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PII: S0048-9697(20)31020-2

DOI: <https://doi.org/10.1016/j.scitotenv.2020.137509>

Reference: STOTEN 137509

To appear in: *Science of the Total Environment*

Received date: 2 October 2019

Revised date: 13 February 2020

Accepted date: 21 February 2020

Please cite this article as: A.C. da Encarnação Paiva, N. Nascimento, D.A. Rodriguez, et al., Urban expansion and its impact on water security: The case of the Paraíba do Sul River Basin, São Paulo, Brazil, *Science of the Total Environment* (2020), <https://doi.org/10.1016/j.scitotenv.2020.137509>

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**Urban Expansion and its impact on water security: The case of the Paraíba do Sul
River Basin, São Paulo, Brazil**

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Abstract

Increasing demand for water is one of the most challenging problems that human societies face today and has encouraged new studies to examine water security and water management. Seeking to discuss this important issue in the Brazilian context, we analyzed the impacts of urban expansion on water security in a basin located in the most populated region of Brazil. To quantify increased water demand, we combined urban sprawl and regional population increase projections. In this context, our study contributes to discussions on water security by addressing the importance of integration between water and urban planning. Simulations indicate good performance in reproducing actual water system conditions. The findings demonstrate that urban expansion in the region is

mainly driven by road proximity. Urban occupation is projected to increase in 170% by 2050, increasing water demands for domestic use in 38%. Results indicate the feasibility of including landscape and socioeconomic constraints in order to obtain potential domestic water demand scenarios by using land use and land cover change modelling to assess urban expansion and population growth. For the study region, our findings suggest that although urban sprawl increases water demand, urban supply will not be compromised given the large volume of available water in the basin. However, the indirect consequences of urban sprawl, such as industrialization and agricultural intensification, may compromise the quality of this resource and require better water use management in the region.

Keywords: Water supply, Urbanization, Population growth, Land use modelling.

1. Introduction

The concept of water security involves sustainable water use, a strive for economic well-being, social equity and water-associated risks reduction (Hoekstra et al., 2018), as well as populational water supply security and production activities in a state of unbalanced water resource supply and demand (Jepson et al., 2017). This is an ample concept, encompassing geopolitics (Empinotti et al., 2019) and human health (Vörösmarty et al., 2010), and can be applied in many forms and types of governance (Jepson et al., 2017). Studies have associated this issue with climate change impacts and adaptation, water management and urban growth (Frone and Frone, 2015; Ghosh et al., 2019; Shao et al., 2012; van Ginkel et al., 2018; Xiao-jun et al., 2014; Yomo et al., 2019).

Studies surrounding climate variability and climate change have shown that these issues will have a vast impact on global water supply and accessibility due to disturbances to

hydrological cycles and climate patterns (van Ginkel et al., 2018). These scenarios are aggravated when human actions are considered. This is especially true when considering land use and cover change (LUCC) as it generates impacts on water resources. Today, LUCC processes are one of the main causes of disturbances to natural systems (Sakai et al., 2004) and, therefore, research on the issues surrounding LUCC has increased in different scientific fields around the world. There is a known correlation between LUCC and water supply, which has been shown to have consequences on water flows, energy, carbon balance in the atmosphere, and local biodiversity dynamics (Carriello et al., 2016; Sakai et al., 2004) at different kinds, intensities, and scales (Coe et al., 2009; Hayhoe et al., 2011; Siqueira Jr et al., 2015). Water security relies significantly on water supplies as an ecosystem service (Geng et al., 2014), which is, in turn, influenced by LUCC (Bennett et al., 2009).

In this context, urbanization is considered to be one of the most drastic forms of LUCC as it impacts the environment in a number of ways (Ghosh et al., 2014; Maiti and Agrawal, 2005). Population growth is one of the major urban expansion drivers (Shukla et al., 2013; Tomás et al., 2016), generally associated with high rates of rural to urban migration (Tomás et al., 2016; Wilson and Chakraborty, 2013). According to the United Nations (UNESCO, 2018), 55% of the world's population lives in urban areas, and estimates indicate that this percentage could reach up to 68% by 2050.

Regarding the hydrological dynamics, urban development expands impermeable surfaces, reduces the vertical circulation of water and underground flow recharges, increases surface runoff, and reduces evapotranspiration (Fletcher et al., 2013). An increase in direct runoff volumes and a decrease in water basin response times result in larger peak flows to drainage systems and channels, which enhance the risk of floods (Thomson et

al., 2005). Such changes in water pathways lead to a baseflow reduction, further aggravating water shortage during hydrological droughts (Calow et al., 2010).

Urbanization can also impact water quality from trash and pollutants being dragged from urban surfaces to drainage systems, and from sewage being dumped into channels (Paul and Meyer, 2001). Urbanization of drainage basins causes deforestation and catchment degradation, morphological alterations to rivers and extinction of river channels, increased soil erosion, increased river silting and sedimentation, and environmental pollution (Shukla et al., 2013). Water pollution reduces water availability, increasing water treatment costs, while sediment deposition in reservoirs decrease storage capacity, and both result in decreased water security (Hoekstra et al., 2018).

In addition to water availability decreases, urbanization also enhances pressure on water systems, as it leads to increased water demands (Wada et al., 2016, Dutta et al., 2010) which, alongside decreased water stocks and quality, enhance issues concerning water security (Deng et al., 2013). High demands and reduced water supply can, in turn, lead to decreased water quality and accessibility (Groppo et al., 2008; Qin et al., 2014; Shukla et al., 2013), making human populations more vulnerable to water availability fluctuations and less resilient to future changes (Ghosh et al., 2019). Therefore, to ensure water security, improvements in public policies towards urban planning are paramount (Empinotti et al., 2019).

Consequently, urban expansion can increase water demands, enhancing pressure on local water resources (Dutta et al., 2010). High demands and reduced water supplies can lead to decrease water quality and accessibility (Groppo et al., 2008; Qin et al., 2014; Shukla et al., 2013) and, therefore, require improvement of efficient public policy responses toward urban planning to ensure the water security (Empinotti et al., 2019).

Globally, water use has been increasing at a rate of 1% per year since the 1980s, driven by population growth, socioeconomic development and consumption patterns (Unesco, 2019). Water demand is expected to continue increasing by 20 to 30% above the current level by 2050, especially in the industrial and domestic consumption sectors (Unesco, 2019). In Brazil, demand for water has been increasing since in the last years and is directly linked to economic development and urbanization in the country (Brasil, 2010). In Brazil, it is estimated that 84% of the country's population lives in urban areas (Brasil, 2010). In more populated areas, such as Brazil's Southeast region, there has been significant population growth over the past 30 years, which has caused huge demand for water withdrawal for domestic consumption, and driven the demand for other diverse uses, such as industrial use (Kelman, 2015). Recently, in 2014, an exceptional drought in Southeastern Brazil resulted in a water crisis (Coelho et al., 2016; Nobre et al., 2016), affecting the metropolitan area of the state of São Paulo, comprising a population of over 20 million inhabitants, which highlighted the deficiencies in resource management and the increasing dispute for water (Kelman, 2015). Moreover, by the beginning of 2020, the water supply of Rio de Janeiro was also seriously affected by quality problems related to intense urbanization and lack of sewage treatment in municipalities surrounding the metropolitan area (Associated Press, 2020).

This study was carried out in the Paraíba do Sul River Basin, which is located in Brazil's Southeast region. The Paraíba do Sul River Basin is responsible for supplying water to the entire Paraíba Valley, and about 75% of the total water consumption for 13 million inhabitants of the Rio de Janeiro metropolitan area, through a river diversion constructed in the 50s. In addition, in the wake of the 2014 water crisis, a new diversion was implemented, aiming at increasing the water security of the metropolitan São Paulo area during extreme droughts (Kelman, 2015). Therefore, water availability in the Paraíba do

Sul basin acquired a strategic character as a safe source of drinking water not only for the basin population, but also for the two main Brazilian metropolitan areas.

In this paper, we explore the feedbacks between urban expansion and water consumption to determine how they influence future water security. Specifically, we aimed to assess if the projected expansion of urbanized areas within the basin alongside increasing water demands, can compromise water security for human consumption in the Paraíba do Sul basin in the next decades. To this end, we use a cellular automata model to project urban expansion which, combined with population growth, allowed for the estimation of water demands for domestic use in the Paraíba do Sul basin until 2050.

2- Study Area

Our analysis was restricted to the part of the Paraíba do Sul River Basin that is located in the state of São Paulo, in the Vale do Paraíba Paulista meso-region (VPP). This region is composed of 39 municipalities and has a population of approximately 2.5 million inhabitants (Brasil, 2010). In addition to being the most densely populated area of the basin, this drainage area includes water withdrawals for the Metropolitan Regions of both Rio de Janeiro and São Paulo, the two most populated cities in Brazil. The basin is part of the Southeast/Midwest subsystem, which contributes about 60% of Brazil's total stored energy (Brasil, 2018). Currently, the multiple uses of water are distributed among domestic and rural consumption, animal consumption, electricity generation, industry, agriculture and mining (Table 1). According to Brazilian National Water Agency (ANA) (Brasil, 2019), the demand for urban supply has increased in recent decades and represents 49% of all water withdrawn from the basin, followed by withdrawals for industries (19%) and irrigation (18%). The volume of withdrawn water has increased by

about 7% over the last 20 years. At the same time, industrialization and urbanization have placed the Paraíba do Sul river basin in critical environmental conditions (Gomes et al., 2018; Silva et al., 2016).

The intensification of population growth in the Vale do Paraíba do Sul occurred in the early nineteenth century with the introduction of coffee cultivation to the region (Carriello et al., 2016). After the decline of coffee cultivation, a number of developments including: construction of the *Central do Brasil* railroad and the *Presidente Dutra* highway, in addition to industrial development in the valley enabled the states of Rio de Janeiro and São Paulo to integrate economically with the region (Carriello et al., 2016; Silva et al., 2016). Consequently, this integration has made the Paraíba Valley one of the axes of great importance for communication and development in the region and the country (Andrade et al., 2016). Today, the Paraíba Valley accounts for approximately 5% of state GDP (Gross Domestic Product) in São Paulo (Brasil, 2010).

In this paper, we adopt the territorial divisions defined by the Brazilian Institute of Geography and Statistics' (IBGE) (Figure 1), based on mesoregions and micro-regions, in order to facilitate the analysis of the different patterns of urban areas. This division was defined by the structure of industrial production, agriculture, mineral extraction and fishing, and includes urban and rural activities (Brasil, 1990).

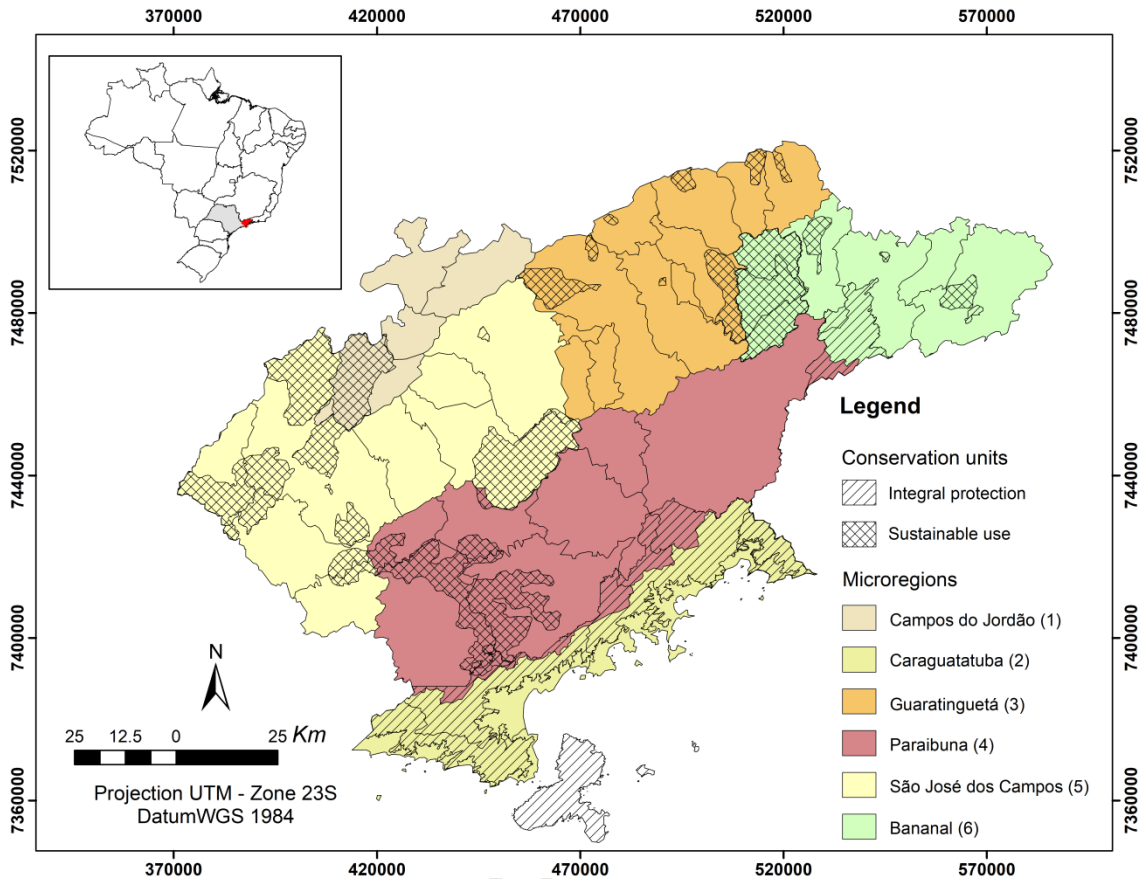


Figure 1 – Location of Vale do Paraíba Paulista and its subdivisions according to IBGE's Regional Division of Brazil in Micro-regions.

3- Methodology

3.1- Database

Inputs for the land use model consisted of a set of variables that represent the biophysical, access and use characteristics that are present in the Paraíba Valley region (Table 2), as these were understood to be key variables that explain urban expansion in the region.

LUCC maps (Figure S. 1.) refer to the years 2005 and 2010 and their classes are: Pasture, Urban, Vegetation, and Water. All data were converted from shapefiles to raster format with 90 m resolution, in UTM-WGS84 projections. Both types of information were reclassified. The Conservation Unit was divided into two classes: Sustainable Use (US)

and Full Protection (FP). The Full Protection conservation unit inhibits the formation of new urban areas, given that human settlements and any exploitation of natural resources are prohibited (Brasil, 2000). Brazilian law establishes that human settlements are permitted in Sustainable Use conservation units, provided that there is compatibility between nature conservation and the sustainable use of natural resources (Brasil, 2000).

The distances from each point to the highways, railroads, hydrography and dam polygons were estimated according to their Euclidean distance in the vector bases. Next, we created *cube maps* where all data were included in order to calculate the probability of a certain land use class transition in each pixel (Soares-Filho et al., 2002).

3.2. Modelling

In order to simulate future urban expansion scenarios and their impacts on water security, we performed two models routines (Figure 2): one simulated LUCC in the study area and the other estimated the withdrawal of water and consumption dynamics in the VPP, based on scenarios of urban expansion.

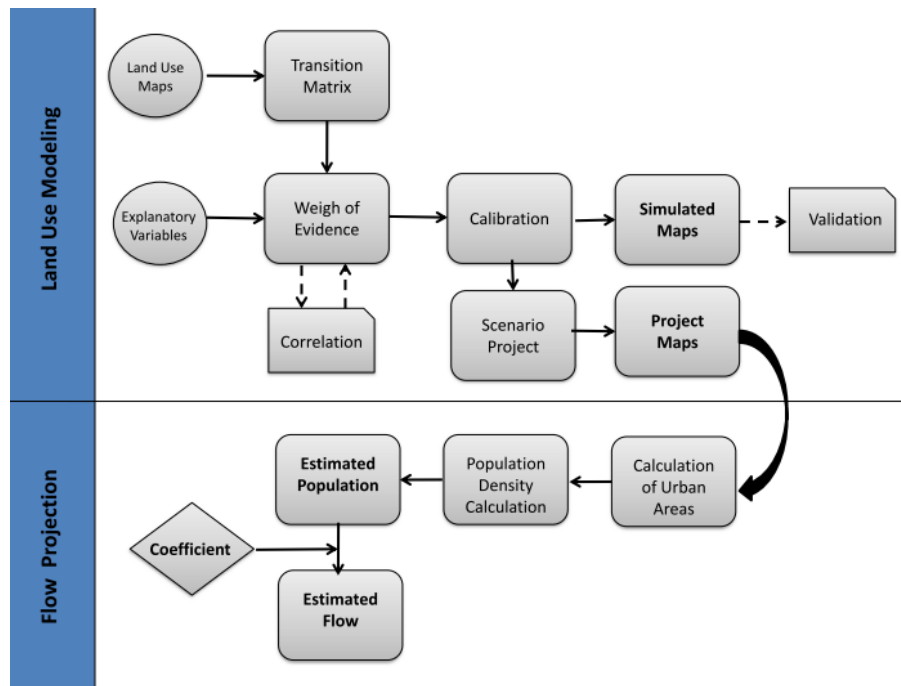


Figure 2 – Diagram of the steps performed in our analysis.

3.2.1. - Land use modeling

In recent decades, cellular automata models, including local interactions into the landscape, have been applied to incorporate spatial expansion representations of urban growth (Fang et al., 2005; He et al., 2008; Yeh and Li, 2006). For LUCC modelling, we used the Environmental system modeling platform Dinamica EGO 4 4.0.10, (<https://csr.ufmg.br/dinamica/>) (Soares-Filho et al., 2009). The model is based on the cellular automata approach (White et al., 2000) and uses a sequence of algorithms that consider that the state of a cell can change according to predefined rules for each model interaction. We developed maps of the explanatory variables that drove LUCC dynamics and guided the process of classifying cells with high and low probability of change (Soares-Filho et al., 2009). Dinamica EGO models generate transition probability maps, simulated landscape maps, and dynamic maps of explanatory variables (Soares-Filho et al., 2002).

Our modelling process focused on two specific transitions of land-use change: pasture to urban and vegetation to urban. In the first step, we generated transition matrices that were calculated from two maps, one from 2005 and the other from 2010, identifying transition rates. Due to the different patterns of urban expansion that we observed throughout the study area, we divided our analysis according to micro-regions estimating local parameters and coefficients and, consequently, analyze the impacts at different sub-regional scales (Soares Filho et al., 2009).

To analyze the influence of each exploratory variable on LUCC transitions, we performed *Weight of evidence* analyses. Evidence weights were also calculated according to micro-regions. Consequently, for each micro-region and transition a representative group of explanatory variables and their corresponding evidence weights were derived. From these results, tables were generated with the level of significance of the probability of each category for certain LUCC transitions to occur. Positive values of the weight of evidence favor certain types of transitions, whereas negative values indicate low probability of occurrence (Soares-Filho et al., 2009).

3.2.1 Calibration

To calibrate the model we cross-examined the initial land use map (2005), the set of explanatory variable maps, the evidence weights, and the transition matrix. In the following step, we adopted two algorithms available in Dinamica EGO, which are responsible for allocating cells and the shape of patches: the *expander* – to expand and contract existing patches, and the *patcher* -to create new patches.

3.2.2. Validation

To validate the model, we carried out an analysis of similarities between the input land use maps and the simulated land use map. Following Soares-Filho et al (2009), we adopted the Reciprocal Similarity Comparison method (Almeida et al., 2008), which accounts for the minimum fuzzy similarity between changes to both maps by applying Fuzzy Kappa (Hagen, 2003) with a *function of exponential decay* in multiple moving windows of different sizes (Khatibi et al., 2017). This method resulted in a similarity map that is calculated from the observed land use map, the simulated map, and the maximum and minimum similarity values. To validate the model we only considered the maximum similarity since one of the objective of this paper is to use the quantification of urban expansion to estimate the population of the VPP.

3.3- Scenarios

The transition rates from historical land use and land cover maps were used as baselines for the generation of future scenarios. In other words, the parameters derived from the simulations between 2005 and 2010 were used in projection the “urban” class for the years 2025, 2030, 2035 and 2050.

3.4- Water flow modelling

To estimate water flow we used a sequence of equations who estimate population growth and water consumption, while taking into consideration the urban area projected by the LUCC models. Because IBGE projections generate information aggregated at the state level, while this study required urban population at a finer scale. We projected population density growth rates based on the observation of the national census for each of the micro-regions, and then combined with their corresponding urban sprawl estimating urban population. All variables were calculated for the years 2025, 2035 and 2050. We

calculated the amount of withdrawn water by considering the per capita urban withdrawal coefficient for the state of São Paulo (the methodology for these data is described in the National Electric System Operator - (Brasil, 2005).

Population was estimated based on average population density data (inhabitants/km²) (Eq. 1) and urban area (Eq. 2). Population density data was obtained from the 1991, 2000 and 2010 IBGE census. Urban area was estimated from the urban expansion scenarios generated by the Dinamica EGO model:

$$D_t = \frac{H}{A_t} \text{ (Eq. 1)} \quad \text{e} \quad D_u = \frac{H}{A_u} \text{ (Eq. 2)}$$

where,

D_t = Total population density, H = number of inhabitants, A_t = Total area (urban + non-urban), D_u = Urban population density, A_u = Urban area.

Thus, the urban population density (Eq. 3) was estimated by the formula:

$$D_u = \frac{D_t \cdot A_t}{A_u} \text{ (Eq. 3)}$$

The amount of withdrawn water (Eq. 4) was calculated by analyzing the per capita income in each micro-region.

$$Q_u = Pop_{u,a} \cdot CP_{(Fxn)} \text{ (Eq. 4)}$$

Where, Q_u = withdrawal flow, $Pop_{u,a}$ = inhabitants; $CP (Fxn)$ = *per capita* coefficient. In this study the population range that was attributed to each micro-region was defined by its average population.

The consumed flow (Eq. 5) is the difference between the withdrawal flow and the return flow (Eq. 6). ABNT NBR 9649 recommends that, in the absence of observed values, a 0.8 return coefficient be adopted for urban supply (Brasil, 2019).

$$Q_{u,c} = Q_u - Q_{u,r} \text{ (Eq. 5)}$$

$$Q_{u,r} = Q_u \cdot K_{r_{urb}} \text{ (Eq. 6)}$$

Where, $Q_{u,r}$ = return flow from urban supply, $K_{r_{urb}}$ = coefficient of return from urban supply, $Q_{u,c}$ = consumption flow from urban supply.

Municipalities that are located in the VPP region but do not use water from the basin for human supplies were excluded from the flow calculations, namely: Monteiro Lobato (located in the micro-region 1) and all the municipalities in micro-region 2. By contrast, the cities of Guararema and Santa Isabel are not part of the VPP but draw water from the basin for human supply and were, therefore, included in the calculations. Flow projections for these cities are presented in Table 5 as “Additional cities”, considering the projections of withdrawal and consumption of water for public supply until 2035 included in the Investment Plan Reports for each municipality (SABESP, 2018). It should be noted, however, that this projection does not extend until the year 2050.

4- Results

4.1- LUCC Modelling

The highest LUCC transition between 2005 to 2010 was from pasture to urban (Table 3). This transition occurred mainly in micro-regions 3 and 5, which are the most populated micro-regions in the study area (Figure 8). The lowest rates for this transition were

observed in micro-regions 1 and 6, which are located in mountains areas that are legal environmental protection areas, therefore making urban occupation difficult. In region 2, which is located on the coast, the vegetation to urban transition was noticeable. Micro-region 6, which presented the smallest transition for the two studied conversions, has a low population density, with about 12.7 inhabitants/km² (Brasil, 2010).

In the Pasture/Urban and Vegetation/Urban (Table 4) transitions, positive weight of evidence values were observed in all regions for the variable “distance to urban area”. The variable “highway distance” favored urbanization in all the micro regions studies. The variable “rail distance” favored the transition in regions 1, 3 and 5, regions where the railroad is present. The variables “distance from the river” and “distance from the dam” also influenced urban sprawl in the regions along the river drainage network (3, 4, 5 and 6). We observed that pasture/urban conversion in micro-regions 4 and 6 are predominant, given the presence of the Serra do Mar Conservation Unit. In the case of vegetation/urban conversion variable PI repelled the transition in all micro-regions, especially micro-regions 3, 5 and 6, where the Serra do Mar and Mantiqueira conservation units are located.

Comparing the maps quantitatively, the LUCC model adequately represented urban expansion dynamics (Fig. 3) with an error of approximately 5%: in 2010, the observed urban area was 83440.72 ha, while the simulated area was 88173.15 ha.

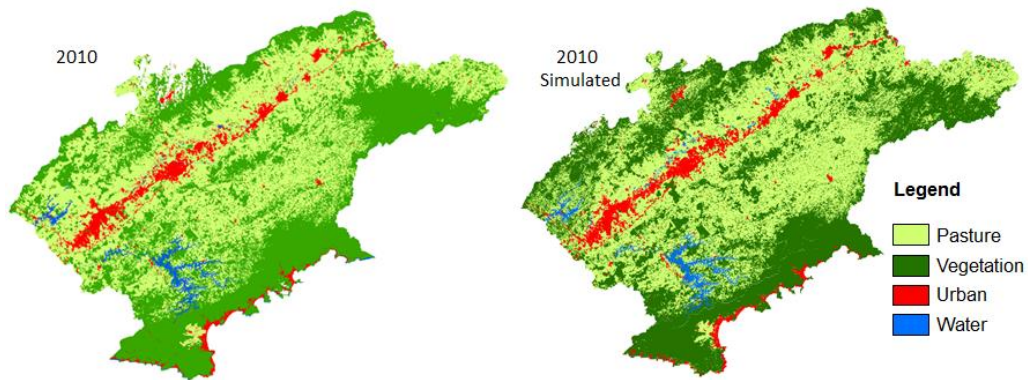


Figure 3 – Comparison of observed and simulated 2010 land use and land cover maps.

Validation results from a comparison of the simulated and the observed (2010) maps show maximum similarity (Figure 4) values above 50% in the 3x3 window and at 91% in the 11x11 window.

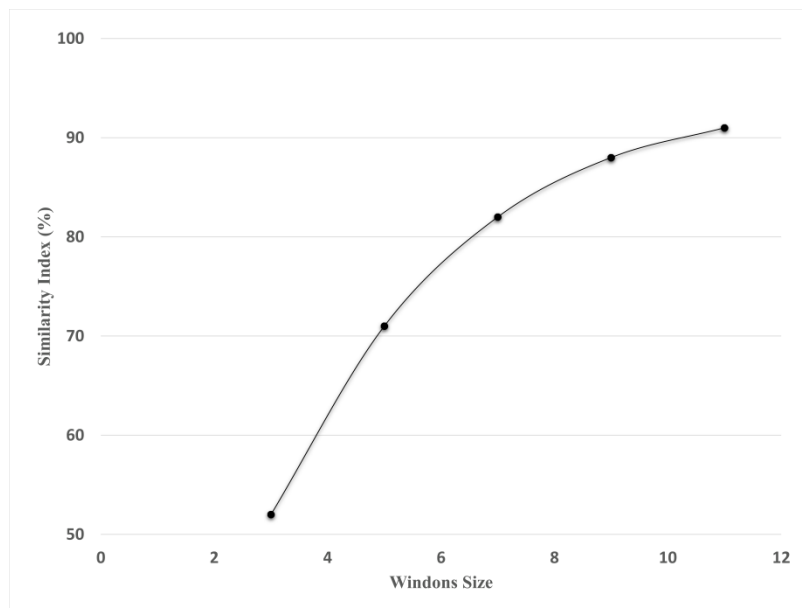


Figure 4 – Maximum similarity indices derived for observed and simulated land use and land cover maps for 2010.

4.2- Urban expansion scenarios

The urban expansion scenarios only considered the transitions from pasture and vegetation to urban, whereas the other classes remained static. Figure 7 presents the

evolution of urban expansion. The areas corresponding to the years 1990, 2000 and 2010 were estimated based on land use classifications, while the scenarios for the years 2025, 2035 and 2050 were generated by the model. The intensification of projected urban area converged around the Dutra and Coastal Highway axes (Figure 5) was expected since these regions currently have the largest concentrations of urban areas.

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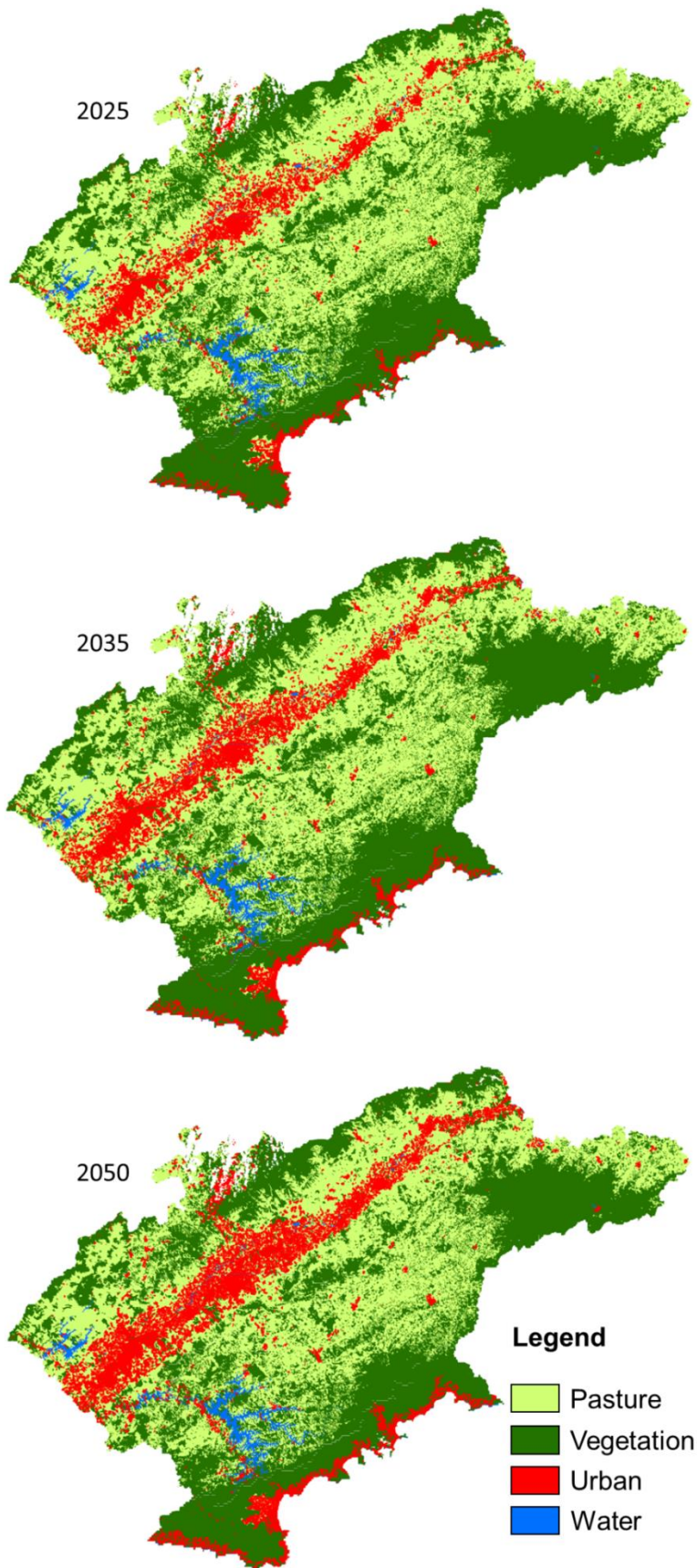


Figure 5 – Urban expansion scenarios simulated for 2025 (top), 2035 (middle) and 2050 (bottom).

4.3- Flow projection

Censuses indicated 15% increase in population density in the region every 10 years (Figure 7). The population projection considered density projections and urban area expansions for each micro-region in the LUCC scenarios, indicating a 40% increase in the region's population by 2050 (Figure 6).

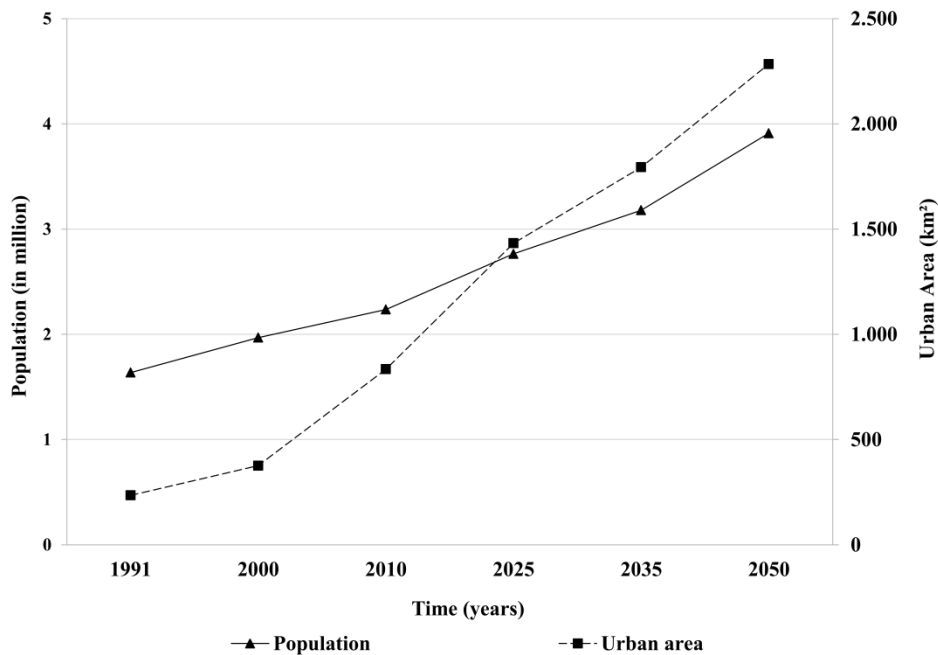


Figure 6 – Projection graph of urban area (ha) and population.

The total withdrawal flow in the region estimated by this method is 6.82 m³/s. Table 5 presents the results of simulated consumption and withdrawal flows for the years 2010, 2025, 2035 and 2050.

In terms of water demand, Table 6 indicates a 38% increase in water withdrawal for urban water supply by 2050 in the VPP. The withdrawal flow increased from 6.82 m³/s in 2010 to 10.99 m³/s in 2050. Urban consumption flow goes up from 1.38 m³ / s in 2010 to 2.19 m³/s by 2050, a 37% increase. Projections by 2050 indicate an average growth of

14% in consumption and withdrawal flows, in line with the increase in urban area projected by land use and land cover scenarios.

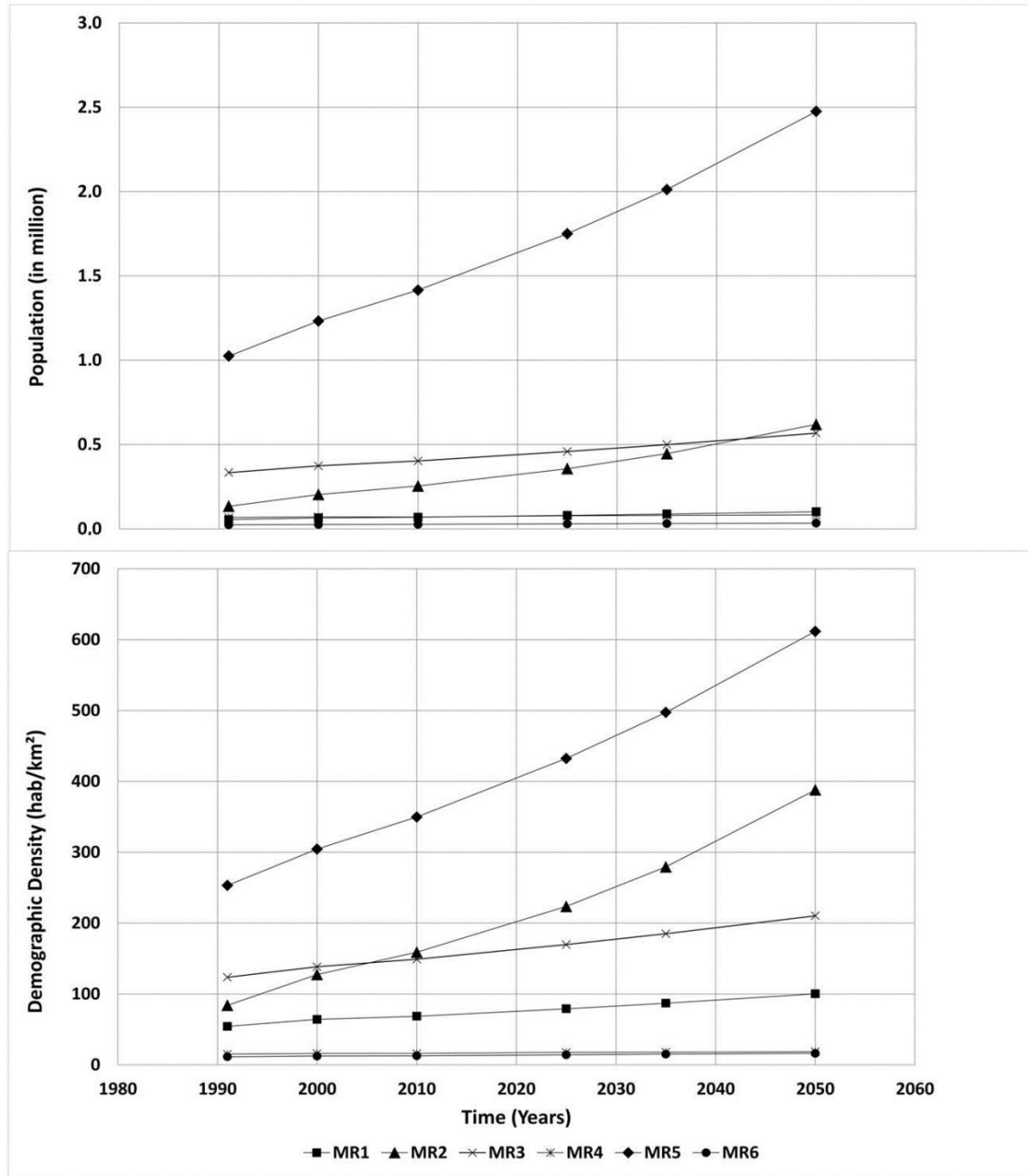


Figure 7 – Projection of demographic density and population for each micro-region (MR1-MR5) of the Vale do Paraíba Paullista.

5- Discussion

5.1- Urban Expansion

The 24% increase in urban area in the VPP between 2005 and 2010 occurred over pasture and vegetation areas, then, these transitions were studied in this paper. Urban sprawl is driven mainly by population growth and migration (Sudhira et al., 2004). The VPP micro-regions 2, 3 and 5 had population growth rates of 20%, 7% and 13%, respectively, between 2000 and 2010, the highest in the region during this period. Also found in these regions were the highest rates of transitions that were studied here.

Micro-regions 3 and 5 showed similar patterns of urban expansion. Both micro-regions have low forest/urban conversion rates due to the presence of consolidated urban centers. This causes the patterns of urbanization to influence pasture/urban conversion in their surroundings. Urban expansion is more likely to increase around urban centers because the easiness of displacement of goods, information and infrastructure (He et al., 2008; White and Engelen, 2000). The presence of a large transport network also influences the expansion in these micro-regions. Proximity to a transport network acts as a connector between urban centers and allows for the circulation of resources (He et al., 2008; Kebbles et al., 1982). The influence of hydrography is associated with the need to meet demand for water resources efficiently, at lower costs (Shukla et al., 2013), and for recreational purposes, such as fishing and boating, sparking interests in real estate (Devide et al., 2014). Additionally, the location of the infrastructure network is benefited by the flat relief, which facilitates human settlements (Dumitrescu and Cruceru, 2013). Conversely, the steepest areas of the Serra do Mar Conservation Unit act as a containment for urban expansion (Andrade et al., 2019).

Micro-region 2 stands out for its large population growth over the last decades and high urban use conversion rate. The factors that influence urban expansion in micro-region 2,

for both transitions, are: highways, sustainable use conservation units and slope. In more recent years the north coast has experienced large economic and urban growth driven by gas and oil exploration, the expansion of ports (e.g., the São Sebastião port), and the consolidation of tourism and urbanization (Marandola JR. et al., 2013). The coastal population in this region increased by 50% from 1991 to 2010 (Brasil, 2010, 1990), and this expansion was concentrated along major highways (Ruiz Jr. and Oliveira, 2013), there by corroborating the results noted in this study. Moreover, the narrow range of low slope areas between the Serra do Mar and the sea force urbanization to advance toward forests (Marandola JR. et al., 2013).

The urban expansion scenario modeled indicates a population increase of approximately 70% in the urban areas of the VPP for the year 2025 compared to 2010, and an increase of 170% by 2050. This conversion occurs mainly over pasture areas. Previous studies have analyzed the evolution of the urban expansion of the VPP and concluded that urban sprawl is strongly influenced by territorial organization and productive chain organization, as well as physical aspects, such as watersheds and relief, or anthropic aspects, such as rail and road axes (Andrade et al., 2019; Gomes et al., 2018). These results corroborate the findings reported herein regarding the urban expansion driver. However, unlike previous studies, our simulations are the first to offer quantitative future scenarios for the urban expansion of the VPP.

5.2- Population and Water

Results indicate that by 2050 the population of the PPV will increase by about 40%, which will generate an increase in demand in water supply for human consumption of about 60%. In terms of water supply, results show that the increased demand will not have a significant impact on the basin, as the reference flow (Q95) is 83.2m³/s at the

Pindamonhangaba gauge station and 113m³/s at the Queluz gauge station (Agevap, 2018). In terms of water security, even water-abundant regions are subject to a water risk in neighboring areas where water supply does not meet demand (van Ginkel et al., 2018). Since the VPP is legally required to supply water to the Cantareira system for the metropolitan area of São Paulo in case of a water crisis, this can potentially lead to conflicts (Kelman, 2015) with other uses within the VPP. Interbasin water transfers are the preferred resources among decision makers in times of water crises, since they are the cheapest and easiest option (van Ginkel et al., 2018).

The Brazilian National Water Agency (ANA) report on Brazilian water consumption (Brasil, 2019) estimates flow withdrawals of 5.7 m³/s in 2010 in the VPP. This indicates that our method might overestimate the withdrawal flow by 19%, which is a reasonable error considering the uncertainties in water supply and demand measurements (Shang et al., 2006). A previous study carried out by the Paraíba do Sul River Basin Agency (AGEVAP, 2013) estimated water withdrawals increases for the VPP as 6.6, 8.3 and 9.3 m³ s⁻¹ for 2010, 2025 and 2035 respectively, close to the estimates reported herein.

Thus, the assessment of population and water demand projections based on urban expansion projections from a cellular automata model produce estimates within the bounds defined by the uncertainties of water measurements and census population data. In agreement with the literature, our study demonstrates the feasibility of using land use and land cover change simulated by automata cellular models to assess potential public policy impacts on ecosystem services concerning natural resources sustainability (Albert et al., 2016; Geng et al., 2014; Sun et al., 2018; Yao et al., 2016).

This approach, based in cellular automata model, allows for the inclusion of local interaction effects between the different land uses in the landscape in order to project urban growth (Santé et al., 2010) and consequent water resource pressures.

The advantage of this approach is that it can be applied to other locations because it is entirely based on available census data. Therefore, it can be an effective decision-making tool when it comes to water resource management.

5.3- Limitations and perspectives

Although the study successfully demonstrated the trend of increasing water demand of the VPP, the method presents certain limitations. First, the urban sprawl model estimates applied herein did not include sociodemographic and socioeconomic variables such as income and education, and other variables that influence residential water usage, such as the presence of gardens or swimming pools, and tourism, among other things (i.e., Chang et al., 2017; Shi et al., 2018; Villar-Navascués and Pérez-Morales, 2018). Since neither the withdrawal estimate, nor the consumption use of constant water withdrawal coefficient consider the seasonality of supply, it is necessary to reevaluate estimates in cases of extreme climatic events for better assessment of risks (Otto et al., 2018). Furthermore, the withdrawal/consumption in rural areas was disregarded because land use maps do not quantify the rural population. However, water withdrawal in rural areas is minimal compared to urban areas. In addition, water security analyses carried out in the present study were based on quantitative deficit assessments, without accounting for water quality, water and wastewater treatments capabilities, freshwater accessibility and the distribution system efficiency. More comprehensive water security definitions include sustainability use and water resource protection, including access not only for humans but

also for the environment, as well as protection against flood and droughts. These approaches integrates both human and natural systems, and risk-based analyses environmental needs for water security (Wheater and Gober, 2015).

Our study focuses on water demands for domestic uses only, which is a priority use according to Brazilian laws, without considering potential agriculture impacts, such as rice farming, silviculture and eucalyptus plantations, traditional basin activities leading to high water consumption (Cabral et al., 2010; Tuong et al., 2005). Potential impacts concerning the expansion of these activities should also be assessed through environmental land use and land cover scenario modelling, since their expansion depend on socioeconomic variables (Rezende et al., 2018). Increased water transfers from the Paraíba do Sul River Basin through diversions to the Rio de Janeiro and São Paulo metropolitan areas may also affect the basin's water availability (Kelman, 2015). Finally, potential climate change impacts in the basin's hydrologic response add another uncertainty factor to future scenarios.

Interactions between human societies and natural systems constitute a highly complex, dynamic and a changing system (Sivapalan et al., 2012). Although there is broad knowledge about the anthropic effects on water systems, human responses to changes are difficult to assess and simulate. Considering that the knowledge of human adaptation strategies toward water resource management are still incipient (Baldassarre et al., 2015; Garcia et al., 2016; Pande and Sivapalan, 2017), projections should not be considered a de facto prediction of the future, but rather a plausible scenario to facilitate the exploration of adaptation strategies.

6- Conclusions

In this article we discuss the application of an approach that generates land use and land cover change projections to obtain future potential scenarios of water demand for domestic use, and its effects on water security due to urban expansion. Model simulations were validated for a historical period (2010) comparing the current withdrawal flow with the model simulation. The approach showed good performance, leading to more reliable future projections, in spite of the limitations due to the simplifications adopted in the modelling framework.

In the urban expansion model, results indicate that the transition will occur over pastures and forests. The explanatory variables distance to urban area, distance to highways, distance to railways (in the regions where the railroad is present), and slope presented the highest values of positive evidence weights in the two transitions. Protected Conservation Units are the biggest barriers to urban development. These results demonstrate that land-use transitions to urban areas are more intense in densely populated areas and less intense where there are protected areas or physical barriers. LUCC modeling is considered satisfactory since it captures the crowding effect, which states that urban expansion occurs in neighborhoods where consolidated urban centers already exist.

As for the flow projection, we estimated a 38% increase in water withdrawal and consumption for urban supply by 2050. This does not directly represent major risks to water availability in the region due to the large volume of water available in the basin. However, population growth and urban expansion lead to indirect consequences, such as industrialization and agricultural intensification, and a reduction of forested areas, which can compromise the quality of water supply and have unintended consequences on water demand. Therefore, better management of water use in the basin is needed.

7- Acknowledgments

This study was carried out with the support of the Coordination for the Improvement of Higher Education Personnel – Brazil (CAPES), Financing Code 001. The authors are also grateful for support from the National Council for Scientific and Technological Development (CNPq), Financing Code 306846 / 2017- 9.

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São José dos Campos – SP, Brazil

February 10, 2020

No **conflict of interest** with other people or organizations that could inappropriately influence or bias the content of the paper.

Sincerely yours,

Ana Carolina da Encarnação Paiva

Journal Pre-proof

São José dos Campos – SP, Brazil

February 10, 2020

To the Editorial Board of the Science of the Total Environment,

I declare that all authors contributed in a relevant way to the development of this research.

Your individual contributions are described below:

Paiva, A. C. E.: Database Survey and Treatment, Methodology, Land Use Modeling (Calibration and Validation), Population Calculation, Flow Calculation, Results Analysis and Main Writing;

Nascimento, N. C.: Methodology (land use modeling), Land use modeling (calibration and validation), result analysis, and writing - review and editing;

Rodriguez, D. A.: Conceptualization, Methodology, Results Analysis, General Article Supervision, and Writing - Review and Editing;

Tomasella, J.: Conceptualization, Methodology, General supervision of article and writing - review and editing;

Carriello, F.: Preparation and editing of land use maps; General supervision of the article.

Rezende, F.: Preparation and editing of land use maps.

All authors of this article have read and approved the final version submitted.

Sincerely yours,

Ana Carolina da Encarnação Paiva

Table 1 – Water Consumption Data for the municipalities in the state of São Paulo that are supplied by the Paraíba do Sul River Basin Source: modified from Brasil (2019).

Consumptive Uses	2000		2010		2017	
	Withdrawal	Consumed	Withdrawal	Consumed	Withdrawal	Consumed
	(m ³ /s)	(m ³ /s)	(m ³ /s)	(m ³ /s)	(m ³ /s)	(m ³ /s)
Human Supply	4,83	0,96	5,49	1,10	6,06	1,21
Rural Supply	0,20	0,16	0,19	0,15	0,19	0,15
Industry	1,62	0,50	2,27	0,49	2,34	0,49
Irrigation	3,37	1,78	1,97	1,23	2,18	1,34
Mining	0,03	0,01	0,04	0,02	0,04	0,02
Thermoelectric	1,00	-	1,00	-	1,00	-
Animal Use	0,45	0,31	0,56	0,39	0,58	0,41
Total	11,49	3,72	11,51	3,38	12,38	3,62

Table 2 – Data used in modeling.

Data	Source
Land Use /Cover Maps (2005 e 2010)	Neves et al. (2018) Rezende et al. (2018)
Highways	Brasil (2018a)
Railroads	Brasil (2001)
Hydrography	Brasil (2018a)
Reservoir	Brasil (2018a)
Conservation Units	Brasil (2018b)
Slope	INPE (2018)

Table 3 – Transition matrix, in hectares.

In/For	Urban (1)	Urban (2)	Urban (3)	Urban (4)	Urban (5)	Urban (6)	Urban (Total)
Pasture	477	2121	3221	817	9028	367	16031
Vegetation	363	2828	360	256	805	59	4670

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Table 4 – Explanatory Variable Weights of Evidence.

Variables	Micro-region											
	1		2		3		4		5		6	
	Pas- ture	Veget- ation	Pas- ture	Veget- ation	Pas- ture	Veget- ation	Pas- ture	Veget- ation	Pas- ture	Veget- ation	Pas- ture	Veget- ation
Distance to urban area	3.24	3.31	2.13	2.61	2.33	4.03	3.86	4.44	1.77	3.73	3.50	5.48
Railroad Distance	3.66	2.24	0.00	0.00	1.92	3.44	0.00	0.00	0.68	2.07	0.00	0.00
Highway Distance	0.89	1.61	4.00	2.25	1.59	2.49	2.17	2.07	1.08	2.64	1.68	2.58
River Distance	0.00	0.00	0.00	0.00	1.68	3.61	1.03	1.21	0.79	2.88	3.43	0.26

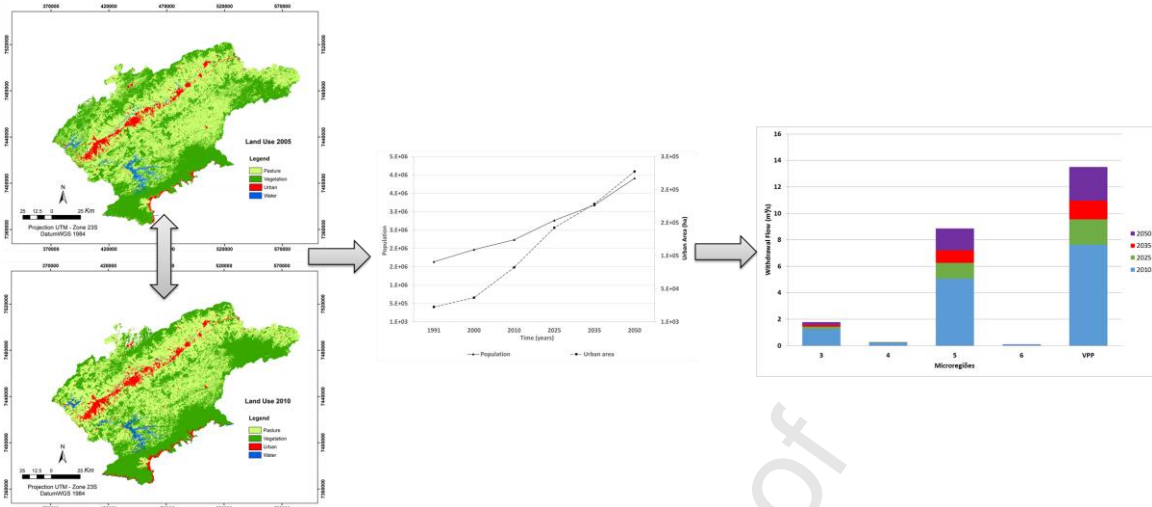
Reservoir Distance	0.00	0.00	0.00	0.00	1.15	3.77	0.38	1.98	-0.96	0.88	2.26	2.14	
Conservation Unit	Protection	2.36	-1.06	-0.65	-0.08	0.00	-9.03	11.19	-1.54	0.57	-12.11	-8.33	-13.08
	Sustainable Use	-0.04	0.15	8.44	3.5	0.00	0.00	0.02	1.15	0.00	0.02	0.00	0.72
Slope	1.30	2.89	-0.79	1.97	1.58	5.56	1.92	12.08	1.03	5.7	1.21	7.36	

Table 5 – Withdrawal and consumption flows for urban supply.

Time (Years)	1		3		4		5		6		Additional Cities		Total	
	Q_u (m^3/s)	$Q_{u,c}$ (m^3/s)	Q_u (m^3/s)	$Q_{u,c}$ (m^3/s)	Q_u (m^3/s)	$Q_{u,c}$ (m^3/s)	Q_u (m^3/s)	$Q_{u,c}$ (m^3/s)	Q_u (m^3/s)	$Q_{u,c}$ (m^3/s)	Q_u (m^3/s)	$Q_{u,c}$ (m^3/s)	Q_u (m^3/s)	$Q_{u,c}$ (m^3/s)
2010	0.01	0.00	1.26	0.25	0.22	0.04	5.06	1.01	0.07	0.01	0.20	0.07	6.82	1.38
2025	0.01	0.00	1.43	0.29	0.24	0.05	6.26	1.25	0.08	0.02	0.23	0.11	8.25	1.72
2035	0.01	0.00	1.56	0.31	0.25	0.05	7.20	1.44	0.08	0.02	0.24	0.12	9.34	1.94
2050	0.02	0.00	1.77	0.35	0.26	0.05	8.85	1.77	0.09	0.02	-	-	10.99	2.19

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Graphical abstract



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Highlights

- 1- To estimate water consumption, we integrated LUCC scenarios with demographic data.
- 2- Results showed good agreement of the estimation of urban sprawl and water consumption.
- 3- The main driver of urban sprawl expansion is the access to the transportation network.
- 4- LUCC scenarios indicate a 38% growth in consumption and withdrawal flows by 2050.

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