

How can Distributed Hydrological Models Inform Decision Making? Multi-Site Calibration of SWAT for a Large Brazilian River Basin

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Key Points:

- We set up a hydrological model coupled to a GIS for a large basin (> 25,000 km²).
- The multisite adjustment strategy was efficient.
- It was possible to adjust the model for subbasins without flow monitoring stations.

Abstract

Although there are numerous modeling tools available for managing water resources, they tend to focus on relatively small watersheds ($<25,000 \text{ km}^2$) and evidence is scarce regarding their applications to large watershed management and planning. The use of hydrological modeling tools in decision making is particularly challenging in large tropical countries such as Brazil. Here we tailored and customized SWAT (Soil and Water Assessment Tool) calibration, validation and sensitivity analysis for large Brazilian watersheds ($>25,000 \text{ km}^2$). Our results show that customized SWAT calibrations successfully simulated flow behaviors across the Rio das Velhas basin, which contains heterogeneous landforms and land uses. The multisite calibration method was adopted because of the large basin area and the availability of flow monitoring stations. As a result of the multi-site calibration, specific regionalized parameters were obtained for each group of sub-basins. Our results showed a good adjustment of the model. NS (Nash & Sutcliffe coefficient) values were 0.73 - 0.97 (calibration) and 0.51 - 0.98 (validation). PBIAS (% bias) was 11.3 to 19.4 (calibration) and -18.6 to 24.6 (validation) and R^2 values were >0.6 in all sub-basins. We conclude that hydrological models coupled with GIS facilitates simulating complex hydrological processes and can improve decision making by Brazilian water resource managers.

1 Introduction

Water management is high on environmental and political agendas (Loch et al., 2020; Lund, 2015). Water provision and water flow regulation directly affect human well-being, particularly across tropical biomes in the Global South (Yan et al., 2020). However, planning and governing tropical landscapes for effective water management in tropical countries is very challenging for several reasons (Haberlandt, 2010; Ponette-González et al., 2015; Souffront Alcantara et al., 2019). First, hydrological cycles encompass a diversity of complex processes that together influence the physical, chemical, biological, and ecological processes. This raises challenges for estimating variations of water-related services across different scales, both geographical (grain and extent) and temporal (dry, and rainy seasons), to inform policymaking and water governance. Second, vegetation cover influences processes in the water cycle through its structural effects on key ecosystem functions in watersheds (Ponette-González et al., 2015) and tropical countries such as Brazil have been experiencing unprecedented land use changes (Souza et al., 2020). Land Use Cover Change (LUCC) influences watershed evapotranspiration regimes, changing retention of precipitation in forest canopies, soil infiltration capacity, and the volume and timing of water runoff (Fletcher et al., 2013; X. Yang et al., 2012). Third, although hydrological modeling integrated with GIS are important tools for dealing with complex processes in highly dynamic land uses across continental extents such as Brazil, there are still issues to overcome to incorporate hydrological modeling in policymaking. Particularly challenging is the use hydrological models for large watersheds and for exploring future scenarios that assist decision making on water resource management in the medium to long term. To explore the consequences of land use change driven by increasing demand for agricultural products, land cover maps for 2050 have been developed. In Brazil, agricultural scenarios include SIMBRASIL (<http://csr.ufmg.br/simbrasil/>) and the Brazilian Land Use Model (BLUM). These spatially explicit estimates of land use patterns for future decades can be used for exploring impacts of land cover patterns on water management.

Hydrological models are widely acknowledged as important decision-support tools among hydrologists (Devia et al., 2015). However, it remains to be demonstrated that they can deliver robust estimates and be performed via relatively simple and straightforward calibration procedures before being widely accepted by governmental bodies and water planning institutions (Haberlandt, 2010; Ponette-González et al., 2015). Three issues still need to be overcome. 1) What are the most appropriate modeling tools and algorithms for targeting specific hydrological processes (runoff, sediment load, etc.)? 2) What are the most appropriate available data for meeting specific model data demands? 3) How does one develop a step by step calibration procedure that effectively estimates processes, but is also feasibly integrated into routine water management institutional practices? Thus, a multi-site calibration, which consists of using two or more fluvimetric stations to calibrate the model, is a strategy that can achieve better results versus models based on one station (C. W. L. de Andrade et al., 2019; Wi et al., 2015). To do so, hydrological models integrated into geographic information systems (GIS) have been widely used in recent years (Khalid, 2018; K. De Mello et al., 2020; Schumann et al., 2000; Schuol et al., 2008). Several improvements have been developing with this integrated approach (Schumann et al., 2000): 1) River basins are characterized by their variations in lithology, morphology, soils and land covers. 2) The estimates of conceptual model parameters are more precisely and accurately quantified. 3) Models are parameterized by sub-basins. 4) Model operations are simplified to make them more widely applicable.

SWAT (Soil and Water Assessment Tool) is a distributed model used worldwide in different contexts. It has been used for estimating soil erosion susceptibility in India by comparing different multicriteria decision-making methods (MCDM) (Bhattacharya et al., 2020). It has been applied to aid understanding the sources and drivers of microbial water quality (Sowah et al., 2020). It is employed for identifying critical erosion-prone areas and selecting best management practices (BMPs). However, most studies using SWAT have focused on relatively small basins, with 20% of studies conducted in basins $<15 \text{ km}^2$, 71% in basins $<1,000 \text{ km}^2$, and only 9% in basins $>10,000 \text{ km}^2$ (Bressiani et al., 2015). In Brazil, SWAT has been used since the 1990s. Between 1999 and 2013 over 100 academic studies used SWAT for exploring its ability to capture the complexity of hydrological processes at basin scales (Bressiani et al., 2015). Despite the large extents of many Brazilian river basins, SWAT has been used mostly in small to medium size watersheds ($2,000 - 16,000 \text{ km}^2$) (Almeida et al., 2018; Pereira et al., 2016). Considering that the management of water resources in Brazil is carried out through large hydrographic basins (average size $\sim 20,000 \text{ km}^2$; ANA, 2020), few studies covered large and heterogeneous basins. Furthermore, when SWAT models were used for large basins the foci were hydropower production (Serrão et al., 2021), water management in drought and high-flow periods (Santos et al., 2018; da Silva et al., 2018), or irrigated agriculture (de Souza Dias et al., 2018). Few studies used SWAT for evaluating land cover change in Brazilian basins (M. P. de Andrade & Ribeiro, 2020). Therefore, there is a need to demonstrate how SWAT can be used for assessing large watersheds as well as land use changes in Brazil.

One essential issue is to customize the highly time consuming and data demanding calibration approaches to facilitate and enhance the robustness of SWAT estimates from small to large geographical extents. This is critical for enhancing SWAT predicting performance as well as for making it possible for water management agencies to consider SWAT cost-effective enough to use hydrological modeling approaches as planning tools. Because of inherent complexities with data availability and model calibration approaches, hydrological modeling in support of water resource planning and management is rare in Brazil (Bressiani et al., 2015).

Calibration issues are particularly problematic in Brazil because of the existing GIS data, such as the coarse scale of soil, lithology and geomorphology maps and the heterogeneity and varying resolution of the mapped hydrographic network. Also, there are relatively few complete hydrological data collection stations for a nation the size of Brazil (K. De Mello et al., 2020). In addition to data issues, there is still the need to explore which calibration approaches likely will make SWAT more robust and appealing to planning and managing large watersheds.

To fulfill these research gaps, the objective of this study is to explore how a distributed and continuous hydrological model coupled with GIS such as SWAT can be used for estimating the dynamics of surface runoff in a heterogeneous and large hydrographic basin ($>25,000 \text{ km}^2$). We particularly aim at exploring how multisite calibration approaches can enhance the performance of runoff estimates in a large basin. We then customize a calibration approach for making SWAT more appealing for use in decision making for large basins in tropical environments.

2 Materials and Methods

2.1 Study area

SWAT coupled into GIS was used to simulate hydrological processes in the Rio das Velhas basin. The study area covers $27,850 \text{ km}^2$ in Minas Gerais state (Brazil) and its tributaries drain water from 51 municipalities (Figure 1). The basin covers most of the Belo Horizonte Metropolitan Area (RMBH), which is the third-largest metropolitan area in Brazil (IBGE, 2020), with approximately 4.8 million inhabitants, which represents 25% of the population of the State of Minas Gerais and 32% of the population of the São Francisco basin (IBGE, 2010, 2020).

This basin covers parts of the Atlantic Forest and Brazilian Savana biomes. Most of the climate in the region is characterized as tropical, with annual average temperatures between 18°C and 22°C , annual total rainfall $\sim 1500 \text{ mm}$ and a five-months dry season (Alvares et al., 2013). There are four geomorphological units in the basin: São Franciscana Depression, São Francisco Plateaus, Quadrilátero Ferrífero (Mountain Range) and Espinhaço Meridional Mountain Range (CETEC, 1983). The most prevalent soil types are Argisols but Latosols, Neossols, Cambisols, Plintossolo and Gleissolo are present (IBGE, 2018). The land use and land cover (LULC) is predominately pasture ($\sim 27\%$), followed by Forest-Evergreen ($\sim 24\%$), Range-Grasses ($\sim 15\%$), Agricultural Land-Generic ($\sim 14\%$) and Range-Brush ($\sim 12\%$). Urban infrastructure occupies about 2% of the total area (Souza et al., 2020).

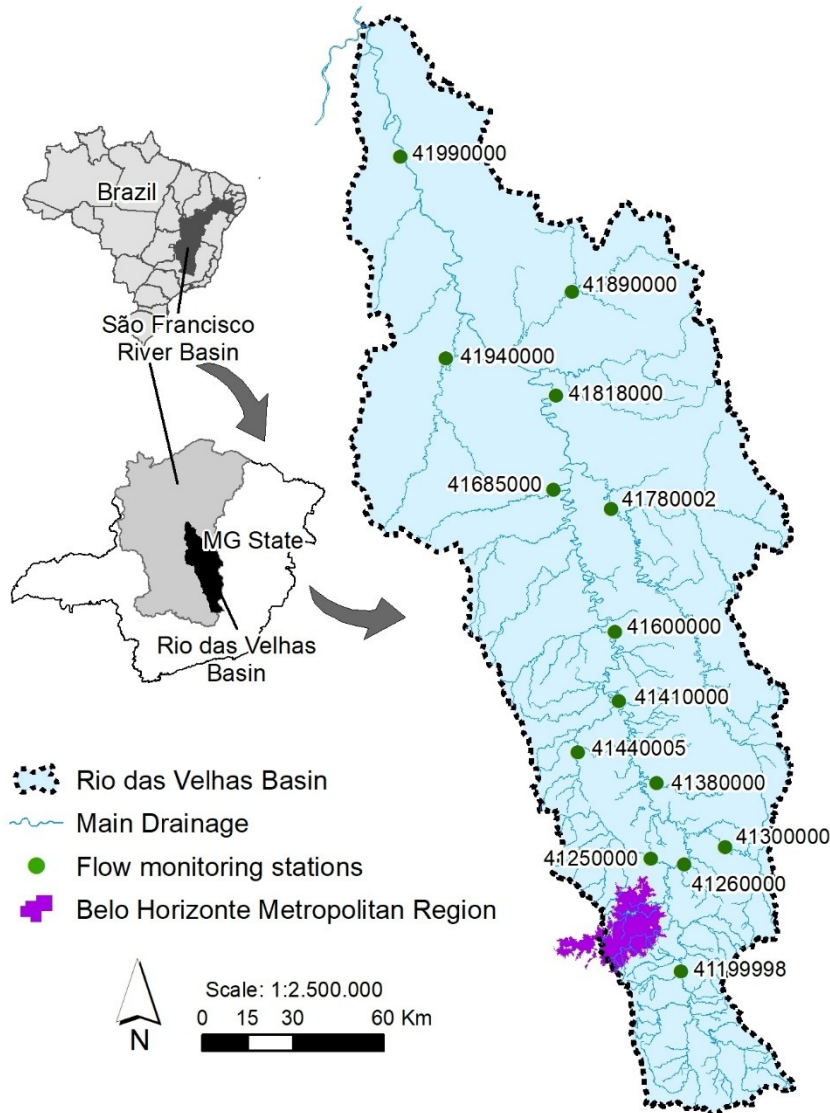


Figure 1. The Rio das Velhas basin & its flow monitoring stations sites.

2.2 Inputing data

We calibrate and test SWAT model using the flow series (1993-2015) obtained from 15 flow monitoring stations available at ANA's HIDROWEB (ANA, 2020) (Table S1; see Figure 1). Simple regression models were used to fill the gaps in the flow series, in the form of potential regression, as recommended by Euclides et al. (1999) (Table S2).

The model used information from four environmental dimensions: climate, relief, soils and land use and cover (Figure 2). The climatic data used in this work were obtained through the analysis of historical series using 5 weather stations (temperature, humidity, solar radiation, wind speed and precipitation) of the National Institute of Meteorology (INMET, 2020) and 29 rainfall stations (daily data from 1993 to 2015) of the National Water Agency (ANA, 2020) (Table S3; Figure 2a). The gaps were filled using the atmospheric state generator model developed for the United States (WXGEN model; Sharpley and Williams, 1990). Therefore, to be applied in the study area, it was necessary to calculate different parameters (Table S4) of atmospheric state and

format them to input to the SWAT model. The relief features (Figure 2b) were taken from the digital elevation model (DEM) generated by the Shuttle Radar Topographic Mission (~30m; USGS, 2015). The land use and cover map (Figure 2c) was generated from the pixel-by-pixel classification of images from Landsat satellites with 30m resolution (Souza et al., 2020). The original land use map classes were made compatible with the SWAT database, resulting in the following land use classes: Agricultural Land-Generic, Barren, Eucalyptus, Forest-Evergreen, Industrial, Pasture, Range-Brush, Range-Grasses, Residential-Medium Density, Wetlands-Non-Forested, and Water (Table S5). The soil characterization (Figure 2d) was obtained through the Brazilian soil map (scale 1:250,000; IBGE, 2018) that was complemented with soils physical-hydro characteristics classified through a survey conducted by experts (Mello et al., unpublished data; Table S6). The GIS data input was inserted in the SWAT model through use of the ArcSWAT module

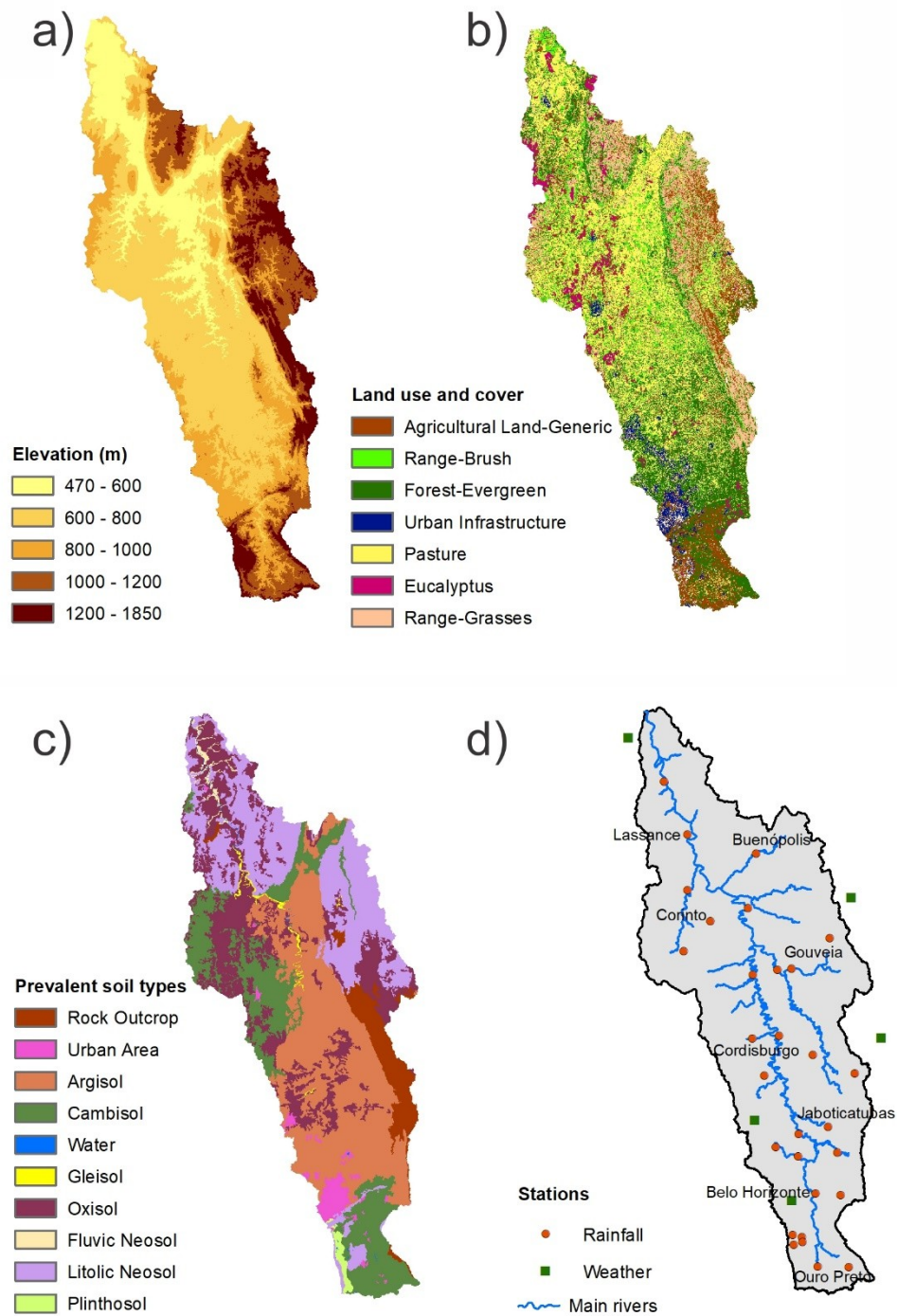


Figure 2. Inputs for SWAT a) topography, b) land use classes, c) soil types and, d) weather stations.

2.3 Hydrological modeling

The entire basin was divided into sub-basins and the confluence of rivers generated through the DEM and by the use of the flow measurement points (each flow monitoring station was assigned as a river mouth sub-basin). The establishment of the minimum contribution drainage area and the size of sub-basins was based on the preliminary tests and recommendations by Jha et al. (2004): minimum drainage area should be between 2% to 5% of the total area for basins between 2,000 km² and 18,000 km², so we used the value of 200 km² (about 1% of the area). Thus, nearly half the sub-basins, particularly those on the mainstem Rio das Velhas and its major tributaries, receive flows from upriver sub-basins and others are aggregates of multiple small tributaries (Omernik et al., 2017). The model is sensitive to the discretization of the hydrographic basin, which makes it an important step. Thus, the Rio das Velhas basin was divided into 80 sub-basins, and grouped according to 15 flow stations, that allowed calibrations, simulation and validation of the hydrologic processes in place (Figure3; Table S7). The main springs are located in sub-basins 79 (Cachoeira das Andorinhas) and 80 (Itabirito river) and the river mouth in sub-basin 1 (Barra do Guaíçu).

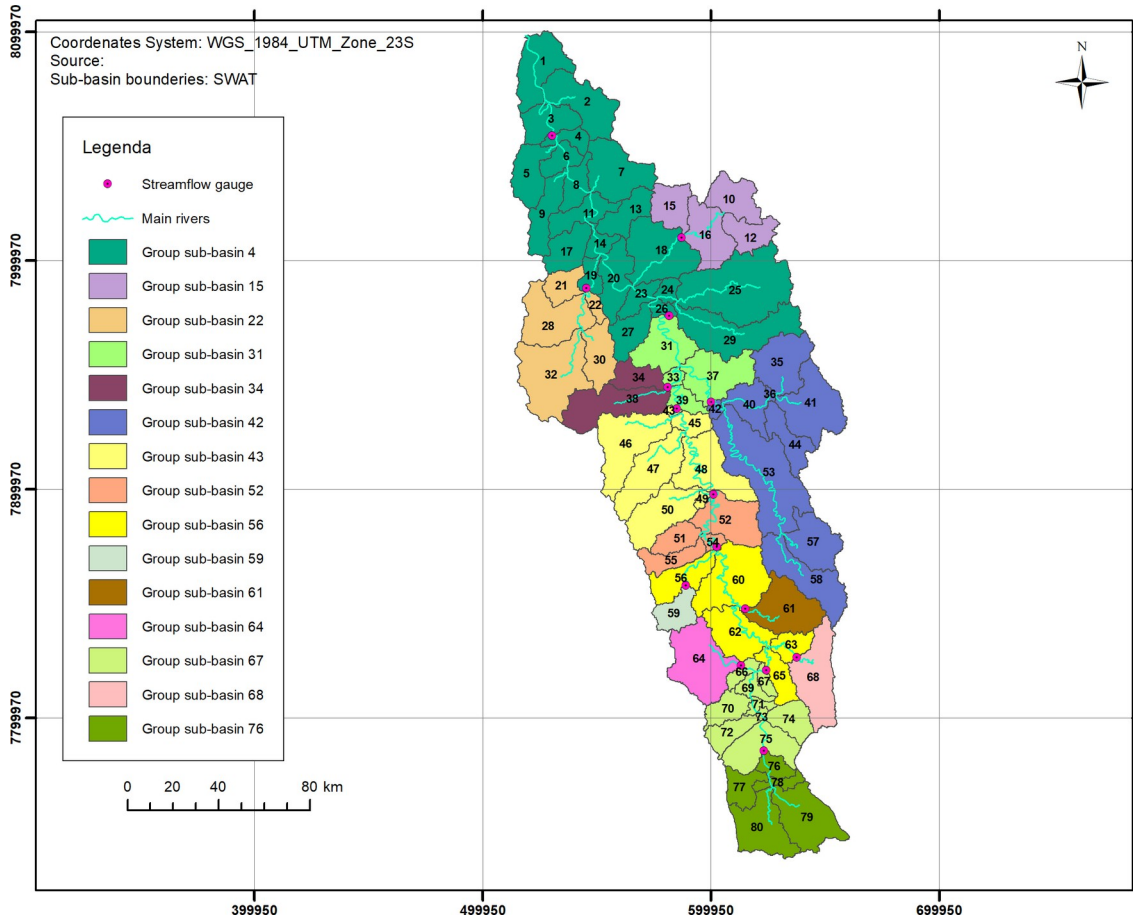


Figure3. Sub-basins and their respective water flow stations group.

Each sub-basin was parameterized by the model generating the hydrological response units (Hydrological Response Units; HRU), which correspond to a single combination of LULC, soil and slope within the sub-basin. The discretization of slope for the definition of HRU was built from 5 classes that homogeneously covered the basin area: <4%; from 4 to 7%; from 7 to 13%; from 13 to 25%; and > 25%. The distribution of HRU in the sub-basins employed the multiple HRU method, which allows creating various combinations of uses and soil type for each sub-basin, according to the level of sensitivity chosen by the user (Neitsch et al., 2011).

The model sensitivity determines the minimum percentage that a slope class needs to occupy in the sub-basin area to create the HRU. This step is important to avoid creating very small HRU that are not representative. The model's default values for sensitivity levels are 20% for land use, 10% for soil type and 20% for slope class (Winchell et al., 2013). After preliminary tests, we adopted the values, 15%, 20% and 20% for land use, soil type and slope class respectively. This means that the classes of land use that occupy an area of less than 15% in the basin will not be considered in the combinations for the creation of HRU, the same applies for soil type and slope class.

The runoff in each sub-basin was estimated by the Soil Conservation Service (SCS) Number Curve method (USDA, 1997). The underground runoff was simulated for two types of aquifers in each sub-basin: (i) shallow (non-confined), which contributed to the runoff in the main channel or sections of the sub-basins; and (ii) deep (confined), which contributed out of the simulated basin. Groundwater flow (Eq. 1) was simulated in a steady regime (Neitsch et al., 2011):

$$Q_{gw} = \frac{8000 \cdot K_{sat}}{L_{gw}^2} \cdot h_{wtbl} \quad (1)$$

where Q_{gw} is the underground (base) flow of the main channel on day i (mm), K_{sat} is the saturated hydraulic conductivity of the aquifer (mm.day⁻¹), L_{gw} is the distance from the underground basin divide to the main channel (m) and h_{wtbl} is the water head of groundwater flow (m). The potential evapotranspiration (PET) was estimated by the Penman-Monteith method and solar radiation, air temperature, relative humidity and wind speed were required as input data. The model calculates the actual evapotranspiration after the PET determination.

2.4 Calibration, validation and uncertainty analysis

2.4.1 Flow series and parameters

The historical flow series were divided following the 70/30 proportion method proposed by Klemeš (1986): (1) years 1995 to 2008 were used for calibration and (2) years 2009 to 2015 were used for validation. The monthly time step was used and both periods (calibration and validation) had rainy and dry years. The years used for initial warm-up were 1993 and 1994 for calibration, and 2007 and 2008 for validation.

In this paper only the flow (runoff) was calibrated. SWAT has twenty-six parameters associated with this variable (Arnold et al., 2012). Such a large number of parameters is a known problem in hydrological models, especially in distributed and semi-distributed models (Brighenti et al., 2016). So a literature search was performed to identify the parameters that tend to be more sensitive, which resulted in selection of 11 parameters.

Those eleven parameters were used throughout the calibration process, namely: base flow recession constant (ALPHA_BF), Manning roughness coefficient (CH_N2), runoff curve number for moisture condition (CN2), calculation of water demand by plants (EPCO), calculation of soil evaporation demand (ESCO), aquifer recharge time (GW_DELAY), water return coefficient from the aquifer to the root zone (GW_REVAP), the limit between water depth in shallow aquifer and the surface (GWQMN), water limit in the shallow aquifer to return to the root zone or percolation to the deep aquifer (REVAPMN), available water capacity in the soil horizon (SOL_AWC), saturated hydraulic conductivity in the soil horizon (SOL_K).

2.4.2 Multisite calibration

SWAT-CUP (Abbaspour, 2015; Abbaspour et al., 2015) was used to proceed with the calibration and validation steps. We opted for the SUFI-2 algorithm among those available in SWAT-CUP, because it is the one that needs the fewest iterations to achieve a satisfactory performance (J. Yang et al., 2008). We adjusted the model by changing the parameter intervals until the model was calibrated. We performed the 100 iterations for calibration using the 1995-2008 data. The validation process was carried out through a new simulation with 100 iterations for each sub-basin previously calibrated, using the period from 2009 to 2015.

The use of few stations to calibrate a model can lead to poor spatial accuracy (Daggupati et al., 2015), so we chose a multi-site calibration for the Rio das Velhas basin because of its size (~28,000 km²) and the availability of 15 flow measurement stations. We used the 15 stations, parameterized individually or stepwise, because this method proves to be efficient (C. W. L. de Andrade et al., 2019; Franco & Bonumá, 2017; Wi et al., 2015).

Thus, the stations upstream were initially calibrated so that the values of the parameters obtained in the calibration of these sub-basins were fixed. Therefore, in subsequent calibration steps those values did not change. Then the stations further downstream were calibrated until all stations in the basin were calibrated (Figure 4). Respecting this calibration order is important because although the calibration is individual, the processes in the basin are integrated and always from upstream to downstream (Wi et al., 2015). Otherwise, when calibrating the upstream basin, the flow values in the downstream basin will be changed again, increasing the computational effort and compromising model performance. The non-instrumented sub-basins were grouped to receive the same parameter values of an instrumented sub-basin with which it had a hydrological connection. (Figure 3).

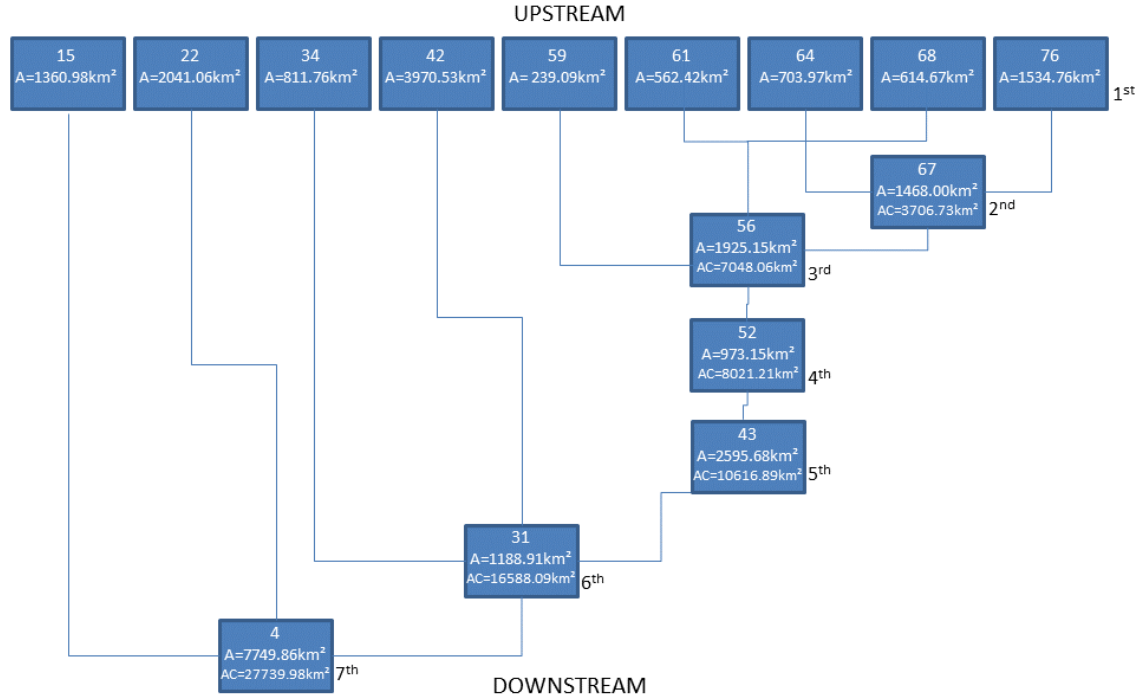


Figure 4. Calibration order of the Rio das Velhas sub-basins.

2.4.3 Performance analysis

The performance of the model was evaluated (calibration and validation) by the Nash and Sutcliffe coefficient (NS; Equation 2). Values of NS close to one (Table 1) indicate that the result is satisfactory:

$$NS = 1 - \frac{\sum_{i=1}^n (E_m - E_s)^2}{\sum_{i=1}^n (E_m - E)^2} \quad (2)$$

where E_m is the observed event, E_s is the event simulated by the model, E is the average of the observed event and n is the number of events.

The percent bias (PBIAS; Equation 3) of the simulated data being above or below than the observed data was calculated. The optimal value of this statistical index is zero (Table 1) and values with low magnitude indicate simulation accuracy. Positive values indicate a tendency to underestimate the results simulated, whereas negative values indicate overestimation of the simulated values (Gupta et al., 1999).

$$PBIAS = \frac{\sum_{i=1}^n (E_m - E_s)}{\sum_{i=1}^n E_s} \times 100$$

Table 1. Classification of the model performance according to Nash and Sutcliffe coefficient (NS) and percent bias (PBIAS) (Moriassi et al., 2007)

Model performance	NS	PBIAS
Very good	$0.75 < NS \leq 1.00$	$PBIAS < \pm 10\%$
Good	$0.65 < NS \leq 0.75$	$\pm 10\% < PBIAS < \pm 15\%$
Satisfactory	$0.50 < NS \leq 0.65$	$\pm 15\% < PBIAS < \pm 25\%$
Unsatisfactory	$NS \leq 0.50$	$PBIAS > \pm 25\%$

Additionally, we used the coefficient of determination (R^2), obtained from the linear regression between the measured and observed values. R^2 values > 0.6 are considered acceptable for monthly simulations in modeling using SWAT (Bonumá et al., 2014; Santhi et al., 2001).

3 Results

In this modeling and using calibration data from 1995-2015, we underestimated the base flow and overestimated flow peaks, thus raising the need for further calibration (Figure 5, Figure S1). Further calibrations included use of the minimum and maximum values for each parameter as well as the “best parameters” or optimal values, which are obtained using the best fit between the calibrated and the simulated flows (Table S8). When we used multi-site calibration, the values of the calibrated range and the optimal values were obtained for each group of sub-basins (see Figure 3). Thus, each of these groups has specific calibration estimates, consistent with the characteristics of that region.

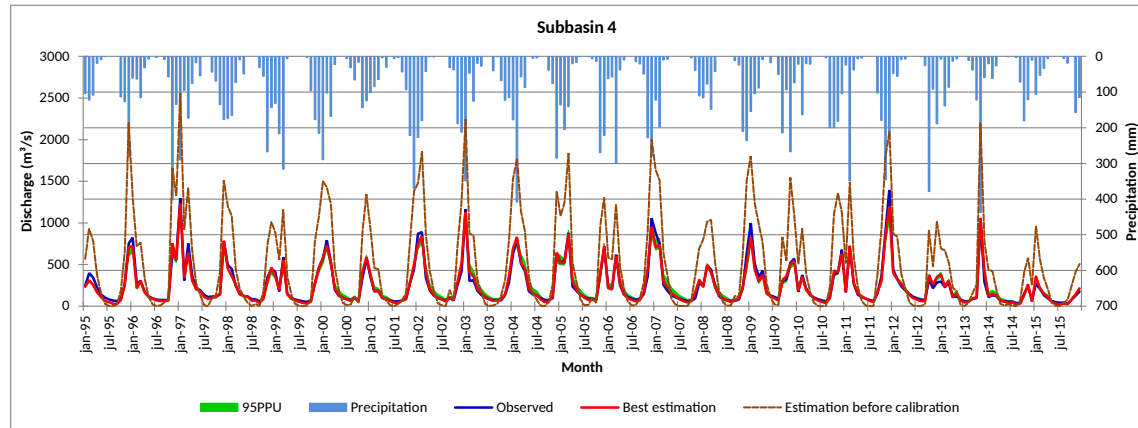


Figure 4. Observed and simulated flows before and after calibration to sub-basin 4

After calibration and validation the NS values ranged from 0.73 to 0.97 (calibration) and from 0.51 to 0.98 (validation). PBIAS ranged between -11.3 and 19.4 (calibration) and between -18.6 and 24.6 (validation), which are considered satisfactory to very good (Moriassi et al., 2007). The R^2 values also remained above 0.6 in all sub-basins, as recommended by Bonumá et al. (2014) and Santhi et al. (2001) (Table 2). Among the 100 iterations performed, it is noteworthy that these statistics were related to the iteration that best fitted the observed data.

305 **Table 2.** Verification of the model after calibration / validation

Sub-basin	Order of calibration	Pre-calibration			Calibration			Validation		
		NS	PBIAS	R ²	NS	PBIAS	R ²	NS	PBIAS	R ²
15	1 st	0.59*	-14.27**	0.62	0.73***	12.2**	0.76	0.51*	-2.1***	0.62
22	1 st	-2.96	-149.28	0.79	0.77***	17	0.79	0.81***	-18.6*	0.85
34	1 st	-20.46	-394.8	0.71	0.78***	10.7**	0.78	0.57*	-15.6*	0.65
42	1 st	0.42	-51.29	0.90	0.92***	-11.3**	0.94	0.86***	-14.3**	0.87
59	1 st	-6.28	-115	0.81	0.78***	-4.8***	0.81	0.90***	-7.0***	0.90
61	1 st	-1.06	-87.37	0.88	0.85***	13.2**	0.86	0.90***	8.2***	0.91
64	1 st	-4.38	-91.25	0.76	0.76***	19.4*	0.85	0.77***	24.6*	0.85
68	1 st	-1.45	-59.31	0.78	0.84***	1.3***	0.88	0.73**	-2.4***	0.80
76	1 st	-2.34	-34.95	0.85	0.88***	-3.1***	0.88	0.92***	-3.2***	0.92
67	2 nd	-4.33	-87.49	0.87	0.94***	-2.5***	0.95	0.90***	-16.2*	0.93
56	3 rd	-3.68	-83.52	0.89	0.91***	7.8***	0.93	0.97***	4.7***	0.97
52	4 th	-3.97	-83.73	0.89	0.93***	2.4***	0.93	0.98***	4.3***	0.98
43	5 th	-3.69	-86.37	0.88	0.93***	-0.1***	0.93	0.85***	0.2***	0.95
31	6 th	-2.27	-93.33	0.90	0.96***	-6.8***	0.97	0.94***	-12.0**	0.96
4	7 th	-1.82	-99.53	0.91	0.97***	2.3***	0.98	0.97***	1.8***	0.97

306 NS and PBIAS model performance: *Satisfactory; **Good; ***Very good. All R² values are acceptable.

307 As shown in Table 2, the pre-calibration results were unsatisfactory for all stations,
 308 except for station 41890000 (sub-basin 15) which presented NS and PBIAS considered
 309 "satisfactory" and "good", respectively. The PBIAS values were all negative and above 25,
 310 which is the limit value for the model to be satisfactory, indicating a strong tendency to
 311 overestimate peak flows. The sub-basins located upstream, which were the first group to be
 312 calibrated (sub-basin 15 to sub-basin 76), showed lower performance of their estimates than the
 313 lower sub-basins. Over the analyzed period (1995 to 2015), the simulated flow graphs showed
 314 that the calibrations of the sub-basins further downstream resulted in better adjustments (Figure
 315 S2).

316 **4 Discussion**

317 This work explores how SWAT, a well-known hydrological model can be used for
 318 planning and managing water resources in the context of heterogeneous, dynamic land uses and
 319 large watersheds (>25,000 km²). From the different approaches to calibration available in SWAT
 320 we developed stepwise and multi-site procedures to effectively tailor and customize the use of

SWAT so it can more likely be used for water resource management. We also stress limitations, advantages, and, ways forward to effectively use SWAT as a tool for informing water resource planning and management in continental-extent countries, such as Brazil.

4.1 Multi-step procedure for multi-site calibration in large watersheds

Management and planning of water resources in Brazil has been carried out by planning units of similar size as the Rio das Velhas basin. Although SWAT has been mostly used in small to medium watersheds worldwide, our results show that through tailored and customized calibration, hydrological models such as SWAT coupled with GIS proved efficient in modeling runoff in large basins ($\sim 30,000 \text{ km}^2$). Our results highlight that using multiple flow monitoring stations and multi-site calibration approaches are useful calibration approaches for managing water resources in countries of continental dimensions such as Brazil.

Even without calibration, the model was able to represent the general pattern of the hydrography, with peaks and recessions, although overestimating peak flows and underestimating base flows occurred as expected in the pre-calibration phase (Abbaspour et al., 2015). In general, it is possible to enhance modeling estimates through calibration, changing the values of some specific parameters, such as decreasing the value of runoff curve number for moisture condition (CN2) and increasing the values of available water capacity in the soil horizon (SOL_AWC) and calculation of soil evaporation demand (ESCO), in the case of overestimated peaks, or decreasing the values of limit between water depth in shallow aquifer and the surface (GWQMN) and water return coefficient from the aquifer to the root zone (GW_REVAP) and increasing the water limit in the shallow aquifer to return to the root zone or percolation to the deep aquifer (REVAPMN), when the base flow is very low (Abbaspour et al., 2015; Rouholahnejad et al., 2014).

After calibration, NS, PBIAS and R^2 were within the confidence levels of 95%. In line with other studies, our results also highlight the importance of the SWAT calibrations (C. W. L. de Andrade et al., 2019; Durães et al., 2011). After calibration, the PBIAS values were improved, ranging from satisfactory to very satisfactory. NS values improved through the calibration process as well. Before calibration only one sub-basin had satisfactory estimates, but after calibration NS was satisfactory for all stations. The results of the validation, confirm the pattern of improvement in the performance of model statistics, this indicating that the calibration of the model can be extrapolated to other periods.

Adopting multi-site calibration for a large and very heterogeneous basin was important for many reasons. Our results were thereby individually calibrated and regionalized for each group of sub-basins (see Figure S2). In this way, the calibration data provided a level of detail that favors water management and planning at the sub-basin scale, instead of the basin as a whole. If it is necessary to calculate the flow from any river in a sub-basin, it will be possible to use the calibrated parameters for the group to which that sub-basin belongs. Despite the advantages of using multi-site calibration, this approach requires considerable processing capacity because it was necessary to perform several iterations for each station. Therefore, the strategy adopted was to test the calibrations first by running 20 iterations, and only when the results obtained were close to those desired, did we perform 100 iterations. In this way, it was possible to considerably reduce the processing time.

When proceeding with stepwise multi-site calibration, it was noted that for the first stations to be calibrated, it was more difficult to achieve good adjustments, and even so, the results were inferior to those obtained in the stations calibrated afterwards (Figure 5 shows the order of calibration). This occurs because as values were first calibrated upstream, the flow was automatically adjusted downstream, making the calibration more effective at later stages and, consequently, in larger and larger sub-basins. Extreme anthropogenic alterations (e.g., chemical spills, urbanization) and natural stochastic events (e.g., floods, torrents, fire, droughts) are more intense in smaller catchments (e.g., Coles et al., 2012; Shiau, 2003), so it is typically easier to model flows in large basins than in small ones.

The performance values obtained in our study for NS (ranged from 0.73 to 0.97 in calibration and 0.51 to 0.98 in validation) and PBIAS (-11.3 and 19.4 in calibration and between -18.6 and 24.6 in validation) are in line with previous work (Durães et al., 2011; Githui et al., 2009). However, if we analyze the most instrumented sub-basin in this study (sub-basin 4, with ~25,000 km²), we observed a NS of 0.97 (calibration and validation) and PBIAS of 2.3 and 1.8, to calibration and validation, respectively. Other studies in relatively large basins showed poorer results. For example, Durães et al. (2011) studying the 14,000 km² Paraopeba River basin, also in Minas Gerais reported NS values of 0.77 and 0.79 in the calibration and 0.76 and 0.82 in the validation. Githui et al. (2009) used the SWAT model to simulate the flow in a 13,000 km² basin located in Kenya. Calibration was performed for a period of 5 years (1980 to 1985), with a monthly time step (NS of 0.76 in calibration and 0.74 in validation) and daily (NS of 0.71 in calibration and 0.63 validation). Their model adjustment for the monthly calibration was higher than for the daily calibration.

4.2 Limitations and advantages of this approach

Although robust estimates were achieved there are some issues concerning the input data. One of the problems relates to the entry of weather data. Although the model assigns the value of the nearest measurement station to each sub-basin, this value is not interpolated and instead simply represents the value of the nearest station. Szcześniak & Piniewski (2015) assessed the effect of entering interpolated precipitation data on the calibration results in 11 medium-sized sub-basins and concluded that in basins with a low density of measurement stations and with low coefficient of variation of daily precipitation, the use of interpolation methods improved estimates.

Also, in general, climatic series have flaws in their historical series, and in our case, they were filled with the atmospheric state generator model available in SWAT (WXGEN) (Sharpley & Williams, 1990). Despite being a widely used method to generate climate data, it generates uncertainties just like any other model (Herman et al., 2018). The same can be said of the series of flow monitoring stations, which were filled in through regressions (Esmaealzadeh & Dariane, 2014).

Another sensitive point relates to soil data available in Brazil. As explained in the methods, because there is not appropriate pedological data available for our study area we used data from basins near the Rio das Velhas basin (see Table S6). For overcoming data gaps, others using SWAT in Brazil employed data from other basins or estimated them from pedotransfer equations (Bonumá et al., 2014; Machado & Vettorazzi, 2003). Soil mapping is a very weak environmental layer in Brazil (K. De Mello et al., 2020). Currently, the country has only general soil surveys, with low-resolution maps; < 5% of the nation has soil maps on a resolution of

1:100,000 or greater, which reinforces the Brazilian government's initiatives to map the territory and generate data with different degrees of detail to support public policies such as the PronaSolos project (www.embrapa.br/pronasolos).

However, despite the uncertainties involved in SWAT modeling, after sufficient calibration the model adequately simulated flows in the Rio das Velhas basin, indicating that it is a tool that can be used in the management of water resources in large hydrographic basins. Besides, the methodological approach used (creation of sub-basins; inputting layers of soil type, slope and land use; climatic data; delimitation of HRU; simulation; calibration; and validation) can be developed in other hydrological models coupled in GIS.

Maps and models are simplified representations of systems and processes that attempt to capture key variables of complex systems. Therefore, they have associated important limitations for exploring different outcomes useful for evaluating different management scenarios (Gregory, 2000). In this work, SWAT was selected not only for its ability to simulate the dynamics of surface runoff and the flow regime but also because it is available to the public free of charge and easily used in GIS tools. Training workshops on SWAT are frequently held in Brazil, which facilitates expanding the knowledge of the use of the tool and to clarify the doubts of the modelers (Bressiani et al., 2015). The model is distributed, and therefore the main basin can be divided into sub-basins. This approach accounts for spatial variation of the parameters, which is extremely important in modeling of large basins (Wood & O'Connell, 1985). In addition, the tool is versatile and effective, and can provide reasonably accurate results (Nash and Sutcliffe efficiency values > 0.5) with moderate data entry effort (Arnold & Fohrer, 2005; Chaplot et al., 2004; Heuvelmans et al., 2005). Finally, it presents a wide range of water use and quality management applications, including use for selecting best management practices (BMPs; Behera & Panda, 2006).

4.3 Implications for water resource management in Brazil

Although there are numerous modeling tools available for managing water resources, evidence is scarce on the use of these tools to inform water management and planning globally. Use of hydrological modeling tools in decision making is particularly challenging in tropical countries. Here we tailored and customized SWAT calibration and validation in the context of large watersheds in Brazil. Despite the widespread acknowledgment that hydrological models are important tools for estimating variations of water-related services across different scales, both geographical (grain and extent) and temporal (dry, and rainy seasons) the use of hydrological models in decision making and water resource management is lagging. Modeling is even more important in countries such as Brazil that have been experiencing unprecedented land use changes and that are likely to experience fundamental climate changes. Changes in vegetation influence processes in the water cycle through their structural effects on key ecosystem functions in watersheds (Ponette-González et al., 2015) influencing watershed evapotranspiration regimes, changing retention of precipitated water in tree canopies and soil infiltration capacity, all of which affect the volume of water runoff (Fletcher et al., 2013; X. Yang et al., 2012). Integrating hydrological modeling and GIS are important tools for dealing with such complex processes in highly dynamic land uses at continental extents, but there are still issues to overcome to incorporate hydrological modeling uptake in policymaking. By customizing the calibration and validation approaches of SWAT we offer decision-makers in Brazil a step-by-step guide for overcoming the limitations of the use of models in water management and planning.

Because the objective of this paper was estimating monthly flows, we calibrated and validated the hydrological model for use in managing a basin's water resources in the long term. Daily time steps are more appropriate when the goal is to ascertain the immediate responses of a basin. According to a survey by Moriasi et al. (2007), most SWAT applications used daily or monthly time steps. They also indicated that, typically, the shorter the time step, the poorer the adjustment (eg, daily versus monthly and yearly). In our study, 15 control stations with flow simulations for a period of 20 y were used, so daily simulations considerably more time and data processing capacity.

Throughout our paper we presented possible solutions to overcome data scarcity: we reduced model complexity by using 11 of 26 possible water flow parameters, yet we showed that this customized approach parametrized the model captured hydrological processes at the large extent of the Rio das Velhas watershed. So we believe that multisite calibration has better distributed errors across the entire watershed.

With this calibrated model in place, water management institutions can explore ex-ante management practices such as the number and size of permits for water use. In the Rio das Velhas basin, 19 municipalities have grants for water supply, but the maintenance of minimum flows in the basin's rivers is essential to ensure this supply and to support aquatic ecosystem structures and functions (siga.cbhvelhas.org.br). Therefore, water resource management agencies can use models such as ours to assist planning for anticipated future water shortages that could affect over 5 million people. These tools are particularly useful to analyze the effects of: demographic growth, land-use changes, water resource availability versus future demands, potential conflicts amongst water users, rationing uses, and increasing the quantity and quality of available water resources. All these issues are mandated in water resource planning according to Law 9.433/97 (Brazil, 1997).

The water supply of the Belo Horizonte Metropolitan Region (RMBH) is an integrated system, incorporating three reservoirs in the Paraopeba River basin and the Upper Rio das Velhas basin with direct surface capture. These systems account for approximately 60% and 40% of the water supply for the RMBH, respectively (ARSAE, 2013). During droughts, when river flows decrease, the Paraopeba reservoirs can be used to maintain supply. During rainy periods, when the reservoirs fill, the Rio das Velhas basin can become the main source of water. Hydrological modeling can be a very useful tool in this decision-making process through modeling scenarios about water available and exploitation.

Another important contribution of our modeling was to include land use as layer for defining sub-basins. This is very important because of the highly dynamic land use changes occurring in the study basin. Future land use maps developed by SIMBRASIL or BLUM can be used as a layer in SWAT simulations to explore the consequences of those land use patterns in providing water in the future.

5 Conclusions

The SWAT multi-site calibrated model was able to accurately reproduce the hydrological processes of a large and heterogeneous basin. The adjustments obtained proved to be consistent with other studies carried out in large basins in Brazil and worldwide. Despite the limitations previously presented, we found that the use of SWAT coupled to the GIS facilitated simulating complex hydrological processes. That modeling can serve as a tool to better target decision

494 making by Brazilian water resource management agencies and reduce the impacts of
 495 anthropogenic interventions on water flow regimes.

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501 **Data Availability Statement**

502 The model inputs is publically available at *[insert zenodo or dryad repository]*.

503 **References**

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