Acta Universitatis Agriculturae Sueciae

Doctoral Thesis No. 2021:64
Faculty of Natural Resources and Agricultural Science

Impacts of land use change on river streamflow and water quality in a semi-arid catchment

Assessment of a catchment under rapid and uncontrolled urbanisation

Benjamin Gossweiler Herrera

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SWEDISH UNIVERSITY
OF AGRICULTURAL
SCIENCES

DOCTORAL THESIS
Uppsala 2021

Acta Universitatis Agriculturae Sueciae
2021:64

ISSN 1652-6880
ISBN (print version) 978-91-7760-805-9
ISBN (electronic version) 978-91-7760-806-6

Swedish University of Agricultural Sciences, Uppsala
Print: SLU Service/Repro, Uppsala 2021

Impacts of land use change on river streamflow and water quality in a semi-arid catchment. Assessment of a catchment under rapid and uncontrolled urbanisation

Abstract

The ongoing degradation of water quality and streamflow in rivers and streams worldwide is mainly due to human action through global land use change, particularly urbanisation. Population growth and economic development are major drivers of urbanisation, which causes environmental problems such as high water demand and solid waste and wastewater generation. This thesis describes the impacts of three decades of unregulated urbanisation and land use change on water quality and streamflow in the semi-arid Rocha River catchment in Bolivia. Remote sensing and geographic information systems (GIS) based on Landsat imagery were used to detect land use change, while an index-based approach was developed to classify and compare river water quality and locate priority source areas (PSAs) of pollution. Correlation analysis was used to examine relationships between different land uses and water quality. The Soil and Water Assessment Tool (SWAT) model was employed to simulate streamflow and total nitrogen and total phosphorus transport in the catchment, based on monthly data. The results showed strong increases in the area of human settlements, forest and cropland, while semi-natural land area generally decreased. Water quality decreased over time and from catchment headwaters to outlet, and human settlements were identified as PSAs of pollution. Human settlements were also associated with decreasing water quality ($p<0.01$) and pollution from PSAs ($p<0.05$). SWAT modelling proved good (Kling-Gupta efficiency, KGE) for streamflow, satisfactory for total phosphorus, and poor for total nitrogen. Simulated mean annual streamflow (13.9-23.3 $m^3 s^{-1}$), total nitrogen (270.3-550.7 ton $year^{-1}$) and total phosphorus (83.1-170.5 ton $year^{-1}$) loads increased over time, with nutrient transport increasing overall from catchment headwaters to outlet. These deleterious impacts of urbanisation-related land use change in the Rocha River catchment demonstrate the need for effective remedial measures, including continuous monitoring, pollution mitigation and water quality restoration.

Keywords: Landsat, maximum likelihood, long-term variations, point and non-point pollution sources, hydrological modelling, nutrient transport, Cochabamba, Bolivia

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Impactos del cambio de uso de la tierra en el caudal y calidad de agua. Evaluación de una cuenca bajo urbanización rápida y descontrolada.

Resumen

La degradación de la calidad del agua y el caudal de ríos y arroyos en el tiempo se debe principalmente a la acción humana por el cambio del uso de la tierra en el mundo. El crecimiento poblacional y desarrollo económico impulsan la urbanización, que a su vez plantea problemas ambientales como la demanda de agua, generación de residuos sólidos y aguas residuales. Esta tesis tiene como objetivo mejorar la comprensión de cómo la urbanización no regulada y el cambio de uso de la tierra (1990-2020) impactan la calidad del agua y caudal, en la cuenca semiárida del río Rocha. Se utilizaron la teledetección y sistemas de información geográfica (SIG) para detectar cambios de uso de la tierra usando imágenes Landsat. Se utilizaron índices para clasificar y comparar la calidad del agua de los ríos y para localizar áreas prioritarias de generación de contaminación (APGC). Se utilizó la correlación para explicar la relación entre diferentes usos de la tierra y categorías de calidad del agua. Además, el modelo de la herramienta de evaluación del suelo y el agua (SWAT) simuló el caudal, transporte de nitrógeno total (NT) y fósforo total (FT) en la cuenca con base en datos observados mensualmente. Los resultados mostraron aumentos de asentamientos humanos, bosques y cultivo, mientras que los usos de la tierra semi-naturales en general disminuyeron. La calidad del agua disminuyó en el tiempo y desde la cabecera hasta la salida de la cuenca, y los asentamientos humanos se identificaron como APGC. Además, los asentamientos humanos se relacionaron ($p < 0{,}01$) con la disminución de la calidad del agua y ($p < 0{,}05$) con las APGC. El modelamiento SWAT fue bueno (Eficiencia Kling-Gupta) para el caudal y satisfactorio para el fósforo total y pobre el nitrógeno total. El caudal medio anual simulado (13,9 a 23,3 $m^3\ s^{-1}$), TN (270,3 a 550,7 ton año^{-1}) y TP (83,1 a 170,5 ton año^{-1}) en carga aumentan con el tiempo y el transporte de nutrientes aumentó desde la cabecera hasta la salida de la cuenca. Estos impactos nocivos están relacionado con la urbanización y demuestran la necesidad de monitoreo continuo, mitigación y la restauración de la calidad del agua.

Palabras clave: Landsat, máxima verosimilitud, variaciones a largo plazo, fuentes de contaminación puntual y difusa, hidrología, nutrientes, Cochabamba, Bolivia

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Dedication

To my beloved sons Samuel and Caleb

Contents

List of publications

This thesis is based on the work contained in the following papers, referred to by Roman numerals in the text:

I. Gossweiler, B., Wesström, I., Messing, I., Romero, A. & Joel, A. (2019). Spatial and temporal variations in water quality and land use in a semi-arid catchment in Bolivia. Water 11(11): 2227.

II. Gossweiler, B., Wesström, I., Messing, I., Villazón, M. & Joel, A. (2021). Impact of land use change on non-point source pollution in a semi-arid catchment under rapid urbanization in Bolivia. Water 13(4): 410.

III. Gossweiler, B., Wesström, I., Messing, I., Grusson, Y., Villazón, M. & Joel, A. Assessment of streamflow and nutrient transport by continuous modelling using SWAT in a semi-arid catchment in Bolivia. (Manuscript).

The contribution of Benjamin Gossweiler Herrera to the papers included in this thesis was as follows:

I. Planned the study together with the co-authors. Performed data curation and collection, formal data analysis and interpretation, with assistance from the co-authors. Wrote the manuscript, with revisions by the co-authors.

II. Planned the study together with the co-authors. Performed data collection, formal data analysis and interpretation, with assistance from the co-authors. Wrote the manuscript, with revisions by the co-authors.

III. Planned the study together with the co-authors. Performed formal data analysis and interpretation, with assistance from the co-authors. Wrote the manuscript, with revisions by the co-authors.

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Abbreviations

ArcGIS	Aeronautical reconnaissance coverage geographic information system
BOD	Biological oxygen demand
CASA	Water and Environmental Sanitation Center
COD	Chemical oxygen demand
DEM	Digital elevation model
DI	Distance indicator
DO	Dissolved oxygen
GIS	Geographical information system
HRU	Hydrologic response unit
IPI	Prati’s Implicit Index of Pollution
KGE	Kling-Gupta efficiency
Landsat TM	Land satellite thematic mapper
LCI	Land cover indicator
NPSP	Non-point source pollution
NSF-WQI	National Sanitation Foundation Water Quality Index
OLI/TIRS	Operational Land Imager/Thermal Infrared Sensor
PET	Poteltial evapotranspiration
PNPI	Potential Non-point Pollution Index

PSA	Priority source area
QUAL2E	The enhanced stream water quality model
RoI	Runoff indicator
SENAMHI	National Meteorology and Hydrology Service of Bolivia
SWAT	Soil and Water Assessment Tool model
WQI	Water quality index

1. Introduction

A major threat to Earth system processes is the ongoing development of human settlements, which includes landscape transformation and natural resource extraction or exploitation for basic human needs (Lade *et al.* 2020). These activities strongly affect local patterns of forest, climate system, ecosystem functioning, fire regimes, flooding and biodiversity (Steffen *et al*. 2018; Ruddiman *et al*. 2015; Smith & Zeder, 2013). Moreover, human activities are determined by climate, which in natural conditions can vary depending on the Earth's "energy budget" (Strapasson *et al*. 2017).

In 2009, Stockholm Resilience Centre established a set of quantitative planetary boundaries of Earth system processes within which humanity can continue to develop and thrive for generations to come (Kim & Kotzé 2020; Heck *et al*. 2018; Rockström *et al*. 2009). Among these processes, "land-system change" and "climate change" are reported to be at increasing risk, while "freshwater use" is still within safe boundaries (Folke *et al*. 2021; Steffen *et al*. 2015).

Hydrological system components such as surface runoff, infiltration, interflow and evapotranspiration are significantly influenced by land use changes (Sajikumar *et al*. 2015). Transformation from pervious surfaces (cropland, shrubland, grassland and forest) to impervious surfaces (paved and urbanised areas) reduces water infiltration into the ground, while it increases surface runoff and introduces variation in water flow by causing e.g. periods of high streamflow (Miller *et al*. 2014). Changes in rainfall and increasing global temperatures can also modify the transformation and transport characteristics of nutrients and pollutants in stream water (Giri *et al*. 2016). In turn, local and regional socio-economic development can be threatened due to increased frequency of floods or droughts as a consequence of the combined effect of land use changes and climate variability. Water quality and quantity are also affected by these factors, which together are responsible for most watershed characteristics.

An example of an affected watershed is that of the Rocha River, which passes through the metropolitan area of Kanata in Cochabamba, Bolivia. The river received its name from a Spanish captain who changed the path of the watercourse to irrigate cropland that Spain had acquired from Sipe Sipe natives. Over the course of time, various canal and dam construction projects have been carried out to prevent flooding in Cochabamba city (Urquidi 2011). In the past 30 years, the Rocha River has been experiencing deteriorating water quality and decreasing streamflow, due to rapid population growth and uncontrolled urbanisation within its catchment. Most of the river's reaches have been utilised for disposal of municipal and industrial wastes since the city was founded. At present, the city's requirements for water supply and wastewater treatment are not met, since aquifers (groundwater) and mountain lakes have been overexploited and the city's sewage systems date from the 1970s.

In addition, limited access to accurate water quantity and quality data for the Rocha River and failure by the scientific community and decision makers to identify pollution sources have become important issues. The main reasons for these shortcomings are the high cost of data acquisition, lack of monitoring programmes and lack of political support for evidence-based decision-making on water-related problems.

The knowledge gap concerning spatial and temporal variations in water quality and quantity influenced by land use changes such as urbanisation in the Rocha River catchment is hampering the development of best-practice strategies to reduce the risk of contamination and devise optimal management options. At the same time, there is a historical lack of data from long-term environmental monitoring regarding water resources in the region. Therefore, economic resources and time are wasted and efforts to develop effective mitigation programmes for pollution control and water quality and quantity improvement are undermined.

There is thus an urgent need to improve understanding of the current status and variability in water quality and quantity in the main Rocha River waterway and the associations with land use changes and climate change. Such knowledge could also help to land use planning tools with sufficient quality and generalisability to be extrapolated to other areas with similar natural and man-made impacts.

2. Objectives

The overall aim of this thesis was to improve understanding of how decades of unregulated urbanisation and land use change affect streamflow and water quality in a semi-arid catchment. The overall hypothesis was that unregulated urbanisation has led to increasing sources of pollution, water quality impairment and restricted streamflow in the Rocha River catchment.

Specific objectives were to:

- Evaluate the relationship between land use changes and surface water quality (Paper I).
- Assess whether non-point source pollution at catchment scale can be explained by land use, potential for surface runoff and distance from the river network (Paper II).
- Evaluate streamflow and pollutant transport under different land uses and periods (Papers I & III).

The research questions related to these specific objectives were:

- In what ways do land use changes contribute to changes in surface water quality?
- Can the effects on surface water quality of pollution from different sources be quantified with limited water quality data and landscape characteristics?
- Can the SWAT model be used effectively to simulate variations in streamflow and nutrient transport under changing land uses over periods with limited water quality data?

3. Background

In catchment management and environment sustainability, spatial and temporal variations in streamflow and water quality caused by land use change are important issues to address. Developing an understanding of interactions between different pollution sources is a critical first step in assessing pollutant load dynamics and interactions with streamflow.

Human-related factors (population, economics, system policy, technical measures etc.) are to a large degree responsible for land use change, as a direct manifestation of human modification of the Earth system's natural environments. Such human factors are generally active worldwide and in particular in developing countries, strongly influencing land use change (Lambin *et al*. 2001). Population growth is leading to rapid and uncontrolled urban expansion and urbanisation in rural areas around the world, resulting in conversion of agricultural land and forest into urban consolidated settlements for socio-economic activities and housing (Meyer & Turner, 1994). The environmental impacts of land use change are contributing to atmospheric composition, regional climate changes, hydrological cycle transformation, nutrient loading from agriculture to natural ecosystems, biodiversity decline and habitat fragmentation (Foley *et al*. 2005).

The problem of limited access to high quality, long-term monitoring data in developing countries leads to uncertainties in conventional statistical assessments. An alternative is the use of suitable models that can represent reality and describe how a catchment will behave when conditions change. Hydrological modelling can provide reasonable frameworks for streamflow and water quality assessment at catchment scale, with acceptable accuracy. A proper evaluation of hydrological conditions could lead to adequate water monitoring and water quality restoration programmes for prevention and mitigation of future pollution.

3.1 Land use

Land use is characterised by the arrangements, activities and inputs people undertake in a certain place to produce, change or maintain it (Di Gregorio 2005). Human activities such as agricultural expansion, fuelwood consumption, intensive agriculture, wood extraction, forestry, animal husbandry and urbanisation are common land uses.

Unplanned changes in land use have become a serious problem especially in developing countries, where little attention has been given to unwanted environmental impacts, especially related to water pollution and land degradation (Fathizad *et al*. 2017). Globally, cropland, pastureland, tree plantations and urban areas have expanded in recent decades, accompanied by large increases in energy, water and fertiliser consumption, disease transmission and considerable losses of biodiversity. Positive outcomes of land use change are opportunities to produce food, feed and fibre for human use, and to provide habitable areas for people (Foley *et al*. 2005).

Temporal and spatial patterns of different land use changes reflect changes in human socio-economic activities. Therefore, land use changes due to physical, chemical or biological conversions occurring in historical patterns are a result of land management. Land use change comprises two major processes (Davis *et al*. 2019). The first process is a change in land cover associated with expansion or contraction of the area of land used for different purposes (e.g. pasture, cropland, urban). The second process is a change in the type of management on existing land cover (e.g. changes in irrigation, fertiliser use, crop type, harvesting practices or impermeable surfaces). Land use change related to management can occur without changing the extent of different land covers.

Around 2005, built-up area covered by settlements and infrastructure occupied 1-3% of land on Earth, and this area is projected to increase to 3-5% by 2050. The increase in built-up area has been accompanied by environmental problems, with increases of 78% in carbon emissions, 60% in residential water use and 76% in wood used for industrial purposes (Grimm *et al*. 2008). In this context, land use change to build cities and support their populations drives local to global alterations in biogeochemical cycles, climate, hydrological systems and biodiversity. This expansion tends to occur on agricultural land, while agriculture expands onto forest land. Cropland comprises about 10% of the world land area and, from 1961 to 2007, overall cropland area increased by about 11% (Bringezu *et al*. 2014).

Remote sensing technology and geographic information systems (GIS) based on multi-spectral and multi-temporal satellite imagery provide a flexible environment for displaying, storing and analysing digital data and field observations (Zhu *et al*. 2012). This technology has been successfully used to map and monitor land use changes, in approaches ranging from simple unsupervised approaches to various complex supervised classifications, and from pixel-based methods to sub-pixel and object-oriented methods (Jensen 2015).

3.1.1 Land use change and impact

Historically, human settlements tended to be associated with water sources such as river, creeks and lakes. River were generally preferred, since they are sources of water and food and a way to get rid of wastes. River plains also provide flat land for infrastructure development and transport facilities (Steffen *et al*. 2015). Urbanisation modifies the original landscape (increased area of hard surfaces, watercourse modification, lake drainage and land clearance for agriculture) to satisfy the needs of urban residents and to provide e.g. a water supply, wastewater treatment and basic sanitary services to avoid contamination (Inostroza *et al*. 2013). As a consequence, many rivers worldwide are degraded to such an extent that they can no longer provide services or resources for which they were the original source, and act only as a channel to evacuate wastewaters (Grimm *et al*. 2008).

During recent decades, the effects of urban expansion have been extensively studied by a large number of researchers from a variety of disciplines. Within hydrology, urban expansion is blamed for increasing surface runoff and, consequently, raising peak flow volumes and increasing the flood risk (Semadeni-Davies *et al*. 2008; Whitford *et al*. 2001). The main effects of urban expansion on surface hydrology and the water balance are caused by conversion of vegetated land cover into sealed or hard surfaces, such as buildings, roads and parking lots. These changes alter several hydrological processes at various spatial and temporal scales (Poelmans *et al*. 2010). Without an integrated approach involving skills in the fields of water engineering, hydrogeology, public health and sanitation, and without adequate design and construction, the extensive use of rivers as sewage disposal systems may cause severe groundwater contamination ((Taylor & Owens 2009; Zingoni *et al*. 2005). Stream ecological function and biotic richness also decrease, with increased dominance of pollution-tolerant species. This causes declines in the abundance and diversity of fish, invertebrates and macrophytes (Paul & Meyer 2008). According to Nie *et al*. (2011), thorough assessment of the impacts of land use changes on hydrology is the basis for watershed management and ecological restoration.

3.2 Water quality

Water quality is usually assessed based on physical, chemical and biological variables and the results indicate the suitability of water to sustain various uses or processes (Meybeck *et al*. 1996). Assessment of these variables by field monitoring of rivers is included in monitoring programmes, to provide basic data for detecting trends and information for devising mitigation actions. The quality of water regarding use is described in terms of the concentrations and forms of organic and inorganic material present in the water, together with streamflow, sediments and nutrient loads.

Water quality is displaying ongoing deterioration worldwide. It is affected by a wide range of natural influences (topography, atmosphere, geology, hydrology and climate) and human influences (land use change, mining, livestock farming, pollution, and erosion), which disrupt ecosystems and/or restrict water use. Furthermore, access to wastewater services for an increasing global population is an important problem (Uddin *et al*. 2021).

3.2.1 Sources of pollution

Water quality degradation is generally caused by point sources (including domestic, industrial and commercial discharges) of wastewater, and by non-point sources (precipitation and stormwater runoff from human settlements and agricultural areas), or both. These sources are affected by e.g. crop sequences, topography, soil type and climate, and can be enhanced by erosion, salinisation, soil compaction, reductions in soil organic matter and landslides. Mitigation and restoration measures, such as best management or conservation practices at catchment scale, then need to be given priority (Bouma & McBratney 2013).

Point sources are relatively easy to identify, quantify and control (sanitary sewage systems and wastewater treatment plants), while non-point source pollution cannot be traced back to a single origin and is confined to certain areas that can produce pollution (Novotny 1999; Carpenter *et al*. 1998). The main concern with point source pollution is to properly collect and analyse water samples, while with non-point source pollution identification and evaluation of priority source areas (PSAs) of the pollution are of great significance (Shrestha *et al*. 2008). The most difficult water quality problem to handle is pollution from non-point sources, due to the complicated hydro-meteorological and biochemical processes involved and the spatial variability affecting pollutant transport and transformation (Lam *et al*. 2010).

3.2.2 Water quality assessment

Assessment of water quality in water bodies plays an important role for appropriate water resources management, reducing environmental risks and health risks, and enabling suitable wastewater and solid waste load allocation and decision-making for pollution monitoring systems (De la Mora-Orozco *et al*. 2017). The list of variables that can be used to assess quality in a water sample is vast, but a proper assessment can be made by including a certain number of variables relevant for actual future use of the water. A convenient alternative is use of a water quality index (WQI), which is a single dimensionless number that describes water quality in a simple form by aggregating the value of selected measured variables. The following general steps are used to develop a WQI: i) selection of variables, ii) calculation of sub-index values, iii) establishment of weights and iv) aggregation of sub-indices to the final index (Abbasi & Abbasi 2012).

Indices are used in water quality monitoring and assessment, resource allocation, public information, research and development and environmental planning (Sener *et al*. 2017; Ewaid & Abed, 2017; Salcedo-Sanchez *et al*. 2016; Kannel *et al*. 2007; Debels *et al*. 2005). In addition, indices make the transfer and utilisation of data easier and clearer, and more spatially and temporally comparable (Lumb *et al*. 2013). Thus, WQIs have been applied worldwide for water quality characterisation, evaluation and classification, and for evaluation of spatial and temporal changes in water quality (Uddin *et al*. 2021; Lumb *et al*. 2013). The National Sanitation Foundation Water Quality Index (NSF-WQI) and Prati's Implicit Index of Pollution (IPI) are examples of indices commonly used for point pollution sources, while the Potential Non-point Pollution Index (PNPI) for diffuse pollution is an example of an index used in non-point pollution source assessment.

3.3 streamflow and nutrient transport

Water resources can be affected by land use changes, especially urbanisation and agricultural expansion. In addition, climatic variability affects runoff and streamflow, as a response to changes in the hydrological cycle (Santhi *et al*. 2001). Changes in precipitation and temperature can modify transport of water pollutants (Giri *et al*. 2016). The study of streamflow variations is important for sustainable utilisation of water resources and local ecological preservation, while nutrient transport can explain water quality dynamics within a catchment.

A modelling approach integrating field measurements and conditions that control hydrology and water balance components, including pollutant loads and transport, can provide efficient solutions to quantify the long-term water quality impacts of land use and climate changes. A hydrology model can develop methodologies for accurately estimating runoff, streamflow and pollution transportation at a range of scales, which is the basis for regional environmental management (Miller *et al*. 2007).

The Soil and Water Assessment Tool (SWAT) model has been widely used all around the world to predict streamflow discharge and nutrient load and transport from catchments of various sizes (Arnold *et al*. 2012). SWAT is a semi-distributed, process-oriented hydrological model (Neitsch *et al*. 2011). It is a continuous time model, which simulates water and nutrient cycles with a daily time step. In addition, the computational efficiency of SWAT is convenient for parametric adjustment and multiple simulations implemented in minimal time (Gassman *et al*. 2014).

Applications of the SWAT model in recent years include description of calibration and validation processes, water balance component and nutrient load simulation, hydrology and water quality modelling, and land use and climate change effects on stream flow and water balance. However, SWAT data requirements (frequency, quantity and quality of observed streamflow sediments and nutrients) and selection of simulation parameters are based on catchment hydrological dynamics (Chahinian *et al*. 2011). The model has some limitations, e.g. no sub-daily simulation, difficulties in modifying input files, no flood and sediment routing simulation, and difficulties in modelling floodplain erosion and snowmelt erosion (Neitsch *et al*. 2002).

4. Materials and Methods

4.1 Description of studied catchment

The Rocha River catchment is located in the eastern Andes of South America, in the central part of Bolivia (Figure 1). The river flows east to west for more than 80 km, passing through the cities of Sacaba and Cochabamba.

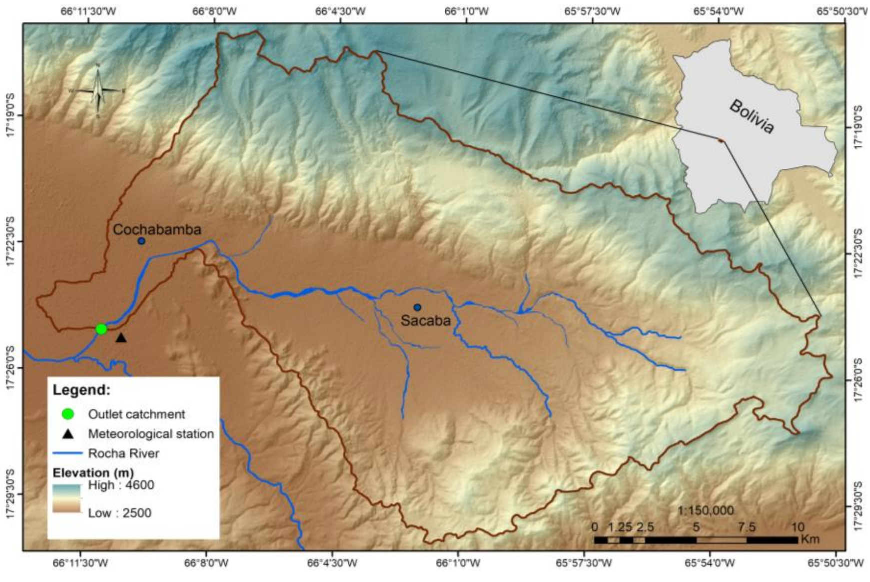
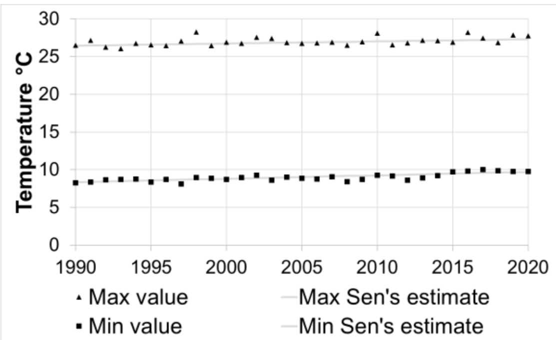


Figure 1. Geographical location and boundaries (dark brown line) of the Rocha River catchment in central Bolivia.

The catchment is characterised by mountain ranges in the north and east, hilly land in the south, a valley in the middle part into which the river system network drains, and piedmont as a transition zone between mountain and valley (Stimson *et al.* 2001; UN-GEOBOL 1978). Soil textures are dominated by sandy loam in the mountains, sandy loam in hill and piedmont areas, and silty loam and sandy clay loam in the valley (Ongaro 1998). Erosional features such as gullies, rills and pipes are also present (Metternicht *et al.* 1998). The altitude ranges between approximately 2500 m above sea level (asl) in the western part of the valley bottom) to 4500 m asl in mountain ranges in the north-western part of the catchment.

Vegetation in the catchment is mostly xerophytic, dominated by shrubs and grasses, but forest is also present. Crops are mainly rainfed, but irrigation is applied in some places, using water from irrigation systems or directly from the river (Metternicht *et al.* 2005). Rocha River water irrigates an estimated 500-900 hectares of cropland in the catchment, mainly potatoes and various vegetables (MMAA 2013).

The climate in the catchment is semi-arid (Köppen climate classification), based on data for the period 1990-2020 collected at Aeropuerto-Cochabamba meteorological station (Amaya *et al.* 2018) (Figure 2). Mean annual temperature in that period was 18°C (min. 9°C, max. 27°C) and mean annual rainfall was 440 mm (range 254-691 mm). Mean annual minimum temperature (p<0.001) and maximum temperature (p<0.05) showed significant increasing trends in the period, while mean annual rainfall showed high variation and no significant trend (p=0.321) (Figure 2). Overall, mean annual minimum temperature increased significantly by 1.5°C and maximum temperature by 1.2°C, while mean annual rainfall increased overall by 1.5 mm (non-significant) in the study period.



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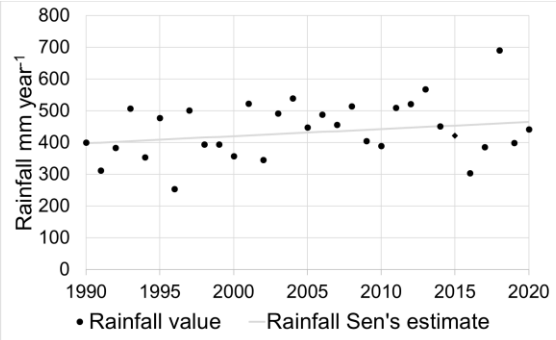
b. 

Figure 2. Mean annual maximum and minimum (a) temperature and (b) rainfall in the Rocha River catchment 1990-2020 (Aeropuerto-Cochabamba meteorological station) and associated Sen's slope estimates.

There is increasing demand for water supply and adequate infrastructure for wastewater treatment in the Rocha River catchment, led by increasing population growth and expanding industrial activities in Cochabamba and Sacaba cities and their surroundings (Trohanis *et al.* 2015). Wastewater treatment facilities are scarce and have operational and maintenance problems (Cossio *et al.* 2019). Untreated effluents are discharged into the river, and thus point and non-point pollution sources are major threats to water resources. Water for human consumption comes from groundwater and a few mountain lakes and reservoirs (Renner &Velasco 2000).

4.2 Data collection and sampling

The National Meteorology and Hydrology Service of Bolivia (Servicio Nacional de Metereología e Hydrología, SENAMHI) provided climate and hydrological data from the ASSANA-Aeropuerto meteorological station close to the study catchment outlet and from the hydrometric station Puente Cajón installed in the Rocha River main channel at the catchment outlet.

No continuous records of monitored water quality and streamflow data were available for the catchment. However, grab sample data were found in available historical physico-chemical and biological local reports for the years 1991, 1997, 2005, 2011 and 2014. The following criteria were applied when selecting data from historical local reports: a) Similar objectives regarding pollution evaluation and classification, b) similar water quality variables analysed, c) similar standard techniques for water quality sampling and d) similar certified laboratories in Bolivia performed the analyses. The analyses were performed by the CASA (Water and Environmental Sanitation Center) Laboratory, University Major of San Simon, Cochabamba city (1991, 1997, 2017) or by SPECTROLAB, Technical University of Oruro, Oruro city (2005, 2011, 2014).

Sampling in 2017 for this thesis work was carried out in accordance with techniques and methods used in previous studies, in order to maintain consistency throughout the whole dataset. Direct measurements were carried out of pH using a pH meter (ExStik pH100) and of turbidity using a turbidity meter (HI93703), while a field spectrometer (Photometer YSI 9500) was used for measuring nitrate and phosphate concentrations in river water every two weeks. As a complement, streamflow was measured using a Universal Current Meter (OTT 300801 Hydromet).

Data sampled in 2017 were collected from measuring stations located at the outlet of six sub-catchments (Figure 3). The stations were selected based on the underlying conditions that they: (a) were representative of the study area with regard to land use types in the upstream contributing area, (b) covered a higher number of water quality-related variables sampled in former studies and c) applied a higher frequency of sampling (Telci *et al.* 2009; Chilundo *et al.* 2008). The stations were used to divide the catchment into sub-catchments by the hydro-processing method (Maathius & Wang 1998) in ArcMap ver. 10.4, a module of ArcGIS Desktop software (Environmental System Research Institute 2019). Thus, the water flow contribution to each outlet was accumulated from the corresponding upstream sub-catchment.

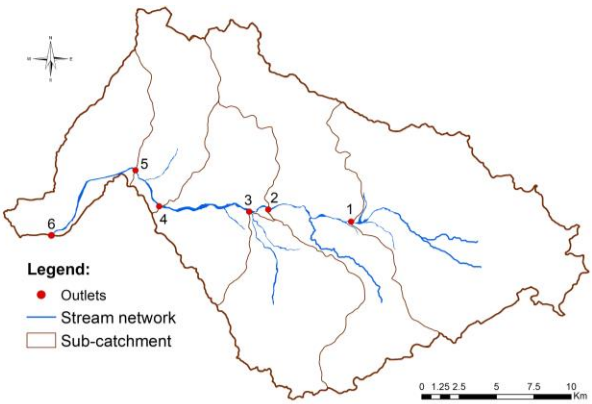


Figure 3. Sub-catchments of the Rocha River catchment and sub-catchment outlets where the six measuring stations were located.

4.3 Land use change analysis

Land use was assessed by image digital classification based on Landsat imagery, downloaded from the United States Geological Survey (USGS; http://glovis.usgs.gov). The Landsat-5 TM (Thematic Mapper) images for 1991, 1997, 2005 and 2011 and Landsat-8 OLI/TIRS (Operational Land Imager/Thermal Infrared Sensor) images for 2014 and 2017 were processed in ArcMap. The images were re-projected (zone 19 in the Southern Hemisphere), the coordinate system (World Geodetic System - WGS 1984) was rectified (Universal Transversal Mercator – UTM) to 1:50,000 scale and then the classification was performed.

A general categorisation was applied to identify land uses present in the study area on field visits. The following land uses were considered:

- Human settlements, made up of civil structures or constructed facilities such as buildings and houses, roads and other artificial areas.
- Cropland, including rain-fed crops (maize, wheat, potato and other native tubers) and irrigated crops (potato, beans, orchard vegetables, alfalfa, oats and barley).
- Forest, composed of several native species (*e.g. kewiña*, *puya*, *molle*, *Alnus*, *Acacia* and *quiswara*) and exotic species (mostly pine and eucalyptus).
- Shrubland, dominated by sclerophyllous bush vegetation including scattered small trees.
- Grassland, semi-natural pastures with grazing by several species (*e.g.* sheep, goats, some cows and llamas in higher parts of the catchment.
- Sparsely vegetated areas, susceptible to erosion and intense runoff due to the lack of vegetation cover.
- Lakes, known as ‘tropical high-altitude mountain lakes’ used for domestic water supply and agriculture.
- Transitional woodland/shrubland zone, consisting of herbaceous vegetation with scattered trees on alluvial fans where groundwater exploitation is carried out to provide a water supply for human settlements.

The Maximum Likelihood classification algorithm included in ArcMap ver. 10.4 was applied in order to obtain the resulting land use classification maps, by calculating the following discriminant functions for each pixel in the Landsat image (Congalton & Green 2019; Richards 2013):

$$g_i(x) = \ln p(w_i) - 1/2 \ln|C_i| - 1/2(x - m_i)^T C_i^{-1}(x - m_i) \quad (1)$$

where i is the number of classes, x is the n-dimensional data (n is the number of bands), ln is the natural logarithm, $p(w_i)$ is the probability that class w_i occurs in the image and is assumed the same for all classes, $|C_i|$ is the covariance matrix in class w_i, T is the threshold if defined, $C_i^{-1}$is the inverse matrix and $m_i$is the mean vector.

Digital image classification accuracy was assessed by comparing the resulting 2017 land use map against ground truth checkpoints (as samples from independent datasets) taken in field work. One hundred (100) site points per land use were obtained by stratified random sampling and verified in the field with a Global Positioning System (GPS) receiver (PROMARK 120). Thereafter, a contingency matrix was calculated to obtain overall accuracy, which indicates the percentage of total pixels in the image that are correctly classified. Producer's and user's accuracy were also computed, where producer's accuracy indicates how well real features on the ground are correctly shown on the classified map and user's accuracy shows whether the class on the map is actually present on the ground (Congalton & Green 2019). In addition, Cohen's Kappa coefficient (*K*) was calculated, to indicate the agreement between two raters who each classify items into mutually exclusive categories, calculated as (Cohen 1960):

$$K = \mathfrak{f}_{(o)} - \mathfrak{f}_{(e)}/1 - \mathfrak{f}_{(e)} \quad (2)$$

where $\mathfrak{f}_{(o)}$ is the observed proportion of agreement and $\mathfrak{f}_{(e)}$ is the proportion of agreement that is expected to occur by chance. Resulting K values are categorised by strength of agreement, defined by: <0.20 = poor, 0.20-0.40 = fair, 0.40-0.60 = moderate, 0.61-0.80 = substantial, and >0.80 = almost perfect agreement (Landis & Koch 1977).

Land use change was detected by post-classification pixel-by-pixel area-based comparison of classified images from different dates, to produce change information summarised in a 'from-to' change detection matrix and thus interpret the changes more efficiently (Congalton & Green 2019; Jensen 2015). The following formula was used:

$$\mathrm{LU}_{Change} = ((LU_{Final}/LU_{Initial})^{(1/\mathrm{n})}) - 1 \quad (3)$$

where LU_{Change} is land use annual growth rate change, LU_{Final} is final land use, $LU_{Initial}$ is initial land use and n is number of years represented in the analysis.

4.4 Water quality evaluation

Water quality indices have been widely used to characterise water quality in terms of environmental impacts, suitability for irrigation and drinking. The WQI approach aggregates different variables characterising the status of water into a single value (Horton 1965). Hence, water quality of a specific source is assessed using physical, chemical and biological variables that can be harmful if their concentrations are outside defined limits.

The National Sanitation Foundation Water Quality Index (NSF-WQI) is a standardised method for classifying and comparing the quality of various water bodies in an attempt to alleviate the subjective element in water quality evaluation. In development of the index, expert judgment was incorporated, calculated as (Brown *et al.* 1970):

$$NSF\text{–}WQI = \sum_{i=1}^{n} q_i w_i \qquad (4)$$

where q_i is the quality class for the nth variable and w_i is the relative weight for the nth variable such that the combined value is 1. This index consists of nine variables, with a weight factor for each corresponding to relative importance in the index calculation (Table 1). The variable values are measured and transferred to a curve chart, where a numerical value of q_i is obtained (Ott 1978).

Table 1. *Weighting values of variables used to determine National Sanitation Foundation Water Quality Index (NSF-WQI).*

Variable	Weight
Dissolved oxygen	0.17
Faecal coliforms	0.16
pH	0.11
Biochemical oxygen demand	0.11
Phosphate	0.10
Nitrate	0.10
Delta temperature	0.10
Turbidity	0.08
Total solids	0.07

The value of NSF-WQI ranges from 0 (heavily polluted water) to 100 (no pollution in water), *i.e.* decreasing water quality is indicated by decreasing NSF-WQI values.

Prati's Implicit Index of Pollution (IPI) is a numerical expression of the degree of pollution that takes into account the various pollutants present at the same time. It increases with degree of pollution and transforms concentrations into level of pollution (Prati *et al.* 1971). For the study area, IPI was modified by Romero *et al.* (1998) based on Rocha River water quality characteristics, focusing on 13 organic pollution variables since there were no heavy industries or intensive agriculture in the catchment at that time. In this thesis, the following variables from among the original 13 were considered: dissolved oxygen, biological oxygen demand (BOD), chemical oxygen demand (COD) and nitrate. The concentrations of the selected variables were transformed into levels of pollution expressed through equations in new units that are proportional to the polluting effect relative to other factors. Then IPI was calculated as the arithmetic mean of the four determinant index (i) scores as:

$$IPI = 1/4 \sum_{i=1}^{4} I_i \qquad (5)$$

where I_i is the degree of pollution in dimensionless units. The equations used for transformation of variable concentrations (Y) into pollution units are presented in Table 2.

Table 2. *Equations used for calculation of Prati's Implicit Index of Pollution (IPI).*

Variable	Units of pollution	Equation
Dissolved oxygen	0-50%	$I_1 = 4.2 - 0.437\left(^{100-Y}/_{5}\right) + 0.042\left(^{100-Y}/_{5}\right)$
	50-100%	$I_1 = 0.08(100 - Y)$
	>100%	$I_1 = 0.08(Y - 100)$
Biological oxygen demand	mg L^{-1}	$I_2 = {}^{Y}/_{1.5}$
Chemical oxygen demand	mg L^{-1}	$I_3 = 0.1Y$
Nitrate	mg L^{-1}	$I_4 = 2^{2.1\log(^{Y}/_{4})}$

The value of IPI ranges from 0 (no polluted water) to >16 (heavily polluted water), *i.e.* decreasing water quality is indicated by increasing IPI values.

The Potential Non-point Pollution Index (PNPI) for diffuse pollution tool proposed by Munafò *et al*. (2005) assesses pollutant dynamics and water quality. Diffuse contamination pressure exerted on water bodies deriving from different land units is expressed in the index as a function of three indicators, land cover indicator (LCI, potential non-point pollution due to land use), runoff indicator (RoI, potential of water to move as surface runoff) and distance indicator (DI, distance to river network) (Figure 4). In this thesis, LCI was calculated from land use information and nitrogen and phosphorus (loads and emissions), a ready-to-use table was used to estimate RoI based on runoff coefficient and DI was calculated by the geodesic straight perpendicular (Euclidean) distance.

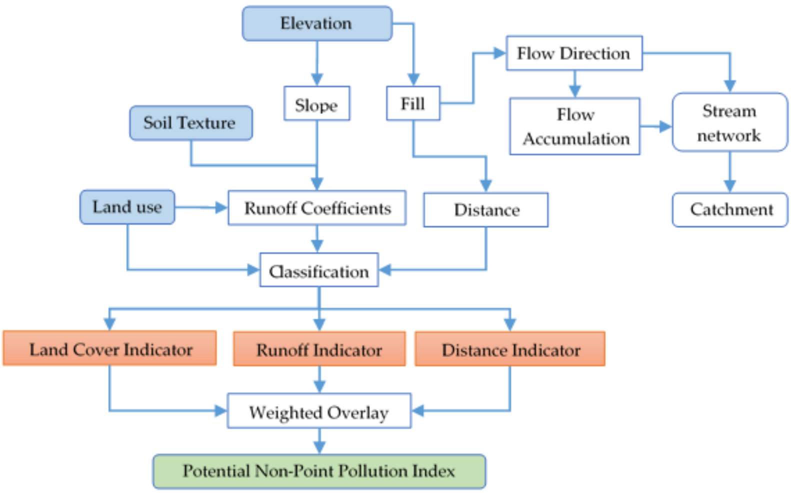


Figure 4. Workflow involved in calculation of Potential Non-point Pollution Index (PNPI).

All indicators were calculated for 1997 and 2017, to assess temporal change. Expert knowledge is incorporated into PNPI to allocate values to each indicator weighting. In this way, potential pollution contribution from different hotspot areas and pollutant mobility are determined by the ability of areas to retain and transport water (Cecchi *et al*. 2009).

Implementation of PNPI was conducted in ArcMap (Figure 4) by the weighted sum tool, to create a PNPI map showing PSAs of pollution. Weighted sum is a multi-criteria analysis tool that provides the ability to weight (by relative importance) and combine multiple inputs (representing multiple indicators) to create an integrated analysis (Fishburn 1970):

$$PNPI = \sum_{i=1}^{k} w_i * \mathrm{x}_i \tag{6}$$

where k is the total number of indicators (= 3), w_i is a coefficient of weights for each indicator and x_i is the corresponding indicator. In the present work, the indicators were weighted based on the rank sum method (Stillwell *et al.* 1981) with values presented by Munafò *et al.* (2005) (Equation (7)). However, values obtained using Equation (8) were also tested, in an attempt to optimise the value with regard to local conditions.

$$PNPI_m = LCI \times 5 + RoI \times 3 + DI \times 2 \tag{7}$$

$$PNPI_c = LCI \times 6 + RoI \times 1 + DI \times 3 \tag{8}$$

4.5 Relationship between land use and water quality

The relationships between water quality index values, *i.e.* NSF-WQI and IPI values, and land uses (percentage area) were explored by correlation analysis, to test whether WQI values were related to upstream land use at catchment level. Accumulated average PNPI values for each sub-catchment were compared against concentration values of nitrate and phosphate as measured water quality variables at the six sub-catchment outlets in 1997 and 2017. The null hypotheses tested was that measured nitrate or phosphate concentration values were not related to PNPI values.

The statistical Mann-Kendall trend test (S for number of samples <9 and Z for number samples >9) was carried out to verify possible trends and their significance for WQI during the period of analysis. Positive values indicated an increasing trend in WQI values, negative values indicated a decreasing trend, and values close to zero indicated no trend. This test was chosen because it is non-parametric (normality not required) and it has low sensitivity to abrupt breaks due to non-homogenous time series (Hirsch *et al.* 1982). Values of Z close to 1 indicate a significant monotonic trend or serial correlation over time. The null hypothesis assumes that values do not show any trend, whereas the alternative hypothesis assumes that there is an increasing or decreasing monotonic trend. The Theil-Sen slope estimator (Q) was used to identify the true slope of linear trends, *i.e.* change per unit magnitude. All statistical analyses were carried out using the R statistical software version 3.6.1 (R Development Core Team 2011).

4.6 Water balance and nutrient transport

The Soil and Water Assessment Tool (SWAT) model was used to assess catchment streamflow, water balance components and nutrient transport. SWAT is a semi-distributed model, capable of continuous simulation over long periods (Neitsch *et al*. 2011), which produces predictions based on physical information: (1) hydrology, (2) soil erosion and sediment transport, (3) nutrient transport and (4) plant growth and management (Gassman *et al*. 2014). The hydrological cycle as simulated by SWAT is based on the water balance equation (Neitsch *et al*. 2011):

$$SW_t = SW_0 + \sum_{i=1}^{t} (R_{day} - Q_{surf} - E_a - W_{seep} - Q_{gw}) \quad (9)$$

where SW_t is the final soil water content, SW_0 is the initial soil water content on day i, t is the time (days), R_{day} is the amount of precipitation on day i, Q_{surf} is the amount of surface runoff on day i, E_a is the amount of evapotranspiration on day i, $Wseep$ is the amount of water entering the vadose zone from the soil profile on day i, and Qgw is the amount of return flow on day i. All units are in mm of H_2O.

Nitrogen- and phosphorus-related processes tracked and modelled by SWAT are described in detail by Neitch *et al.* (2011). These are modelled based on the respective nutrient cycle (Santhi *et al.* 2006; Neitsch *et al.* 2005). Instream nutrient dynamics have been incorporated into SWAT using the kinetic routines from the in-stream Enhance Stream Water Quality Model (QUAL2E) (Brown & Barnwell 1987).

In the first step, catchment delineation was carried out using ArcSWAT 2012 (Olivera *et al*. 2006) based on digital elevation model (DEM) to automatically extract the stream network, delineate the study area and then divide it into sub-catchments. In the next step, Hydrologic Response Units (HRUs) were defined by overlaying land use, soil data and the DEM information transformed into slope classes (Neitsch *et al*. 2005). The model was set up including elevation band to reflect temperature changes and the Hargreaves method was used for potential evapotranspiration (PET) estimation, based on incorporated climate data (1990-2020). In the final step, geodatabase tables were generated (soil, weather, sub-catchment and HRUs among others) to store input values and to run a default simulation.

In order to achieve accurate SWAT simulations, model calibration was performed based on observed streamflow and in-stream total nitrogen and total phosphorus data at the catchment outlet. The Kling-Gupta efficiency (KGE) objective function (Gupta *et al.* 2009) was used to evaluate the accuracy of predictions (Abbaspour *et al.* 2018). KGE is computed as:

$$KGE = 1 - \sqrt{(r-1)^2 + (\alpha - 1)^2 + (\beta - 1)^2} \quad (10)$$

where r is the linear correlation coefficient between observed and simulated records, α is a measure of the variability in the data values (equal to the standard deviation of simulated over the standard deviation of observed), and β is a equal to the mean of simulated over the mean of observed. Optimal performance is indicated by a KGE value equal to 1, while good, satisfactory and poor performance is indicated by a KGE value of 0.7-1, 0.4-0.7 and <0.4, respectively (Brocca *et al*. 2020).

The impacts of land use change and climate variability on hydrological components were evaluated based on the calibrated SWAT model. Inputs such as DEM (elevation), soil maps (soil texture data) and the calibrated SWAT parameters were kept constant, while land use and climate data were changed (Munoth & Goyal 2020; Aboelnour *et al*. 2019; Zhang *et al*. 2017).

Meteorological data from 1990 to 2020 were divided into five periods (1990-1993, 1994-2001, 2002-2008, 2009-2013 and 2014-2020), considering the five available land use maps (from 1991, 1997, 2005, 2011 and 2017).

5. Results and Discussion

5.1 Land use changes 1991-2017

The results from comparisons of land use maps and the corresponding ground truth in 2017 are presented in Table 3. Results from former studies (ERM 2013) helped in definition of classes, as did direct observations (lakes) and researcher experience and knowledge.

Table 3. *Contingency table of supervised land use classification of 2017 versus ground truth images (TWS = transitional woodland-shrubland).*

	Human settlements	**Cropland**	**Forest**	**Shrubland**	**Grassland**	**Sparsely vegetated**	**Lakes**	**TWS**	**User's accuracy (%)**
Human settlements	84	2	1	0	5	2	1	7	82
Cropland	3	82	2	0	14	7	3	0	74
Forest	1	3	87	12	1	0	0	11	76
Shrubland	0	2	8	78	11	7	0	4	71
Grassland	3	4	1	4	67	8	3	6	70
Sparsely vegetated	2	6	1	2	2	74	1	8	77
Lakes	0	0	0	0	0	0	92	0	98
TWS	7	1	0	4	0	2	0	64	82
Producer's accuracy (%)	84	82	85	78	67	74	92	64	

Lakes showed the highest values of producer's and user's accuracy, indicating that this class was relatively accurately classified, while grassland was least accurately classified and in some cases confused with other classes, such as cropland and shrubland. The overall accuracy was 78.5% and calculated *K* was 0.76, indicating substantial agreement of image classifications with field observations.

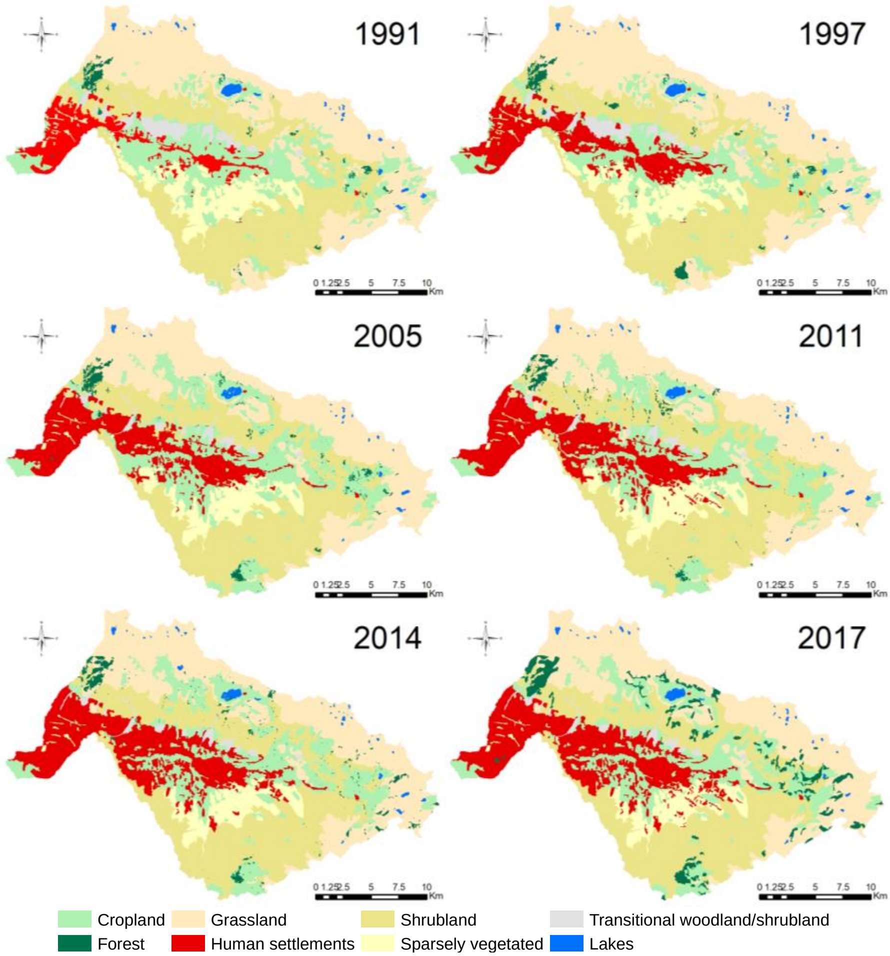


Figure 5. Land use maps of the Rocha River catchment for the years 1991, 1997, 2005, 2011, 2014 and 2017.

Land use geographical distribution maps (Paper I) for the years 1991, 1997, 2005, 2011, 2014 and 2017 are presented in Figure 5, where a clear feature is expansion of human settlement land use (in red). Other increasing land uses were forest and, to a smaller extent, cropland, while grassland and shrubland decreased in area. Sparsely vegetated areas, transitional

woodland/shrubland and lakes remained largely unchanged, with only slight variations. The dominant land uses in the study catchment were grassland and shrubland (both 29% on average), cropland (18% on average) and human settlements (13% on average).
Land use percentage coverage in the catchment in the years 1991, 1997, 2005, 2011, 2014 and 2017 is presented in Figure 6. Human settlement land use expanded most in the period, gradually increasing from 7% in 1991 to 16% in 2017, while grassland and shrubland areas, which declined the most, gradually decreased from 32% and 30%, respectively, in 1991 to 27-28% in 2017. Cropland increased from 16-18% in 1991 to 20% in 2005, and then decreased to 17% in 2017. Forest increased from 1% in 1991 to 3% in 2005, then decreased to 1-2% in 2011-2014 and increased again to 5% in 2017.

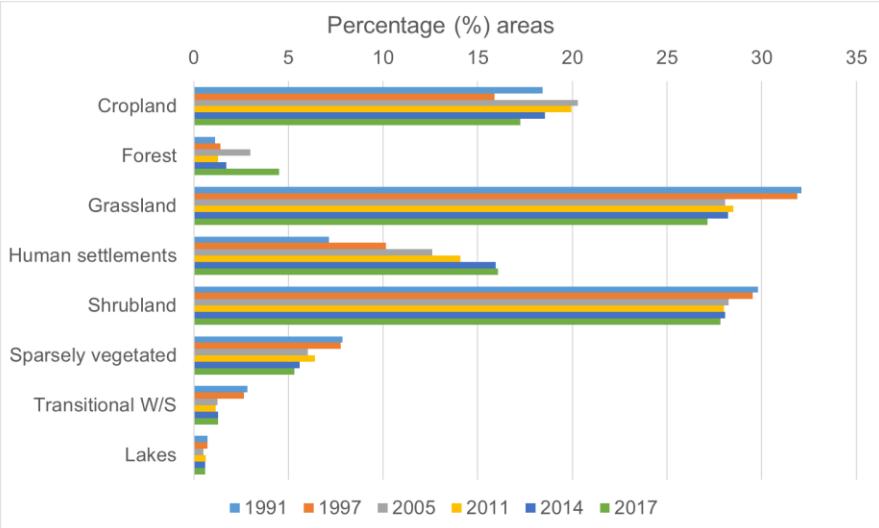


Figure 6. Land use percentage coverage in the Rocha River catchment in the years 1991, 1997, 2005, 2011, 2014 and 2017.

This increase in land conversion to human settlements can be explained by the increase in human population growth and economic activities during the period. According to national census data, population growth rate was 5.6% between 1992 and 2001, 2.8% between 2001 and 2012 and 3.5% between 2012 and 2017 (INE 2013). This has made the catchment the most densely populated in Bolivia, with a population of approximately 1.3 million people.

The annual rate of change in percentage area of the different land uses in the periods 1991-1997, 1997-2005, 2005-2011, 2011-2014, 2014-2017 and

1991-2017 is displayed in Figure 7. Forest showed the highest annual growth rate (38%) in the period 2014-2017, but the lowest (-13.3%) in 2005-2011. Overall, the highest annual rates of positive change were shown by forest and cropland (1997-2005), followed by human settlements (in all periods). In general, transitional woodland/shrubland zones in 1997-2005 (-9%) and sparsely vegetated areas in 1997-2005 (-3.1%) and 2011-2014 (-4.4%) showed important negative annual rates of change in percentage area in the study catchment.

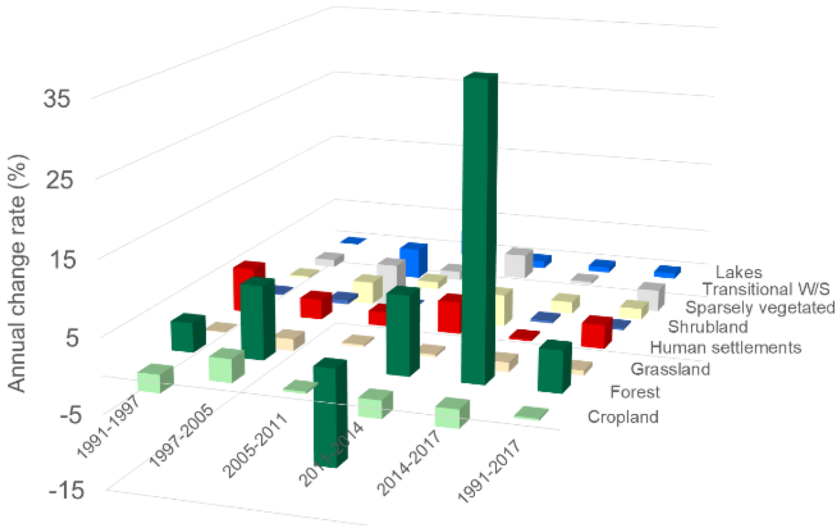


Figure 7. Annual rate of change in percentage area of different land uses in the Rocha River catchment in the periods 1991-1997, 1997-2005, 2005-2011, 2011-2014, 2014-2017, and 1991-2017.

The annual land use change rate calculations provided a synoptic and quantitative view of spatial and temporal changes in land uses in the catchment. Increments seen in forest and cropland reflected government incentives to increase agricultural production (GAMS 2010) and the outcomes of independent afforestation programmes related to catchment management (Weise & Klette 2018; USER 2018; Robledo *et al.* 2003). The increasing process of urban expansion and population growth over time have converted adjacent land uses into human settlements, while at the same time the forested area in the catchment has increased.

Land use change between 1991 and 2017 in a from-to change detection matrix is presented in Table 4. The results revealed that 21% (by area) of the original land uses in 1991 had been transformed or changed by human actions into new land uses in 2017, while 79% had experienced no change. Specific land use changes from 1991 to 2017 into human settlements were: from cropland 5.6%, from shrubland 1.6%, from transitional woodland/shrubland zones 1.1%, from sparsely vegetated areas 1.0% and from grassland 0.1%. In a similar way, grassland (0.9%), sparsely vegetated areas (0.2%), forest (0.2%) and lakes (0.1%) were transformed by human intervention into cropland. The diagonal in Table 4 (in bold) indicates areas with no change between 1991 and 2017, *e.g*. 6.8% of the human settlements in 1991 were identical in 2017. Grassland (26.3%) and shrubland (27.3%) had the highest percentage of unchanged area, while forest (0.7%) and lakes (0.5%) had the lowest.

Table 4. *From-to land use change matrix showing percentage land use areas in the Rocha River catchment between the years 1991 and 2017 (TWS =transitional woodland/shrubland).*

		Land use percentage area 2017							
		Cropland	Forest	Grassland	Human settlement	Shrubland	Sparsely vegetated	TWS	Lakes
Land use percentage area 1991	Cropland	**11.5**	0.2	3.8	5.6	0.2	1.1	0.2	0.1
	Forest	0.2	**0.7**	2.6		1.0			
	Grassland	0.9		**26.3**	0.1				0.2
	Human settlements				**6.8**		1.0	1.1	
	Shrubland		0.1		1.6	**25.3**			
	Sparsely vegetated	0.2			1.0		**4.9**	0.2	
	TWS				1.1			**1.3**	
	Lakes	0.1		0.1					**0.5**

5.2 Water quality assessment

A statistical summary of the complete dataset of water quality variables for all sub-catchment stations (1-6) and years (1991, 1997, 2005, 2011, 2014 and 2017) is presented in Table 5, where permissible values according to USEPA (2017) are included in the far right-hand column for comparison. The variables within/below permissible limits were pH, nitrate, mean and median turbidity, median BOD and median COD medians. However, mean and median DO, faecal coliforms (FC), phosphate, delta temperature, total solids (TS) and mean BOD and COD were outside the permissible limits.

Table 5. *Values of water quality variables (number of samples = 68) measured at stations 1-6 in the Rocha River catchment between 1991 and 2017, compared against permissible limits according to USEPA (2017): dissolved oxygen (DO), faecal coliforms (FC), biological oxygen demand (BOD), chemical oxygen demand (COD), delta temperature (ΔTem.) and total solids (TS).*

Variable	Units	Min.	Mean	Max.	Median	Std. dev.	USEPA (2017)
DO	% Sat.	2.5	33.8	123.0	19.8	30.5	> 50
FC	CFU mL^{-1}	$4.0x10^0$	$3.1x10^6$	$6.3x10^7$	$8.6x10^4$	$9.2x10^6$	1000
pH		6.0	7.7	9.0	7.7	0.6	6–9
BOD	mgO_2 L^{-1}	0.3	56.2	439.7	24.3	93.6	30
COD	mgO_2 L^{-1}	0.5	117.8	659.1	32.1	174.2	60
Phosphate	mg L^{-1}	0.0	13.2	111.0	2.4	19.7	1
Nitrate	mg L^{-1}	0.0	5.2	23.5	1.4	6.5	50
ΔTem.	°C	-6.5	4.2	15.5	3.9	3.9	±3
Turbidity	NTU	2.0	144.0	630.2	93.5	149.4	< 200
TS	mg/L^{-1}	7.5	627.4	2475.2	487.9	579.8	< 100

The average values of water quality variables by station and within years are presented in Table 6. The variables that increased most over time were faecal coliforms, BOD, COD, phosphate, nitrate, turbidity, and TS. Other variables, such as DO, pH and delta temperature, showed decreasing values.

The concentration of most variables generally increased from catchment headwaters to outlet, *i.e*. from station 1 to 6, with the exception of station 5, which had higher values than station 6. The increases were higher at stations 4, 5 and 6 than at stations 1, 2 and 3.

In the correlation matrix (Table 7), significant (p<0.05 and p<0.01) positive relationships were found between most variables. Significant negative relationships were found between DO and all variables except pH and delta temperature. Variables such as pH and delta temperature showed no significant relationship with other variables (Table 7).

Table 6. *Average values of water quality variables at stations 1-6 in the Rocha River catchment in different study years between 1991 and 2017: dissolved oxygen (DO), faecal coliforms (FC), biological oxygen demand (BOD), chemical oxygen demand (COD), delta temperature (ΔTem.) and total solids (TS).*

	DO	**FC**	**pH**	**BOD**	**COD**	**Phosphate**	**Nitrate**	**ΔTem.**	**Turbidity**	**TS**
Year										
1991	72.5	$4.9x10^5$	8.0	11.3	44.1	1.9	0.1	5.5	57.2	504.1
1997	44.0	$7.4x10^5$	7.2	14.3	52.7	3.1	2.3	3.8	118.7	460.0
2005	41.0	$3.9x10^6$	7.9	28.1	11.1	1.1	8.2	5.7	74.1	240.9
2011	31.0	$1.5x10^6$	7.9	65.1	110.3	4.4	26.0	3.8	164.8	561.2
2014	14.2	$9.0x10^5$	7.8	117.4	208.0	11.9	24.9	2.2	136.8	935.3
2017	11.2	$1.1x10^7$	7.7	108.2	282.1	9.0	19.0	4.5	276.4	1098.5
Station										
1	67.9	$9.9x10^3$	7.9	5.4	3.8	0.8	0.1	4.6	37.2	271.2
2	39.0	$1.0x10^6$	7.4	12.4	10.8	2.0	2.7	6.4	46.1	584.6
3	21.3	$2.8x10^6$	8.1	11.9	23.2	3.9	10.4	1.9	126.3	464.9
4	30.4	$8.3x10^6$	7.3	25.1	157.2	5.6	19.7	3.5	228.1	695.6
5	23.5	$2.2x10^6$	7.8	167.5	235.0	8.7	25.1	4.6	167.3	832.4
6	24.1	$2.8x10^6$	7.8	96.9	218.9	8.9	16.1	3.8	214.7	800.8

Table 7. *Correlation coefficient matrix of water quality variables in all samples: dissolved oxygen (DO), faecal coliforms (FC), biological oxygen demand (BOD), chemical oxygen demand (COD), delta temperature (ΔTem.) and total solids (TS).*

	DO	**FC**	**pH**	**BOD**	**COD**	**Phosphate**	**Nitrate**	**ΔTem.**	**Turbidity**	**TS**
DO	1	-0.37*	-0.01	-0.43**	-0.52**	-0.61**	-0.57**	-0.05	-0.44*	-0.36*
FC		1	-0.03	0.52**	0.53**	0.57**	0.41**	0.06	0.54**	0.43**
pH			1	0.03	-0.01	-0.03	-0.15	-0.03	0.02	0.08
BOD				1	0.80**	0.64**	0.65**	-0.04	0.54**	0.56**
COD					1	0.56**	0.74**	-0.02	0.62**	0.68**
Phosphate						1	0.50**	0.04	0.67**	0.43**
Nitrate							1	0.05	0.52**	0.71**
ΔTem.								1	0.08	0.02
Turbidity									1	0.62**
TS										1

*Significant at $p<0.05$, **Significant at $p<0.01$.

5.2.1 National Sanitation Foundation Water Quality Index

The NSF-WQI values obtained (Paper I) are summarised in Figure 8. Water quality was acceptable (green bars) in river headwaters at station 1 from 1991 to 2014 and at station 2 in 1991, whereas it was slightly polluted (yellow bars) at station 3 and 4 and polluted (orange bars) at stations 3 to 6 until 2005. In 2011, station 6 had heavily polluted water (black bars) which continued until 2017 and included stations 4 and 5 from 2014.

Trend analysis of variations in long-term NSF-WQI over time showed significant ($p<0.05$) decreasing trends (Z=-2.44; Q=-0.7), indicating decreasing water quality from 1991 to 2017 (Figure 8). NSF-WQI also showed a significant ($p<0.001$) decreasing trend (Z=-5.14; Q=-1.3) from station 1 to 6 (Figure 8). The trends indicated water being increasingly polluted over time and from headwaters down to the outlet.

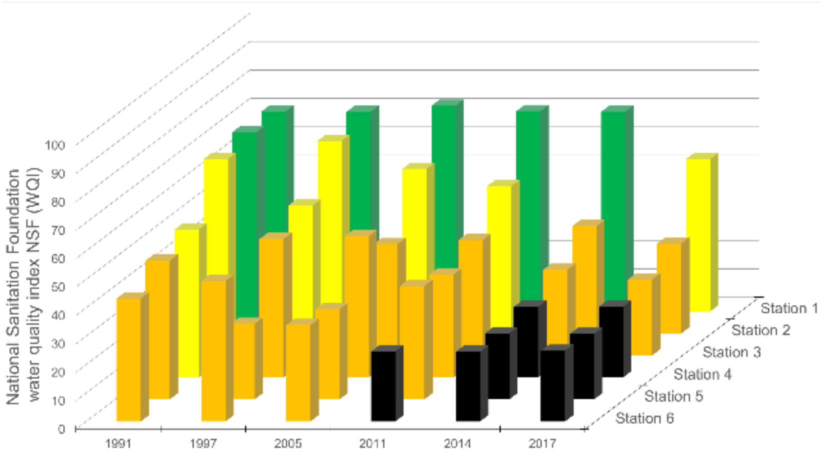


Figure 8. Change in National Sanitation Foundation Water Quality (NSF-WQI) values in the Rocha River over time and by station.

5.2.2 Prati's Implicit Index of Pollution

The IPI values obtained (Paper I) are summarised in Figure 9. Based on the values, river water was not polluted (blue bars) at stations 1 to 3 (headwaters) in 1991, whereas it gradually became slightly polluted (yellow bars) and polluted (orange bars) from 1991 to 2014, and at stations 2-3 even became very polluted (red bars) in 2017. River water at stations 4 to 6 was slightly to very polluted in 1991 but gradually became heavily polluted (black bars), at stations 5 and 6 from 2011 and at station 4 from 2014.

Trend analysis of variations in the long-term IPI over time showed significant (p<0.001) increasing trends (Z=0.3; Q=0.47), indicating decreasing water quality from 1991 to 2017 (Figure 9). The IPI values also showed a significant (p<0.001) increasing trend (Z=6.0; Q=0.55) from stations 1 to 6, indicating decreasing water quality from headwaters to outlet.

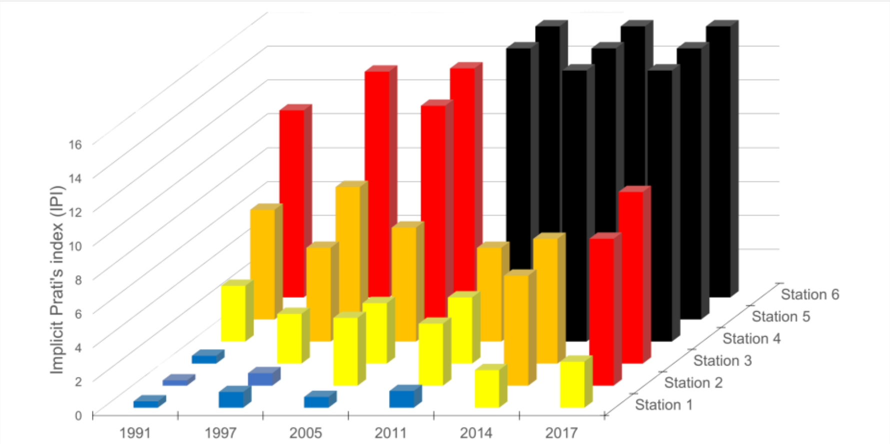


Figure 9. Change in Priti's Implicit Index of Pollution (IPI) values in the Rocha River over time and by station.

The trends in NSF-WQI and IPI confirmed that Rocha River water became increasingly polluted from 1991 to 2017 and from station 1 to 6 (headwaters down to the catchment outlet). Samples considered in WQI calculation usually correspond to the dry season, and thus the effect of elements (nutrients or pollutants) can be considered to be at its maximum.

Differences arising between the NSF-WQI and IPI values (Figures 8 and Figure 9), and their respective translation into pollution load, were partly caused by the different numbers of variables included in NSF-WQI (nine variables) and IPI (four variables), the inclusion of COD in IPI (lacking in NFS-WQI), and its organic pollution orientation (Romero *et al.* 1998). Other contributing factors were differences between weighting rank values in NSF-WQI (Table 1) and pollution unit transformation equations used in IPI (Table 2). However, both indices showed significant temporal and spatial variability from upstream sub-catchments all the way down to the outlet of the Rocha River catchment.

The increasing pollutant load gradient from upstream (station 1) to downstream at the catchment outlet (station 6) in the study period, with clear increments in COD and BOD values, was most probably related to sewage water. The low DO values found were related to organic matter abundance, as verified during field work in 2017 and as stated in previous local reports (CGE 2011; PDC 2005) and studies (Romero *et al.* 1998).

Water quality deterioration in the catchment (decreasing NSF-WQI and increasing IPI) in the study period was most likely caused by industrial spills, illegal wastewater discharge, construction waste and phosphate in detergents, as found in other studies (Shi *et al.* 2019; Carstens *et al.* 2019). Moreover, deficiencies in sanitation can lead to discharge from septic tanks and leaking sewers directly into the riverbed.

5.2.3 Potential Non-point Pollution Index

The geographical distribution in 1997 and 2017 of the land cover indicator (LCI) used (Paper II) in calculation of PNPI is presented in Figure 10. In that diagram, areas with higher LCI values (above 0.6) correspond to high-density (>70 persons per ha) human settlements around the main Rocha river reaches in the lower catchment and lower LCI values (below 0.4) correspond to grassland and shrubland present at higher elevations. The higher LCI values around human settlements are most likely related to the inefficient sewerage systems and water treatment plants in and around the cities of Sacaba and Cochabamba, since only a small proportion of the sewage generated is treated (Trohanis *et al.* 2015). The association between higher LCI values and denser human settlements has been used in previous evaluations (Cecchi *et al.* 2007; Ciambella *et al.* 2005; Munafò *et al.* 2005).

The eight general land uses considered (see Figure 5) were based on integration of contextual information related to pollution potential generation (*e.g.* fertiliser inputs, management, pollutant or nutrient load and export) for each land use weighting procedure, as done in previous studies (Wu *et al.* 2019; Zhang & Huang 2011; Wesström & Joel 2010). A greater number of classes can be used, supported by expert knowledge weighting (Cecchi *et al.* 2007), when information is available.

Land use weighting was based on nitrogen and phosphorus loads, as they are the most studied indicators directly related to non-point pollution (Shen *et al.* 2011; Chesters & Schierow 1985). For this purpose, the well-known dynamics between nitrogen and phosphorus (Jacbos *et al.* 2018; Van Drecht *et al.* 2009), and information from the literature (Cecchi *et al.* 2007) were adapted to local conditions and combined on a GIS interface to obtain LCI (Figure 10). However, difficulties arose during land use characterisation regarding pollution potential, estimation of pollution emission/generation, sewage and solid waste assessment and quantifying effects of surface runoff variation.

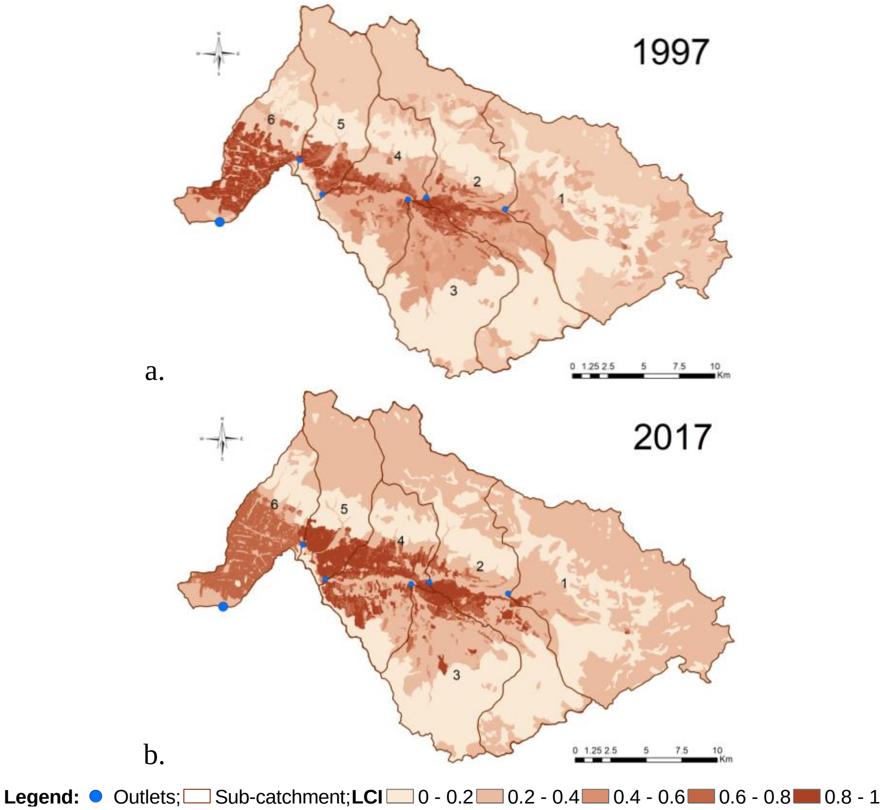


Figure 10. Land cover indicator (LCI) values for the Rocha River catchment in (a) 1997 and (b) 2017.

The distribution in 1997 and 2017 of the runoff coefficient (RoI) used (Paper II) in calculation of PNPI is presented in Figure 11, where higher RoI values (>0.6) correspond to the interactions of hard surfaces with slope >10% and with clay and silt soil texture (low water permeability). On the other end of the scale, lower values (<0.4) correspond mostly to forest, shrubland/grassland (semi-natural vegetation covers) and cropland, interacting with >45% sand soil texture (high water permeability rates) and slope <5%. RoI was determined through GIS and remote sensing, which are adequate techniques when dealing with data-scarce regions in large-scale analyses (Gebresellassie 2017; Rawat & Singh 2017).

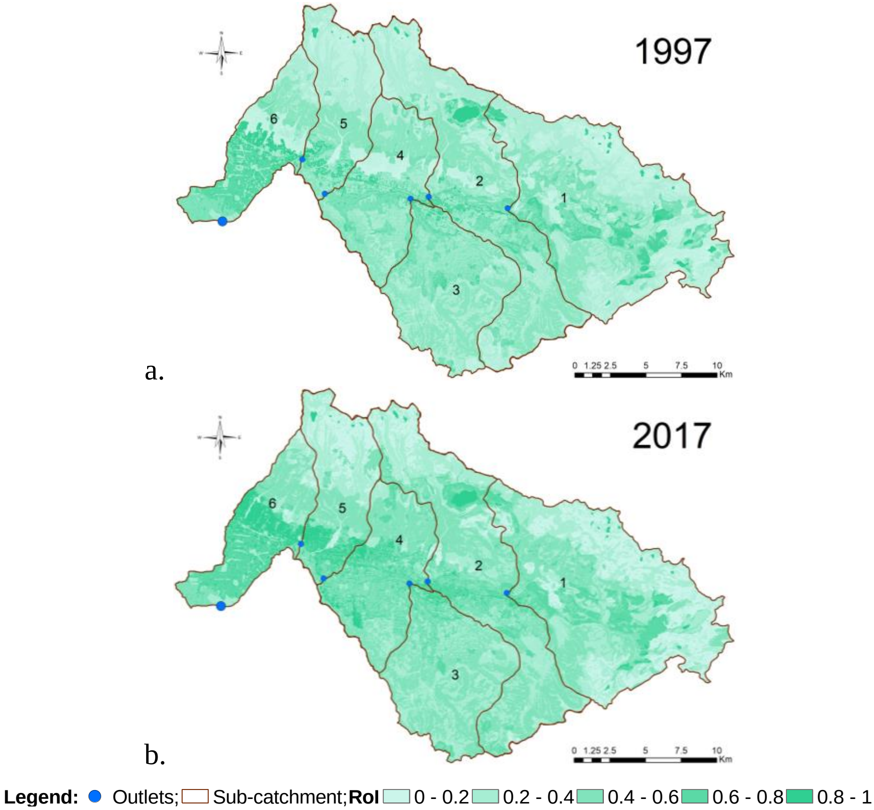


Figure 11. Runoff indicator (RoI) values for the Rocha River catchment in (a) 1997 and (b) 2017.

The movement of pollutants from land surfaces to the Rocha River stream network is controlled by surface runoff due to topography, soil characteristics and rainfall pattern. The main source of recharge for river streamflow is precipitation, but illegal domestic sewage water and industrial spills to the river act as additional sources and can be considered the only inputs during dry periods. Higher amounts of precipitation in the rainy season can contribute to increased surface runoff and pollutant wash-off from adjacent areas to the main river (Ochoa-Tocachi *et al.* 2016). On the other hand, lower precipitation in the dry season can contribute to pollutant concentrations impairing water quality (De Oliveira *et al.* 2017; Zhu *et al.* 2015).

The distribution (1997 and 2017) of the distance indicator (DI) values (Paper II) used in calculation of PNPI are shown in Figure 12. Areas with the highest DI values (>0.8) in Figure 12 correspond to areas with numerous river network tributaries (distance <520 m) located on steep slopes, while the lowest values (<0.2) correspond to a few river tributaries (distance >2166 m) on gentle slopes. Modelling of DI reflected the fact that about 70% of the study catchment consisted of mountainous terrain and 30% of fluvial plains. A previous study in a region with fewer mountainous areas (33%) and more fluvial plains (67%) also found high DI values for a dense stream network along major river tributaries (Zhang & Huang, 2011). Thus, high DI values mainly depend on the density of the river stream network (large number of tributaries) and high runoff in mountainous topography. Similar findings have been made by Wu and Lu (2019), who assigned higher DI values to shorter distances to the river network, and lower values for longer distances.

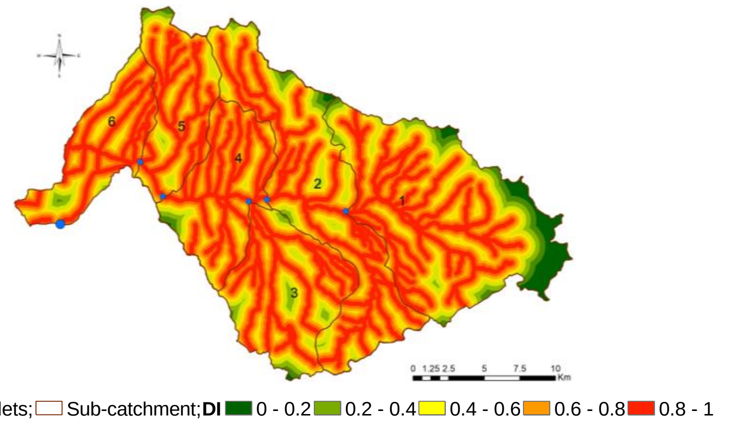


Figure 12. Distance indicator (DI) values in the Rocha River catchment (both 1997 and 2017).

The distributions of PNPI resulting (Paper II) from Equation (7) ($PNPI_m$ = LCI × 5 + RoI × 3 + DI × 2) and Equation (8) ($PNPI_c$ = LCI × 6 + RoI × 1 + DI × 3) are presented in Figure 13, where areas with higher PNPI values (>0.6) correspond to higher population densities (>120 persons/ha), higher pollutant mobility and shorter distances to river network. Areas with lower

PNPI (<0.4) correspond to semi-natural land uses (forest, shrubland, grassland and lakes), lower pollutant mobility and longer distance to river. The cities of Sacaba and Cochabamba are located in areas with higher PNPI values (>0.6), while lower values (<0.4) surround the central part towards the edges of the catchment (except the western part) (Figure 13).

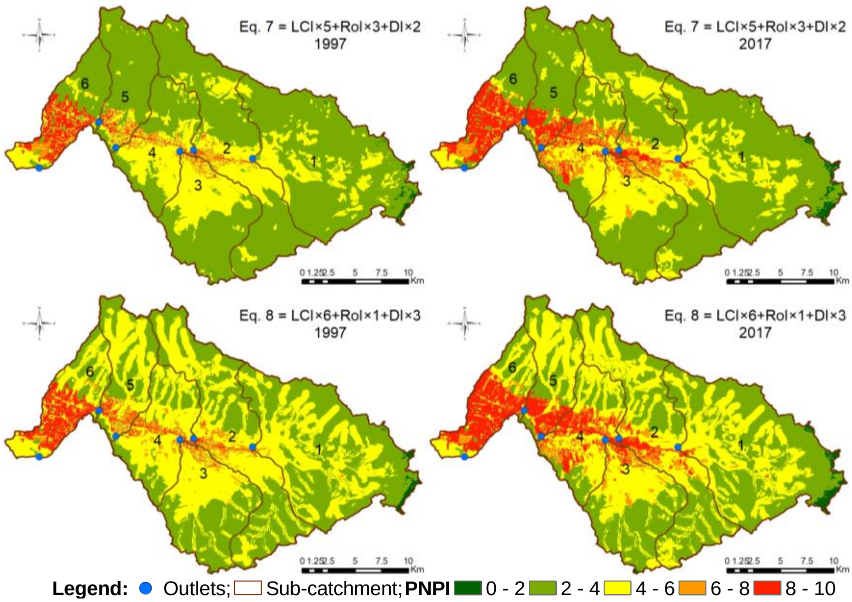


Figure 13. Spatial distribution of Potential Non-point Pollution Index (PNPI) classes in the Rocha River catchment in 1997 and 2017, calculated based on Equations (7) and (8).

As can be seen in Table 8, the catchment area was dominated by the PNPI 2-4 and 4-6 classes, representing 85-95% of the catchment between 1997 and 2017 (the former decreasing and the latter increasing with time) (Paper II). The lowest PNPI class (0-2) occupied less than 1% of catchment area throughout, and the highest (8-10) class occupied less than 2% in 1997, but this increased to 6% in 2017.

The weighted sum integrated in ArcGIS 10.4 improved PNPI calculation compared with previous studies using map algebra integration of LCI, RoI and DI (Puccinelli *et al.* 2012; Munafò *et al.* 2005; Li & Yeh 2004). Indicator weights differed between Equations (7) and (8) based on relative importance of the indicators in generation of potential pollution, but LCI was identified as the most important indicator, as proposed by Munafò *et al.* (2005).

Table 8. *Percentage of Rocha River catchment area occupied by different Potential Non-point Pollution Index (PNPI) classes in 1991 and 2017, calculated based on Equations (7) and (8) (CI = land cover indicator, RoI = runoff coefficient, DI = distance indicator).*

PNPI class	**Eq. (7): LCI×5+RoI×3+DI×2**		**Eq. (8): LCI×6+RoI×1+DI×3**	
	1997	2017	1997	2017
0-2	1%	1%	1%	1%
2-4	66%	61%	46%	44%
4-6	27%	25%	46%	41%
6-8	4%	9%	5%	8%
8-10	2%	4%	2%	6%

The weighted sum integrated in ArcGIS 10.4 improved PNPI calculation compared with previous studies using map algebra integration of LCI, RoI and DI (Puccinelli *et al.* 2012; Munafò *et al.* 2005; Li & Yeh 2004). Indicator weights differed between Equations (7) and (8) based on relative importance of the indicators in generation of potential pollution, but LCI was identified as the most important indicator, as proposed by Munafò *et al.* (2005).

The higher PNPI values obtained were related to higher potential pollution generation explained by lacking or ineffective sewage systems in human settlements, in agreement with Trohanis *et al*. (2015). Solid waste generation and inadequate disposal, soil erosion and surface runoff in sensitive areas (waste disposal sites, septic system failures and construction sites) were other contributing factors. Similar results have been reported by Puccinelli *et al*. (2012), Cecchi *et al*. (2007) and Munafò *et al*. (2005). In contrast, Wesström and Joel (2010) found that urban areas in a highly developed country (Sweden) were associated with lower PNPI values, since all urban water discharges were properly treated, and higher PNPI values were related rather to intensive cropping systems in agriculture.

The PNPI values obtained were aggregated into micro-catchments (Figure 14) to identify PSAs that could be utilised as decision support for recommendations on appropriate management measures to reduce pollution potential in different parts of the catchment.

A proper representation of landscape features (land use, runoff and distance to stream network) at multiple levels (catchment, sub-catchment, micro-catchment) for the indicators LCI, RoI and DI can be considered advantageous when calculating PNPI and subsequently identifying PSAs. It is also possible to use PNPI analysis in limited or data-scarce regions due to its simple, effective and less time- and resource-demanding approach (Munafò *et al.* 2005). Future studies should examine how landscape features and detailed hydrological, chemical and geographical processes interact in PSA prediction with scarce data. For example, local landscape patterns and rainstorm-driven events in parts of the year can be considered to reduce non-point pollution, by capturing runoff in some areas (Lu & Wu 2019). Wetland areas can act as sinks and/or sources of sediments and pollutants in surface runoff, allowing these to settle and become trapped and later remobilised (Walega & Wachulec 2018; Wang *et al.* 2016).

All three water quality indicators tested (NSF-WQI, IPI, PNPI) were confirmed in Papers I and II to be useful tools for assessing spatial and temporal changes in river water quality. These indices provide quantifiable values of the degree of pollution and they combine information on several variables into a single value (Debels *et al.* 2005).

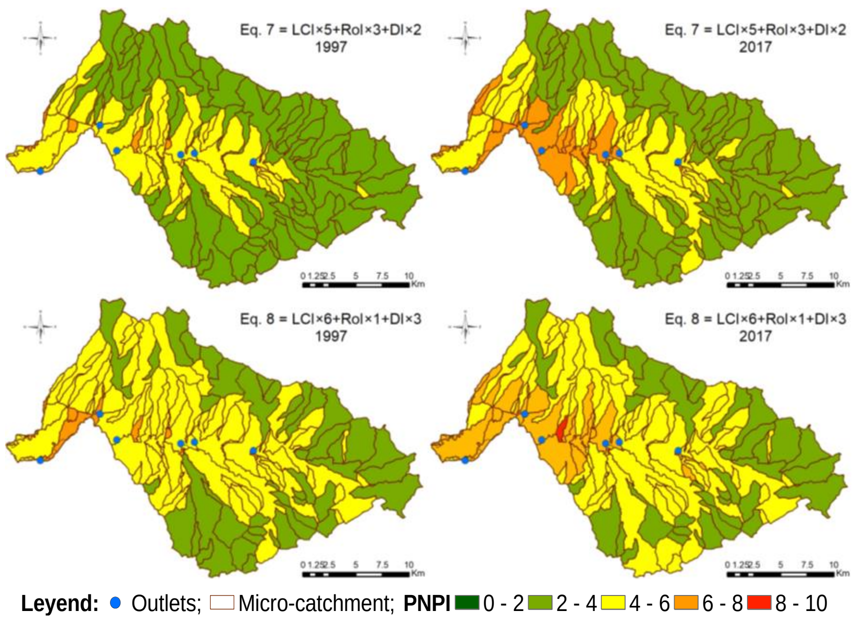


Figure 14. Spatial distribution of Potential Non-point Pollution Index (PNPI) classes at micro-catchment level in the Rocha River catchment in 1997 and 2017, calculated based on Equations (7) and (8).

This allows the general status of water to be evaluated, classified and compared (bringing data from several studies into one database to track changes), irrespective of period (Kannel *et al.* 2007; Giri & Qui 2006).

5.3 Relationship between land use and water quality

The relationships between the NSF-WQI and IPI values and the percentage area of different land uses in the catchment (Paper I) are shown in Table 9. Significant ($p<0.001$) negative relationships (i.e. deteriorating water quality) were found between NSF-WQI and human settlement area, and corresponding significant ($p<0.001$) positive relationships (deteriorating water quality) between IPI and human settlement area. However, significant negative relationships (improved water quality) were found between IPI and sparsely vegetated areas ($p<0.001$), IPI and cropland ($p<0.05$), IPI and shrubland ($p<0.05$), and IPI and transitional woodland/shrubland ($p<0.05$). Finally, a significant ($p<0.05$) positive relationship (improved water quality) was observed between NSF-WQI and cropland.

Table 9. *Correlation coefficient (Spearman's rho) for relationships between water quality indices (NSF-WQI and IPI) for stations 1-6 and land use (% of sub-catchment areas) 1991-2017.*

Land use	**National Sanitation Foundation Water Quality Index (NSF-WQI)**		**Prati's Implicit Index of Pollution (IPI)**	
	rho	*p-value*	*rho*	*p-value*
Cropland	*0.39*	*0.016**	***-0.44***	***0.006****
Forest	0.05	0.974	0.16	0.343
Grassland	0.25	0.133	-0.11	0.533
Human settlements	***-0.72***	***0.001*****	***0.89***	***0.001*****
Shrubland	0.18	0.283	*-0.49*	***0.001*****
Sparsely vegetated	0.24	0.153	***-0.53***	***0.001*****
Transitional W/S	-0.22	0.195	*-0.36*	*0.031**

**Significant at $p<0.001$, *significant at $p<0.05$.

The stations, and their related sub-catchments, were a source of variation in WQI values, as they varied in land use proportions and change during the study period. Human settlements were positively related to water quality decline, as found in previous studies (Souza *et al.* 2019; Carstens *et al.* 2019;

Chu *et al*. 2013; Haidary *et al.* 2013). Thus, urbanisation, increasing population and lack of sanitation are the major threats to water quality in the study catchment, due to the lack of adequate public policies for water management (Shi *et al.* 2019).

The relationships between the PNPI values obtained with Equations (7) and (8) in 1997 and 2017 and nitrate and phosphate concentrations measured in the six sub-catchments (Paper II) are shown in Table 10. The results revealed significant (p<0.05) relationships between phosphate in 2017 according to both equations.

The nitrate and phosphate concentrations (used for validation) within sub-catchments increased due to (i) sewage water discharge (houses, industries and other economic activities), (ii) runoff from fertilised land and (iii) surface runoff from hard surfaces in human settlements. The significant correlations (p<0.05) found for phosphate (Table 10) can be explained by better stability and higher concentrations compared with nitrate. Similar results were found in a previous study where low water quality status was compared against nitrogen loss potential (Zhang & Huang, 2011).

Table 10. *Coefficient of correlation (Pearson's r) between Potential Non-point Pollution Index (PNPI) and measured mean nitrate and phosphate concentrations (n=3 in 1997, n=2 in 2017) at the outlet of the six Rocha River sub-catchments in 1997 and 2017.*

PNPI equation		**1997**				**2017**			
		Nitrate		Phosphate		Nitrate		Phosphate	
		r	*p*-value	*r*	*p*-value	*r*	*p*-value	*r*	*p*-value
(7)	LCI×5+RoI×3+DI*2	0.44	0.385	0.12	0.820	0.50	0.317	0.85	0.034*
(8)	LCI×6+RoI×1+DI×3	0.52	0.290	0.18	0.735	0.51	0.306	0.85	0.034*

*Significant at p<0.05.

It is possible to improve validation results by collecting samples in different periods of the year, to better represent the effects of hydrological regime and human settlement dynamics (de Souza *et al.*, 2019). An alternative to improve the correlation between PNPI and nitrate and that between PNPI and phosphate used for PNPI model validation could be to compare PNPI results with outputs from physically based models (Munafò *et al.*, 2005). However, this will increase the requirements on the data (collection, quality evaluation, time and technical skills), hampering the use of PNPI for identification of PSAs using multi-criteria analysis and GIS implementation and representation in data-scarce regions.

5.4 Streamflow and nutrient simulationLorem ipsum

5.4.1 SWAT model calibration and performance

The 18 most influential parameters in streamflow simulations, as identified by sensitivity analysis (Paper III), are presented in Table 11. The parameters are ranked in order of their sensitivity and include the calibrated values in SWAT-CUP by the SUFI-2 algorithm for the Rocha River catchment.

Table 11. *Sensitivity ranking of influential Rocha River streamflow parameters and their calibrated values.*

Rank	Parameter	Meaning	Value
1	CN2	SCS runoff curve number	-0.34[r]
2	ESCO	Soil evaporation compensation factor	0.30[v]
3	EPCO	Plant uptake compensation factor	0.67[r]
4	GWQMN	Threshold depth of water in shallow aquifer for percolation to occur	505[a]
5	GW_REVAP	Groundwater “revap” coefficient	0.03[v]
6	RCHRG_DP	Deep aquifer percolation fraction	0.28[a]
7	SOL_AWC	Available water capacity of the soil layer	0.45[r]
8	SOL_K	Saturated hydraulic conductivity	-0.21[r]
9	SLSUBBSN	Average slope length	0.36[r]
10	HRU_SLP	Average slope steepness	-0.38[r]
11	CANMX	Maximum canopy storage	18.65[v]
12	GW_DELAY	Groundwater delay	43.95[v]
13	ALPHA_BF	Baseflow alpha factor	0.14[v]
14	REVAPMN	Threshold depth of water in the shallow aquifer for "revap" to occur	199.50[v]
15	LAT_TTIME	Lateral flow travel time	45.02[v]
16	SHALLST	Initial depth of water in the shallow aquifer	-623.94[a]
17	SOL_Z	Depth from soil surface to bottom of layer	0.47[r]
18	SURLAG	Surface runoff lag time	21.70[v]

“revap” is the water in the shallow aquifer returning to the root zone. [r]Multiply value, [v]replace value, [a]add value in ArcSWAT.

The parameters in Table 11 are similar to those found in previous studies for arid and semi-arid catchments in which, as in the Rocha River catchment, CN2, ESCO and EPCO were the most sensitive parameters (Santhi *et al.* 2006; White & Chaubey 2006; Jha *et al.* 2004). Groundwater parameters (GWQMN, GW_REVAP, RCHRG_DP, GW_DELAY, ALPHA_BF, REVAPMN and SHALLST) were also identified as important model parameters. Adequate simulation of hydrology is the first step toward realistic prediction of nutrient transport (Moriasi *et al*. 2015; Chahinian *et al.* 2011; Van Griensven *et al.* 2006; Santhi *et al.* 2006).

The nutrient simulation in ArcSWAT was influenced by seven parameters relating to total nitrogen and total phosphorus, for which the sensitivity ranking is shown in Table 12. These parameters were related to general catchment characteristics, hydrological response unit characteristics, stream water quality, soil information and soil chemical data.

Table 12. *Sensitivity ranking of influential total nitrogen and total phosphorus parameters and their calibrated values.*

Rank	**Parameter**	**Meaning**	**Value**
Total nitrogen parameters			
1	NPERCO	Nitrogen percolation coefficient	-0.98[r]
2	N_UPDIS	Nitrogen uptake distribution parameter	0.34[r]
3	BC3	Rate constant for hydrolysis of organic N to NH4 in the reach	-0.98[r]
4	SHALLST_N	Concentration of nitrate in groundwater contribution to streamflow	0.34[r]
5	RS4	Rate coefficient for organic N settling in the reach	0.66[r]
6	SOL_NO_3	Initial NO_3 concentration in the soil layer	0.18[r]
7	USLE_K	USLE equation soil erodibility (K) factor	-0.98[r]
Total phosphorus parameters			
1	SOL_ORGP	Initial organic phosphorus concentration	4.43[v]
2	ERORGP	Organic P enrichment ratio	0.07[v]
3	P_UPDIS	Phosphorus uptake distribution parameter	-0.79[r]
4	PHOSKD	Phosphorus soil partitioning coefficient	-0.47[r]
5	PERCOP	Pesticide percolation coefficient	0.51[r]
6	PPERCO	Phosphorus percolation coefficient	14.45[v]
7	PSP	Phosphorus sorption coefficient	0.53[r]

[r]Multiply value, [v]replace value, [a]add value in ArcSWAT.

Total nitrogen parameters (Table 12) were found to be related to general catchment characteristics (N_UPDIS and NPERCO), stream water quality (RS4 and BS3), soil information (USLE_K), groundwater flow (SHALLST_N) and soil chemical data (SOL_K). Total phosphorus simulations were influenced by general catchment characteristics (PERCOP, PHOSKD, PSP, P_UPDIS and PPERCO), HRU characteristics (ERORGP) and soil chemical data (SOL_ORGP) (Table 12) (Moriasi *et al*. 2015; Chahinian *et al.* 2011; Santhi *et al.* 2006).

The performance of the SWAT model, assessed using KGE (in Paper III), in simulating streamflow, total nitrogen and total phosphorus on a monthly basis is shown in Table 13. The KGE values obtained in model calibration and validation were compared against performance evaluation criteria for watershed- and field-scale models recommended by Moriasi *et al*. (2015).

Table 13. *Kling-Gupta efficiency (KGE) values obtained in SWAT model calibration and validation.*

Variable	Calibration	Validation	Performance*	
Streamflow	0.77	0.71	0.7-1	Good
Total nitrogen	0.31	0.33	<0.4	Poor
Total phosphorus	0.53	0.61	0.4-0.7	Satisfactory

*Rating according to Brocca *et al.* (2020).

The SWAT model results based on comparison of observed and simulated values (Table 13) suggested that SWAT can reproduce streamflow good (Figure 15), satisfactory total phosphorus (Figure 17) and total nitrogen poor (Figure 16*)* in the Rocha River catchment.

The results of SWAT modelling for monthly streamflow at Puente Cajón station (catchment outlet) are shown in Figure 15, where temporal variations in calibration and validation periods are indicated. These gaps in the observed values were caused by malfunction and dropouts of the automatic sampler and no comparisons were possible for those occasions. In general, the fit of the model was good, but underestimations of streamflow were obtained when low or no rainfall occurred (*e.g*. May 2017, August and April-September 2019). Some over- or underestimations were obtained at intense rainfall events (*e.g*. January-February 2018, 2019 and 2020), corresponding to a well-plotted peak.

For arid and semi-arid catchments, generally characterised by ephemeral streams, underestimation of major peak rain-rainfall events in SWAT modelling has been reported previously (Chen *et al.*, 2017; Lam *et al.*, 2012; Ouessar *et al.*, 2009). This could be explained by the nature and design of the SWAT model, which works in continuous (daily, monthly or yearly) time steps. Rainfall patterns regarding intensity and duration can affect SWAT model simulation (see *e.g*. the differences between observed and simulated values in March and July 2018 in Figure 15), since rainfall events in the

Rocha River catchment are mainly composed of high-intensity, short-duration summer thunderstorms. Similar discrepancies have been reported in previous studies assessing arid and semi-arid catchments (Mengistu *et al.*, 2019; Pulighe *et al.*, 2019; Nie *et al.*, 2011). The limited study period (2014-2020) applied in SWAT modelling in this thesis encompassed natural variability in rainfall and streamflow, but no extended dry or wet periods could be identified. This may explain the poorer performance during the validation period compared with the calibration period, as also found in previous studies (Merriman *et al.*, 2018; Ozcan *et al.*, 2017; Romagnoli *et al.*, 2017).

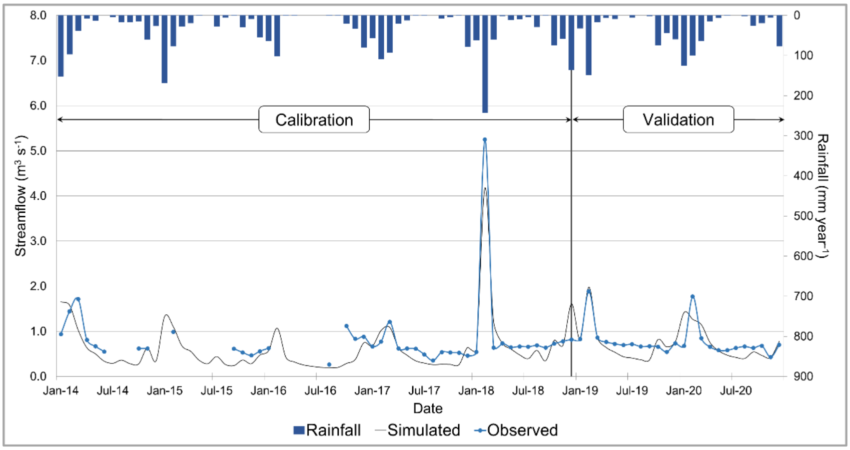


Figure 15. Comparison of observed and SWAT-simulated monthly streamflow and rainfall (2014-2018 calibration, 2019-2020 validation) in the Rocha River catchment.

The poor ability of the SWAT model to predict total nitrogen peaks and recession curves can be seen in Figure 16. A tendency to slightly underestimate the measured values can be seen for most of the simulations, whereas at the peaks in March 2015 and October 2016 total nitrogen seemed to be overestimated (Figure 16).

Nitrogen compounds are in general unstable and easily transform into several components (*e.g.* nitrite (NO_2-), nitrate (NO_3-) and ammonium (NH_4^+) and can be exported from catchments by surface runoff and evaporation by denitrification (N_2O and N_2 gas) (Chahinian *et al.* 2011; Santhi *et al.* 2006; Neitch *et al.* 2005). Uncontrolled discharges to the river may have been the cause of the unsatisfactory model performance in calibration and validation, as may lack of available data.

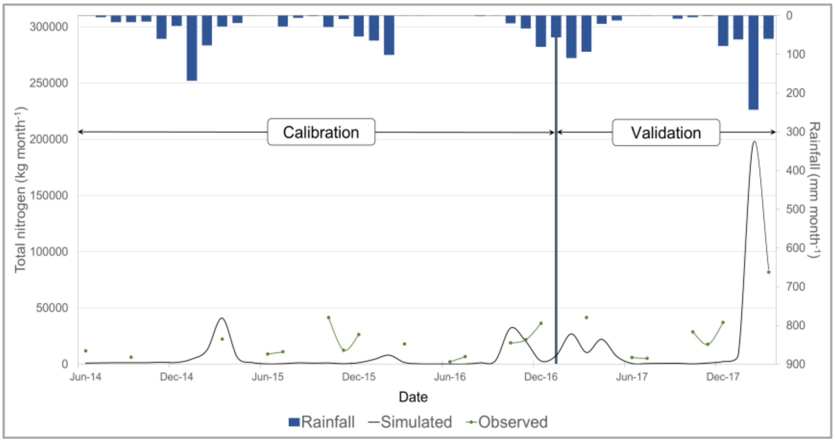


Figure 16. Comparison of observed and SWAT-simulated monthly total nitrogen and rainfall (2014-2016 calibration and 2017-2018 validation) in the Rocha River catchment.

The temporal distribution of total phosphorus in the catchment is shown in Figure 17**.** The values produced by SWAT were underpredictions of total phosphorus load for a few occasions in both the calibration and validation period. Moreover, when high rainfall occurred, high peaks of simulated total phosphorus were predicted in line with streamflow (Figure 17).

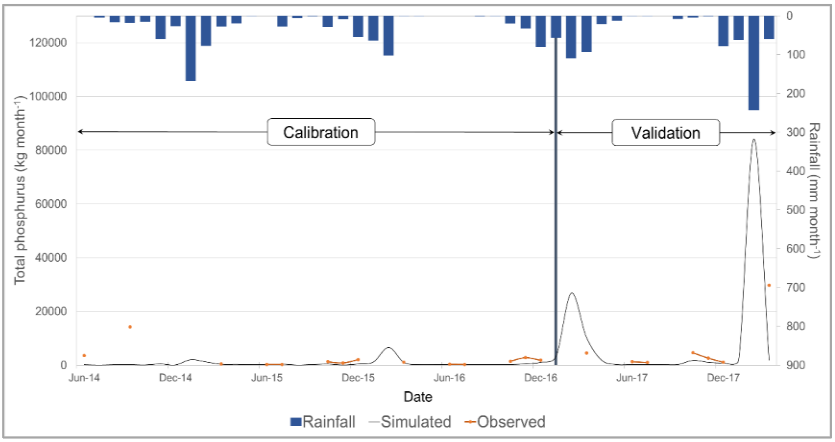


Figure 17. Comparison of observed and SWAT-simulated monthly total phosphorus and rainfall (2014-2016 calibration and 2017-2018 validation) in the Rocha River catchment.

This can be explained by phosphorus compounds generally being more stable than nitrogen compounds. Phosphorus is transported in and out of catchments by surface runoff, both bound to small particles carried in the flow and dissolved in the water (Chahinian *et al.* 2011; Santhi *et al.* 2006; Neitch *et al.* 2005). However, although there was some over- or underestimation, the overall performance was satisfactory.

5.4.2 Water balance components

The SWAT simulated average monthly values of water balance components (Paper III) in the Rocha River catchment over the study period are presented in Table 14.

Table 14. *Simulated average monthly values (all in mm) 1990-2020 of water balance components in the Rocha River catchment.*

Month	Rain	Surface runoff	Lateral flow	Water yield	Evapo-transp.	Potential evapotransp.
January	96	14	5	23	33	65
February	105	22	5	36	38	74
March	62	9	3	25	59	130
April	13	1	1	12	59	168
May	3	0	0	4	20	171
June	3	0	0	1	8	165
July	3	0	0	0	6	171
August	5	0	0	0	7	166
September	8	0	0	0	8	142
October	22	1	0	1	14	127
November	41	2	1	3	24	98
December	81	8	3	11	28	70
Total year	442	56	19	116	304	1547

The results showed that evapotranspiration was the dominant outflow component, comprising 304 mm year^{-1} (potential evapotranspiration was 1547 mm year^{-1}). Evapotranspiration accounted for approximately 68% of annual precipitation (442 mm), with a peak during summer months, while about 26% of annual precipitation became water yield, *i.e.* water discharged in river channels. Surface runoff in the catchment was 56 mm year^{-1}, representing about 13% of annual precipitation, *i.e.* surface runoff was smaller than all other components of the water balance except lateral flow.

Monthly surface runoff showed significant seasonal peaks during summer months (January and February), following heavy storms with associated sediment and pollutant losses. In contrast, transition to an ephemeral state of most river corridors gave negligible water yield values during winter months, as found in previous studies (Pulighe *et al.* 2019; Ozcan *et al.* 2017).

5.4.3 Nutrient transport

Total nitrogen and total phosphorus loads in Paper III by river reach sub-catchment are presented in Table 15. An increasing trend in load values was observed from outlets 1 and 3 to outlets 2, 4, 5 and 6, suggesting cumulative properties of nutrient loads downstream from headwaters to the outlet of the catchment with the increasing volume of water transporting nutrients. A dominant factor in increasing nutrient concentration are the increasing areas of non-point pollution sources (Wu *et al.* 2017; Lam *et al.* 2009).

Table 15. *Simulated average streamflow (m^3 s^{-1}), total nitrogen (ton $year^{-1}$) and total phosphorus (ton $year^{-1}$) loads and percentage contribution to total (%) by sub-catchment in the Rocha River catchment, 1990-2020.*

Sub-catchment	**Streamflow**		**Total nitrogen**		**Total phosphorus**	
	m^3 s^{-1}	%	ton $year^{-1}$	%	ton $year^{-1}$	%
1	6.3	8	156.0	8	49.7	8
2	11.7	15	274.0	15	87.8	15
3	4.0	5	61.1	3	21.9	4
4	17.8	22	404.6	22	130.9	22
5	19.8	24	453.2	25	146.4	25
6	21.2	26	494.7	27	158.4	27
Total	80.9		1843.7		595.1	

Urban activities related to sewage and solid waste disposal have significant effects on generation of non-point pollution. On the other hand, agriculture in the Rocha River catchment is well-known for the lack of heavy fertilisation, which can lead to nutrient retention. Human settlements close to the Rocha River are the main contributors of nutrients in the watershed, and the nutrient loads can be associated with different human activities. Irrigation (mostly flood irrigation) and soil erosion (mainly affecting phosphorus transport) can explain much of the nutrient transport, due to the presence of drainage channels in the agricultural land and subsequent intense runoff (soil loss) in the rainy season.

5.4.4 Modelled changes in streamflow and nutrient loads

The results of the SWAT simulations for annual streamflow and nutrients are shown in Figure 18. There was in general a significant ($p<0.05$) increasing trend in annual streamflow (K=2.1, Q=0.5), total nitrogen (K=2.0; Q=8.6) and total phosphorus (K=1.8, Q=2.6) over time, suggesting that streamflow volume and nutrient loads increased under the influence of land use changes and climate changes in the Rocha River catchment between 1990 and 2020. Changes in irrigation water use accompanying land use change to cropland can make streamflow decrease, while changes in catchment climate can make streamflow decrease or increase (Munoth & Goyal 2020; Aboelnour *et al.* 2019; Zhang *et al.* 2017).

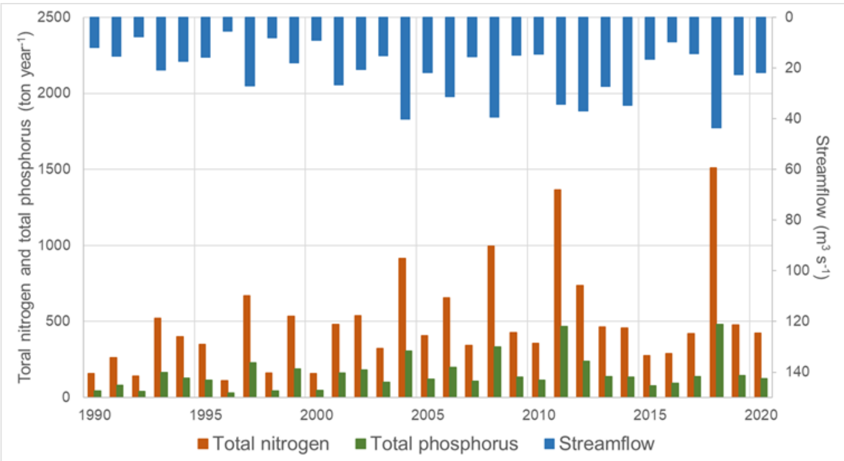


Figure 18. Simulated mean annual streamflow (m^3 s^{-1}) and total nitrogen and total phosphorus (ton $year^{-1}$) in the Rocha River catchment in the study period 1990- 2020.

Mean monthly streamflow, total nitrogen and total phosphorus loads simulated by SWAT as result of different models are presented in Figure 19. Most streamflow was concentrated from December to March, *i.e*. within the rainy season, in all models. In general, the increasing trend in mean annual long-term simulation values seen in Figure 18 was also present within modelled values of monthly averages in Figure 19.

There was a clear trend for an increase in total nitrogen and total phosphorus loads from 1990-1993 to 2014-2020 in February, in line with the increment in streamflow, which in turn corresponded to an increment in rainfall in the same month. An unexpected result was seen for January at 2009-2013 period, where lower values were found for all three variables studied (Figure 19). This can be explained by the reduction in the number of rainy days and the number and intensity of rainstorm concentrated in January in this period. Thus this period may have been related to a drought, since rainfall and streamflow increased in the next period (2014-2020). The increases in 1990-1993, 1994-2001, 2002-2008, 2009-2013 and 2014-2020, which reflected the combined effects of land use change and climate variability, resulted in increases in monthly averages of the studied variables (Figure 18). Reduced streamflow from May to October affected total nitrogen and total phosphorus dynamics, with reduced loads and thus reduced transport.

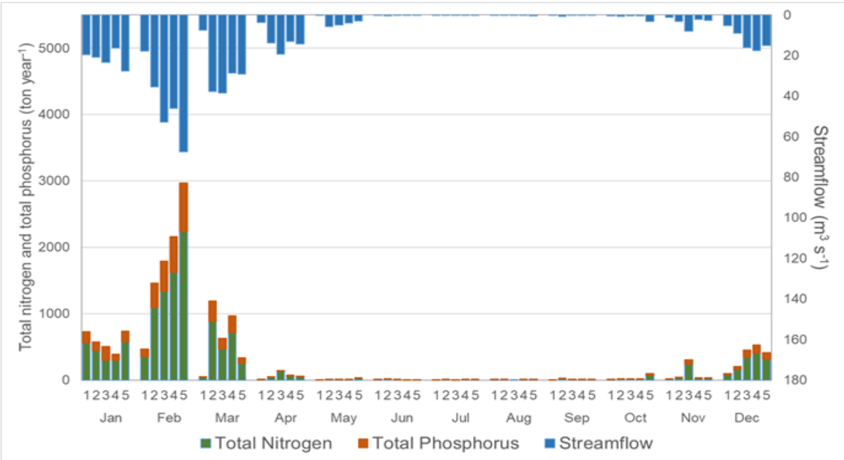


Figure 19. Average monthly streamflow (m^3 s^{-1}) and total nitrogen and total phosphorus loads (ton year^{-1}) in the Rocha River catchment under different periods: 1) 1990-1993, 2)1994-2001, 3) 2002-2008, 4) 2009-2013 and 5) 2014-2020, see section 4.6.

The SWAT model-simulated annual average streamflow, total nitrogen and total phosphorus for land use and climate data for consecutive sub-periods in the period 1990-2020 are presented in Table 16. The results indicated an increasing trend in streamflow between 1990-1993, 1994-2001 and 2002-2008, while decreasing trends were observed between 2002-2008, 2009-

2012 and 2013-2020. Meanwhile, for both total nitrogen and total phosphorus loads an increasing trend between 1990-1993, 1994-2001, 2002-2008 and 2009-2013 was observed, while a decreasing trend was observed between 2009-2013 and 2014-2020. Therefore, the results may indicate impacts of land use change in 2009-2013 (major land use change, human settlement 3.3%) and 2014-2020 (major land use change, forest 2.9%), since decreasing trends were detected. On the other hand, climate variations played a dominant role, particularly the decreasing number of short-duration, high-intensity rain storms and the reduction in total rainfall. However, increases in human settlement area also increased surface runoff and decreased water infiltration by increasing hard surfaces, which had considerable impacts on the studied variables. It is possible that the rainfall reduction from 478.6 mm year^{-1} in 2009-2013 to 442.0 mm year^{-1} in 2014-2020 exacerbated the negative impact of land use change on streamflow, as it decreased from 25.6 m^3 s^{-1} in 2009-2013 to 23.3 m^3 s^{-1} in 2014-2020.

Table 16. *Recorded rainfall (mm year^{-1}) and simulated average annual streamflow (m^3 s^{-1}), total nitrogen (ton year^{-1}) and total phosphorus (ton year^{-1}) by different periods in the Rocha River catchment.*

Period	**Rainfall**		**Streamflow**		**Total nitrogen**		**Total phosphorus**	
	mm year^{-1}	% [a]	m^3 s^{-1}	% [a]	ton year^{-1}	% [a]	ton year^{-1}	% [a]
1990-1993	400.8		13.9		270.3		83.1	
1994-2001	406.9	1.5	15.9	14.3	358.5	32.6	117.5	41.4
2002-2008	469.0	17.0	26.2	88.1	596.8	120.8	193.4	132.6
2009-2013	478.6	19.4	25.6	83.7	671.1	148.3	218.2	162.5
2014-2020	442.0	10.3	23.3	67.4	550.7	103.7	170.5	105.0

[a] Percentage increase in relation to 1990-1993.

The results also suggested that land use and climate had a greater decreasing impact on total phosphorus (57.5%), total nitrogen (44.6%) and streamflow (16.3%) in 2014-2020 compared with the previous period (2009-2013), and a greater increasing impact on total phosphorus (162.5%), total nitrogen (148.3%) both in 2009-2013 and streamflow (88.1%) in 2002-2008 compared with 1991-1993 as the reference period, which illustrates the effect of land use change in the Rocha River catchment. The reduction in total nitrogen and total phosphorus in 2014-2020 may be due to reduced streamflow, but also to a decrease in socio-economic activities, intensification of groundwater pumping for water supply and introduction of stronger regulations on disposal of domestic and industrial sewage waters.

6. Conclusions

This thesis analysed the impacts of land use on streamflow and water quality in the semi-arid Rocha River catchment in Bolivia. The results revealed that unregulated urbanisation has led to increasing sources of pollution, water quality impairment and increased streamflow in the Rocha River. Based on the findings and research objectives, the following conclusions can be drawn:

Land use changes contribute to changes in surface water quality:

- Landsat image classification can be used to produce accurate land use information.
- Water quality declined with increasing area of human settlements, whereas it improved with increases in cropland, transitional woodland/shrubland, shrubland and sparsely vegetated areas.
- Water quality showed a deteriorating trend over time.

Effects on surface water quality from non-point sources pollution can be quantified with landscape characteristics when water quality data are limited:

- A multi-criteria approach including analyses at micro- and sub-catchment scales and GIS-based modelling (PNPI) could be used to identify and rank PSAs that are more likely to produce pollution.
- Increasing PSAs identified were mainly associated with increasing degree of human settlement.

The SWAT model can be effectively used to simulate variations in streamflow and total phosphorus transport under changing land uses over periods with limited water quality data:

- The SWAT model adequately simulated streamflow and total phosphorus load, but not total nitrogen load.

- Simulated average annual streamflow increased from 1990 to 2008, while total nitrogen and total phosphorus loads increased from 1990 to 2013. This can be explained mostly by variation in rainfall and to some extent changes in land use.
- Nutrient transport (total nitrogen and total phosphorus loads) was identified as increasing from headwaters to outlet catchment.

All three water quality indices approaches (NSF-WQI, IPI and PNPI) are useful tools for assessment, planning and implementation of measures to reduce water pollution and improve water quality. SWAT modelling can also be a useful tool, but requires high expertise for modelling and a significant amount of measured data. Therefore, SWAT is a less appropriate approach under conditions such as those in the Rocha River catchment in Bolivia.

7. Future perspectives

The significant relationship found here between water quality indices and the area of different land uses in the study catchment, which was verified by correlation analysis, can be used to complement an efficient control programme comprising continuous monitoring of streamflow and water quality variables. This can help achieve pollution mitigation and water quality restoration, as part of sustainable catchment management.

Human settlements were confirmed to play a major role in pollution generation in the Rocha River catchment, and therefore local politicians should introduce restrictions to effectively control urban sprawl and implement pollution remediation in critical areas. Human settlements should also be divided into sectors, based on PSA of pollution, in order to implement best management practices in the study area.

The methodological indices approach described here may be applicable to other catchments with similar landscape characteristics and hydrological features. It may be particularly useful in data-poor regions. However, future studies should examine in detail how landscape features, hydrological, chemical and geographical processes interact in PSA prediction with limited data.

Initial experiences and results with SWAT modelling showed that it is applicable for predicting streamflow, but needs to be improved for simulation of water quality variables. SWAT model performance may be improved by the following actions:

- Land use information complementation and future change scenarios projection in order to fulfil the model requirements regarding SWAT legend classes related to soil properties.

- Incorporation of climate data analysis, which can also be useful to identify future streamflow, water quality and nutrient transport scenarios.
- Improvement of data on physical soil characteristics and associated soil hydraulic properties by soil sampling and laboratory analysis.
- Better characterisation of nitrogen and phosphorus cycles, including identification of variations in different components (*e.g*. nitrite, ammonia, organic nitrogen, organic phosphorus and mineral phosphorus) and their interaction with hydrology in the catchment.
- Implementation of a water quality monitoring programme, based on the variables required for calculating appropriate indices and including suspended sediment-, organic nitrogen- and phosphorus-related components.
- Flow-related sampling is necessary since variations in concentrations can be expected.

Water balance results from SWAT simulations can be used to define strategies for water management, which can include water capture/collection in future reservoirs. However, improvements in measured data, data quality and modelling performance in characterising hydrological processes are needed to reduce modelling uncertainty. Therefore, uncertainty analysis needs to be included in future model evaluation, as well as acceptability thresholds for simulation results considering study area characteristics.

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Popular science summary

When standing on one of the many bridges that cross the Rocha River, a quick look shows obvious contamination of its waters (dark colour, foam, floating rubbish) and unpleasant odours can often be detected. Over time, flow in the river has decreased. This situation arises frequently around the world in places where increased population and expansion of population centres transform the original landscape to meet the demand for land for housing and resources for human subsistence.

This thesis evaluated the changes in land use that occurred between 1991 and 2017 in the Rocha River catchment in Cochabamba, Bolivia, and the impacts on water quality and flow in the river. The ways in which land use has changed over time under human influences were identified using satellite imagery analysis, while water quality was measured as a single index based on a larger group of variables. Areas prone to produce pollution were mapped by describing human interactions with catchment characteristics, based on geographical modelling. In addition, models were developed to describe streamflow in the river and nutrient dynamics based on different combinations of land use, slope soil and climate conditions over time.

Human settlements in the catchment, which have increased in area over time, were identified as the main sources of pollution generation. The results showed degradation of water quality over time, and from headwaters downstream to the outlet of the catchment. Hydrological modelling worked well to successfully described streamflow, it was not as accurate in describing water quality. This means that more effort should be given to collection of data on water quality. The simulation results confirmed that accumulated nutrients/pollutants have degraded water quality over time and downstream in the Rocha River.

Resumen científico popular

Parado en uno de los muchos puentes construidos para cruzar el rio Rocha y luego de una rápida vista, se puede observar la evidente contaminación (colores oscuros, espumas y basura) y hasta olores desagradables, mientras que el caudal ha disminuido en el tiempo. Esta situación se repite frecuentemente al rededor del mundo en lugares donde el aumento de la población y la expansión urbana transforman el paisaje en demanda de territorio para nuevas casas y recursos para la subsistencia humana.

Esta tesis evaluó los cambios en el uso de la tierra entre 1991 y 2017 y los impactos el caudal y la calidad del agua en la cuenca en el río Rocha en Cochabamba, Bolivia. El cambio de uso de la tierra se identificó mediante análisis de imágenes satelitales y la calidad del agua se midió con un índice basado en un grupo variables. Las áreas propensas a producir contaminación se mapearon describiendo las interacciones humanas con las características de la cuenca, en base a modelos geográficos. Además, se desarrollaron modelos para el caudal en el río y la dinámica de los nutrientes basados en diferentes combinaciones de uso de la tierra, suelo, pendiente y condiciones climáticas a lo largo del tiempo.

Los asentamientos humanos, que han aumentado con el tiempo, fueron identificados como las principales fuentes de generación de contaminación. Los resultados mostraron una degradación de la calidad del agua a lo largo del tiempo y desde las cabeceras aguas abajo hasta la salida de la cuenca. El modelado hidrológico funcionó bien para describir el caudal, pero no fue tan preciso para describir la calidad del agua. Esto significa que se deben hacer más esfuerzos para recopilar datos sobre la calidad del agua. Los resultados de la simulación confirmaron que los nutrientes / contaminantes acumulados han degradado la calidad del agua con el tiempo y aguas abajo en el río Rocha.

Populärvetenskaplig sammanfattning

Stående på en av de många broar som byggdes för att korsa floden Rocha kan man efter en snabb titt se den uppenbara föroreningen av vattnet (mörka färger, skum och skräp) och dessutom känna en obehaglig lukt. Flödet har minskat under flera år. Så blir det ofta runt om i världen på platser där befolkningsökningen och utbredningen av bebyggelse förvandlar det ursprungliga landskapet för att möta efterfrågan på ny mark för bebyggelse.

I denna doktorsavhandling undersöktes de förändringar i markanvändning under åren 1991, 1997, 2005, 2011, 2014 och 2017, som har påverkat vattenkvaliteten och flödet i Rochaflodens avrinningsområdet i Cochabamba, Bolivia. Förändringar i markanvändning mättes med fjärranalystekniker och geografiska informationssystem, medan vattenkvaliteten utvärderades genom olika. Prioriterade områden för uppkomst av föroreningar identifierades genom flerkriterie-analys och GIS-modellering. Med hjälp av mark- och vattenbedömningsverktyget (SWAT) utvecklades modelleringstekniker baserat på olika kombinationer av förändringar av markanvändning och klimat över tid.

Resultaten visade att områden med ökad bebyggelse över tid var den främsta källan till föroreningar. På samma sätt bekräftades försämringen av vattenkvaliteten över tid från uppströms till utloppet av avrinningsområdet. Modellering återgav flöde och transporten av fosfor bra, men inte transporten av kväve. Resultaten av simuleringarna bekräftade att ackumulering av näringsämnen har försämrat vattenkvaliteten över tid och att det har skett en ökning av transporten nedströms i floden.

Acknowledgements

I would like to acknowledge the Swedish International Development Cooperation Agency (SIDA), Swedish University of Agricultural Sciences (SLU) and San Simon University (UMSS) for support and funding for this thesis work.

I would like to thank my supervisors Ingrid Wesström and Ingmar Messing for their dedicated support and guidance. I really appreciate the criticisms, enthusiasm and scientific support during the production of this thesis. Thanks to Ana M. Romero, Mauricio Villazón and Youen Grusson for the knowledge sharing and support with analysis. I would also like to express my gratitude to Carmen Ledo in Bolivia for her understanding and support and to Abraham Joel in Sweden for his invaluable advice, helpful discussion, and guidance to complete the thesis and for accommodation in Sweden. I learned a lot from you all in these years.

I express my gratitude to the CLAS, Center at UMSS, the National Meteorology and Hydrology Service of Bolivia (SENAMHI), the Basin Departmental Service of Cochabamba (CDC), The International Science Programme and the Soil and Environment Department at SLU.

Thanks to friends in Ultuna, Cochabamba and all the other places I visited during this work. I thank you for your support, and, memories.

My eternal gratitude to Claudia, Samuel and Caleb for your love, support, strength and understanding during all this time away from home. Thanks also to my Loida, Carito, Luana y Loidita for thinking of me.

Acta Universitatis Agriculturae Sueciae

Doctoral Thesis No. 2021:64

This thesis describes the impacts of land use change on streamflow and water quality in the Rocha River catchment. Geographic modelling, index-based approach and hydrologic modelling were used to assess land use change, water quality, predict streamflow and nutrient loads. The results showed increases in man related land uses and streamflow while water quality decreased from headwaters to outlet over time.

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Online publication of thesis summary: http://pub.epsilon.slu.se/

ISSN 1652-6880
ISBN (print version) 978-91-7760-805-9
ISBN (electronic version) 978-91-7760-806-6