

<https://doi.org/10.1590/2318-0331.282320230034>

Managing water resources in complex tropical basins: tailored SWAT ecohydrological modeling to the Rio das Velhas, Brazil

Gestão dos recursos hídricos em bacias tropicais complexas: uma abordagem customizada da modelagem eco-hidrológica SWAT para o Rio das Velhas, Brasil

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Received: April 20, 2023 - Revised: August 06, 2023 - Accepted: September 01, 2023

ABSTRACT

Hydrological modeling in decision-making is particularly challenging in tropical countries such as Brazil. There are numerous modeling tools; however, many applications have focused on watersheds with a total area of <20,000km². Here we tailored a customized SWAT (Soil and Water Assessment Tool) ecohydrological model application using the SWAT CUP tool for calibration and validation of the Rio das Velhas, a relatively large, complex Brazilian basin (~28,000km²). The Rio das Velhas is the longest tributary of the São Francisco River and contains heterogeneous landforms, soils, vegetation, and land uses. A multisite calibration method obtained specific regionalized parameters for each sub-basin group for successfully simulating Rio das Velhas streamflows. Our results showed a suitable adjustment of the model. Nash-Sutcliffe (NS) model performance values were 0.73-0.97 (calibration) and 0.51-0.98 (validation). The percent bias (PBIAS) was -11.3 to 19.4 (calibration) and -18.6 to 24.6 (validation), and the coefficient of determination values (R²) were >0.6 in all sub-basins on a monthly basis. We also explored how four contrasting land use scenarios affected four water-flow variables (surface runoff, base flow, percolation, and total streamflow). Our results show that by using multiple flow-monitoring stations and multisite calibration approaches, ecohydrological models can be useful for managing basin-extent water resources in countries of continental dimensions such as Brazil.

Keywords: Water resources management; Water governance; GIS spatial tools; Rio das Velhas.

RESUMO

O uso de ferramentas de modelagem hidrológica na tomada de decisão é particularmente desafiador em países tropicais como o Brasil. Existem inúmeras ferramentas de modelagem disponíveis; entretanto muitas aplicações destas ferramentas são focadas em bacias hidrográficas com área total <20.000 km². Neste trabalho, adotamos e customizamos o modelo ecohidrológico SWAT (Soil and Water Assessment Tool) usando a ferramenta SWAT CUP para calibração e validação do Rio das Velhas, uma relativamente grande e complexa bacia brasileira (~ 28.000 km²). O Rio das Velhas é o maior afluente da bacia do rio São Francisco e contém formas de relevo, solos, vegetação e usos da terra heterogêneos. Usando um método de calibração multi-site, parâmetros regionalizados específicos foram obtidos para cada grupo de sub-bacias para simular com sucesso as vazões do Rio das Velhas. Nossos resultados mostraram um bom ajuste do modelo. Os valores do coeficiente de performance Nash-Sutcliffe (NS) foram 0,73-0,97 (calibração) e 0,51-0,98 (validação). A porcentagem de viés (PBIAS) foi de -11,3 a 19,4 (calibração) e -18,6 a 24,6 (validação) e os valores do coeficiente de determinação (R²) foram >0,6 em todas as sub-bacias considerando uma escala mensal. Também exploramos as maneiras pelas quais quatro cenários contrastantes de uso da terra impactam às quatro variáveis de vazões avaliadas (escoamento superficial, fluxo de base, percolação e fluxo total). Nossos resultados mostram que, usando múltiplas estações de monitoramento de vazão e abordagens de calibração multi-site, os modelos ecohidrológicos podem de fato ser úteis para gerenciar os recursos hídricos da extensão da bacia em países de dimensões continentais como o Brasil.

Palavras-chave: Gestão de recursos hídricos; Governança da água; Ferramentas espaciais SIG; Rio das Velhas.



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INTRODUCTION

Water management is high on environmental and political agendas (Carvalho et al., 2019; Loch et al., 2020). Water provisioning 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 at least four key 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 physical, chemical, biological, and ecological processes. Furthermore, current computational development has produced many alternative tools and algorithms for calibration, simulation, and validation of modeling those hydrological cycles (Gharari et al., 2013; Ghoreishi et al., 2021; Moreira et al., 2020).

Second, the availability of spatially explicit environmental databases (i.e., geospatial information) and free software expand the analytical possibilities for water resources management (Macedo et al., 2018). 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.

Third, vegetation cover influences processes in the water cycle through its structural effects on essential ecosystem functions in watersheds (Ponette-González et al., 2015). This is key for tropical countries such as Brazil, which are experiencing unprecedented land use changes (Souza Junior 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; Yang et al., 2012). 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 (2023) and the Brazilian Land Use Model (BLUM). These spatially explicit estimates of land use patterns for future decades can be used for exploring the impacts of land cover patterns on water management.

Fourth, although ecohydrological modeling integrated with GIS is essential for dealing with complex processes in highly dynamic land uses across continental extents such as Brazil, there are still issues to overcome to incorporate ecohydrological modeling in policymaking. It is particularly challenging to use ecohydrological modeling for relatively large river basins and explore future scenarios that assist decision-making in water resource management in the medium to long term.

Ecohydrological 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 perform accurately 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 and is feasibly integrated into routine water management institutional practices?

Thus, a multisite calibration, which consists of using two or more fluviometric stations to calibrate the model, is a strategy that can achieve better results versus models based on one station (Andrade et al., 2019; Wi et al., 2015). To do so, ecohydrological models integrated into geographic information systems (GIS) have been widely used in recent years (Khalid, 2018; De Mello et al., 2020; Schumann et al., 2000; Schuol et al., 2008). Four improvements have been made in developing this integrated approach. 1) River basins are characterized by their lithology, morphology, soils, and land cover variations. 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.

Numerical hydrological models have been implemented in geographic information systems (GIS) frameworks; however, the Soil and Water Assessment Tool (SWAT) ecohydrological model (Arnold & Fohrer, 2005; Arnold et al., 2012a, 2012b) is the most used worldwide in scientific works (Paul et al., 2021). Furthermore, SWAT stands out for (1) allowing multisite modeling (Arnold et al., 2012b); (2) being open source (Arnold et al., 2012b); (3) facilitating deployment in several GIS and statistical softwares (e.g., ArcGis, Qgis, and R; Soil & Water Assessment Tool, 2023b); (4) being actively supported by the scientific community (Soil & Water Assessment Tool, 2023a); (5) being regularly updated (Tan et al., 2020); (6) being widely used in the academic and management world (Paul et al., 2021; Tan et al., 2020); and (7) being used worldwide in different contexts (i.e., watersheds with various sizes, different land uses and cover, regulated catchments, etc; Soil & Water Assessment Tool, 2023c).

There are many examples of SWAT's versatility. SWAT 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 understand the sources and drivers of microbial (Sowah et al., 2020) and chemical (Schilling & Wolter, 2009) water quality in USA watersheds. It was used in an integrated approach to estimate streamflow, soil loss, and water contamination in the Tiete watershed of Sao Paulo, Brazil (Santos et al., 2020). It helped determine critical erosion-prone areas for selecting best management practices (BMPs) and conservation programs for a USA reservoir (White et al., 2010).

However, despite the large extent of many Brazilian river basins, more than 75% of studies using SWAT in Brazil have focused on basins <20,000 km² (Soil & Water Assessment Tool, 2023c). In Brazil, SWAT has been used since the 1990s, and between 1999 and 2013, over 100 academic studies used SWAT to explore its ability to capture the complexity of hydrological processes at basin scales (Bressiani et al., 2015). Considering that land use changes are the greatest threat to water resources in Brazil (De Mello et al., 2020) and the water resources management in the country is carried out through large hydrographic basins (average size ~ 20,000 km²; Agência Nacional de Águas, 2020), it is necessary to demonstrate how SWAT can be used for assessing large basins and land use changes in Brazil. Particularly important is to explore how major drivers of land use change, associated with both native vegetation

loss (urbanization and agricultural expansion) and native vegetation gain (forest recovery) might influence streamflows in such large basins and the ways in which these might be accounted for in watershed planning and management.

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 improving SWAT predictive performance and making it possible for water management agencies to consider SWAT cost-effective enough to use as an ecohydrological modeling and planning tool. Because of inherent complexities with data availability and model calibration approaches, ecohydrological 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 resolution (map scale > 1:500,000) 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 (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, we explored how a distributed and continuous ecohydrological model coupled with GIS such as SWAT can be used to estimate surface runoff dynamics in a heterogeneous and relatively large hydrographic basin (~28,000 km²). We mainly aimed to explore how multisite calibration approaches can enhance the performance of runoff estimates in a large basin as a function of varying land use change scenarios. We then customized a calibration approach to make SWAT more appealing for decision-making for large tropical basins.

MATERIALS AND METHODS

Study area

We used SWAT coupled with GIS to simulate hydrological processes in the Rio das Velhas basin, the longest tributary of the São Francisco River. The study area covers 27,850 km² 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 (Instituto Brasileiro de Geografia e Estatística, 2020), with approximately 4.8 million inhabitants representing 25% of the population of Minas Gerais and 32% of the population of the São Francisco basin (Instituto Brasileiro de Geografia e Estatística, 2010, 2020).

This basin covers parts of the Atlantic Forest and Brazilian Savanna biomes. Most of the region's climate is tropical (Cwb, Cwa, and Aw Köppen climate types), with annual average temperatures between 18°C and 22°C, annual total rainfall of ~1500 mm, and a six-month dry season (April to September) (Alvares et al., 2013). The basin comprises four distinct geomorphological units (Fundação Centro Tecnológico de Minas Gerais, 1983; United States Geological Survey, 2015). 1) The headwaters are situated in the southern part

of the Quadrilátero Ferrífero, with elevations ranging from 800 to 1875 m. 2) The mainstem flows through the São Franciscana Depression (470-800m). 3) The São Francisco Plateaus border the western region (800-1000m). 4) The Espinhaço Meridional Mountain Range dominates the eastern side (1000-1875m). The most prevalent soil types are Argisols (~ 30%), but Latosols (~ 22%), Neosols (~ 22%), Cambisols (~ 17%), and Plinthosols and Gleisols (~ 1%) also occur (Instituto Brasileiro de Geografia e Estatística, 2018). The land use and land cover (LULC) is predominately Pasture (~ 27%), followed by Forest-Evergreen (~ 24%), Range-Grasses (~ 15%), Agricultural Land-Generic (~ 14%), and Range-Brush (~ 12%). Urban infrastructure occupies about 2% of the total area (Souza Junior et al., 2020).

Datasets and their sources

We calibrated and tested the SWAT ecohydrological model using the flow series (1993-2015) obtained from 15 streamflow monitoring stations available at ANA's HIDROWEB (Agência Nacional de Águas, 2020) (Supplementary Material 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. (2005) (Supplementary Material S2).

The model used information from four environmental dimensions: climate, topography, soils, and land use and cover (Figure 2). The climatic data were obtained through the analysis of historical series using five weather stations (temperature, humidity, solar radiation, wind speed, and precipitation) of the National Institute of Meteorology (Instituto Nacional de Meteorologia, 2020) and 29 rainfall stations (daily data from 1993 to 2015) of the National Water Agency (Agência Nacional de Águas, 2020) (Supplementary Material S3; Figure 2d). The gaps were filled using the weather generator model developed for the United States (SWAT WXGEN model; Sharpley and Williams, 1990). Therefore, to be applicable to the study area, it was necessary to calculate different climatic parameters (Supplementary Material S4) and format them for input to the SWAT model. The topography features (Figure 2a) were taken from the digital elevation model (DEM) generated by the Shuttle Radar Topographic Mission (~30m; United States Geological Survey, 2015). The land use and cover map (Figure 2b) was generated from the pixel-by-pixel classification of satellite images from Landsat (30m resolution) and Sentinel (10m resolution) through machine learning algorithms such as deep learning and convolutional neural networks (Souza Junior 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 (Supplementary Material S5). The soil characterization (Figure 2c) was obtained through the Brazilian soil map (scale 1:250,000; Instituto Brasileiro de Geografia e Estatística, 2018) that was complemented with soil physical-hydro characteristics classified through a survey conducted by experts in the upper Rio das Velhas basin (Mello et al., 2020; Supplementary Material S6). The GIS data were inserted in the SWAT model using the ArcSWAT interface (Winchell et al., 2013).

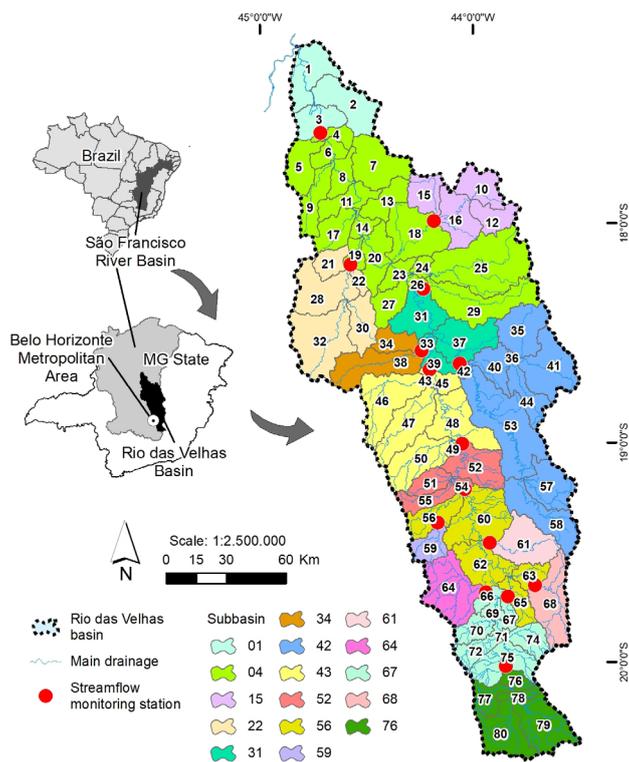


Figure 1. The Rio das Velhas basin, the sub-basins, and their respective streamflow stations group and streamflow monitoring stations.

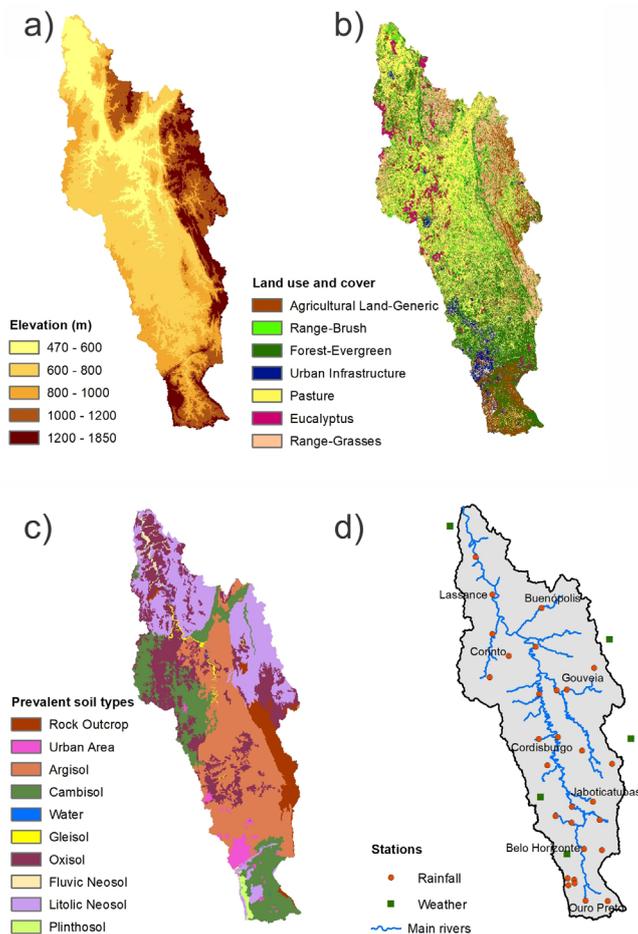


Figure 2. Inputs for SWAT a) topography, b) land use classes, c) soil types, and d) weather stations.

Hydrological modeling

The entire basin was divided into sub-basins (hydrologic units), and the confluence of rivers was generated through the DEM and using the streamflow measurement points (each streamflow 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 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 are simply hydrologic polygons, particularly those on the mainstem Rio das Velhas and its major tributaries, which receive streamflows from upriver sub-basins, and others are aggregates of multiple small tributaries (Omernik et al., 2017). The model is sensitive to the accuracy of the basin's sub-basins, making it an important step. Thus, the Rio das Velhas basin was divided into 80 sub-basins and grouped according to 15 streamflow stations that allowed calibrations, simulation, and validation of the hydrologic processes occurring (see Figure 1; Supplementary Material S7). The main springs are in sub-basins 79 (Cachoeira das Andorinhas) and 80 (Itabirito river) and the river mouth is in sub-basin 1 (Barra do Guaçu).

Each sub-basin was parameterized by the model generating the hydrological response units (Hydrological Response Units; HRUs), corresponding to a single combination of LULC, soil, and slope within the sub-basin. The slope classes for defining HRUs were based on 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 HRUs in the sub-basins employed the multiple HRU method, which facilitates creating various combinations of uses and soil types for each sub-basin, according to the level of sensitivity chosen by the user (Neitsch et al., 2011).

Model sensitivity determines the minimum percentage a slope or land-use class needs to occupy in a sub-basin to create a HRU. This step is important to avoid creating very small, unrepresentative HRUs. 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 15%, 20%, and 20% for land use, soil type, and slope class, respectively. This means that the categories of land use and cover that occupy an area of more than 15% (i.e., Forest-Evergreen, Pasture, or Range-Grasses) in the basin were considered in the combinations for the creation of HRUs; similarly, 20% for soil type (i.e., Argisol, Oxisol, or Litolic Neosol) and 20% for slope class (i.e., <4%, 7 to 13%, or 13% to 25%) were used to create HRUs. This process generated a total of 701 HRUs.

Runoff in each sub-basin was estimated by the Soil Conservation Service (SCS) Number Curve method (United States Department of Agriculture, 2004). Subsurface flow 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) aquifer, which contributed flow out of the simulated subbasin. Groundwater flow (Equation 1) was simulated in a steady-state regime (Neitsch et al., 2011):

$$Q_{gw} = \frac{8,000 \cdot K_{sat}}{L_{gw}^2} \cdot h_{wtbl} \quad (1)$$

where Q_{gw} is the underground (base) flow of the main channel on a day i (mm), K_{sat} is the saturated hydraulic conductivity of the aquifer (mm.day⁻¹), L_{gw}^2 is the distance from the underground basin divide to the main channel (m), and h_{wtbl} is the water head of groundwater flow (m). Potential evapotranspiration (PET) was estimated by the Penman-Monteith method, which requires solar radiation, air temperature, relative humidity, and wind speed as input data. The model calculates the actual evapotranspiration after the PET determination.

Calibration and validation

Flow series and parameters

The historical streamflow series were divided following the 70/30 proportion method proposed by Klemeš (1986) and widely used in hydrologic modeling studies (Paul et al., 2021): (1) years 1995 to 2008 were used for calibration and (2) years 2009 to 2015 were used for validation. An aggregated monthly time step for the streamflow comparisons was used, and both periods (calibration and validation) had rainy and dry years. The years used for the initial warm-up period included 1993 and 1994 for calibration and 2007 and 2008 for validation.

In this study, only streamflow (runoff) was calibrated. SWAT has twenty-six parameters associated with this variable (Arnold et al., 2012a). There are many input parameters, but most of them do not influence the hydrologic output. Thus, we performed a literature search to identify the parameters that tend to be more sensitive, which resulted in selecting 11 parameters (Abbaspour et al., 2015; Gharari et al., 2013; Ghoreishi et al., 2021; Moreira et al., 2020).

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 II (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 the 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), and saturated hydraulic conductivity in the soil horizon (SOL_K) (Supplementary Material S8).

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 (Yang et al., 2008). We used an interactive approach to adjust the model, changing the parameter intervals until the model was calibrated (Arnold et al., 2012b). We executed 100 iterations for calibration using the 1995-2008 data. The validation process was carried out through a new simulation with 100 iterations for each previously calibrated sub-basin, using the period from 2009 to 2015.

We employed 100 iterations based on preliminary tests, as they demonstrated that values beyond 100 iterations (i.e., 200, 500, and 1,000) did not yield significant improvements in adjustments that would warrant the additional computational effort involved.

The use of few stations to calibrate a model can lead to poor spatial accuracy (Daggupati et al., 2015), so we chose a multisite calibration for the Rio das Velhas basin because of its size (~28,000 km²) and the availability of 15 streamflow measurement stations. We used the 15 stations, parameterized individually or stepwise, because this method proves efficient (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 3). Respecting this calibration order is essential because, although the calibration is gauge specific, 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 as an instrumented sub-basin with a hydrological connection (Figure 3a). Additionally, we grouped the sub-basins in the three major upstream areas to understand which specific characteristics may have influenced the hydrologic processes between those areas (Figure 3b).

Performance analysis

Model performance was evaluated (calibration and validation) by the Nash and Sutcliffe coefficient (NS; Equation 2):

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

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. Values of NS close to one (Table 1) indicate satisfactory results.

The percent bias (PBIAS; Equation 3) of the simulated data was calculated as above or below that of the observed data. 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 simulated results, whereas negative values indicate overestimating the simulated values (Gupta et al., 1999).

$$PBIAS = \left[\frac{\sum_{i=1}^n (E_m - E_s) * 100}{\sum_{i=1}^n E_m} \right] \tag{3}$$

Additionally, we used the coefficient of determination (R^2) obtained from linear regression between the measured and observed values. R^2 values >0.6 are considered acceptable for monthly simulations in modeling using SWAT (Moriassi et al., 2015).

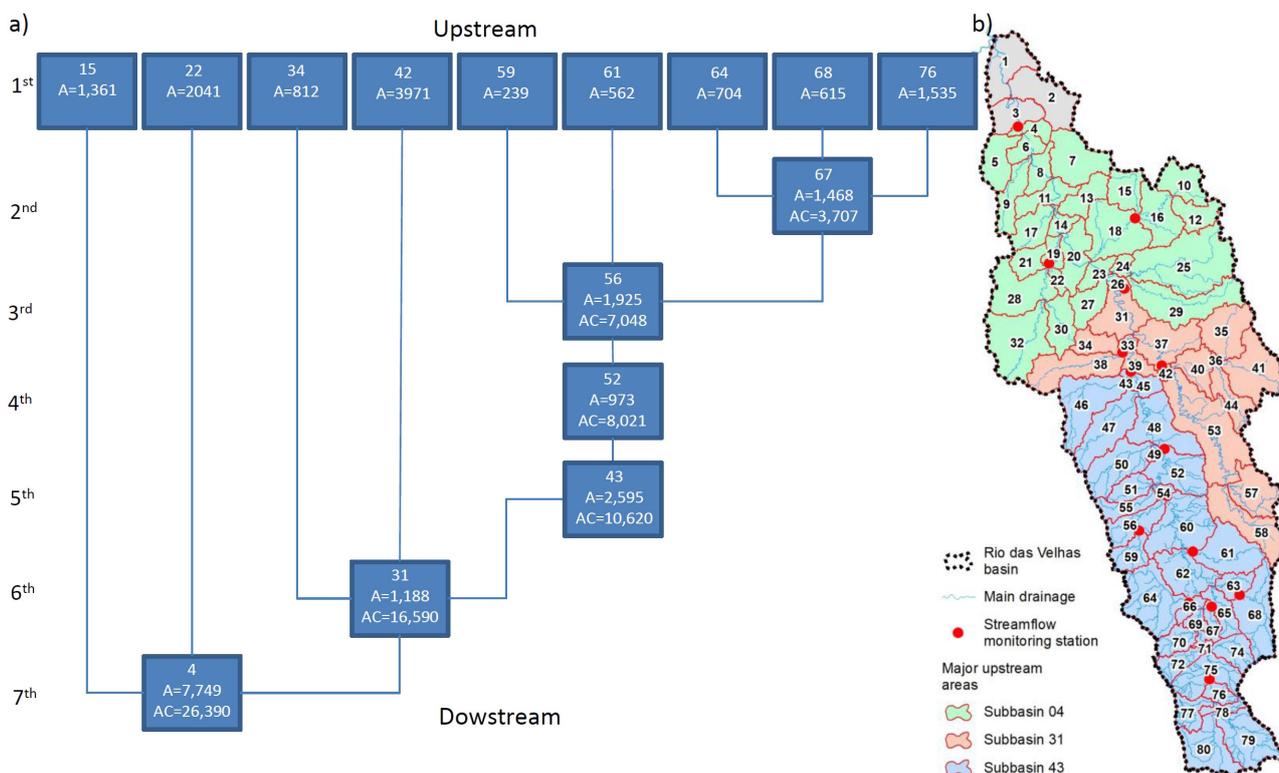


Figure 3. a) Calibration order of the Rio das Velhas sub-basins. A: subbasin area (km²); AC: accumulated upstream subbasin area (km²). b) three major upstream areas, subbasins, and respective water flow stations group.

Land use and land cover change scenarios

We used four scenarios to assess the extent to which land use changes can be associated with water balance, runoff, and total discharge. In the scenarios, we explored how major drivers of land use change associated with native vegetation gain (to the level of human occupation in the 16th century) and native vegetation loss (extreme urbanization and agricultural expansion) might influence streamflows in the basin. Scenario 1 (S1) is the “baseline” scenario that includes the land use map in the year 2018. The second scenario (S2) explores a pristine circumstance where original native vegetation (i.e., forest-evergreen, range-brush, and range-grasses) replaces all anthropogenic land uses. In this case, the anthropogenic uses observed in 2018 were replaced by the natural coverage according to the original distribution through inference based on topography, geomorphology, climate, and land cover. The third scenario (S3) reflects an extreme increase of agricultural lands across the landscape. In this scenario (S3), agricultural land use replaces forest-evergreen, range-brush, and range-grasses. Finally, in the fourth scenario (S4) urban infrastructure replaces forest-evergreen, range-brush, and range-grasses (Table 2).

The water balances for each scenario with the average annual values of the components of precipitation, evapotranspiration, surface runoff, percolation, lateral flow, base flow, capillary rise, and aquifer recharge were generated using the SWAT Check software. We used the relations among (1) surface runoff/total flow; (2) base flow/total flow; and (3) surface runoff/percolation to assess the influences of the land cover scenarios in the water balance (White et al., 2014). Furthermore, we evaluated the statistical differences among streamflow estimates across the four scenarios differentiating wet and dry seasons using t-tests on paired samples.

RESULTS

Using overall streamflow data from 1995–2015, we initially underestimated the base flow and overestimated peak flows, highlighting the need for additional calibration (Figure 4, Supplementary Material S9). Subsequent calibrations included using the minimum and maximum values for each parameter and optimal values, which were obtained using the best fit between the calibrated and the simulated flows (Supplementary Material S10). When we used multisite calibration, the calibrated range and the optimal values were obtained for each group of sub-basins (Figure 3).

Table 1. Classification of model performance according to Nash and Sutcliffe coefficient (NS) and percent bias (PBIAS) (Moriassi et al., 2007, 2015).

Model performance	NS	PBIAS
Very good	$0.75 < NS \leq 1.00$	$PBIAS \leq \pm 10\%$
Good	$0.65 < NS \leq 0.75$	$\pm 10\% < PBIAS \leq \pm 15\%$
Satisfactory	$0.50 < NS \leq 0.65$	$\pm 15\% < PBIAS \leq \pm 25\%$
Unsatisfactory	$0.0 < NS \leq 0.50$	$\pm 25\% < PBIAS \leq \pm 30\%$
Unacceptable	$NS \leq 0.0$	$PBIAS > \pm 30\%$

Table 2. Land use and land cover in simulated scenarios in the Rio das Velhas basin.

	Baseline (S1)	Natural (S2)	Agricultural (S3)	Urbanization (S4)
Agriculture	14.47%	0%	51.35%	14.47%
Urban Infrastructure	2.41%	0%	2.41%	39.29%
Natural vegetation cover ¹	36.88%	100%	0%	0%
Others	46.24%	0%	46.24%	46.24%

¹ Forest-evergreen, range-brush, and range-grasses.

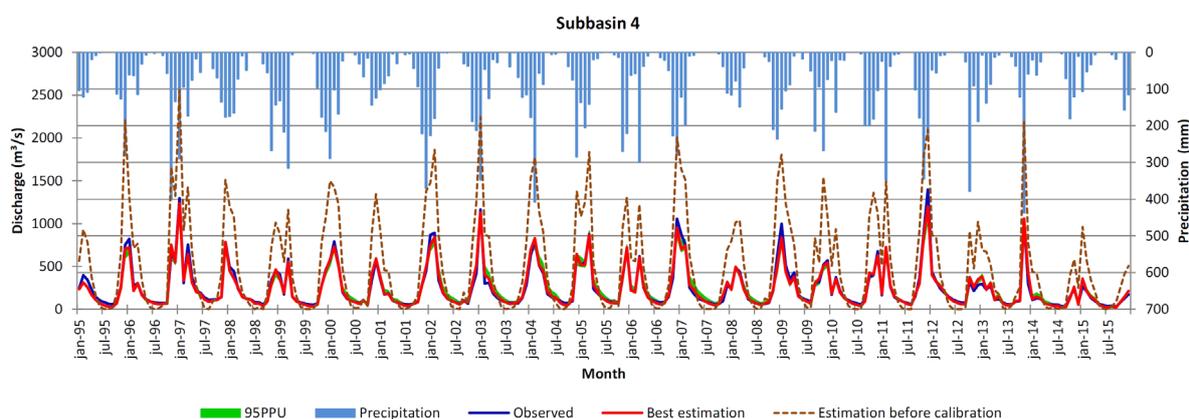


Figure 4. Observed and simulated flows before and after calibration to sub-basin.

Thus, each of these groups has specific calibration estimates consistent with the characteristics of that region. The major difference between the three main groups of sub-basins is related to climate type (Table 3). Sub-basin groups 31 and 43 have the same predominant soils and slope class (Argisols and 13-25% slopes). The same natural vegetation cover (forest-evergreen, range-brush, and range-grasses) and altitude class (600-800 m) are dominant in all three sub-basin groups.

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), Moriassi et al. (2015) and Santhi et al. (2001) (Table 4).

As shown in Table 4, the pre-calibration results were unsatisfactory for all stations, except for station 41890000 (sub-basin 15), in which NS and PBIAS were “satisfactory” and “good,” respectively. The remaining PBIAS values were all negative and considerably above an absolute value of 25, the limit for the model to be satisfactory, indicating a strong tendency to overestimate peak streamflows (also shown in Figure 4). The upstream sub-basins, which were the first group to be calibrated (sub-basin 15 to sub-basin 76), showed lower performance than the lower sub-basins because the calibration started in the headwater sub-basins and proceeded towards the basin outlet. Over the analyzed period (1995 to 2015), the simulated streamflow graphs showed that the calibrations of the downstream sub-basins resulted in better adjustments (Supplementary Material S11).

The simulations of the four land-use scenarios revealed differing proportions amongst water balance components (total

flow, base flow, surface runoff, and percolation) (Table 5). The sum of the lateral flow, base flow, and surface flow was considered as total flow. Ratio (1) refers to how much of the total flow was composed of surface runoff, and the higher this ratio, the greater the runoff generated in the basin. The ratio for the “urbanization” scenario (S4) is higher than for the “agricultural” (S3), modeled, and natural scenarios (S2), respectively, indicating that more intensive land use generates more surface runoff and less groundwater flow. Ratio (2) is the relationship between baseflow and total flow, so a high ratio indicates that a large part of the total flow was comprised of subsurface flow pathways. In this case, we found that the highest value for ratio 2 occurred in the natural scenario (S2), followed by “baseline” (S1), “agricultural” S3, and “urbanization” (S4), reinforcing the results from ratio 1. Ratio 2 indicates that more intensive land use generates less subsurface flow relative to total flow. Ratio (3) describes the ratio between surface runoff and percolation, which means that the higher this ratio, the more surface runoff is generated, and less water infiltrates the soil. Like ratio (1), it is higher for the “urbanization” scenario (S4), followed by the “agricultural” scenario (S3), the “baseline” scenario, and lastly, the “natural” scenario. Again, ratio (3) indicates that the less natural scenarios favor the generation of surface runoff and less soil infiltration, which is undesirable for aquifer recharge and maintaining base flows.

Almost 80 sub-basins showed significantly different simulated average flows (paired t-test, italicize $p < 0.01$) between the adjusted model and the land use change scenarios, both in the dry and wet seasons (Table 6). In general, there was a decrease in the average flow in the dry period with increasing anthropogenic land covers (back-to-nature > baseline > agricultural > urbanization). On the

Table 3. Principal characteristics of the three major sub-basin groups.

Three major subbasin groups	Number of HRUs	Predominant class				
		Soil type	Climate type	Land use and cover	Elevation class	Slope class
04	276	Neosol	AW	Natural cover	600-800m	< 4%
31	144	Argisol	CWb	Natural cover	600-800m	13-25%
43	259	Argisol	CWa	Natural cover	600-800m	13-25%

Table 4. Verification of the model before and after calibration and 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	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

All coefficient of determination (R^2) values are acceptable. Nash-Sutcliffe (NS) and percent bias (PBIAS) model performance: *Satisfactory. **Good. ***Very good.

Table 5. Proportional rates between simulated water flows in the Rio das Velhas basin under different scenarios.

	Baseline (S1)	Natural (S2)	Agricultural (S3)	Urbanization (S4)
(1) Surface runoff/Total flow	0.178	0.154	0.192	0.479
(2) Base flow/Total flow	0.379	0.415	0.363	0.210
(3) Surface runoff/Percolation	0.190	0.153	0.208	0.847

Table 6. Simulated average flows in the dry (April to September) and wet (October to December) seasons for the 15 adjusted sub-basins in the Rio das Velhas basin. Baseline (S1); Natural (S2); Agricultural (S3); Urbanization (S4). Significant differences in mean flows (italicize $p < 0.01$) between land use change scenarios and baseline are in bold.

Sub-basin	Area Km ²	Dry				Wet			
		S1	S2	S3	S4	S1	S2	S3	S4
15	1,361	2.65	2.88	2.65	2.76	33.98	37.55	36.61	35.34
22	2,041	7.51	6.73	7.16	6.05	24.15	22.43	25.66	32.19
34	812	0.94	1.66	1.16	1.12	4.36	6.16	4.84	7.46
42	3,971	22.76	21.89	22.01	21.91	122.88	120.36	124.26	132.11
59	239	1.73	1.88	1.61	0.76	3.89	3.28	3.75	5.17
61	562	1.31	0.99	1.45	1.24	9.35	8.14	9.39	11.58
64	704	2.07	2.55	2.28	1.82	10.4	8.48	15.45	9
68	615	2.88	3.22	1.5	2.62	14.57	14.8	14.15	17.86
76	1,535	21.61	22.15	21.21	17.72	40.88	40.56	41.06	45.14
67	3,707	35.84	38.86	35.51	29.17	83.88	79.13	81.89	99.7
56	7,048	47	52.14	45.59	35.52	124.92	120.06	121.5	160.1
52	8,021	57.56	65.09	41.28	55.79	138.62	136.21	134.78	174.23
43	10,620	81.38	92.27	79.66	58.04	171.6	179.08	169.65	213.35
31	16,590	107.28	118.16	105.2	83.33	299.36	306.02	299.68	358.16
4	26,390	127.98	139.2	125.74	103.41	405.94	417.32	413.41	497.45

other hand, average streamflows and runoff in the wet season, increased with increased land use intensity.

DISCUSSION

We explored how SWAT can be used for planning and managing water resources in relatively large (~28,000 km²), heterogeneous basins experiencing dynamic land use changes. We developed stepwise and multisite procedures to effectively tailor and customize the use of SWAT so it can more likely be used for water resource management. Additionally, the model effectively estimated the flow responses to changes in land use and land cover. Below, we discuss limitations, advantages, and ways forward to implement SWAT to inform water resource planning and management in continental-extent countries, such as Brazil.

Multi-step procedure for multisite calibration in large basins

Management and planning of water resources in Brazil are carried out by planning units of similar size areas as the Rio das Velhas basin. Our results show that tailored and customized calibration of ecohydrological models coupled with GIS efficiently modeled runoff in our study area. Using multiple streamflow monitoring stations and multisite calibration approaches improves water flow modeling.

Even without calibration, the model represented the general pattern of the hydrographic peaks and recessions but overestimated peak flows and underestimated base flows, as expected in the pre-calibration phase (Abbaspour et al., 2015; Tan et al., 2020). Changing the values of some parameters improved model estimates. For example, we decreased the value of the runoff curve number for moisture condition II (CN2), the distance between the shallow aquifer depth and the surface (GWQMN), and the water return coefficient from the aquifer to the root zone (GW_REVAP). On the other hand, we increased the values of available water capacity in the soil horizon (SOL_AWC) and the water limit in the shallow aquifer to return to the root zone or percolation to the deep aquifer (REVAPMN) when the base flow was very low (Abbaspour et al., 2015; Rouholahnejad et al., 2014). We also recalculated soil evaporation demand (ESCO) in the case of overestimated peaks.

In line with other studies, our results also highlight the importance of SWAT calibrations (Andrade et al., 2019; Durães et al., 2011). After calibration, NS, PBIAS, and R² were within 95% confidence levels. The PBIAS values were greatly improved, ranging from satisfactory to very satisfactory. Before calibration, only one sub-basin had satisfactory NS estimates, but NS was satisfactory for all stations after calibration. The validation results improved model performance, indicating that the calibrated model can be extrapolated to other periods.

For many reasons, adopting multisite calibration for a large and very heterogeneous basin was important. Our results were individually calibrated and regionalized for each sub-basin group

(see Supplementary Material S10). In this way, the calibration data provided a level of detail that favors water management and planning at the sub-basin extent instead of the entire basin. 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 multisite calibration, this approach requires considerable processing capacity because it is necessary to perform several iterations for each station. However, by checking the results step by step and then performing the maximum of iterations reduced processing time considerably.

When proceeding with stepwise multisite calibration, we saw that it was more difficult to achieve good adjustments for the upstream stations than for the downstream stations (see Table 4). This occurs because as streamflows were calibrated upstream, the modeled streamflows were automatically adjusted downstream, facilitating the calibration of downstream flows and in ever larger sub-basins. Also, 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.

Comparing the model calibration and validation performance with literature values facilitates further understanding of model improvements, despite basin differences. The performance values obtained in our study for NS (0.73 to 0.97 in calibration; 0.51 to 0.98 in validation) and PBIAS (-11.3 and 19.4 in calibration; -18.6 and 24.6 in validation) are in line with previous work (Arnold et al., 2012b). However, if we analyze the most instrumented sub-basin in this study (sub-basin 4, ~25,000 km²), we observed a NS of 0.97 (calibration and validation) and PBIAS of 2.3 and 1.8, for calibration and validation, respectively. Other studies of relatively large basins showed poorer results. For example, Durães et al. (2011), studying the 14,000 km² Paraopeba River basin 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 ecohydrological model to simulate the flow in a 13,000 km² basin in Kenya. Calibration was performed for 5 years (1980 to 1985), with monthly and daily time steps. Their model adjustment for the monthly calibration (NS of 0.76 in calibration and 0.74 in validation) was higher than for the daily calibration (NS of 0.71 in calibration and 0.63 validation).

Land use and cover change scenarios

Through SWAT simulations, we observed that scenarios with increased agricultural and urban areas at the expense of native forest areas caused changes in the basin water balance. Among them, runoff increased, and infiltration and base flow decreased, as expected. In addition, the current scenario differed from the natural scenario, in which modeled surface runoff decreased and infiltration and base flow increased. Other authors have found similar results using SWAT to simulate different land use scenarios in Brazil (Andrade et al., 2017; Perazzoli et al., 2013; Rodrigues et al., 2015). Although the simulated scenarios are extreme, the results facilitate us seeing the applied theory by quantifying the impacts of increased anthropogenic interventions seasonally.

The percolation of water to the deep aquifer supports base streamflows in the periods. During droughts, it is critically important for sufficient base flows to maintain the watercourse permanence, ecosystems, and ecosystem services. However, greater human intervention drives base flows in the opposite direction (Hudak, 2004). On the other hand, in the wet season, increased soil impermeability (represented by the average value of the curve number) hinders infiltration and increases surface water runoff. This is not ideal because what is desired in rainy periods is for sufficient water to infiltrate to maintain dry season streamflows and dampen peak flows to minimize flooding (Paul & Meyer, 2008).

Limitations and advantages of this approach

Although robust estimates were achieved, there are five input-data issues. First, the model assigns uninterpolated precipitation data to the value of the nearest measurement station for each sub-basin. Szcześniak & Piniewski (2015) assessed the effect of entering interpolated precipitation data on the calibration results in 11 medium-sized sub-basins. They concluded that in basins with few measurement stations and having low variation of daily precipitation, interpolated methods improved estimates. Second, climatic series have flawed or gaps in historical data. In our case, they were filled with the weather generator model available in SWAT (WXGEN) (Sharpley & Williams, 1990). Despite being a widely used method to generate climate data, it generates uncertainties like any other model (Herman et al., 2018). Third, the streamflow data series from monitoring stations contained missing data that were filled through regression models, which again include uncertainties (Esmaealzadeh & Dariane, 2014). A fourth issue is the national-extent soils data. Because no pedological data were available for our entire study area, we used data from the upper Rio das Velhas basin (see Supplementary Material S6). To overcome 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 an extremely imprecise data layer in Brazil (De Mello et al., 2020). Currently, the country has only general soil surveys with low-resolution maps; < 5% of the nation's soils are mapped at a resolution of 1:100,000. Fifth, only about half the sub-basins are true watersheds, meaning that those sub-basins create misleading estimates of true watershed land use, discharge, and water quality (Omernik et al., 2017). Modeling could be improved by joining upstream true watersheds and downstream HUC sub-basins into true watersheds, by using digital elevation modeling to determine true watersheds of various sizes, or by mapping landscape portions where surface flows drain directly into a particular stream or river segment ('catchments'), but excluding any upstream contributions (Hill et al., 2016).

Further analyses of uncertainty propagations in the model can contribute to understanding the output variability, which is crucial for making water resource decisions. However, the current model is a useful tool for managing water resources in the Rio das Velhas basin given sufficient calibration and adequately simulated flows. Besides, the methodological approach used (creation of sub-basins, ottobasins, Hill 'catchments', or true watersheds; inputting layers of soil type, slope, and land use; climatic data;

delimitation of HRUs; 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 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 flow regimes but also because it is effective, user-friendly, well-documented, available to the public free of charge, and supported by GIS tools. Training workshops on SWAT are frequently held in Brazil, which facilitates expanding the knowledge of the tool's use and clarifying the doubts of the modelers (Bressiani et al., 2015). The model is distributed; therefore, the main basin can be divided into sub-basins or true watersheds. This approach accounts for spatial variation of the parameters, which is extremely important in modeling large basins (Wood & O'Connell, 1985). In addition, the tool is versatile and effective and can provide reasonably accurate results (NS efficiency values > 0.5) with moderate data entry effort (Arnold & Fohrer, 2005; Chaplot et al., 2004; Heuvelmans et al., 2005). Finally, it offers a wide range of water body management applications, including selecting best management practices (BMPs; Behera & Panda 2006).

Implications for water resource management in Brazil

Although numerous modeling tools are available for managing water resources, evidence is scarce on the use of these tools to inform water management and planning globally. Hydrological modeling tools in decision-making are particularly challenging in tropical countries. Here we tailored and customized SWAT calibration and validation in the context of large hydrologic units in Brazil. Despite the widespread acknowledgment that hydrological models are essential 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 critical in countries such as Brazil, which is experiencing unprecedented land use changes and only beginning to experience fundamental climate changes. Changes in vegetation influence processes in the water cycle through structural effects on key ecosystem functions in watersheds (Ponette-González et al., 2015). Changes in watershed evapotranspiration regimes, resulting in changed retention of precipitated water in tree canopies and soil infiltration capacity, affect the volume and timing of water runoff (Fletcher et al., 2013; 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. However, there are still issues to overcome to incorporate hydrological modeling 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 using models in water management and planning.

Throughout our study, 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 for parametrizing the model adequately

captured hydrological processes in the Rio das Velhas basin. With this calibrated model, 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 water supply permits, and maintaining minimum flows in the basin's rivers is essential to ensure this supply and support aquatic ecosystem structures and functions (<https://siga.cbhvelhas.org.br>). Therefore, water resource management agencies can use models such as ours to assist in planning for anticipated future water shortages that could affect over 5 million people. These tools are particularly useful for analyzing the effects of demographic growth, land-use changes, and 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 (Brasil, 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 (Agência Reguladora de Serviços de Abastecimento de Água e Esgotamento Sanitário do Estado de Minas Gerais, 2013). During droughts, when river flows decrease, the Paraopeba reservoirs can be used to maintain supply. When the reservoirs fill during rainy periods, the Rio das Velhas basin can become the primary water source. Hydrological modeling can be useful in this decision-making process by modeling water availability and exploitation scenarios.

Another important contribution of SWAT ecohydrological modeling is to include land use as a layer for defining hydrologic response units (HRUs) and, consequently sub-basins or watershed potentials. 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. Furthermore, the model is flexible regarding insertion of climate heating scenarios in the context of watershed management (Bressiani et al., 2015).

CONCLUSIONS

The SWAT multisite calibrated model effectively replicated the relatively large and heterogeneous basin's hydrological processes. The study results showed that the SWAT ecohydrological model was an effective tool that could help manage land use that directly affects the amount of water and its multiple potential uses. Multisite calibration improved the accuracy and precision of the model, and it can be used to predict how changes in land use can influence water availability and improve water resources management. However, water resource management must consider future climate scenarios, and thus an adequately calibrated hydrological model can be very useful in land and water use planning. The adjustments obtained proved to be consistent with other studies carried out in large basins in continental-sized countries such as Brazil, China, and India. Despite the previously presented limitations, we found that using SWAT coupled with a GIS facilitated the simulation of complex hydrological processes. That modeling can serve as a tool to better target decision-making by Brazilian water resource

management agencies and reduce the impacts of anthropogenic interventions on water flow regimes.

ACKNOWLEDGEMENTS

This research was supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq, research productivity grants 309763/2020-7 and 313566/2021-6 to DRM and SMCR), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES, Finance Code 001) and Fulbright Brasil to RMH.

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Editor in-Chief: Adilson Pinheiro

Associated Editor: Fernando Mainardi Fan

SUPPLEMENTARY MATERIAL

Supplementary Material S1. Streamflow Monitoring Stations

Supplementary Material S2. Flow series faults correction

Supplementary Material S3. Weather and rainfall stations

Supplementary Material S4. SWAT weather generator model parameters (SWAT WXGEN model)

Supplementary Material S5. Compatibility between Mapbiomas legend and SWAT database

Supplementary Material S6. Parameters of soils physical-hydro characteristics

Supplementary Material S7. Relationship between sub-basins and streamflow monitoring stations

Supplementary Material S8. Model start values for sensitivity levels

Supplementary Material S9. Observed and simulated flows before and after calibration

Supplementary Material S10. Calibrated values by subbasin

Supplementary Material S11. Adjustment results to streamflow simulated vs observed values by subbasin

This material is available as part of the online article from <https://doi.org/10.1590/2318-0331.282320230034>