Modelling freshwater quality scenarios with ecosystem-based adaptation in the headwaters of the Cantareira system, Brazil

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10 Abstract. Although hydrologic models provide hypothesis testing of complex dynamics occurring at catchments,

11 freshwater quality modelling is still incipient at many subtropical headwaters. In Brazil, a few modelling studies

12 assess freshwater nutrients, limiting policies on hydrologic ecosystem services. This paper aims to compare

13 freshwater quality scenarios under different land-use/land-cover (LULC) change, one of them related to

14 Ecosystem-based Adaptation (EbA) in Brazilian headwaters. Using the spatially semi-distributed Soil and Water

- 15 Assessment Tool (SWAT) model, nitrate, total phosphorous and sediment were modeled in catchments ranging
- 16 from 7.2 to 1037 km². These headwaters were selected for the Brazilian Payment for Ecosystem Services (PES)
- 17 program in the Cantareira System, which has supplied water to 9 million people in Sao Paulo. We considered
- 18 SWAT modelling of three LULC scenarios : (i) recent past scenario ("S1"), with historical LULC in 1990, (ii)
- 19 current land use scenario ("S2"), with LULC for the period 2010-2015 with field validation, and (iii) future land

20 use scenario with PES ("S2+EbA"). This latter scenario proposed forest cover restoration through EbA following

21 the River Basin Plan by 2035. These three LULC scenarios were tested with a selected record of rainfall and

22 evapotranspiration observed in 2006-2014, with the occurrence of extreme droughts. To assess hydrologic services,

- 23 we proposed the Hydrologic Services Index (HSI), as a new composite metric comparing water pollution levels
- 24 (WPL) for reference catchments, and related to the grey water footprint (greyWF) and water yield. On the one
- 25 hand, water quality simulations allowed for the regionalization of greyWF at spatial scales under LULC scenarios.
- According to the critical threshold, HSI identified areas as less or more sustainable catchments. On the other hand,
- 27 conservation practices simulated through the S2+EbA scenario envisaged not only additional and viable best
- 28 management practices, but also preventive decision making at the headwaters of water supply systems.

Key words: water quality modelling; ecosystem-based adaptation; SWAT; grey water footprint; land-use/land cover change; Brazil.

31

32 1 Introduction

Basin Plans comprise the main management tool and they plan sustainable use of water resources in both spatial and temporal scales. For sustainable water allocation, river plans are based on accurate data on actual water availability per basin, taking into account water needs for humans, environmental water requirements and the

basin's ability to assimilate pollution (Mekonnen et al., 2015). However, adaptive management options such as 36 37 ecosystem-based adaptation (EbA; see CBD, 2010; BFN/GIZ, 2013) and the water footprint (WF) (Hoekstra & 38 Chapagain, 2008) have rarely been incorporated into Brazilian Basin Plans. Moreover, integrated qualiquantitative simulations and indicators of human appropriation of freshwater resources are seldom used in river 39 40 plans. The concept of Ecosystem-based Adaptation (EbA) is addressed as 'using biodiversity and ecosystem services to help people adapt to the adverse effects of climate change', which was defined by the Convention on 41 42 Biological Diversity - 10th Conference of the Parties (CoP) (CBD, 2010). Detailed definitions of EbA applied to 43 the Cantareira's Headwaters can be found in Taffarello et al (2017). The WF is still an environmental indicator 44 used in watershed plans. For example, Spain uses WF as an indicator in Basin Plans (Hoekstra et al., 2017; Velázquez 45 et al., 2011; Aldaya et al., 2010). The clean water plan of Vancouver (June/2011) established the reduction of the 46 WF as a sustainable action in its water resources management (MetroVancouver, 2011; Zubrycki et al., 2011). The 47 Colombian government was the first to publish a complete and multi sectorial evaluation of WF in its territory. 48 Although this study, entitled Estudio Nacional del Agua (Colombia, Instituto de Hidrología, Meteorología y 49 Estudios Ambientales, 2014), was not included in the national water management plan, the strategic plan of 50 Magdalena Cauca basin incorporates the greyWF to assess agriculture pollution (Colombia, 2014). In Brazil, a

51 glossary of terms released by the Brazilian National Water Agency (ANA, 2015) includes the concept of WF to

52 support water resources management.

The WF (Mekonnen & Hoekstra, 2015; Hoekstra et al., 2011) measures both the direct and indirect water use within a river basin. The term water use refers to *water withdrawal*, as the consumptive use of rainwater (the green

55 water footprint) and of surface/groundwater (the blue water footprint), and *water pollution*, i.e., the flow of water

56 used to assimilate the pollutant loads (the grey water footprint (greyWF) (see Chapagain et al. 2006). Given that

57 water pollution can be considered a non-consumptive water use, the greyWF is advantageous by quantifying the

58 effects of pollution by flow, instead of by concentration, making water demand and availability comparable.

59 Water footprint assessment comprises four phases: (1) Setting goals, (2) Accounting, (3) Sustainability

assessment, and (4) Response formulation. At the WF response formulation phase, the EbA options, represented

by Best Management Practices (BMP) at the catchment scale, could represent a trade-off on greyWF (Zaffani et

62 al., 2011). That is, BMP adopted in the catchment scale could contribute indirectly to decreasing the level of water

63 pollution. Thus, the EbA would compensate the greyWF of a certain river basin (Taffarello, 2016).

64 In the context of water security associated with land-use/land-cover (LULC) change, many existing conflicts over

water use could be prevented (Winemiller et al., 2016; Aldaya et al., 2010; Oki & Kanae, 2006). For example,

66 LULC influences water quality, which affects the supporting¹ and regulating² ecosystem services (Mulder et al.,

67 2015; MEA, 2005) and needs to be monitored for adaptive and equitable management on the river basin scale

- 68 (Taffarello et al., 2016a). In spite of discussions regarding the lack of representativeness of data used in early
- 69 studies with greyWF (Wichelns, 2015; Zhang et al., 2010; Aldaya et al., 2010; Aldaya & Llamas, 2008), we argue

¹Examples of supporting services: nutrient cycling, primary production and soil formation.

²Examples of regulating services: self-depuration of pollutants, climate regulation, erosion control, flood attenuation and water borne diseases.

70 that the greyWF method may account for hydrologic services and provide a multidisciplinary, qualitative-71 quantitative integrated and transparent framework for better water policy decisions. Understanding these 72 catchment-scale ecohydrologic processes requires not only low-frequency sampling, but also automated, in situ 73 high-frequency monitoring (Bieroza et al., 2014; Halliday et al., 2012), as well as using ecohydrologic models 74 to protect water quality and quantity. However, freshwater quality modelling associated with EbA, greyWF and 75 LULC is still incipient in many river catchments. In Brazil, approximately only 5% of modelling studies evaluate 76 nutrients in freshwater (Bressiani et al., 2015), which limits the policies on regulating ecosystem services. 77 In this research, we propose the regulating ecosystem services to be addressed by the greyWF because it considers 78 the water volume for self-purification of receiving water bodies affected by pollutants (Zhang et al., 2010). The 79 working hypothesis of the paper is related to how conservation practices addressed by EbA impact hydrology and 80 the ecosystem services, such as maintaining, restoring or improving both the water yield and the freshwater quality, use ecohydrological modeling in different catchment scales. On the other hand, we hypothesized that incentives 81 82 of EbA policies can affect water yield and water quality through non-linear tradeoffs, with high spatiotemporal 83 complexity, which can be assessed by modeling, but previously supported by in-situ monitoring variables for setup 84 boundary conditions of simulation runs. In these scales, the greyWF can evaluate the changes in the regulating 85 hydrologic services. Among the three water footprint components, in this study we assessed greyWF for nitrate, 86 total phosphorous and sediments in 20 sub-basins in the headwaters of the Cantareira Water Supply System. The 87 aim of this study is to compare freshwater quality scenarios, one of them related to EbA options through BMP and 88 to assess greyWF under different LULC changes: (S1) historic LULC of 1990; (S2) current LULC for the period 89 2010-2015; and (S2+EbA) future LULC based on EbA with S2 as a baseline. This method is addressed using 90 Nested Catchment Experiments (NCE), (see Taffarello et al., 2016a and 2016b) at a range of scales from small 91 catchments of 7.7 km² to medium-size basins of 1200 km² at subtropical headwaters responsible for the water 92 supply of Sao Paulo Metropolitan Region (SPMR). This paper consists of four sections. The first section provides 93 a brief description of the context, gap, hypothesis and our research goals. The second section describes the 94 simulation methods used in the watershed scale and development of three LULC scenarios. We then propose some 95 ecosystem-based adaptation (EbA) approaches related to water pollution. Finally, in the fourth section, we discuss 96 how the grey water footprint for nitrate or total phosphorous could be an EbA option for improving decision-97 making and water security in subtropical catchments under change.

98 2. Material and Methods

99 2.1. The case-study area

Two of the most vulnerable areas in the Brazilian South-East are the Upper Tietê (drainage area 7,390 km²) and Piracicaba-Capivari-Jundiaí - PCJ (drainage area 14,178 km²) watersheds, particularly due to their high population: 18 Mi inhabitants in the Upper Tietê River basin, and 5 Mi in PCJ (Sao Paulo, 2017; IBGE, 2010).

- 103 In an attempt to ensure public water supply, the government built the Cantareira System, an inter-basin transfer,
- 104 in two stages: a) between 1968 and 1974, at the end of a 35-year period that underwent a severe drought in the

Piracicaba watershed, and b) in 1982, with the inclusion of two additional reservoirs that regularized the increasing
 rainfall from the mid-1970s until 2005 (Zuffo, 2015).

107 The study area comprises the part of the Cantareira System that drains into the Piracicaba river and which is the headwater of the Piracicaba basin (Figure 1). This basin is located on the borderline of the state of Minas 108 109 Gerais and Sao Paulo. This part of the water supply system, in the Piracicaba watershed, consists of three main 110 reservoirs, named after the rivers, damming the Jaguari-Jacareí, Atibainha and Cachoeira watersheds (drainage areas are 1230 km², 392 km² and 312 km², respectively). These rivers are main tributaries of the Piracicaba river, 111 112 which is a tributary of the Tiete River system on the left bank of the Parana Basin. The Cantareira System consists of two more reservoirs out of the Piracicaba river basin, Paiva Castro and Águas Claras, which are not part of our 113 114 study area.

115 With respect to the water quality, the headwaters of the Cantareira System are classified as "class 1" for 116 Jacareí, Cachoeira and Atibainha watersheds, and "class 2" for the Jaguari watershed, according to the CONAMA Resolution Nº 357/2005 (Brazil, 2005) and Sao Paulo Decree Nº 8468/1976 (Sao Paulo, 1976), which means that, 117 with the exception of the Jaguari watershed, the others can be used with only a simple treatment. Regarding the 118 119 water volume, this region has been intensely impacted by a severe and recent drought (Taffarello et al., 2016a; Escobar, 2015; Whately & Lerer, 2015; ANA, 2015; Porto & Porto, 2014). As a result of this serious water crisis, 120 121 a new water policy on the average flow of the transfer limits of the Piracicaba watershed to the Upper Tiete 122 watershed was postponed from 2014 to May, 2017 (ANA, 2015). The Cantareira System is located in the Atlantic 123 Forest biome, considered a conservation hotspot because of its rich biodiversity. In spite of that, 78% of the original 124 forest cover of the Cantareira watershed has been deforested over the past 30 years (Zuffo, 2015). In 2014, the native forest cover was 10% in Extrema, 12% in Joanópolis and 21% in Nazaré Paulista (SOS Mata 125 126 Atlântica/INPE, 2015). To counteract deforestation, some environmental/financial trade-offs have been developed 127 in the Cantareira headwaters to protect downstream water quality and the regulation of water flows. These are 128 Ecosystem-based Adaptation (EbA) initiatives, in which rural landowners receive economic incentives to conserve 129 and/or restore riparian forests and implement soil conservation practices (see Chapter 3 of this thesis). The first Brazilian EbA approach was the Water Conservator Project, created in 2005 and implemented in Extrema, Minas 130 131 Gerais (Richards et al., 2015; Pereira, 2013). The Water Producer/PCJ Project was developed from 2009 to 2014 132 in the Cantareira System region (Guimarães, 2013), using EbA scenarios and local actions adopting the concept of Payment for Hydrological Ecosystem Services (Pagiola et al. 2013; Padovezi et al., 2013) through public-133 private partnerships, strengthening EbA in Brazil.

134

136 2.2. Databases and model adopted

137 **Figure 2** shows the method developed and applied to assess the regulating hydrologic services through grey WF,

- as well as the spatial data used in this study. The simulations were enhanced by model parameterization with
- 139 qualitative and quantitative primary data (Mohor et al., 2015a; Mohor et al., 2015b; Taffarello et al. 2016b) from
- 140 six field campaigns between 2012 and 2014, in partnership with ANA, CPRM, TNC-Brazil, WWF, USP/EESC

- 141 and municipalities. This can reduce uncertainties of the model, facilitate data interpretation and provide consistent
- 142 information. We installed three data collection platforms (DCP) in catchments at Posses, Cancã and Moinho, and
- 143 level and pressure sensors (see Table 1, and Figure 8) in paired sub-basins (*i*) with high original vegetation cover,
- and (ii) in basins that receive payment for ecosystem services due to participating in the Water Producer/PCJ
- 145 project.
- 146 We obtained and organized secondary data from the region upstream of the Jaguari-Jacareí, Cachoeira and
- Atibainha reservoirs. We then set up a database originating from several sources: Hidroweb (ANA, 2014); Basic
 Sanitation Company of the State of Sao Paulo (SABESP); Integrated Center for Agrometeorology Information
- 149 (CIIAGRO, 2014); Department of Water and Power (DAEE); National Institute of Meteorology (INMET) from
- 150 the Center for Weather Forecasts and Climate Studies (CPTEC/INPE).
- Supplement Table S1 summarizes all hydrologic, pedological, meteorological and land-use data used as input for the delineation and characterization of the watersheds. The topographical data used was the Digital Elevation Model "ASTER Global DEM", 2nd version, 30-m (Tachikawa, et al., 2011), available free of charge at: http://gdex.cr.usgs.gov/gdex/.
- 155 The changes in hydrologic services can be evaluated by a large number of models (Carvalho-Santos et al, 2016; Duku et al, 2015; Quilbé & Rousseau, 2007), especially those more user-friendly for stakeholders and policy 156 157 makers. Simulations in this watershed-scale ecohydrologic model (Williams et al, 2008; and Borah & Bera, 2003) 158 allow for the quantification of important variables for ecosystem services analysis and decision-making. Some 159 examples of ecohydrologic models with progressive applications in Brazilian basins are SWAT (Bremer et al., 160 2016; Francesconi et al., 2016; Bressiani et al., 2015), the models reviewed by de Mello et al. (2016), Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) (Sharp, 2016; Tallis et al., 2011) and Resource 161 162 Investment Optimization System (RIOS) (Vogl et al., 2016).
- The Soil and Water Assessment Tool SWAT-TAMU (Arnold et al., 1998; Arnold and Fohrer, 2005) is a public domain conceptual spatially semi-distributed model, widely used in ecohydrologic and/or agricultural studies at a river basin scale (Krysanova & Whyte, 2015; Krysanova & Arnold, 2008). It divides the basin into sub-basins based on an elevation map and the sub-basins are further subdivided into *Hydrologic Response Units* (HRU). Each HRU represents a specific combination of land use, soil type and slope class within the sub-basin. The model includes climatic, hydrologic, soil, sediments and vegetation components, transport of nutrients, pesticides, bacteria, pathogens, BMP and climate change in a river basin scale (Srinivasan et al., 2014; GASSMAN et al., 2014: Arnold et al. 2012)
- 170 2014; Arnold et al., 2012).
- 171 There have been at least 2,600 published SWAT studies (SWAT Literature Database, mid-2016). In the SWAT
 172 *Purdue Conference*, held in 2015, 118 studies were presented, of which only 8% assessed the transport of nutrients
 173 in watersheds (SWAT Purdue, Book of Abstracts, 2015). Research using SWAT, not only for quantity but also for
 174 water quality and ecosystem service assessments (Francesconi et al., 2016; Abbaspour et al., 2015; Duku et al.,
 175 2015; Dagupatti & Srinivasan, 2015; Gassman et al., 2014) and also as an educational tool for comparing
- 176 hydrologic processes (Rajib et al., 2016) have increased in recent years.
- 177

178 2.3. Model Set-up

- The initial model set-up used the ArcSWAT interface, integrated to ArcGIS 10.0 (Environmental Systems
 Research Institute ESRI, 2010, ArcSWAT 2012.10.15 in ArcGIS 10).
- 181 Discretization in sub-basins was carried out, where possible, at the same as NCE sites of field investigations.
- 182 The delimitation of the basin using ArcSWAT requires a drainage area threshold, determined to 7.1km², dividing
- the geographical space to represent the 17 sampling sites in the research field as sub-basins, plus the limits of the
- 184 three reservoirs' drainage areas, which resulted in 20 sub-basins (**Table 1 and Figure 1b**). We highlight that the
- basin was designed up to the confluence of the Jaguari and Atibaia Rivers, forming the Piracicaba river, to integrate
- all areas of interest in the same SWAT project.
- The definition of the HRU was carried out using soil maps of the state of São Paulo. (Oliveira, 1999) and land use maps were developed by Molin (2014; et al. 2015) from LANDSAT 5 TM imagery for 2010, using a 1:60,000 scale. The procedure defined 49 HRUs inside the 20 sub-basins, i.e. 49 different combinations of soil type, soil cover and slope classes in our study area.
- 191 Next, we adapted the land use map developed by Guimarães (2013), which represents a 2010 land use scenario
- 192 for the Cantareira System restoring the most fragile degraded parcels (greatest potential for sediment production),
- to agree with the land use classes of Molin (2014). Additionally, we assumed that the Second Scenario of
- 194 Guimarães (2013), who used the INVEST model to provide the ecological restoration benefits in the Cantareira
- 195 System, could be achieved in 2035, considering the investments provided in the PCJ River Plan (Cobrape, 2011)
- 196 to recover riparian forests. It is worth mentioning that in the PCJ Basin Plan, this is called "Trend Scenario".
- 197 Since in the region the restoration of riparian forests is mostly due to Water-PES projects, which was
- recognized as an Ecosystem-based Adaptation (EbA) (CBD, 2010; BFN/GIZ, 2013; Taffarello et al., 2017), we identify the third scenario as S2+EbA. Thus, **Figure 3** shows the land-use changes over time. In the "Trend
- 200 Scenario" (PCJ-COBRAPE, 2011), the municipalities covered by the Cantareira System could reach a 98%
- 201 collection rate, a collected sewage treatment rate of 100% and BOD_{5,20} removal efficiency of 95% (PCJ-COBRAPE,
- 202 2011). Some studies have suggested including other parameters such as dissolved oxygen, nitrate and phosphate
- 203 polluting loads, as well as sediments to assess the water quality (Cruz, 2015; Cunha et al., 2014). Regarding the
- 204 treatment costs for drinking water supply, ecosystem-based adaptation options, such as watershed restoration, seem
- to be more cost-effective than many technologies for water treatment (Cunha; Sabogal-Paz & Dodds, 2016).
- 206

207 2.4. Calibration & validation

We used the SWAT CUP 5.1.6.2 interfaces and Sequential Uncertainty Fitting (SUFI-2) algorithm for calibrating
the quantity and quality parameters and also for validating the simulations in the sub-basins. Quantitative
calibration was performed in stations that had more than two full years of observed data, i.e., 8 stations, namely:
Posses outlet, F23, F24, F25B, F28, Atibainha reservoir, Cachoeira reservoir, Jaguari and Jacarei reservoirs (Table
A common test period for all LULC scenarios was selected, in our case, the test period ranged from 01 Jan,
2006 to 30 June, 2014. This period has the rain-anomaly of drought conditions from 2013 to 2014.

- The calibration period was from October, 2007 to September, 2009, the only period with observed data in all of
- the above 8 stations. Validation took place from January, 2006 to September, 2007 and from October, 2009 to
- June, 2014. Calibration and validation of SWAT at the stations with over 2 years of data were rated as "good",
- 217 according to the classification by Moriasi et al. (2007), since the Nash-Sutcliffe Efficiency (NSE) criterion (Nash
- 218 & Sutcliffe, 1970) was greater than 0.65, except for the Posses outlet, which presented the logarithmic Nash-
- 219 Sutcliffe (NSElog) (using the logarithm of streamflow, a criterion that gives greater weight to smaller flow rates)
- of less than 0.5, rated as "unsatisfactory". The Percent Bias (Pbias) statistics indicates the bias percentage of simulated flows relative to the observed flows (Gupta et al., 1999). Thus, when the Pbias value is closer to zero, it
- results in a better representation of the basin, and in lower estimate tendencies (Moriasi et al., 2007). As a general
- rule, if | Pbias | < 10%, it means a very good fit; 10% < | Pbias |< 15%, good; 15% < | Pbias | < 25%, satisfactory and | Pbias | > 25%, the model is inappropriate. On the other hand, the NSE coefficient translates the application efficiency of the model into more accurate predictions of flood flows, using the classification: NSE > 0.65 the model is rated as very good; 0.54 < NSE < 0.65 the model is rated as good and between 0.5 and 0.54, it is rated as
- satisfactory.
- In the results obtained for different basin scales (Figure 4), the Pbias and NSE coefficients (including NSE of 228 logarithms) indicate adequate quantitative adjustments. As the SWAT simulations include more than 200 229 230 parameters, based on research from the literature (Duku et al., 2015; Bressiani et al., 2015; Arnold et al., 2012; 231 Garbossa et al., 2011), we selected approximately 10 parameters (see Table 3) to complete the calibration to 232 simulate streamflow processes and nutrient dynamics. These parameters refer to key processes which represent 233 soil water storage, infiltration, evapotranspiration, flow channel, boundary conditions (see Mohor et al., 2015b) 234 and main water quality processes at hillslopes. Although our calibration is mainly focused on water yield as total 235 runoff, freshwater quality features through pollutant loads were performed in the scenarios. Further comments 236 related to the existing literature for selected model parameters are depicted in Section S.3 with comments on sensitivity 237 analysis to select model parameters used in this paper (Supplementary Material).
- Moreover, to reduce the uncertainty of our predictions, we used approximately 2500 primary data derived from an earlier stage of this research (Taffarello et al., 2016a). As a parameterization result of field investigations and ecohydrologic modelling, **Figure 5** shows parts of the calibrated model performance (lines) against field observations (dots with experimental uncertainty) for flow discharges, nitrate and total phosphorus loads for catchment areas ranging from 7.1 to 508 km². Finally, other water quality variables were studied based on data from field sampling.
- 244 We highlight some SWAT model limitations when we compare the simulated to observed water flows, especially 245 in the dry season. For example, when the model was discretized on a daily resolution, the adherence level between
- the observed and simulated flows was considered good. However, the model did not fit well to the observed values
- 247 during the drought period (Feb/2014-May/2014). These differences were more significant for water quality
- parameters, such as nitrate and total phosphorous. We point out that the macronutrient loads found in May, 2014
- 249 were clearly higher than the loads we found in previous sampling, which occurred in wetter periods (Taffarello et
- al. 2016). For the sample collected in May, the model significantly underestimated the pollutant loads of nitrate.
- 251 This behaviour, arising from the recent and most severe drought faced by the Cantareira System (Nobre et al.,

252 2016; Marengo et al., 2016; Taffarello et al. 2016-a; Escobar, 2015; The Economist, 2015; Porto & Porto, 2014), shows the need for the improvement of the SWAT model performance, especially to capture nonlinearities having impacts on regulating ecosystem services during extreme flows. For EbA scenarios, we planned to set up field investigations and SWAT calibrations (see Figure 5, this paper) using the extreme conditions of the 2013–14 drought through freshwater quality monitoring at the headwaters of the Cantareira System (see Tafarello et al., 2016-a).

253 2.5. The scenarios and a new index for hydrologic service assessment

Differences in flow rates and water quality (for the variables nitrate, phosphate, BOD_{5.20}, turbidity and faecal 254 255 coliforms) for the 20 sub-basins were evaluated using flow and load duration curves for the three scenarios 256 proposed in this study: (i) recent past scenario (S1), including the recorded past events for land use in 1990, (ii) 257 current land use scenario (S2), which considered land uses for the 2010-2015 period as the baseline, and (iii) future land use scenario (S2+EbA), supposing a forest cover conversion in the protected areas, through EbA 258 options, according to the PCJ River Basin Plan by 2035. Using these curves, from the methodology shown by 259 Hoekstra et al. (2011), and based on Duku et al. (2015) and Cunha et al. (2012), we estimated the grey water 260 footprint (greyWF). Next, we developed a new ecohydrologic index to assess the regulating hydrologic services 261 in relation to the greyWF. This new indicator encompasses the former theory related to environmental 262 sustainability of the greyWF, according to Hoekstra et al. (2011). In this study, as a relevant local impact indicator, 263 Hoekstra et al. (2011) proposed to calculate the 'water pollution level' (WPL) within the catchment, which 264 measures the degree of pollution. WPL is defined as a fraction of the waste assimilation capacity consumed and 265 calculated by taking the ratio of the total of greyWF in a catchment ($\sum WF_{grey}$) to the actual runoff from that 266 catchment (R_{acl}), or, in a proxy manner, the water yield or mean water yield or long-term period (Q_{lp}). This 267 assumption is that a water pollution level of 100 per cent means that the waste assimilation capacity has been fully 268 consumed. Furthermore, this approach assumes that when WPL exceeds 100 %, environmental standards are 269 violated, such as: 270

271
$$WPL[x, t] = \frac{\sum WF_{grey}[x, t]}{R_{act}[x, t]},$$
(1)

It is worth mentioning that for some experts, the aforementioned equation can overestimate the flow necessary to dilute pollutants. For that reason, new insights of composite indicators or thresholds are recommended, as follows. The above assumption could overestimate WPL because it would fail considering the combined capacity of water to assimilate multiple pollutants (Hoekstra et al., 2012; Smakhtin et al., 2005). Conversely, in this study, we define an alternative indicator related to the three following fundamentals. First, the WPL should be extended to a composite index, thereby representing weights of each pollutant related to the actual runoff, here as a proxy of long-term runoff, i.e.:

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284
$$WPL_{composite}[x, t] = \frac{\sum\{w[x,t] * WF_{grey}[x,t]\}}{R_{act}[k,t] \neq Q_{lp}[x,t]},$$
 (2)

 $285 \quad \sum w[x, t] = 1$

 $286 \qquad 0 \le w[x, t] \le 1$

287

For this new equation, weights should be assessed, either from field experiments or even from simulation outputs. Second, we define a threshold value of WPL composite regarding the reference catchments in non-developed conditions which suggest more conservation conditions among other catchments of the same region, as *WPL*_{reference}. For this study, we selected *Domithildes* catchment as the reference catchment with conservancy measures. From this reference catchment, we define the composite reference index for the water pollution level as *WPL*_{composite,ref} and, derived from it, the Hydrologic Service Index, as a non-dimensional factor of comparison between WPL for reference and non-reference catchments, as follows:

295
$$HSI[x,t]_{greyWF} = \frac{WPL[x,t] - WPL_{composite,ref}}{WPL_{composite,ref}},$$
(3)

296 3. Results

In the following section, we present the results from field observations, useful not only for ecohydrologic parameterization, but also to elucidate features regarding greyWF and hydrologic services. Next, we compare the water yield and greyWF outputs from simulations under LULC scenarios, including EbA options, to finally propose a new hydrologic services indicator.

301 3.1. Data from field sampling

- Some of the water quality and quantity variables from our freshwater monitoring are useful to assess the hydrologic services, thus they are presented in **Table 4**. These variables were selected due to their relationship with anthropic impacts on the water bodies and because of their importance for sanitation
- Among the water quality variables sampled in the field step of the research (see Taffarello et al., 2016a; Taffarello et al., 2016b), we highlight turbidity because it indicates a proxy estimation about the total suspended solids in lotic environments (UNEP, 2008), related to the LULC conversion and reflects the changes in the hydrologic services. **Figure 6** shows the direct correlation between turbidity and size of the sub-basins. Turbidity can indirectly indicate anthropic impacts in streams and rivers (Martinelli et al., 1999). The lower turbidity mean values were observed in two more conserved sub-basins (which presented higher amounts of forest remnants): 2 NTU in the *reference Cancã catchment* (Domithildes) and 5 NTU in *Upper Posses*.
- Otherwise, we found a positive relationship between nitrate concentrations and both discharge and mean water level (**Figure 7**). It can be inferred that higher concentrations of macronutrients would be found in downstream areas. This trend can be associated to the nutrient migration (Cunha et al., 2013) and land-use change (Zaffani et al., 2015), as well as point source pollution. In addition, the absence of the riparian forest in 70% of protected area (36.844 ha) of the Cantareira System (Guimarães, 2013) can increase the sediment transport from riparian areas to rivers and make pollutant filtration more difficult, leading to higher nitrate concentrations downstream.

319 3.2. LULC change scenarios

- 320 The variations in LULC affect freshwater quality which, in turn, affect the dynamics of aquatic ecosystems
- 321 (Zaffani et al., 2015; Botelho et al., 2013; Hamel et al., 2013; Bach & Ostrowski, 2013; Kaiser et al., 2013). These
- 322 changes impact the hydrologic services, especially regulating and supporting ecosystem services (Mulder et al.,
- 323 2015; Molin et al., 2017).
- 324 The LULC of each sub-basin, according to a past-condition scenario (S1, in 1990), a present-condition (S2, in
- 325 2010) and a future (S2+Eba, in 2035) LULC scenario, using the same weather input datafiles, is shown in Table
 326 5.
- We evaluated the effects of LULC change scenarios in 20 catchments in the Jaguari, Cachoeira and Moinho subbasins, South-East Brazil. Concerning the land-use change, the main soil use 25 years ago was: pasture (in 50% of the sub-basins) and native vegetation (in 45% of the sub-basins). According to ISA (2012) and Molin (2014), the 5% of the remaining area were divided into vegetables, eucalyptus, sparse human settlements, bare soil and mining. The main activity in the past (1990) was extensive cattle raising for milk production by small producers in the region (ANA, 2012; Veiga Neto, 2008).
- 333 By assessing the temporal trends of increment or reduction of native remnants, we examined the periods 1990-334 2010 versus 2010-2035. From 1990 to 2010, the percentage of forest increased by 50% in the Domithildes sub-335 basin, which was the reference catchment of the Water Producer/PCJ project, (see Taffarello et al., 2016a), 336 Moinho, Cachoeira dos Pretos, F34, B. Jacareí, B. Atibainha, B. Cachoeira, Pq Eventos, F25B and B. Jaguari (Figure 9). Concerning the period from 2010-2035, the model was set up considering an increase in native 337 vegetation in all sub-basins from forest remnants in 2010, and from the new BMP practices of reforestation with 338 339 native species in 20 sub-basins by 2035 (Figure 9). The hydro-services in the Posses and Salto catchments and in 340 the Cachoeira sub-basin will be increased by 2035 as a function of the efforts on EbA which currently exist in the
- 341 region (Richards et al., 2017; Richards et al., 2015; Santos, 2014).

342 3.3. Water yield as a function of soil cover

- In this research, we chose to use quali-quantitative duration curves for integrated assessment of availability and quality of water. The flow-and-load duration curve, comparable to histograms of relative cumulative frequencies of flows and loads of a waterbody, is a simple and important analysis in hydrology (Collischonn & Dornelles, 2013). In quantitative terms, the flow duration curve shows the probabilistic temporal distribution of water availability (Cruz & Silveira, 2007), relating the flow in the river cross section to the percentage of time in which it is equalled or exceeded (Cruz & Tucci, 2008).
- The three scenarios S1, S2 and S2+EbA resulted in different flow values for the 20 sub-basins (**Figure 10**). Based on the arithmetic mean of time series of monthly water yields, related to catchment areas, and assessed for all modelled sub-basins (N=20), the results show average values of water yield: 31.4 ± 25.2 L/s/km² for S1 (1990), 14.9 ± 11.5 L/s/km² for S2 (2010) and 21.4 ± 15.3 L/s/km² for S2+EbA (2035), respectively. This very high variation can be due to the complexity of river basin systems and the various sources of uncertainty in the
- 354 representation of ecohydrologic processes.

- The three analyzed scenarios and the ecohydrologic monitoring provide different types of information for the same catchments.
- 357 The 52% decrease of water yield between S1 (1990) and S2 (2010) scenarios, as $(14.9 31.3)/31.3 \times 100$ might be
- related to a marginal increase in the Eucalyptus cover. In fact, from 1990 to 2010, eucalyptus cover increased +6.8
- 359 % in total land cover, but +181% in relative terms. Another possible explanation is the decrease in native vegetation
- from 1990 to 2010, with -1.8 % in total land cover, but -4.3%, in relative terms.
- 361 In parallel, we evaluated the water yield. Thus, the flow-and-load duration curves summarize the flow and pollutant
- 362 load variability, thereby showing potential links and impacts for aquatic ecosystem sustainability (Cunha et al.,
- 363 2012; Cruz & Tucci, 2008). From these curves, we obtained two different behaviours for the studied sub-basins
- 364 (**Figure 10**):
- Behaviour I: the water yield in 2010 reduced in relation to 1990 and the water yield in 2035 might exceed the
 1990 levels. The examples are: *Upper Jaguari, Cachoeira* sub-basin (including the *Cachoeira dos Pretos, Chalé Ponto Verde, Ponte Cachoeira, F24 outlet*) and *Moinho* catchments;
- 368 Behaviour II: the water yield after 2010 was reduced until 2035 and this water yield recuperation was not possible 369 for the values in 1990. Examples, in decreasing size of drainage areas, are: Atibainha, B. Jaguari, F25B, Parque de Eventos, F23, B.Atibainha, F34, F30, Salto, Posses Outlet, Domithildes, Portal das Estrelas (Middle Posses). 370 On the one hand, according to Figure 11, the water yield of S1 is inversely proportional to the land use of mixed 371 372 forest cover. The water yield in S2 indicates a constant value of approximately 17 L/s/km². Moreover, for the S2+EbA scenario, which incorporates the EbA approach through BMP, the water yield is approximately 17 373 374 L/s/km², but with a slight increase in the water yield when the percentage of forest cover is higher than 50%. 375 Presumably, this slight increase in the water yield would be related to the type of best management practices 376 (BMP) of the recovery forests, which still did not achieve evapotranspiration rates of the climax stage. In the 377 riparian forest recovery, evapotranspiration rates are lower and, thus, a greater amount of precipitation reaches the 378 soil and rivers through the canopy. This process could benefit other hydrologic components, such as runoff, 379 increasing water flows into the rivers. This effect can possibly explain the behaviour I catchments (see Fig. 10). 380
- 381 3.4. Relationships between land-use/land-cover change and grey water footprint
- For an integrated assessment of hydro-services, we analysed the spatio-temporal conditions of load production at 382 383 the sub-basin scale (see more information on Section S.4 "Comments on differences in land-use/land-cover in subbasins studied", in Supplementary Material). As we studied rural sub-basins, water pollution is mainly produced 384 by diffuse sources, such as fertilizers and agrochemicals. In this context, we evaluated the evolution of greyWF to 385 show nitrate (N-NO₃), total phosphorus (TP) and sediment (Sed) yields (indicated by turbidity) of scenarios S1, 386 S2 and S2+EbA. First, we calculated the nitrate loads generated from the 20 sub-basins in the three scenarios. 387 Second, we did the same for total phosphorous loads and sediment yields. Third, considering the river regime, we 388 389 calculated the greyWF for nitrate, total phosphorous and sediments in each sub-basin to develop a new composite 390 index that assesses the sustainability of hydrologic services.

- 391 Concerning nitrate, the sampled concentrations were low. In addition, SWAT simulations also brought very low
- 392 outputs, and the greyWF-NO₃ varied from 0.11 L/s/km² (in *Atibainha* subbasin in S2 (2010) scenario) to 2.83
- 393 L/s/km² (in *Middle Posses* catchment, *Portal das Estrelas*, under S2+EbA (2035) scenario). Considering Brazilian
- 394 water quality standards for nitrate, the maximum allowed concentration is 10 mg/L (Brasil, 2005). These low
- amounts of nitrate loads make the greyWF-NO₃ fall to low values in the three analyzed scenarios (between 1 and
 10%; Figure 12a).
- In relation to total phosphorous (TP), the load duration curves from S1, S2 and S2+EbA scenarios showed
 disparities. For example, the greyWF-TP decreased in all sub-basins between 1990, 2010 and 2035. From 2010
 to 2035, the model predicts a new behaviour for the greyWF-TP.
- 400 Results of the greyWF for TP, NO₃ and sediments enabled us to infer hydrological regionalization for nutrient
- 401 loads. Among the 20 sub-basins studied, we selected 2 sub-basins as study cases to illustrate the links between
- 402 LULC and greyWF: (1) the Upper Jaguari and (2) Domithildes. The reasons for selecting the two sub-basins
- 403 among the 20 sub-catchments are detailed in Section S.5 of Supplementary Material

404 3.4.1 Case study I: Upper Jaguari sub-basin

The Upper Jaguari (**Figure 13**) has 302 km² and is the second most upstream sub-basin within the Cantareira System (downstream of only *F28* sub-basin, with 277 km²). Comparing scenario 1990 (S1) and 2010 (S2), the results showed evidence that the native forest decayed approx. 10 %. Indeed, scenario 2035 (S2+EbA) still assumes a very small decrease in the native forest. This decrease may be due to the increase in secondary forests by BMP, which could stabilise the native forest LULC by 70% until 2035. The mean annual simulated water yields, in spite of high variability of simulated scenarios, pointed out values of 18 L.s⁻¹.km² (1990, S1), 13 L/s/km² (2010, S2) and 21 L/s/km² (for 2035, S2+EbA).

412 3.4.2 Case study II: Domithildes headwater

- 413 The Domithildes catchment (9.9 km²) is located in the Cancã catchment. Similar to Upper Jaguari, Domithildes
- 414 is one of the most conserved sub-basins, mainly with native forests. The native forest fraction remained constant
- 415 (see Figure 14) from S1 (51% in 1990) to S2 (52% in 2010). However, unlike the Upper Jaguari sub-basin (see
- 416 **Figure 13**), native vegetation could increase by 56% in S2+EbA (2035). Due to the fact that Domithildes was
- adopted as a reference basin for Water Producer/PCJ, the augmented fraction of native forest by 2035 could showan increase of secondary forest.
- 419 Regarding water yield, the *Domithildes* catchment was classified as a second type of 'subbasin behaviour' (Section
- 420 3.3). There is a positive increment of water yield between 2010 (~18 L/s/km²) and 2035 (~23 L/s/km²), although
- 421 this situation may not achieve values obtained for S1 conditions in 1990 (~ 29 L/s/km²).

422 3.5. Results of a new index for hydrologic service assessment

- 423 A new index for hydrologic service assessment was developed as a simple relation between greyWF and water
- 424 yield, using a fraction between water demand (numerator) and availability (denominator). Some authors commonly

- 425 use this fraction as a direct approach to water scarcity (i.e. Smakhtin, et al., 2005; Hoekstra et al, .2013; McNulty
- 426 et al., 2010; among others). Therefore, we first assessed greyWF by respective drainage basins (Figure 15). Then,
- 427 we calculated the water pollution levels.
- 428 The results in Figure 16 show the composite water pollution level (WPLcomposite) versus drainage areas and
- 429 compared with the HSI. The baseline *WPLcomposite, ref* is related to the *Domithildes* catchment (horizontal, dotted
- 430 line in Figure 16). This line divides the graph into two regions: less sustainable basins (HSI>0) and more
- 431 sustainable basins (*HIS*<=0). More sustainable basins (*HIS*<0) are *Salto*, *Cachoeira* nested catchments (*Cachoeira*
- 432 dos Pretos, Chalé Ponto Verde and Ponte Cachoeira), as well as F28, F24 and the Upper Jaguari basin.

433 **3.6.** Comparison of field investigation and modelled scenarios

Field, experimental data (Taffarello et al., 2016-a) with modelled scenarios of land-use and land-cover change,
including the EbA hypothesis were integrated into a summary figure in the Supplementary Material (see
Suppementary Figure S.1).

437

438 4.Discussion

This section discusses field data, LULC change scenarios, GWF and water yield, not only in general aspects, butalso in selected catchments, mentioned in Section 3.

441

442 4.1 On field data

443 Other conserved subbasins also presented low mean values of turbidity (< 6.5 NTU): intervention Cancã catchment 444 (5 NTU), and Cachoeira dos Pretos (6 NTU). We found the highest turbidity above 40 NTU, which is considered the maximum established water quality standard for Brazilian Class 1 (BRASIL, 2005): at Parque de Eventos (283 445 446 NTU), at F23 (180 NTU) and at Salto outlet (160 NTU). However, these three sampling sites are located at water 447 bodies of Class 2, where the maximum turbidity allowed is up to 100 NTU (BRAZIL, 2005). Due to these areas having the highest urbanization among the sampled sites, they are in non-compliance with Brazilian environmental 448 449 standards. Arroio Júnior (2013) found a decreasing relation between turbidity and drainage areas in another 450 catchment located in Sao Paulo state. Temporal turbidity patterns show that on the one hand in 11 out of 17 451 monitored sites, the higher values of turbidity occurred in December, 2013, the only field campaign with significant precipitation (35.3 mm) and with a higher antecedent precipitation index (API = 123.7mm). This can 452 453 be due to carrying allochthone particles, which are drained into rivers by precipitation. Similarly, Arroio Júnior 454 (2013) also observed higher turbidity in the rainy season (December, 2012) which can lead to erosive processes. On the other hand, Zaffani et al. (2015) showed that turbidity did not vary over the hydrologic year in medium-455 456 sized, rural and peri-urban watersheds ranging from 1 to 242 km². In this case, other factors may have had an 457 influence, such as deforestation, seasonal variability, soil use type, sewage and mining (CETESB, 2015; Tundisi, 458 2014).

461 In the S2 Scenario (2010), the main soil use is pasture in 58% of the sub-basins and forest in 40% of them. From 462 1990 to 2010, there was a significant conversion of soil cover, with a slow reduction of pasture areas (-2%) and 463 native remnants (-5%) and with a progressive increase of eucalyptus (Eucalyptus sp.), an exotic forest in Brazil. Eucalyptus soil use varied from +1%, within Posses up to +31% in the Chalé Ponto Verde sub-basin in 2010. 464 465 Eucalyptus cover, however, did not achieve 10% of the soil uses in any of the simulated sub-basins in 1990. In the 466 third scenario (S2 + EbA), we hypothesized incentives of public policies for forest conservation and restoration, 467 due to the strengthening of EbA in the Cantareira System. This could lead to an increase in native vegetation reaching percentages of 15% in the Posses outlet and 69% in the F28 sub-basin. In this scenario, the higher 468 469 percentages of native vegetation would occur in the sub-basins F28, Upper Jaguari and Cachoeira dos Pretos. 470 Despite this general increase in native forest cover, we highlight the deforestation which occurred in the F23 subbasin in the Camanducaia river. Currently, although the basin has 34% of native forest cover, this rate has tended 471

472 to decrease since 1990. The *F23 outlet* (sub-basin 2) had 37% of native forest cover in 1990, which then became 473 34 % in 2010 and the S2+EbA Scenario predicts that F23 could reach 36.2% of native forest by 2035, returning to 474 the percentages found in 1990. Another critical situation is the *Posses outlet* (SWAT sub-basin 6). Despite the 475 conservation efforts which have been made in the region through the *Water Conservation* project (see Richards et 476 al., 2015; Santos, 2014; Pereira, 2013), the current percentage of native remnants is 13%, which may be 16% 477 in 2035, however not achieving the rate in 1990 (22%). This can potentially disrupt the regulating and provision

477 In 2033, however not achieving the rate in 1990 (22%). This can potentiarly disrupt the regulating and provision
 478 hydrologic services provided by Posses sub-basin and needs to be evaluated in depth.

479 Spatio-temporal patterns of the main soil uses which compete with forest cover are analysed: pasture and 480 eucalyptus. First, related to pasture, it can be observed that it was the main use in the past in 60% of the sub-basins 481 (in 1990) and, currently, it has become the majority LULC, approximately 40%. Our scenarios indicate that due 482 to EbA strengthening, encouraging the links between environmental conservation and forest restoration, 20% of 483 the sub-basins could be mainly occupied by pasture (sub-basins 2, 4, 6 and 7). This rate is reasonable, considering 484 rural sub-basins. Moreover, the reduction in pasture in the Cantareira System was more evident in the 1990-2010 485 period than in the 2010-2035 scenario. This can be explained by, at least, three factors: i) rural landowners 486 awareness of the relevance of converting pasture to native forest to generate and maintain ecosystem services in 487 the Cantareira System (Saad, 2016; Extrema, 2015; Mota da Silva, 2014; Padovezi et al., 2013; Goncalvez, 2013; 488 Veiga-Neto, 2008); ii) seasonal changes in the ecosystem structure which can increase the ecosystem resilience 489 (Mulder et al., 2015) and an observed significant increase, mainly in the 1990-2010 period, of non-native species 490 plantations.

Second, regarding the eucalyptus cover, the future scenario shows an increasing threat to the regulating and 491 492 supporting services as a result of the exotic forest in expansion. In 2035, eucalyptus cover may include, on average, 493 12% of the total area of the 20 catchments studied here. This is significant in comparison with 10% in 2010 and only 2% in 1990 for the same catchments. The scenario for 2035 shows that the maintenance of hydrologic services 494 495 deserves attention, because eucalyptus monoculture can potentially impact not only the headwaters, but entire landscapes, threatening the ecosystem dynamics. Moreover, these plantations, with an average wood yield of 50 496 497 to 60 m³ of Urograndis per hectare, need high quantities of agrochemicals, due to the low diversity of the population and low adaptation to climate change (Kageyama & dos Santos, 2015). Inshort, here we highlight the 498

499 threat on biodiversity that has been brought by alien species in headwaters and the changes that it can promote on 500 native species (Hulme & Le Roux, 2016) which, in turn, impact the ecosystem services.

501

502 4.3 On water yield and LULC

503 On the other hand, we observed in Posses, Salto, Jaguari, Cancã and Atibainha catchments an inverse situation 504 (behaviour II). This effect can be related to the hydrologic response produced by: (a) type of catchment; (b) size 505 of catchment; (c) the low soil moisture in the red-yellow latosol (Embrapa, 2016), which did not favour high evapotranspiration rates; (d) the riparian forest, originating from the EbA or Water-PES actions, that should still 506 507 be at the initial stages, not achieving a climax in 20 years (this explanation therefore assumes that the baseline of 508 PES actions was in 2015, although there are examples of restored forests in Extrema-MG with high evapotranspiration rates, as can usually be found in climax forests); and (e) unpredictability, non-linearity and 509 510 uncertainty (Ferraz et al., 2013; Lima & Zakia, 2006).

511 The role of the forest in the hydrologic cycle in river basin scales has been debated for centuries. Riparian native forests, eucalyptus and riparian forests in recuperation (shown here as orchard) have different hydrologic 512 responses. There is still a lack of knowledge regarding the influence of different types and phases of vegetation on 513 the hydrologic processes. Bayer (2014) found that the vegetation height and leaf area index are inversely 514 515 proportional to the water flows, which corroborate previous studies (Hibbert, 1967). Riparian forest restoration 516 increases the mean evapotranspiration, reducing the water yield (Molin, 2014; Salemi et al., 2012; Lima & Zakia, 2006; Andreassian, 2004). Restoration increases the water storage capability into the catchment throughout the 517 riparian zone, contributing to the higher water flow in the dry season (Lima & Zakia, 2000). This can lead to 518 unexpected results regarding water yield. Furthermore, at small catchments of temperate climate, researchers 519 520 estimated that deforestation in 40% of the catchments would increase the runoff of 130 ± 89 mm.year⁻¹ considering 521 the entire water cycle in the catchment scale (Collischonn & Dornelles, 2013). In addition, there is high dispersion 522 in the results based monitoring (usually, in paired catchments or Nested Catchment Experiment - NCE), which 523 makes it more difficult to predict the flow as a result of soil use conversion. Similarly, we found high dispersion 524 in the comparison between water yields versus different land cover in 20 sub-basins of the subtropical climate

525 (Figure 11).

526 BMP have been in progress since 2005 in the Posses Outlet (sub-basin 6, Table 5) and Middle Posses (Portal das Estrelas, N° 7), and since 2009 in Domithildes, F30 and Moinho catchments (Subbasins 9, 11 and 20, respectively). 527 These BMP originated from the Water Conservator and Water Producer/PCJ projects. In these cases, we 528 529 recommend that public agencies take care when defending PES as inductors of more water availability (ANA, 530 2013). Parts of these results and previous investigations, which were made through NCE (Taffarello et al., 2016a), 531 point out the opposite, i.e., in the more conserved catchments, we found lower water yields. Despite the fact that there are many Water-PES programs in Brazil (Pagiola, von Glehn & Taffarello, 2013; Guedes & Seehusen, 2011), 532 533 measurements of the effect on water yield under forest restoration are still lacking in tropical and subtropical conditions (Taffarello et al., 2016a; Salemi et al., 2012). However, the benefits of riparian forests on water quality, 534 535 margin stability, reduction of water erosion and silting are clear in the scientific literature (Santos, 2014; dos Santos et al., 2014; Studinski et al., 2012; Udawatta et al., 2010). 536

537

538 4.4 On GWF, LULC and water yield in selected catchments: Upper Jaguari and Domithildes

The discussion of the variability in GWF and water yield is based on the hydrologic conditions simulated in the test period from 2006 to 2014. In turn, this test period was selected due to high availability of rainfall stations under operation, which would potentially better perform distributed modelling at several sub-basins using SWAT. For the three scenarios simulated, the relationships between the native forest cover and mean water yield are different from each other.

544 On the one hand, in Upper Jaguari ("Alto Jaguari"), for scenario S1 (1990), the higher the native forest cover, the lower the water yield. This scenario behaviour is extended at experimental sites, and even strongly documented in 545 546 the literature (Salemi et al, 2012; Smarthust et al., 2012, Collischon & Dornelles, 2013). For scenario S2 (2010) the water yield seems not fully related to native forest LULC, oscillating around an average value of 18 L/s/km². 547 548 In scenario S2+EbA (2035), however, there is a slight increase in water yield when native forest cover is higher 549 than 50%. This proportional relation between water yield and forest cover in the S2+EbA is both controversial and contrary to results published by some authors (e.g. Collischonn & Dornelles, 2013; Salemi et al., 2012). For 550 551 example, monitoring data shows a reduction in the water yield with higher native forest land cover (Taffarello et 552 al., 2016a). Salemi and co-authors, in a review on the effect of riparian forest on water yield, found that riparian 553 vegetation cover decreases water yield on a daily to annual basis.

554 Furthermore, the greyWF-NO₃ of the Upper Jaguari basin showed 0.14 L/s/km² for scenario S1 (1990), increased 555 to 0.23 L/s/km² for scenario S2 (2010) and could grow to ca. 0.54 L/s/km² in S2+EbA scenario (in 2035). However, 556 this result is different from the one expected in the hypothesis testing through modelling. The null hypothesis states 557 that increasing native forest cover is correlated to decreasing nutrient loads flowing to streams. The results, 558 modelled by SWAT, predicted an increase in the greyWF by 2035. The simulated increase in the native forest (approx. +5%) appears to be insufficient for buffering nitrogen loads from animal excrements such as mammals 559 560 or zooplankton. For a more in-depth analysis, other factors that influence the greyWF should be evaluated 561 thoroughly.

562 On the other hand, in "Domithildes" catchment (reference catchment), other factors, such as native vegetation, 563 could influence the hydrologic cycle decreasing water yields in the 2010 scenario (S2). One explanation of this 564 water yield decrease could be the positive LULC of *Eucalyptus sp.* to +5% in 2010 (S2). Regardless of other 565 factors, +1% of eucalyptus land-use fraction in *Domithildes* will represent -2 L/s/km² of water yield, or -63 mm 566 per year, in the same range of results reported by Salemi (2012) and close to Semthurst et al (2015).

567 Comparing seasonal water yields, the results showed higher variability around monthly flow averages for the 568 S2+EbA (2035) scenario. These deviations in monthly flows by the S2+Eba (2035) scenario were higher in wetter 569 months between November and March. The regulation of water yield, in both rainy and dry conditions, is more 570 effective when quantified through variance (Molin, 2014). In spite of these uncertainties, scenarios modelled by

571 SWAT estimated the highest mean monthly water yield in February (38 L/s/km²) and the lowest mean monthly

- 572 water yield in September and October (8 L/s/km²). On the one hand, the results showed that a growing rate of
- 573 native vegetation LULC since 2010 would serve to attenuate both e-flows peaks, especially in the rainy season
- 574 (see flow duration curves), and pollutant filtration (see duration curves of N-NO₃ loads). On the other hand, the
 - 16

- 575 more native forest cover, the lower the water yield (Bayer, 2014; Molin, 2014; Burt & Swank, 1992). Thus, the
- 576 progressive increase of water yield from 2010 to 2035, compared to a higher total forest cover, could indicate other
- 577 factors, such as forest connectivity, forest climax and secondary factors such as BMP, that could produce non-
- 578 linear conditions of water yield from the local scale to the catchment scale.

579 5. Conclusions and Recommendations

Although the water-forest system interaction is a classic issue in Hydrology, the impacts of vegetation on qualiquantitative aspects of water resources need to be better understood.

582 Supported by field experiments and quali-quantitative simulations under different scenarios including EbA options 583 with BMP, our results showed evidence of nonlinear relationships among LULC, water yield, greyWF of nitrate, total phosphorus and sediments, which irreversibly affect the composite of water pollution level (WPL), the 584 585 definition of WPL of reference (here established at Domithildes catchment) and the hydrologic service index 586 (HSI). Although there was a coherent and proportional relation between the observed mean river velocity and 587 observed specific flow, experimental evidence still depicted outliers, not only in reference catchments with EbA/PES-Water options, but also in intervention catchments with no EbA/PES-Water options. This evidence 588 points out illustrative examples of how complex LULC options from EbA would be exhaustively sensed into 589 590 hydrological parameters and simulation scenarios using SWAT or other distributed models. Despite using a semi-591 distributed model for assessing non-point sources of pollution mainly tested under different LULC scenarios, our 592 results showed that the intrinsic nature of flow-load duration curves, LULC and greyWF are constrained to high uncertainties and nonlinearities both from *in-situ* sampling and from processes interactions of modelling. Our 593 594 results show the need to evaluate many uncertainty sources, such as: model sensitivity analysis, observed 595 streamflow data, ecohydrologic model performance, residual analysis, etc. To attain goals of EbA, using HSI 596 through greyWF assessment and composite of WPL, some conditions are needed to better fit models to field observations, as follows: (i) monitoring and, if possible, constraining illegal inputs of high-concentrated 597 pollutants, especially from growing urban settlements, (ii) restoring riparian vegetation, especially at HRUs where 598 599 EbA scenarios introduce more sensitivity of water yields and GWF and (iii) modelling EbA effects at HRUs where trapping and removing inflowing sediments are more evident. For the health of river ecosystems, we used HSI, 600 601 flow regimes and WPL composite, as composing alternative environmental flows Although the role of vegetation 602 on streamflow has been widely studied, very few investigations have been reported in Brazil with control 603 nutrient sources, transportation and delivery. Moreover, further field and modelling research is needed when 604 integrating LULC, EbA and greyWF through hydrologically-distributed models. Thus, future research could 605 clarify the influence of vegetation on water quality and the role of anthropogenic and natural drivers in 606 ecohydrologic processes on a catchment-scale.

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TABLES

SWAT sub-basin	Gauge station	Field Modelling		Drainaga	Coordinates	
		observations (2013-2014)	LULC/EbA scenarios	area (km ²)	Lat.	Long.
1	AltoJaguari	Yes	Yes	302.2	-22.820	-46.154
2	F23Basin	Yes	Yes	508.1	-22.827	-46.314
3	F28Basin	Yes	Yes	276.8	-22.806	-45.989
4	Salto Basin	Yes	Yes	15.0	-22.838	-46.218
5	Parque de Eventos	Yes	Yes	926.5	-22.853	-46.325
6	Posses Exut [*]	Yes	Yes	11.9	-22.833	-46.231
7	Portal das Estrelas	Yes	Yes	7.1	-22.820	-46.244
8	F25Basin	Yes	Yes	971.9	-22.850	-46.346
9	Domithildes[**]	Yes	Yes	9.9	-22.886	-46.222
10	Jaguari Basin	No	Yes	1037.0	-22.896	-46.385
11	F30 [*]	Yes	Yes	15.1	-22.935	-46.212
12	Ponte Cachoeira.	Yes	Yes	121.0	-22.967	-46.171
13	Chale Ponte Verde	Yes	Yes	107.9	-22.964	-46.181
14	Cachoeira dos Pretos	Yes	Yes	101.2	-22.968	-46.171
15	Jacarei Basin	No	Yes	200.5	-22.959	-46.341
16	F24	Yes	Yes	293.5	-22.983	-46.244
17	Cachoeira Basin	Yes	Yes	391.7	-46.209	-46.276
18	F34 Basin	Yes	Yes	129.2	-23.073	-46.209
19	Atibainha Basin	No	Yes	313.8	-23.182	-46.342
20	Moinho [*]	Yes	Yes	16.9	-23.209	-46.357

Table 1: Sub-basins delimited in SWAT with drainage areas and geographic locations.

Legend: * indicates new data collection stations installed for experimental monitoring according to ANA/CPRM standards; ** indicates experimental stations for research purposes. Source: Taffarello et al (2016-a)

Gauge station	Area (km²)	Pbias (%)	NSE (-)	NSE Log (-)	Pbias (%)	NSE (-)	NSE Log(-)	Performance level of calibration and validation (Moriasi et al., 2007)
		Calibration		Validation			-	
Posses	13.3	-22.0	0.68	0.52	15.4	0.78	0.38	Unsatisfactory/very good
F28	281.5	5.3	0.80	0.68	14.2	0.72	0.31	Very good/good
F24	294.5	-13.3	0.69	0.71	-1.7	0.65	0.34	Satisfactory/satisfactory
Atibainha	331.7	-14.5	0.60	0.55	1.7	0.71	0.54	Satisfactory/good
Cachoeira	397.3	-26.6	0.49	0.31	-46.7	0.27	0.05	Unsatisfactory/unsatisfactory
F23	511.2	-1.8	0.88	0.90	12.0	0.84	0.77	Very good/ very good
F25B	981.4	3.6	0.91	0.89	11.4	0.77	0.72	Very good/ very good
Jag+Jac	1276.9	-12.0	0.83	0.87	-8.4	0.82	0.73	Very good/ very good

Table 2: Characteristics of quantitative calibration and validation of SWAT in studied catchments (Moriasi et al.,2007). Area delimited by Digital Terrain Model (adapted from Mohor, 2016):

	Description	Parameter	Fitted values
Water Quantity	Initial SCS curve number (moisture condition II) for runoff potential.	CN2	<0.25
	Soil evaporation compensation factor.	ESCO	<0.2
	Plant uptake compensation factor.	EPCO	<1.0
	Maximum canopy storage (mm).	CANMX	Varies by vegetal cover
	Manning's coefficient "n" value for the main channel.	CH_N2	0.025
Water Quality	Nitrate percolation coeficiente	NPERCO	0.2
	Minimum value of the USLE C coefficient for water erosion related to the land cover	USLE_C	Varies by land use (< 0.4)

Table 3: Calibrated SWAT parameters in the headwaters of the Cantareira Water Supply System.

FIGURES



Figure 1: Location of Cantareira Water Supply System in the Piracicaba and Upper Tietê watersheds.



Figure 2: Methodological scheme for assessing hydrologic services based on greyWF.



Figure 3: Land-use change during 1990 (Scenario S1), 2010 (Scenario S2) and 2035 (Scenario S2+EbA) in the headwaters of the Cantareira Water Supply System:



Figure 4: Model calibration related to drainage areas of catchments in the Cantareira System.



Figure 5: Comparison between flow discharges (upper part) and nitrate loads (lower part), through observed (dotted lines), simulated by SWAT (solid lines) and field validation through instantaneous experimental samples (marked points with uncertainty intervals) at monitored stations of *Posses Outlet* (left part), *F23 Camanducai*a (center part) and *F24-Cachoeira* (right part). The uncertainty bars were determined using instantaneous velocities measured in the river cross-sections during 2013/14 field campaigns (see Taffarello et al, 2016-a). The uncertainty bars represent the minimum and maximum values of measured streamflow and pollutant loads in a cross section of the river during a field campaign of headwater catchments.



Figure 6: Experimental sampling of turbidity (size of circles), observed flows and mean velocities in river cross sections of 17 catchments in Cantareira System headwater (Oct, 2013 - May, 2014). This illustration shows the high interdependence and complexity to integrate any standard parameterization, at a regional scale, of the SWAT model, linking potential scenarios of LULC, water yield and freshwater quality in medium-size basins and headwaters



Figure 7: Multidimensional chart of hydraulic and water quality variables sampled in field campaigns in the headwaters of the Cantareira Water Supply System between Oct, 2013 - May, 2014.



Figure 8: Study area divided into sub-basins for hypothesis testing using semi-distributed SWAT model.



Figure 9: Native forest cover in S1 (1990), S2 (2010) and S2+EbA (2035).



Figure 10: Flow duration curves under three LULC scenarios: S1(1990), S2(2010) and S2+EbA(2035) at headwaters of the Cantareira Water Supply System.



Figure 10: Flow duration curves under three LULC scenarios: S1(1990), S2(2010) and S2+EbA(2035) at headwaters of the Cantareira Water Supply System(cont.).



Figure 11: LULC scenarios for specific water yield for 20 drainage areas at Jaguari, Cachoeira and Atibainha watersheds, according to S1 (1990), S2 (2010) and S2+EbA (2035) scenarios.



Figure 12: Fraction of water yield (mean Q) compromised by the grey water footprint of nitrate (GWF-NO3), total phosphorous (GWF-TP) and sediments (GWF-Sed) versus drainage area (a), and versus selected sub-basins (b).



Figure 13: Synthesis chart of case study *Upper Jaguari* sub-basin (drainage area = 302 km²). Left, upper chart: localization at the drainage areas of Cantareira System: Center, upper chart: LULC conditions for scenarios S1 (1990), S2 (2010) and S2+EbA (2035): Right, upper chart: comparison of water yields simulated for conditions of S1, S2 and S2+EbA: Left, lower chart: water yield scenarios compared with intra-annual regime of S2+EbA scenario: Center, lower chart: comparison of duration curves of flows for S1, S2 and S2+EbA conditions: Right, lower chart: duration curves of N-NO3 loads for S1, S2 and S2+EbA



Figure 14: Synthesis chart of case study *Domithildes* catchment (drainage area = 9.9 km^2). Left, upper chart: localization at the drainage areas of the Cantareira System: Center, upper chart: LULC conditions for scenarios S1 (1990), S2 (2010) and S2+EbA (2035): Right, upper chart: comparison of water yields simulated for conditions of S1, S2 and S2+EbA: Left, lower chart: water yield scenarios compared with intra-annual regime of S2+EbA scenario: Center, lower chart: comparison of duration curves of flows for S1, S2 and S2+EbA conditions: Right, lower chart: duration curves of N-NO3 loads for S1, S2 and S2+EbA.



Figure 15: Relationships between Grey Water Footprint for Nitrate (a) and Total Phosphorous (b) according to three LULC scenarios (1990, 2010 and 2035) and size of the drainage areas of headwaters in the Cantareira Water Supply System.



Figure 16: Hydrologic Service Index (circle ratio) related to drainage area of river basin (horizontal axis) and composite of water pollution index (vertical axis) for S2+EbA scenario: Equal weights of nitrate, total phosphorus and dissolved sediments are expressed in *WPLcomposite*