve the 592 performance of all other variables. However, we have identified that this did not happen

in our experiments. This can be due to uncertainties in model structure, in 593 parameterization, in the observations, or the integration techniques in model calibration 594 595 (Dembele et al., 2020). Previous studies have also found significant advantages in using 596 RS-based model calibration to identify structural model issues (e.g., Werth et al., 2009; 597 Willem Vervoort et al., 2014; Winsemius et al., 2008), detect uncertainties in input data (e.g., Milzow et al., 2011), identify deficiencies in model parameterization (e.g., Franks 598 599 et al., 1998; Koppa et al., 2019), or increase model reliability (e.g., Koch et al., 2018; 600 Manfreda et al., 2018).

601 According to Figure 4b and Supplementary Material (Figure S1), calibration with 602 discharge improved estimates of almost all variables. However, calibration with discharge deteriorated the performance for vegetation ET time series. Vegetation ET 603 estimated by MOD16 varies at maximum 30mm/month. MGB calibration with 604 605 discharge led to ET variations of 100 mm/month, reaching around 30 mm/month in the 606 driest periods, while MOD16 estimates are limited to a minimum of 100 mm/month in 607 these periods (time series in Figure 4b). However, one can notice that not even the 608 seasonality between MGB and MOD16 time series agree. This could be due to relatively high uncertainties in vegetation ET estimates from MOD16 for the Amazon 609 610 basin (around 23 mm/month, according to Gomis-Cebolla et al., 2019). Nonetheless, it 611 could also be related to model structural and/or parameter deficiencies, in which case the model might be "right for the wrong reasons". In order to identify the source of this 612 613 ET inconsistency, we have compared MOD16 and MGB results to in-situ measurements 614 of ET in Purus River Basin, provided by Gomis-Cebolla et al. (2019) and Maeda et al. 615 (2017). We found a much stronger agreement both in seasonality and in amplitude of in-616 situ observations with MOD16 observations than with MGB model output. Hasler & 617 Avissar (2007) and Pan et al (2020) have already warned about the overestimation of

dry season water stress in hydrological models, probably related to 618 the 619 misrepresentation of soil water availability for plants. This was also found by Maeda et 620 al. (2017), which highlighted that ET was not water-limited because of the plants' 621 access to deep soil water, which has also been previously documented by Nepstad et al. 622 (1994). They found that, in the Southern Amazon ecotone, deep root water intake plays a key role in maintaining ecosystem productivity during dry season. MGB model is 623 probably misrepresenting these processes, which would remain unknown if it were only 624 625 compared to discharge time series.

Even though the calibration with discharge observations was not able to accurately estimate ET, calibration with the remaining variables (except for soil moisture) was able to improve ET estimates. For instance, in Figure 3b, ET and water level presented low correlation (r = 0.08), but calibration with water level improved ET estimates by S =16.9% (cal period) and S = 25.6% (eval period). However, in Figure 3b, ET and TWS presented high correlation (r=0.47), but calibration with TWS improved ET estimates by only S = 7.9% (cal period) and S = 13.1% (eval period).

633 In general, calibration with TWS did not present much influence on any of the variables. 634 In spite of some improvements, skill scores were usually low. Consistently, TWS 635 estimates got relatively easily improved by calibration with any variable (except for ET, for cal period; or discharge, for eval period). These results for TWS contrast with 636 637 previous work from Lo et al. (2010), Nijzink et al. (2018), Rakovec et al. (2016), 638 Schumacher et al. (2018), and Werth & Güntner (2010), which highlighted the value of 639 GRACE data when incorporated into hydrological modeling. This can be due to the 640 high seasonality of Purus River Basin, in which TWS does not aggregate much information, biasing the calibration with high correlation values. Even for the initial 641 guess (uncalibrated) setup TWS performances were already very good: KGE values 642

were around 0.8, while for all other variables, except for ET (for which KGE valueswere negative), KGE values were around 0.3 for the uncalibrated setup.

Flood extent and water level performances were improved by calibration with discharge, water level and flood extent, but it did not affect much ET (which actually was degraded with discharge calibration) and soil moisture. This is probably due to the relationship between water level and flood extent with river transport processes (e.g., flood routing and floodplain storage), while ET and soil moisture are more related to vertical hydrological processes (e.g., soil water balance). This highlights the complementarity between variables that relate to different processes.

652 Calibration with soil moisture improves performances of all variables (water level to a
653 lesser extent), except for ET. Consistently, calibration with all variables (except ET) are
654 able to improve soil moisture to some extent.

655

656 3.2.3 What is the added value of complementary RS observations?

657 By calibrating with all variables together except Q (Figure 5b), we found improvements 658 for almost all variables, with the most significant improvements for flood extent (S =659 25% for cal and eval periods) and ET (S = 20% for cal and eval periods). For discharge, performance for the evaluation period was improved (S = 17.4%), which is important 660 661 for estimating discharge in poorly gauged basins. However, for the calibration period, Skill Score for discharge performance was S = 1.7%, which might reflect some 662 663 limitations in retrieving discharge based on the calibration of the RS-derived variables, 664 as discussed previously.

665 Therefore, we chose a specific arrangement of two complementary variables in order to666 check if this calibration setup might lead to better retrievals for discharge and the other

variables. The chosen variables were soil moisture and water level, because of their
complementarity. Based on the Skill Score values in Figure 5-I, calibration with water
level only improves all variables but discharge (and soil moisture to a lesser extent),
while calibration with soil moisture only improves all variables, but ET (and water level
to a lesser extent).

672 The calibration arrangement of water level and soil moisture led to improvements not 673 only to soil moisture and water level themselves, but also to all other variables (ET to a 674 lesser extent). For instance, flood extent was improved by S = 52.6% and S = 34.1%(cal and eval period, respectively). Discharge was improved by S = 59.9%, with a 675 resulting mean KGE = 0.70 for the calibration period (S = 45.0% and mean KGE = 0.35676 677 for evaluation period). These results agree with previous works that found an 678 improvement in model performances by multi-variable calibration of soil moisture and 679 evapotranspiration (e.g., Koppa et al., 2019; López et al., 2017), discharge and 680 evapotranspiration (e.g., Herman et al., 2018; Pan et al., 2018; Poméon et al., 2018), 681 discharge and soil moisture (e.g., Li et al., 2018; Rajib et al., 2016), discharge and TWS (e.g., Rakovec et al., 2016; Schumacher et al., 2018; Werth & Güntner, 2010), and 682 discharge and water level (e.g., Kittel et al., 2018; Schneider et al., 2017; W. Sun et al., 683 684 2012). However, it is difficult to compare this study to previous works, because most of 685 them used discharge observations as constraints. In this study, we avoided the use of 686 discharge observations for multi-variable calibration, in order to analyze the 687 applicability of the RS-based calibration method for poorly-gauged regions.

688 Calibration with water level and soil moisture did not present much influence on ET 689 performance, because of the specificities regarding ET in this watershed, i.e., given that 690 the model setup does not represent deep root water intake during dry season, as 691 discussed previously. By comparing the two frameworks for multi-variable calibration (all except Q versus
h+W calibration), we found that calibration with all variables except Q is useful to some
extent, but consistently selecting complementary variables for model calibration
resulted in best overall performance.

696

697 3.3 Are we getting the right results for the right sets of parameters?

698 When analyzing the dispersions of parameters before and after calibration with each 699 variable (Figure 6 for a few selected parameters, Supplementary Material Figure S2 for 700 all calibrated parameters), it can be observed that the range of parameters varies largely depending on the calibration variable. For instance, Wm is a soil conceptual parameter 701 related to maximum water storage in the soil. In the calibration based on single 702 703 variables (except ET) it converged to low values (300 mm), while in the calibration with ET it reached high values (2000 mm). This probably occurred in order to compensate, 704 705 by overparameterization, a structural error in the model, i.e., the model inability to 706 represent deep root water uptake in dry season. These trade-offs between model 707 parameters during calibration has also been reported and discussed by Koppa et al. (2019). 708

The surface resistance parameter also resulted in a wide range of values depending on the calibration target variable. When calibrated with water level, flood extent, or 'all except Q' experiments, it reached median values higher than 150 s/m, but calibration with h+W led to median values lower than 50 s/m. Surface resistance is a vegetation parameter directly related to ET dynamics, so it is important to note that calibration with ET was able to reduce the dispersion of this parameter, reaching a median value of about 80 s/m (similar to calibration with Q and W). Another interesting result relates to channel Manning's coefficient, which presented different values for each calibration experiment. This agrees with previous findings about Manning parameter being often used as an effective parameter that compensates for neglected hydrodynamic processes as localized channel head losses, poor cross section representation, or non-represented 2D processes (Neal et al 2015).

721 Many previous studies have highlighted the use of multi-variable calibration to narrow 722 parameters' search space (Nijzink et al., 2018; W. Sun et al., 2018), but this was not 723 observed in our results. Based on the limited multi-variable calibration experiments performed here ('all except Q' and h+W), no narrowing in parameters' search space 724 725 was found. For most parameters (except for Wm), calibration with 'all except Q' and 726 h+W resulted in a wide range of values. This can be due to differing convergence sets of 727 parameters between each of the triplicate runs. A more robust experiment comparing 728 more multi-variable calibration strategies (e.g., Q + different R-based variables) might provide better understanding on this topic. 729



Figure 6. Boxplots of dispersion of three model parameters before (Initial) and after the singlevariable calibration (Q – discharge; h – water level; A – flood extent; TWS – total water
storage anomalies; ET - vegetation ET; W – soil moisture), and multi-variable calibration (All
– variables except discharge; h+W – water level and soil moisture). The spread of the values in
the boxplots stems from 300 model runs (100 for each calibration experiment). Description of

parameters is presented in Supplementary Material Table S2. A complete figure with boxplotsfor all parameters is presented in Supplementary Material Figure S2.

739

740 3.4 Spatial Evaluation

For model calibration, we used one streamflow gauge for discharge, one virtual station for water level, and averaged RS data for the whole basin for TWS, ET and soil moisture. However, many recent studies investigated the potential for using RS spatially distributed information in model calibration, for instance with bias-insensitive metrics (Demirel et al., 2018; Zink et al., 2018; Dembele et al., 2020). Here we further analyze how the lumped calibration affected the simulated spatial patterns (Figure 7; Figure S3 in Supplementary Material).

748 For discharge, water level, flood extent and TWS, spatial patterns are well reproduced even when running the model with the initial parameter set, because the spatial patterns 749 750 of these variables are determined by intrinsic characteristics of the basin. Nonetheless, 751 for ET, the spatial patterns are completely different between the initial parameter set and 752 the calibrated setup. In this case, the calibration with spatially aggregated ET was able 753 to recover the spatial representation of MOD16. A similar result was found for soil 754 moisture spatial representation by Demirel et al. (2019), that calibrated a model with spatially aggregated soil moisture and TWS data. 755

756 In summary, these results highlight the overall model capability to retrieve the ET 757 spatial pattern even by using a lumped calibration approach. However, for other 758 variables, the spatial pattern was not considerably affected by the differing model 759 calibration strategies.



Figure 7. Spatial distribution of variables. Columns: RS observation, model run with the
initial parameter set, model run with the best parameter set (calibrated for each
variable), model run with the best parameter set (when calibrated with discharge).
Complete figure is presented in Figure S3 (Supplementary Material).

769 4 Conclusion

We calibrated and evaluated a hydrologic-hydrodynamic model with five different RSbased observations of the water cycle: water levels (Jason-2), flood extent (ALOS-PALSAR), TWS (GRACE), vegetation ET (MOD16), and soil moisture (SMOS), for a study basin in a tropical region with floodplains (Purus River Basin in the Amazon), and analyzed the redundancy and complementarity between different variables and processes.

776 Results showed that calibration with current RS observations was able to improve discharge estimates. For instance, in the uncalibrated setup (a priori parameter sets), 777 778 average performances for discharge were around KGE = 0.30. By calibrating the model with ET from MOD16 (and evaluating for the same time period), discharge average 779 performance was improved to KGE = 0.64, representing a Skill Score of S = 52.9%. 780 Also in the calibration period, a joint scheme of calibration with water level + soil 781 moisture led to discharge improvements of S = 59.9%. When evaluating for a different 782 783 time period, discharge performance was improved by calibration with water level, TWS and a joint scheme of all RS-variables (S = 25.9%, S = 27.9% and S = 17.4%, 784 respectively). We conclude that RS observations are useful to predict discharge 785 estimates. However, the utility of each RS variable might depend on the study area 786 787 characteristics and the time period considered.

Our results also showed that RS-based calibration led to an overall improvement of the water cycle representation. For instance, calibration with water level was able to improve estimates of water level itself, but also flood extent, TWS and ET; calibration with soil moisture was able to improve estimates of soil moisture itself, but also discharge, flood extent and TWS. Moreover, calibration with multiple RS variables was able to highlight deficiencies that might be related to model structure, parameterization, observations, and data integration techniques in model calibration. In the context of model structure, for instance, calibration with ET highlighted the model inability to represent the root water intake in dry season in this region, thus compensating it by misrepresenting other variables. In the context of model parameterization, for instance, we found a wide range of different parameters by varying the calibration target variable.

Besides individual calibration with each RS variable, we conducted two multi-variable calibration experiments: calibration with all variables except discharge, and calibration with water level and soil moisture. Calibration with all variables was useful to some extent, but appropriately selecting complementary variables for model calibration may result in a better overall performance. Even though we used a lumped calibration approach, results highlighted the overall model capability to retrieve ET spatial pattern, but not for TWS and soil moisture.

807 The main conclusions presented here are of great interest for the hydrological 808 community, and agree with previous works in that RS-based calibration is useful to 809 improve the water cycle representation in hydrological models. To further investigate 810 the potentiality of RS data, future developments should test the methodology presented here for multiple basins at contrasting hydro-climatic regions. Here, we assessed an 811 812 Amazonian Equatorial basin, with particular climate and land cover characteristics and an overall spatial homogeneity of rainfall-runoff processes. Other basins with different 813 hydroclimatic regimes could be also assessed, e.g., in arid basins subject to long dry 814 815 periods, more erratic precipitation patterns, and different runoff generation mechanisms 816 than the Amazon, which require different model structures.

Finally, here we used one state-of-the-art RS product for each variable, but future
developments should explore other missions like SWOT for surface water observation
(Biancamaria et al., 2016), as well as considering different products for representing
each variable (e.g., ET could be estimated by GLEAM, MODIS, SSEBop, SEBS,
ALEXI, METRIC, etc., besides MOD16).

822

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