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Soluções baseadas na natureza para aproveitamento de águas urbanas: modelagem da remoção de poluentes em sistema de biorretenção para fins não potáveis

Versão corrigida
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Dissertação apresentada à Escola de Engenharia de São Carlos, Universidade de São Paulo, como parte dos requisitos para a obtenção do título de Mestre em Ciências: Engenharia Hidráulica e Saneamento

Orientador: Prof. Dr. Eduardo Mário Mendiondo

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“A inquietude é o estímulo essencial à pesquisa científica.”

Anderson Vailati Ritzmann

RESUMO

OLIVEIRA, T. R. P. (2021). **Soluções baseadas na natureza para aproveitamento de águas urbanas: modelagem da remoção de poluentes em sistema de biorretenção para fins não potáveis.** Dissertação (Mestrado) - Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos, 2021.

As Soluções baseadas na Natureza (SbN) emergem como uma alternativa viável para a mitigação dos danos causados devido às enchentes, alagamentos e degradação da qualidade da água associados à alta taxa de urbanização e à um sistema tradicional de drenagem urbana ineficiente. Entre as TCs exploradas pela literatura internacional, a biorretenção permite não somente reduzir o escoamento superficial, mas também remover a carga poluidora, permitindo a melhora dos índices de qualidade da água. No entanto, o aproveitamento de águas pluviais após sistemas de biorretenção ainda precisa ser estudado. Assim, o objetivo desta pesquisa é avaliar a eficiência de um sistema de biorretenção, em escala de protótipo, na remoção de poluentes visando o aproveitamento da água da chuva para fins não potáveis. A metodologia se estende em três partes: (1) Caracterização do efluente da biorretenção por meio de experimento em protótipo; (2) Comparação da qualidade do efluente com zona insaturada e zona saturada para avaliar a potencialidade do reuso; (3) Aplicação de um modelo matemático de *E. coli* para calibração e validação inicial de parâmetros qualitativos. A pesquisa colabora no alcance das metas dos Objetivos do Desenvolvimento Sustentável (Objetivo 6 – Água potável e saneamento; Objetivo 11 – Cidades e comunidades sustentáveis e Objetivo 13 – Combate às alterações climáticas) a partir da implantação de uma alternativa adaptativa com a possibilidade de aproveitamento da água da chuva, aumentando a segurança hídrica e com o desenvolvimento de cidades resilientes à eventos extremos de enchentes e secas.

Palavras-chave: Soluções baseadas na natureza. Aproveitamento da drenagem pluvial. Biorretenção. Modelagem de *E. coli*.

ABSTRACT

OLIVEIRA, T. R. P. (2021). **Nature-based solutions for stormwater harvesting: modeling the removal of pollutants in a bioretention system for non-potable purposes.** Master thesis – School of Engineering of São Carlos, University of São Paulo, São Carlos, 2021.

Nature-based Solutions (NbS) emerge as a viable alternative for mitigating the damage caused by floods and water quality degradation associated with a high urbanization rate and a traditional inefficient urban drainage system. Among the NbSs explored in the international literature, bioretention allows not only to reduce surface runoff, but also to remove the polluting load, allowing the improvement of water quality indices. However, the use of rainwater after bioretention systems still needs to be studied. Thus, the objective of this research is to evaluate the efficiency of a bioretention system, on a prototype scale, in the removal of pollutants aiming at the use of rainwater for non-potable purposes. The methodology is divided into three parts: (1) Characterization of the bioretention effluent through a prototype experiment; (2) Comparison of effluent quality with an unsaturated zone and a saturated zone to assess the potential for reuse; (3) Application of a mathematical model of *E. coli* for calibration and initial validation of qualitative parameters. The research collaborates in achieving the Sustainable Development Goals (6 – Clean water and sanitation; 11 - Sustainable cities and communities; 13 - Climate action) through the implementation of an adaptive alternative with the possibility of using rainwater, increasing safety and with the development of cities resilient to extreme events of floods and droughts.

Keywords: Nature-based solutions. Stormwater harvesting. Bioretention. *E. coli* modeling.

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LIST OF ABBREVIATIONS

ABNT	Associação Brasileira de Normas Técnicas / Brazilian Association of Technical Standards
BOD	Biological Oxygen Demand
COD	Chemical Oxygen Demand
CONAMA	Conselho Nacional do Meio Ambiente / National Council for the Environment
CT	Compensatory Techniques
DEAP	Distributed Evolutionary Algorithms in Python
DP	Dissolved Phosphorus
E. Coli	Escherichia coli
EMBRAPA	Empresa Brasileira de Pesquisa Agropecuária / Brazilian Agricultural Research Company
EMC	Event Mean Concentration
INMET	Instituto Nacional de Meteorologia / National Institute of Meteorology
IPCC	Intergovernmental Panel on Climate Change
IWS	Internal Water Storage
LID	Low Impact Development
NBR	Norma técnica brasileira / Brazilian technical standard
NSE	Nash Sutcliff Efficiency
P	Phosphorus
PP	Particulate Phosphorus
PZ	Ponding Zone
RMSE	Root Mean Squared Error
RTC	Real Time Control
SuDS	Sustainable Drainage System
SZ	Submerged zone
TP	Total Phosphorus
U.S. EPA	United States Environmental Protection Agency
USP	Universidade de Sâo Paulo / University of Sao Paulo
USZ	Unsaturated zone
WSUD	Water Sensitive Urban Design

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1 GENERAL INTRODUCTION

Many issues delay the sustainable development of today's society, among them, the increase in the world population and, consequently, the pollution added by the development of human activities. The emission of greenhouse gases has been occurring due to the increase in anthropogenic activities, and this leads to changes in the climate pattern (Wada et al., 2016). Climate change can cause changes in the water cycle, through variations in temperature, evapotranspiration rate, duration, intensity, and frequency of precipitation, resulting in flood events or water scarcity in different regions (Field et al., 2012; IPCC 2014). These changes are likely to get worse in the future, increasing the risk of extreme events and water insecurity (Simonovic, 2017).

The water crisis increases when demand approaches the total of available resources, since the demand for water increases and needs to be allocated to different sectors (e.g.: domestic consumption, industrial, irrigation, etc.) (Kummu et al., 20.16; Roshan & Kumar, 2020). According to Gittins et al., (2021), water reservoirs cannot always withstand collapse through economic or engineering decisions alone. Furthermore, the water crisis can be aggravated not only by the scarcity of water itself, but by the availability of water of sufficient quality for use, or by structural issues of distance and the need for large investments in water distribution systems.

Thus, new alternative sources of water collection and treatment should be studied to supplement the existing water supplies systems and reduce the risk of water scarcity, such as stormwater harvesting (Dandy et al., 2019; Ali et al., 2021). The use of runoff control devices not only to store stormwater, but also to perform a primary treatment of runoff is currently gaining prominence. Antunes et al. (2020) evaluated the implementation of a permeable pavement system for non-potable water uses, achieving a potable water saving of 69.6%. Several studies also assess the performance of biofilters with runoff treatment through plant uptake and filter media for reuse (Payne et al. 2019; Shen et al. 2020; Mehmood et al. 2021; Macedo et al. 2019). Thus, Low Impact Development (LID) practices can be used in multi-purpose systems, as peak flow mitigation and initial runoff treatment for stormwater reuse.

However, for the precise urban waters harvesting, it is necessary to guarantee sufficient quantity and quality. Runoff can contain different types of pollutants depending on the location, as stormwater washes the surface, which may contain naturally deposited atmospheric pollutants, solid wastes, sediments, metals, nutrients, and pathogenic

organisms. According to Ferguson et al., (2003), faecal microorganisms are one of the mainly pollutants of urban waters and, consequently, of waterways. Thus, for safe urban water reuse, studies are needed to assess water quality. Lau et al. (2017) reports on the fit-for-purpose approach where lower quality water for non-potable purposes is used.

This study aims to evaluate the quality of water after a bioretention system focusing on reuse for non-potable purposes, and to investigate through modeling the behavior of *Escherichia coli* (*E. coli*) in bioretention systems.

1.1 RESEARCH HYPOTHESIS

Bioretention system is an alternative for the primary treatment of pollutants in urban waters and can be used as flood and water stress attenuators with the storage to use stormwater as resource for non-potable purposes demand.

1.2 PURPOSE

1.2.1 General purpose

To improve the scientific knowledge on bioretention systems application with multi-purposes such as reducing the risk of floods and using a new water source alternative to meet the demand for water for non-potable purposes and to evaluate the behavior of key pollutant for stormwater harvesting.

1.2.2 Specific purpose

- Assess the quality of the inflow and outflow of a bioretention box targeting pollutants for non-potable uses in accordance with ABNT NBR 15527/2019;
- Analyze water quality with unsaturated zone and saturated zone in a bioretention box in subtropical climate;
- Apply a mathematical model to investigate the behavior of *E. coli* within the bioretention system.

1.3 TEXT ORGANIZATION

This dissertation is organized into 4 chapters. The **first chapter** presents a general introduction to the topic, as well as the hypothesis and objectives of this research. The **chapter two** presents stormwater quality assessment after a bioretention system focusing

on stormwater harvesting. In this chapter, an initial exploratory analysis of the difference in water quality between unsaturated zone and saturated zone in a bioretention system in a subtropical climate was evaluated. The **chapter three** explores the modeling of one of the most common pollutants in urban water, *E. coli*, which is the main pollutant that puts the stormwater harvesting at risk, due to health risks. Finally, the **chapter four** presents general conclusions and recommendations for future studies.

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2 DIFFERENT CONFIGURATIONS OF A BIORETENTION SYSTEM FOCUSED ON STORMWATER HARVESTING IN BRAZIL

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Abstract

Low Impact Development (LID) practices contribute to the reduction of flooding and improvement of water quality. Water crises may be a result of water scarcity and flooding due to climatic changes and the increase of impervious areas, thus stormwater harvesting becomes a sustainable alternative solution for relative water problems. The performance of a bioretention system with the submerged zone (SZ) and unsaturated zone (USZ) was evaluated as an alternative for stormwater harvesting. The study was carried out on a laboratory scale, using a bioretention box to simulate the processes that occur in a real system and in the field. The system was efficient in removing TP (68.5% and 76.5%), COD (71.6% and 56.9%) and NO_2 (28% and 16.6%) in USZ and SZ events, respectively. NH_3 removal (31%) occurred only at SZ events. NO_3 was exported at all events tested, but at values below the Brazilian CONAMA Resolution 357/2005 on the quality of water bodies for supply. The bioretention effluent showed relatively high values of turbidity; however, the pH parameter presented good values in all experiments (> 6.5 and < 7.5), and *E. coli* only in some cases presented satisfactory values to meet the Brazilian Standard for Rainwater Usage for non-potable purposes (< 200MPN/100mL). In general, both configurations provide different improvements for stormwater to support sustainable water resources management. This study presents a comparison between bioretention systems with and without SZ as an initial proposal for improvement in bioretention systems in Brazil, however more experiments must be monitored and new improvements should be tested for reaching restrictive water reuse purposes.

Keywords: Submerged zone; Water quality; Low Impact Development; Stormwater harvesting.

2.1 INTRODUCTION

The increase in impervious surfaces in cities, associated with the intensification of urban activities, results in floods and hence potentialize the generation of pollutants that are carried in the runoff, degrading the water quality of water body receivers (Fletcher et al. 2013). In addition, climate change can increase the occurrence of extreme events (Simonovic 2017). These changes occur when there are variations in temperature, duration, intensity, and frequency of flood events, which affect the hydrological cycle of each region differently (Field et al. 2012), making the population more susceptible to the risk of disasters, such as floods, droughts, and landslides. Thus, cities need solutions that incorporate urban resilience, which are able to absorb, deal with, learn and recover from extreme events e.g., droughts and floods (Simonovic & Peck 2013; Admiraal & Cornaro 2019).

During the 1990s, a variety of new urban drainage approaches sought to control rainfall on-site rather than to produce runoff: Low Impact Development (LID in the United States), Sustainable Drainage Systems (SuDS in the United Kingdom), Water Sensitive Urban Design (WSUD in Australia), and Compensatory Techniques (CT in France and Brazil) (Fletcher et al. 2014; Souza et al. 2012). Low Impact Development practices (LIDs), the term adopted in this article, can be used to achieve sustainability in cities in two main aspects: (a) flood mitigation through adaptation to hydrological extremes due to the impacts of climate changes and modifications in land use, as well as for the reduction of flooding risks due to increasing maximum flows (Yoshizaki et al. 2019); and (b) water quality management to mitigate stormwater runoff pollution, based on improving the quality of runoff with the control of urban diffuse pollution (Ma et al. 2019; Macedo et al. 2019a; Jiang et al. 2019).

Among the existing LIDs, the bioretention system is an on-site practice composed of filtering media and vegetation in the upper layer. The filtering media layer provides the peak flow reduction due to the increase in stormwater infiltration into the soil during rainy events. In addition to aesthetic benefits, plants also promote pollutant removal from stormwater (Akan 2013; Roy-Poirier et al. 2010). The water quality improvement occurs due to biologically active soils with high permeability and plants capable of filtering polluted stormwater and retaining it for growth, thus removing contaminants from the water (Jiang et al. 2019; Trowsdale & Simcock 2011).

There are different design configurations of the bioretention system that can help to increase the efficiency of pollutant removal, e.g., underdrain outlet height, filtering media, and plant selection (Li et al. 2021). Many studies have shown that the elevation of the outlet valve provides the formation of an anaerobic submerged zone (SZ) within the bioretention system, also known as Internal Water Storage. The SZ increases the retention time of stormwater within the system, enhancing nutrient and pathogenic indicator removal, such as total phosphorus (TP), nitrate (NO_3), and *E. coli* (Xiong et al. 2019; You et al. 2019; Wang et al. 2018; Chandrasena et al. 2014). The aerobic unsaturated zone (USZ) occurs in the filtering media as a complement to the submerged zone, but when the underdrain outlet height is located at the bottom of the system, there is no formation of a submerged zone. Therefore, the entire system is classified as USZ. This configuration is equally important for the removal of ammonia by the nitrification process (Shrestha et al. 2018). Zinger et al. (2013) showed that the use of USZ was better in TP removal rates, when compared to the SZ system, but regarding metal removal, there was no significant difference between the systems.

The plant selection is also fundamental for the bioretention quality and hydrological performance (Vijayaraghavan et al. 2021). There are several guidelines for plant selection criteria (Payne et al. 2018; Hunt et al. 2015). Dagenais et al. (2018) stablished four main statements about plant selection in bioretention systems: (a) plants improve the system efficiency for water quality treatment; (b) different species have different effectiveness; (c) native plant species are more effective than exotic ones; and (d) a diversified system is more efficient than a system with a particular species. The selection must be made according to the conditions that the plant will be subject to, such as temperature, humidity, pollution load, etc.

There are several types of filter media for bioretention systems, the main ones are based on mixtures of sand, loam, and clay, and are chosen according to saturated hydraulic conductivity and pollutant retention capacity (Davis et al. 2009). Studies have also analyzed the addition of different types of organic source materials to assess the efficiency in removing pollutants, such as biochar (Søberg et al. 2019; Zinger et al. 2013) and fly ash (Mei et al. 2020; Kandel et al. 2017). Feng et al. (2012) showed that a larger depth of the filter media resulted in metal leaching (iron (Fe), aluminum (Al), chromium (Cr), Zinc (Zn), and lead (Pb)). Therefore, the choice of the configuration of a bioretention system, from the types of plants to the material of the filtering media, can influence the improvement of water quality, mainly to achieve desirable stormwater quality levels.

Despite the improvement in water quality, there are few studies that relate the bioretention system, and its different design configurations, as a viable alternative to increase water security with the reuse of effluent for multiple purposes. In Australia, Feng et al. (2012) evaluated the performance of biofilter columns in removing stormwater pollution. As a result, the systems were efficient for removing metals to meet standards for irrigation. Shen et al. (2020) employed Real Time Control (RTC) strategies to minimize health risks by faecal organisms in stormwater harvesting, mainly in the control of the stormwater volume within the system (as SZ) and the number of days that this stormwater is retained to ensure the treatment. However, in the study by Macedo et al. (2019b), the effluent from a bioretention system with an USZ configuration does not meet Guidelines for Water Reuse in the United States and Australia.

In Brazil, there is still no legislation for stormwater reuse, only a recommendation from the Brazilian Standard for Rainwater Usage for non-potable purposes – NBR 15527/2019 (ABNT 2019), which covers few parameters (turbidity, pH, and *E. coli*). Adopting stormwater reuse can help to provide water supply in the future (Goonetilleke et al. 2017), becoming a sustainable adaptive alternative, helping to achieve the Sustainable Development Goals (6 - Clean water and sanitation; 11 - Sustainable cities and communities and 13 – Climate action) (UN 2020). Therefore, the study of the difference between USZ and SZ configuration in bioretention systems and how it can contribute to stormwater harvesting is a subject that needs further attention.

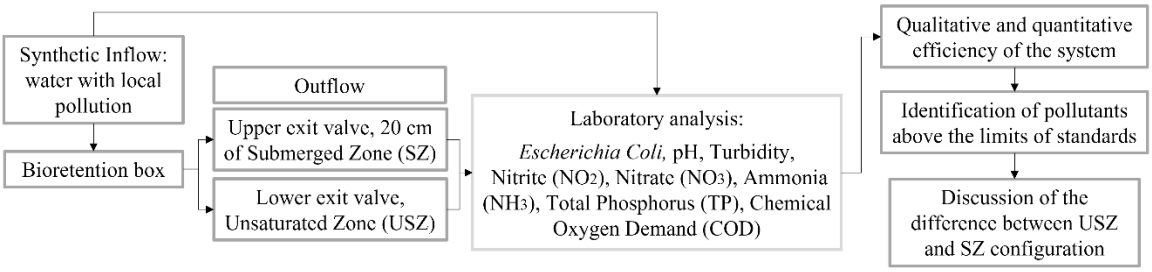
This paper aims to evaluate the performance of removing pollutants from a bioretention system, from the USZ and SZ conditions, for water reuse. We monitored synthetic events in a bioretention box, evaluating the parameters mentioned in the Brazilian Standard for Rainwater Usage NBR 15527/2019 (ABNT 2019). For an extended investigation, we also evaluated typical parameters in urban waters in the city of São Carlos, in Brazil (NO_2, NO_3, NH_3, TP, and COD). To compare these pollutants levels with a standard, we used CONAMA 357/420 (BRASIL, 2005), which establishes the quality standards of rivers and drinking water in Brazil.

2.2 METHODOLOGY

The methodology consists of two main steps: (1) Characterization of the inflow and outflow of a bioretention system, on a bioretention box, with synthetic inflow and different outlet heights; (2) Evaluation of the system efficiency in removing pollutants in terms of

the different outlet heights (with and without submerged zone). Figure 2.1 shows the methodology flowchart of this study. Each step is presented in the next sections in more detail.

Figure 2.1 - Methodology flowchart

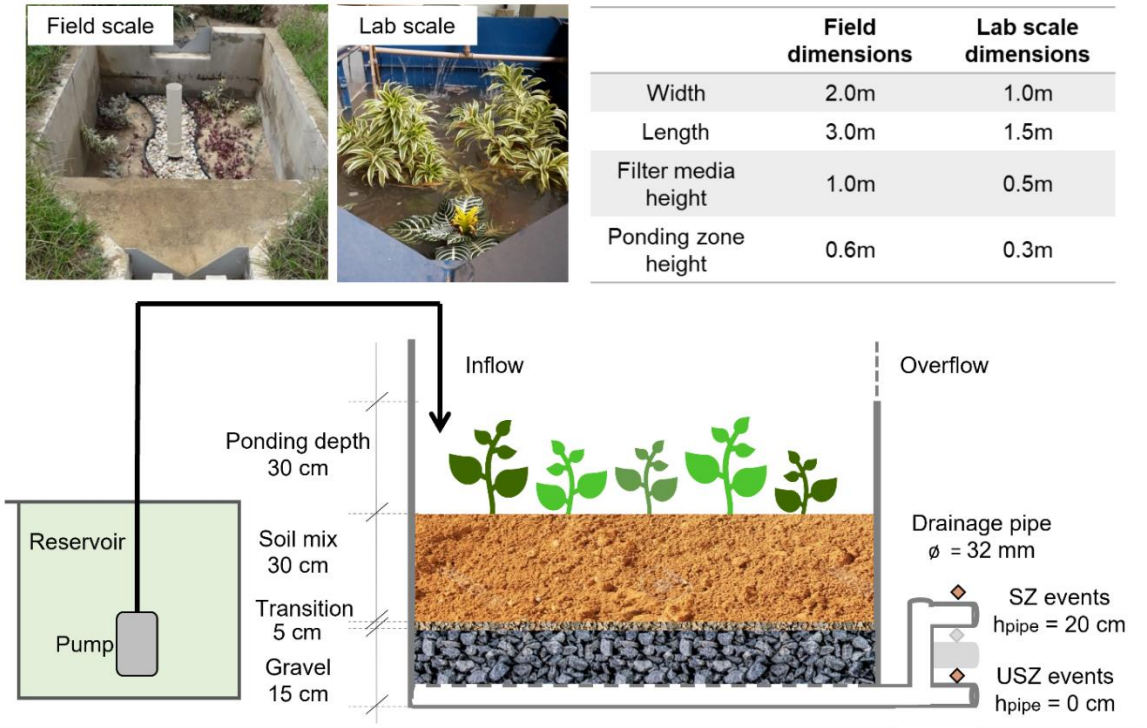


2.2.1 Study site

The city of São Carlos has a subtropical climate and average annual rainfall of 1,361.6 mm, in which the wettest month is January (precipitation around 274.7 mm) and the driest month is July (approximately 28.3 mm) (EMBRAPA 2020). The average temperature of São Carlos varies from 17 °C to 29 °C in the rainy season (November to April) and from 9 °C to 24 °C in the dry season (May to October).

The bioretention box was designed on a scale with a field bioretention system, which receives stormwater runoff from a 94 m^2 roof covering. The dimensions of the laboratory scale bioretention box are equivalent to half of the field system (Figure 2.2). The bioretention box has an area of 1.5 m^2 and 0.75 m in height. The filter media consists of two layers: (1) a mixture of sand and natural soil (20% natural soil for plant fixation and 80% sand), and (2) a layer of gravel at the bottom (average porosity: 0.408). The use of natural soil in the bioretention box follows the recommendations in the Brazilian literature (Macedo et al. 2019b; Melo et al. 2014; Daniel Júnior 2013; Azevedo 2019), as well as the bioretention in the field. Moreover, the system has a drain perforated at the bottom, with a diameter of 32 mm, and outlet valves at different heights. In this study, the lower outlet (outlet drain height = 0 m) and the upper outlet (outlet drain height = 0.2 m, allowing the formation of a submerged zone) were used. According to Macedo et al. (2019a), the local soil has a saturated hydraulic conductivity equal to 5.83 mm/h and is characterized as brown with organic matter. The plants were chosen following the recommendations of Hunt et al. (2015) for the criterion of greater NO_3 removal, considering the small size of the bioretention prototype and landscape criterion. Preference was given to native vegetation of South America (Table 2.1).

Figure 2.2 - Scheme of the lined bioretention box system with different outlet heights. The bioretention box was designed with dimensions on a 1:2 scale with the system in the field. For this study, only the upper exit valve and the lower exit valve of the bioretention box were used in the experiments.



	Field dimensions	Lab scale dimensions
Width	2.0m	1.0m
Length	3.0m	1.5m
Filter media height	1.0m	0.5m
Ponding zone height	0.6m	0.3m

Table 2.1 - Description of the prototype plans. Adapted from Hunt et al. (2015)

Scientific name	Maximum height	Origin	Percentage of Nitrate Removal
Dracaena reflexa	-	India*	64%
Complaya trilobata	0.7 m	South America	95%
Sanchezia nobilis	3 m	South America	87%

* Despite originating in India, this species is common in the study region

2.2.2 Monitoring and collection procedures

The experiments were conducted from May to September 2019 at the University of São Paulo/São Carlos (USP/SC). To simulate the inlet pollution of the experiment, the sweeping method was used according to Maglionico (1998). This method consists of sweeping nearby impermeable areas to collect material (with pollutants) to simulate runoff pollution; therefore, the inlet runoff simulation considered the pollution of the same catchment as the roof covering to represent the deposition of pollutants in the area. The

materials were collected after the formation of the natural sediment deposition of the campus, thus half a bucket (approximately 6 L) of this material was mixed into clean water without chlorine to compose the synthetic inflow water in each experiment. The inflow simulation was calculated to be approximately the daily rainfall that has an exceedance probability of 90% in the city of São Carlos (P90 = 32.5 mm, calculated with the historical series data from 1961 to 2015 obtained by the weather station of the National Institute of Meteorology – INMET for the city of Sao Carlos) during the rainy season. Moreover, we used an intensity - duration - frequency curve (Barbassa, 1991) with a constant duration of 30 minutes and a 5-year return period, resulting in an intensity of 61.9 mm/h. The equivalent precipitation (P_e = 31 mm) is equal to a proportional inflow of 0.4 L/s, considering the dimensions of the bioretention box (Macedo 2020).

In each experiment, the inflow concentration was kept constant through continuous mixing throughout the event. A total of two inlet samples were collected; one every 15 minutes to verify if the concentration of the pollutants remains constant. For the effluent, the samples were collected every 5 minutes, totaling 10 samples, to characterize the outlet pollutograph. The parameters *E. coli*, turbidity and pH were analyzed according to the Brazilian Standard for Rainwater Usage for non-potable purposes - NBR 15527 (ABNT 2019). In addition, we also evaluated the parameters of NO_2, NO_3, NH_3, TP (significant indicators of water contamination for eutrophication), and COD (an indication of organic matter). These parameters are important for assessing the quality of stormwater for reuse for more restrictive purposes. Laboratory analysis were performed following the methodology of the Standard Methods for the Examination of Water and Wastewater (APHA et al. 2015).

2.2.3 Efficiency analysis of the bioretention box

Runoff control and pollutant removal efficiency indicators were calculated to compare the initial configuration performed in the experiments. The water balance for each experiment followed Eq. (1). The efficiency of the system in terms of peak flow attenuation was calculated according to Eq. (2) (adapted from Silveira and Goldenfum 2007) and runoff volume reduction according to Eq. (3). In the characterization experiments, pollutants were analyzed by concentration over time. However, the Event Mean Concentration (EMC) (Eq. 4) was also calculated to compare the quality of effluent with the Brazilian guidelines -

CONAMA 357/420 (BRASIL 2005). The pollutant removal efficiency was calculated from the EMC values (Eq. 5).

$$\Delta S = V_{in} - V_{out} - V_{overflow} \quad (1)$$

$$Eff_{Qp} = \frac{Q_{p.out}}{Q_{p.in}} \times 100 \quad (2)$$

$$Eff_{V} = \frac{V_{out}}{V_{in}} \times 100 \quad (3)$$

$$EMC = \frac{\sum_{t=1}^{T} C(t) \times Q(t) \times \Delta t}{\sum_{t=1}^{T} Q(t) \times \Delta t} \quad (4)$$

$$Eff_{treatment} = \left(\frac{EMC_{in} - EMC_{out}}{EMC_{in}}\right) \times 100 \quad (5)$$

Where: ΔS = Storage volume variation in bioretention [mm]; V_{in} = Total inflow volume [mm]; V_{out} = Total outflow volume [mm]; $V_{overflow}$ = Total overflow volume [mm]; Eff_{Qp} = Peak flow attenuation efficiency [%]; $Q_{p.in}$ = Maximum inflow [L/s]; $Q_{p.out}$ = Maximum outflow [L/s]; Eff_{V} = Volume attenuation efficiency [%]; EMC = Event Mean Concentration [mg/L]; $C(t)$ = Concentration, on time t [mg/L]; $Q(t)$ = Water flow at time t [L/s]; Δt = Time interval [min].

The efficiencies were calculated for each event and grouped into: (1) events using the lower outlet valve, with an unsaturated zone (USZ); and (2) events using the upper outlet valve, with the formation of saturated zone (SZ), to obtain the average efficiency according to the height of the register. After collecting the samples, the parameters of *E. coli*, turbidity and pH were compared with the limits of the Brazilian Standard for Rainwater Usage for non-potable purposes - NBR 15527 (ABNT 2019). However, the recommendations of NBR 15527 do not cover all parameters, making it necessary to consult CONAMA 357/420 (BRASIL 2005) regarding the quality standards of rivers and drinking water to compare the limits of the other parameters. We used the limits of two categories of this legislation: (1) “River class I” referring to water quality from rivers that can be destined for human consumption after simplified treatment, protection to aquatic life, and recreational purposes; (2) “River class II” refers to the water quality of human consumption after conventional treatment, protection of aquatic life, recreational purposes, irrigation of fruits and vegetables and fishing activities.

2.3 RESULTS AND DISCUSSIONS

2.3.1 Characterization of experiments

A total of 7 experiments with synthetic inflow were analyzed to characterize the pollutant concentration before and after the bioretention box. The events Ev.1, Ev.2 and Ev.5 were with USZ; and the events Ev.3, Ev.4, Ev.6 and Ev.7 were with SZ, allowing the formation of a continuous saturated layer of 20 cm throughout the experiment (Table 2.2). The inflow was approximately 0.4 L/s, for 30 minutes.

Table 2.2 - Description of laboratory-scale experiments

Event	Date	Antecedent dry days	Type	Duration (min)	Equivalent precipitation (mm)	Inflow (L/s)
Ev1	27/05/2019	1	USZ	30.0	33	0.40
Ev2	10/06/2019	14	USZ	30.4	33	0.40
Ev3	26/06/2019	16	SZ	31.1	33	0.40
Ev4	06/08/2019	41	SZ	28.8	33	0.40
Ev5	19/08/2019	13	USZ	30.2	32	0.38
Ev6	02/09/2019	14	SZ	20.5	21	0.38
Ev7	30/09/2019	28	SZ	30.0	32	0.38

USZ: Unsaturated zone (lower exit valve)

SZ: Submerged zone (upper exit valve)

In all events, there was a reduction in peak flow and volume, as shown in Table 2.3. Using this event condition (duration = 30 min and return time = 5 years), there was no overflow at the weir, showing that the maximum height of the ponding zone of the prototype (30 cm) has not been reached. The ponding zone increases the efficiency of the technique through temporary storage when the saturation of the filter medium is high, and the infiltration occurs slowly.

Table 2.3 - Water balance and runoff volume reduction and peak flow attenuation efficiencies

Event	Type	Volume in (L)	Volume out (L)	Max Q_{out} (L/s)	Eff_V	Eff_{Qp}
Ev1	USZ	721.4	592.5	0.23	17.9%	41.7%
Ev2	USZ	731.1	655.6	0.19	10.3%	53.8%
Ev3	SZ	747.9	520.7	0.14	30.4%	65.4%
Ev4	SZ	693.3	392.2	0.13	43.4%	68.3%
Ev5	USZ	697.4	456.5	0.21	34.5%	48.3%
Ev6	SZ	473.1	455.3	0.16	3.8%	60.8%
Ev7	SZ	692.3	582	0.18	15.9%	55.0%
				Average USZ	20.9% ± 10.1%	47.9% ± 4.9%
				Average SZ	23.4% ± 16.5%	62.4% ± 3.1%

USZ: Unsaturated zone (lower exit valve)

SZ: Submerged zone (upper exit valve)

In events with an unsaturated zone, the efficiency in reducing peak flow ranged from 41.7% to 53.8%, with an average value of 47.9% ± 4.9%, while in events with a saturated zone, the efficiency varied from 55% to 68.3%, with an average value of 62.4% ± 3.1%. Figure 2.3 shows the average of the hydrographs with maximum and minimum values. The volume retention of the system was slightly higher in the saturated zone experiments, as expected, due to the internal storage of the bioretention. Considering the implantation of a reservoir after the bioretention system, in which water can be harvested and reused for multiple purposes, it is possible to harvest an average of 79.1% ± 10.1% and 76.6% ± 16.5%, in USZ and SZ events, respectively, of the system effluent (depending on the quality) of recurrent precipitation, such as that tested in the experiments. In this approach, only the overflow volume of the reservoir would be directed to the rain drainage system, reducing the volume of possible floods, and increasing the availability of water.

Figure 2.3 - Average hydrographs for all experiments grouped by USZ configuration events and SZ configuration events. The shaded range represents the maximum and minimum runoff flow values obtained from the experiments.

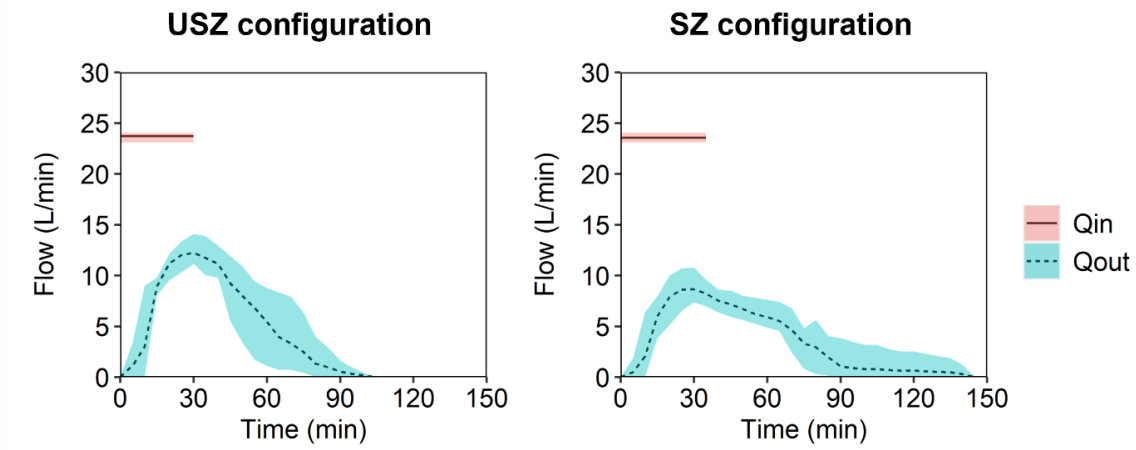
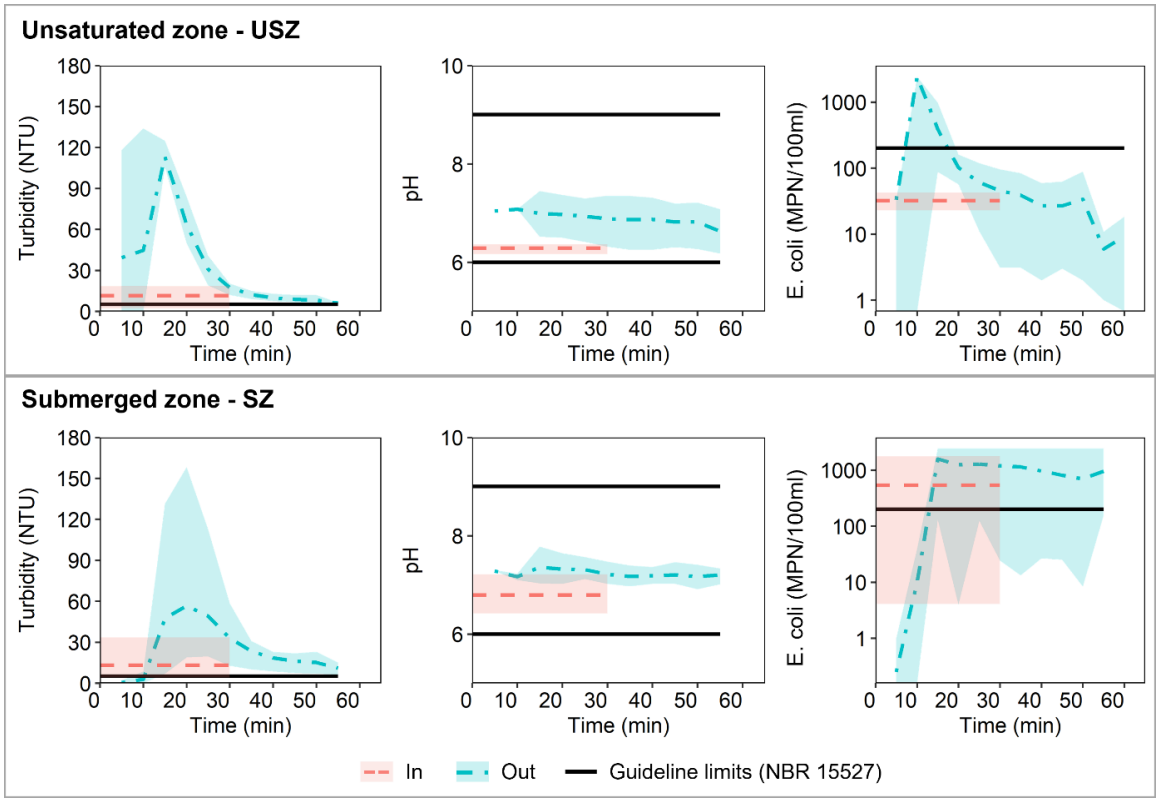


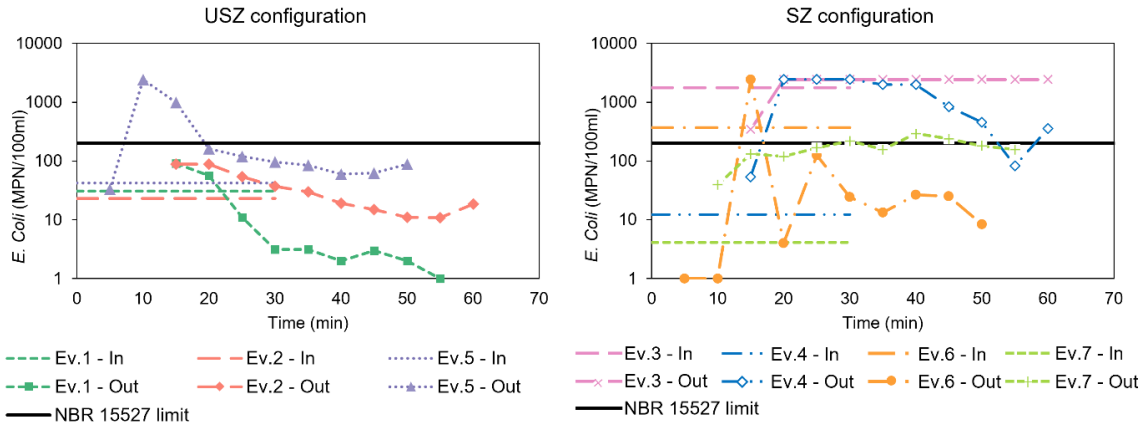
Figure 2.4 shows the average of the water quality results, considering the parameters of NBR 15527 (ABNT 2019): *E. coli* (<200 microorganisms per 100 ml); turbidity (<5 NTU); pH (> 6 and <9), separated in USZ and SZ events. This difference between the events resulted in different values in the pollutant removal. In all experiments, the pH parameter was within the limits of the standard. However, the quality of the system's effluent does not meet the criteria for rainwater reuse due to high turbidity values. Although USZ experiments showed high average values at the beginning, the turbidity values were considerably reduced, reaching close to the standard limit after 40 minutes. The SZ events presented a lower turbidity peak than USZ events, however, the reduction of values occurred more slowly, therefore SZ events did not fit within the measured time interval (50 minutes). This turbidity peak in the first minutes occurs due to the initial stormwater performing a “wash” in the system, and therefore the fine particles of the filter media are taken into the outflow. Regarding the turbidity parameter, some adaptations such as the disposal of the initial volume may be suitable for stormwater harvesting.

Figure 2.4 - Average values over time of turbidity, pH and *E. coli* parameters with the limits of NBR 15527/2019 (ABNT 2019): *E. coli* (<200 microorganisms per 100 ml); turbidity (<5 NTU); pH (> 6 and <9). The data were grouped by USZ configuration events and SZ configuration events.



Regarding the *E. coli* results, the inflow concentration in all USZ events presented similar values (around 40 MPN/100mL), and the Ev.1 and Ev.2 experiments presented outflow concentration values below the limit established by the standard, while the Ev.5 experiment showed a higher value in only two samples. The results of the *E. coli* parameter in SZ events presented the variability of the inflow concentration and each experiment had a different outflow concentration behavior. Ev.3 resulted in all concentration values above the limit of the NBR 15527 standard (ABNT 2019); Ev.4 had a similar behavior, however with only two samples within the standard limit. Ev.4 and Ev.7 presented all outflow concentrations higher than the inflow, but Ev.7, despite this, presented outflow concentrations close to the guideline limit. Ev.6 showed all sample concentrations below the inflow concentration and the standard limit, except for one sample at 15 minutes. This may be the result of errors originating from contamination during the experiment, sample transport, or laboratory analysis. Figure 2.5 shows the *E. coli* results according to event settings.

Figure 2.5 - *E. coli* parameter behavior over time in each experiment grouped by USZ configuration events and SZ configuration events. The NBR 15527/2019 (ABNT 2019) limits were added for comparison.



The results are different from those observed in the literature, which typically indicates the reduction of *E. coli* and bacteria with the increase in the depth of the submerged zone (Chandrasena et al. 2014; Chandrasena et al. 2017; Stott et al. 2017). This can be explained by differences in the initial conditions of the experiments and in the structure of the system (the height of the saturated zone used in this work is 20 cm, which may not be sufficient for significant reductions such as those presented in the work of Chandrasena et al. (2014) who used a saturated zone height of 30 cm). Vegetation selection also influences reducing the concentration of *E. coli* (Shirdashtzadeh et al. 2017; Kim et al. 2012).

The removal efficiency for parameters that are measured in concentration (mg/L) was calculated based on the EMC values (Table 4). Figure 2.6 shows the average quality results of inflow, outflow, and removal efficiencies of the system of the following pollutants: NO_2, NO_3, NH_3, TP and COD in both configurations of the experiments, USZ and SZ. When there is a negative efficiency, it means that the system exported pollutants.

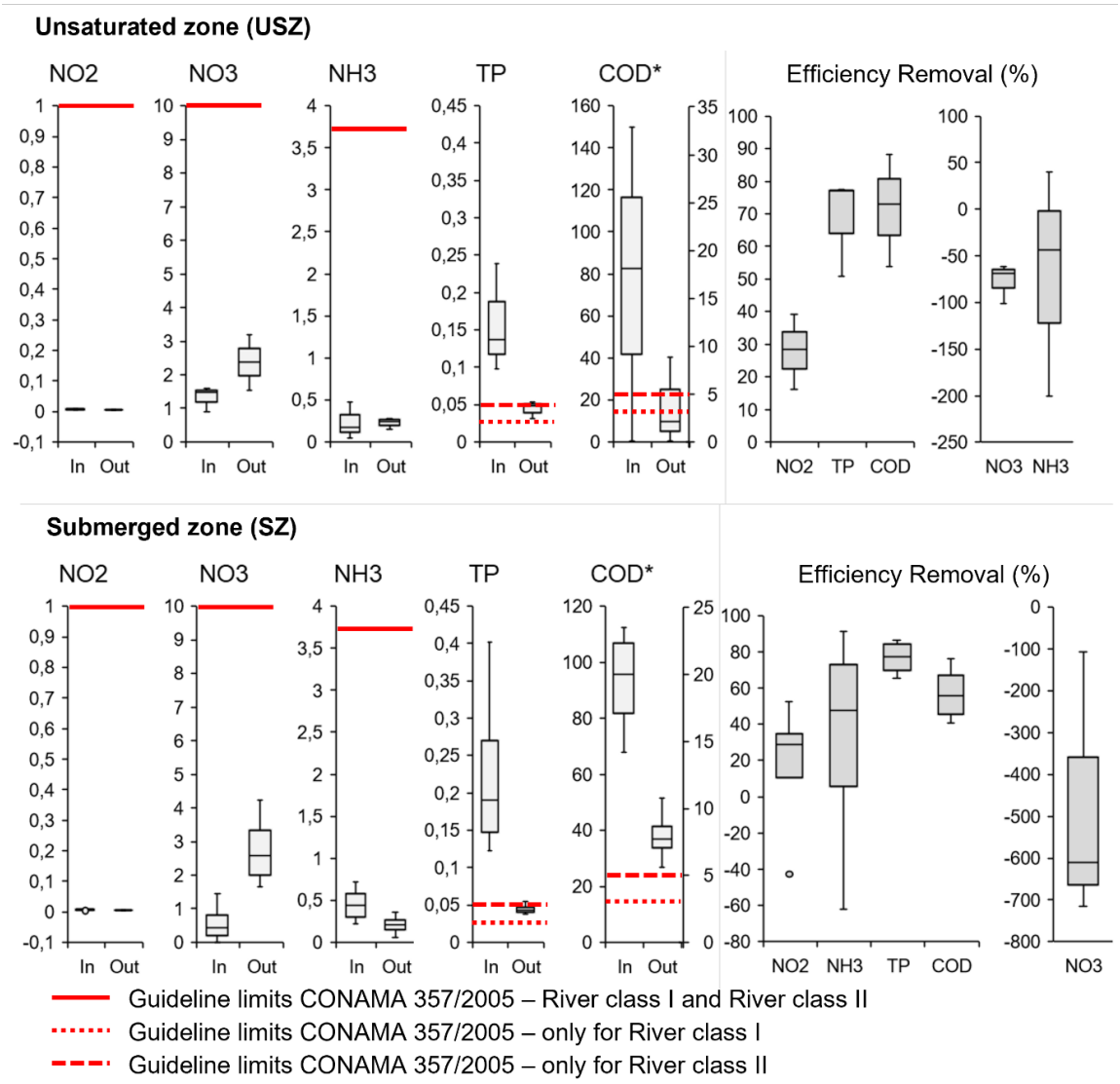
Table 2.4 - Event Mean Concentration of the events

Event	EMC (mg/L)									
	TP		NO_2		NO_3		NH_3		COD	
	In	Out	In	Out	In	Out	In	Out	In	Out
1	0.098	0.048	0.006	0.005	1.58	3.18	0.05	0.15	0.7	0.3
2	0.137	0.031	0.007	0.004	1.48	2.39	0.47	0.28	150.0	40.5
3	0.225	0.037	0.007	0.005	0.00	1.64	0.22	0.36	86.3	51.4
4	0.154	0.045	0.007	0.005	0.60	4.23	0.33	0.24	105.0	37.9
5	0.238	0.054	0.007	0.005	0.91	1.53	0.17	0.25	82.5	9.7
6	0.124	0.042	0.004	0.005	0.26	2.12	0.54	0.18	68.0	35.9
7	0.402	0.055	0.011	0.005	1.46	3.02	0.72	0.06	112.5	26.9
Average SZ	**0.16 ± 0.06**	**0.04 ± 0.009**	**0.007 ± 0.0005**	**0.005 ± 0.0004**	**1.32 ± 0.29**	**2.37 ± 0.7**	**0.23 ± 0.18**	**0.23 ± 0.05**	**77.7 ± 61.0**	**16.8 ± 17.2**
Average USZ	**0.27 ± 0.11**	**0.04 ± 0.006**	**0.007 ± 0.002**	**0.005 ± 0.0**	**0.58 ± 0.55**	**2.7 ± 0.99**	**0.45 ± 0.19**	**0.21 ± 0.1**	**92.9 ± 17.3**	**38 .0 ± 8.7**

USZ: Unsaturated zone (lower exit valve)

SZ: Submerged zone (upper exit valve)

Figure 2.6 - Average inflow and outflow concentrations calculated by the EMC for each parameter. In COD* graphic, the second axis refers to estimated BOD values, through the ratio COD/BOD = 5. The limits of CONAMA 357/2005 - River class I (only requires simplified treatment for drinking water) are: 1 mg/L for NO_2; 10 mg/L for NO_3; 3.7 mg/L for NH_3 (for pH ≤ 7.5); 0.025 mg/L for TP; 3 mg/L for BOD. For the River class II category, the same limits are applied, except for 0.05 mg/L for TP and 5 mg/L for BOD.



In this study, COD values were calculated; however, the CONAMA 357/420 regulation (BRASIL 2005) presents a limit only for the BOD parameter. Thus, we calculated an average COD:BOD ratio from literature studies, which presents COD and BOD values for the Mineirinho River watershed in Sao Carlos municipality. Galavoti (2012) performed a qualitative analysis of the water drained from the zinc roofing tiles in

an experimental peri-urban plot in the city of São Carlos. From the COD and BOD results obtained by Galavoti (2012), the average COD:BOD ratio was calculated by eliminating the experimental sites with BOD values <1, thus we reached a ratio equivalent to 8.6. Martins (2017) monitored 19 events in 2015 in the Mineirinho watershed outlet. According to the results obtained by Martins (2017), the average COD: BOD ratio was calculated for the dry and rainy periods, resulting in 3.5 and 4.8, respectively. Thus, an average COD:BOD ratio value of 5 was chosen for discussion with the legislation limit. Therefore, in USZ events, the estimated BOD removal efficiency would lead to almost all results within the limit for River class II, below 5 mg / L and at least more than half of the data still below 3 mg / L within the most restrictive category River class I. In SZ events, the removal was not sufficient to meet the regulation; however, the estimated BOD entry values were higher than in USZ events. Both types of configurations showed good efficiency in the removal of COD (on average, 71.6% in USZ events and 57% in SZ events), which indicates that more than half of the organic matter from the incoming pollution is retained in the filter media. However, the stored values $(EMC_{in} - EMC_{out})$ are relatively low (average of 60 mg / L).

The system also showed good efficiency in TP removal in the two configurations evaluated. On average, the system reduced TP to 68.5% in USZ events and 74.3% in SZ events. In both configurations, TP removal was sufficient for the effluent to meet the category of River class II. However, TP removal was not enough to meet River class I limits. The phosphorus (P) present in stormwater runoff is in the form of particulate phosphorus (PP) and dissolved phosphorus (DP), in which DP was the most common form. The main way of eliminating phosphorus in bioretention systems occurs by filtration processes of PP (Li & Davis 2016) and geochemical processes of adsorption and chemical precipitation with metallic salts of DP (Hunt et al. 2012; Lucas & Greenway 2008). You et al. (2019) point out that soils composed of metal ions in the bioretention filter may be the key to increasing the removal efficiency of DP due to chemical reactions, thus transforming into PP. Li & Davis (2016) also reported on the relationship between the filter media depth, the reduction in P concentration and the soil adsorption capacity, since a high soil adsorption capacity can represent a lower height of the required filter media depth. Thus, the addition of compounds in the filter media to increase soil adsorption can increase the efficiency of the system.

Regarding the nitrogen series, within the bioretention system, nitrification processes occur in the USZ due to the amount of oxygen present in the soil (mainly because the soil

in question is formed by 80% sand) and denitrification in the SZ due to the creation of an anaerobic zone. The system showed an average NO_2 removal efficiency of 28% ± 9.4% in USZ events and 16.7% ± 37.7% in SZ events. There was export of NO_3 in all experiments, which may be related to the initial concentration of this element in the soil. In addition, the nitrogen treatment in bioretention systems occurs in the interevent (which mainly treats NO_3), thus the biochemical processes will interfere in the next event, while the physical-chemical processes (sorption, which mainly treats NH_4) will interfere in the event itself. According to Osman et al. (2019), the export of NO_3 is always higher than NH_4 due to the interactions of ion charges with the soil. The NH_4 charge is positive (NH_4^+), and it interacts easier with negative soil particles, therefore the NH_4 is also retained by adsorption processes of the filter media. NO_3 has a negative charge (NO_3^-), and therefore interacts less with the soil, being more easily exported from the bioretention during the event. In addition, the increase in nitrification limit denitrification (Osman et al. 2019), that is, the higher removal of NH_4, the higher the formation of NO_3. Thus, regarding the NH_4 parameter, the events with USZ showed a lower average removal efficiency compared to the experiments with SZ.

Nitrate leaching can be explained due to: (1) the number of dry days preceding between one event and another, in which, this period favored nitrification, regardless of the existence or not of the submerged zone during the events. For example, Ev.4 and Ev.7, despite being performed with SZ, were done after a long period (41 and 28 days), therefore the saturated zone may have reduced over the days due to plant evapotranspiration, giving space to the aerobic zone, resulting in reduced NH_4 and increased nitrate formation/export; and (2) in addition, the experiments were carried out without the presence of an internal source of carbon to simulate the behavior of a common bioretention system in Brazil, which may have limited the denitrification process, therefore contributing to the NO_3 leaching. Studies indicate that maintaining an anaerobic condition promoted by the submerged zone with an additional carbon source is suitable for chemical denitrification reactions that occurred within the bioretention system (Luo et al. 2020; Wan et al. 2017; Erickson et al. 2013). However, despite the leaching, these results showed that the values of the nitrogen series are all within the limit of CONAMA resolution 357 for “River class I” (BRASIL 2005).

2.3.2 Stormwater harvesting from a bioretention system

Stormwater harvesting from a bioretention system is still a recent issue that has been studied (Payne et al. 2019; Lim et al. 2015; Vijayaraghavan et al. 2021). The main problem related to the harvest stormwater from biofilters is the need for methods to validate the quality of the system effluent. Zhang et al. (2015) proposed a validation based on three steps: (1) pre-validation, to identify target pollutants and potential removal by the system; (2) validation monitoring of hydraulic and treatment performance and (3) operational monitoring. In this case, the development of RTC strategies for monitoring becomes increasingly important. Another issue is the additional cost, both for implementing the reservoir for water reuse, and for the lined bioretention, to improve water quantity.

The bioretention system works as a primary treatment for stormwater; however, some pollutants are difficult to remove, such as pathogens and nitrogen. Concerning this, the substitution approach refers to the use of lower quality water instead of drinking water for non-potable purposes (Lau et al. 2017). According to Lim et al. (2015), the viral health risk of using harvested urban stormwater for toilet-flushing was below the United States Environmental Protection Agency (U.S. EPA) annual risk benchmark. In addition to what was mentioned throughout this study about changes in the system design, e.g., plant selection, substrate of the filter media and systems with or without a submerged zone; some studies analyze the optimization of the system's operating conditions. Shen et al. (2020) used RTC strategies to improve microbial efficiency through the operating conditions of the system. For example, the system was able to increase the detention time of the stormwater runoff within the submerged zone to improve pollutant removal.

2.4 CONCLUSIONS

The water balance of the bioretention system showed a reduction in peak flow at both outlet heights used for the experiments, with an average of 48% to 62% in the experiments without and with submerged zones, respectively. In addition, the system has an average volume retention efficiency of 20.9% to 23.4%, which means that the system releases 76.6% - 79.1% of the inflow volume that can be temporarily stored with the addition of a reservoir after the bioretention, and sent to the rain drainage system, reducing the occurrence of floods, or reusing them for multiple purposes, increasing water security in times of water crisis. Regarding qualitative aspects, the bioretention showed different values for reducing pollutants depending on the presence or absence of a SZ. In the

experiments with SZ, the high values of turbidity and *E. coli* exceeded the limits of the NBR 15527 resolution (ABNT 2019). The export of NO_3 was also observed; however, the nitrate values were still within the CONAMA resolution 357/420 (BRASIL 2005), on average 74.14% below the limit. In experiments with USZ, the values of the parameters *E. coli* and pH were below the limit of the NBR resolution (ABNT 2019), except for turbidity, and there was no reduction in NH_4 values. Thus, bioretention systems work for flood mitigation and as a sustainable alternative for urban water treatment. However, for harvesting stormwater reuse, some modifications in the design must be tested aiming to improve water quality, as well as the fit-for-purpose approach, in which, based on studies and monitoring, the optimized configuration for each type of water reuse can be defined.

The limitations of this study are related to the control of input quality pollutants, since with the sweeping method, the concentrations of pollutants are not previously defined, therefore it is recommended to carry out experiments with known initial concentrations, as well as the simulation of other types of rainfall, with different durations and return times. Moreover, it is recommended to evaluate other improvement strategies in the bioretention design for removing target pollutants (e.g., adding carbon source to the filter media; plant species selection to reduce *E. coli*), as well as increasing the number of monitoring events with the same operating conditions, (e.g., the same antecedent dry periods to check removal patterns). Thus, an optimized bioretention system can be achieved for removing persistent pollutants from this region. Furthermore, this can contribute to a better understanding of operational conditions, aiming at stormwater harvesting in a sustainable way.

This study contributed to the advancement of sustainable development practices for stormwater management as a viable alternative to ensure water security. As an initial exploratory analysis of water quality between USZ and SZ systems, this study provides an initial guide for future studies regarding pollutant removal efficiencies of a common bioretention system in Brazil. The implementation of a reservoir for reuse contributes to the mitigation of extreme events due to climate change and urbanization, increasing urban resilience in line with the 11th (sustainable cities and communities) and the 13th (climate action) United Nations Sustainable Development Goals (UN, 2020).

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3 MODELING OF E. COLI IN BIORETENTION SYSTEM: CALIBRATION OF QUALITATIVE PARAMETERS

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Abstract

Bioretention systems are efficient in improving the runoff quality, making it a good alternative for primary treatment of stormwater harvesting. One of the problematic pollutants of urban waters is pathogenic organisms, such as *E. coli*. Microbial modeling is an important tool for understanding the behavior of microorganisms in biofilters, however, due to the sensitivity of pathogens, the calibration of parameters is complex. Thus, this work presents a comparison of the values of the main parameters in microbial modeling (adsorption and desorption coefficients and die-off rate), from different events used for calibration. A total of 10 synthetic events were monitored for data collection of the effluent from a bioretention box, which were used in different combinations for calibration. Root Mean Square Error (RMSE) minimization of observed and modeled values was used in the calibration. The results showed low values of RMSE ranging from 1.0 to 6.79 MPN / 100ml, however two events, when calibrated separately, showed a good relationship between modeled and observed concentration. More events must be monitored so that other relations between parameters and antecedent event conditions can be observed.

Keywords: *E. coli*; Die-off rate; Low Impact Development practices.

3.1 INTRODUCTION

Problems related to water resources are increasingly common. The increase in impervious surfaces results in the risk of flooding due to the rapid runoff formation (Kong et al., 2021). Furthermore, population growth and increased demand for water, associated with climate change and environmental issues, promote water scarcity (IPCC, 2019; Hristov et al. 2021). Thus, it is essential to discuss alternative solutions to complement the water demand. According to Goonetilleke et al. (2017), stormwater harvesting can increase water security, saving the excessive demand for water resources and reducing the risk of water scarcity.

However, stormwater runoff does not always have a good quality to be directly reused due to particle deposition on the surface areas of cities (such as roofs, sidewalks, streets, and roads), which are carried during a precipitation event resulting in environmental damage (Fletcher et al. 2013). The main pollutants contained in runoff are heavy metals (mainly Cu, Pb and Zn in high concentrations (Maniquiz-Redillas and Kim, 2016)), solid particles, nutrients (mainly nitrogen and phosphorus), organic matter, and pathogenic microorganisms (Grogan et al., 2021; Eckart et al., 2017; Ma et al., 2019). Among them, the main pollutant that most interferes in stormwater harvesting due to health risk is faecal microbes (Fletcher et al., 2008). Despite that, stormwater runoff can be considered as a viable water source for non-potable purposes, such as toilet flushing and irrigation (Lim et al., 2015).

A bioretention system, also known as a rain garden or biofilter, consists of a filtering layer and an internal storage layer that serve both to reduce the peak flow and pollutants as a result of plant uptake. Several studies have shown the efficiency of bioretention systems in removing *E. coli* due to the saturated zone present within the system (Chandrasena et al. 2014; Stott et al. 2017; Li et al. 2012). This is due to the governing processes of adsorption, desorption, and die-off rate (predation, competition, etc.) (Hathaway et al. 2011). In addition, it is possible to optimize the system to focus on the removal of target pollutants, through plant selection, filtering media type, and the underdrain outlet height (Li et al. 2021).

Modeling is an important tool for understanding the behaviors inside biofilters, however, the simulation of microbiological processes becomes even more complex when analyzing a sensitive pollutant such as *E. coli*. In addition to the governing processes, different factors can affect the microorganism behavior within bioretention systems, such as soil moisture, temperature, evapotranspiration rate, etc., and this significantly compromises the model calibration and validation result.

This study aims to compare the values of different parameters of *E. coli* modeling, from the calibration of events under different initial conditions in a bioretention at a prototype scale. To do this, synthetic events were monitored in a bioretention system on a laboratory scale for data collection and we used the microbiological removal model in biofilters for urban waters developed by Shen et al. (2018) and the Macedo calibration model (2020) to obtain the different modeling results.

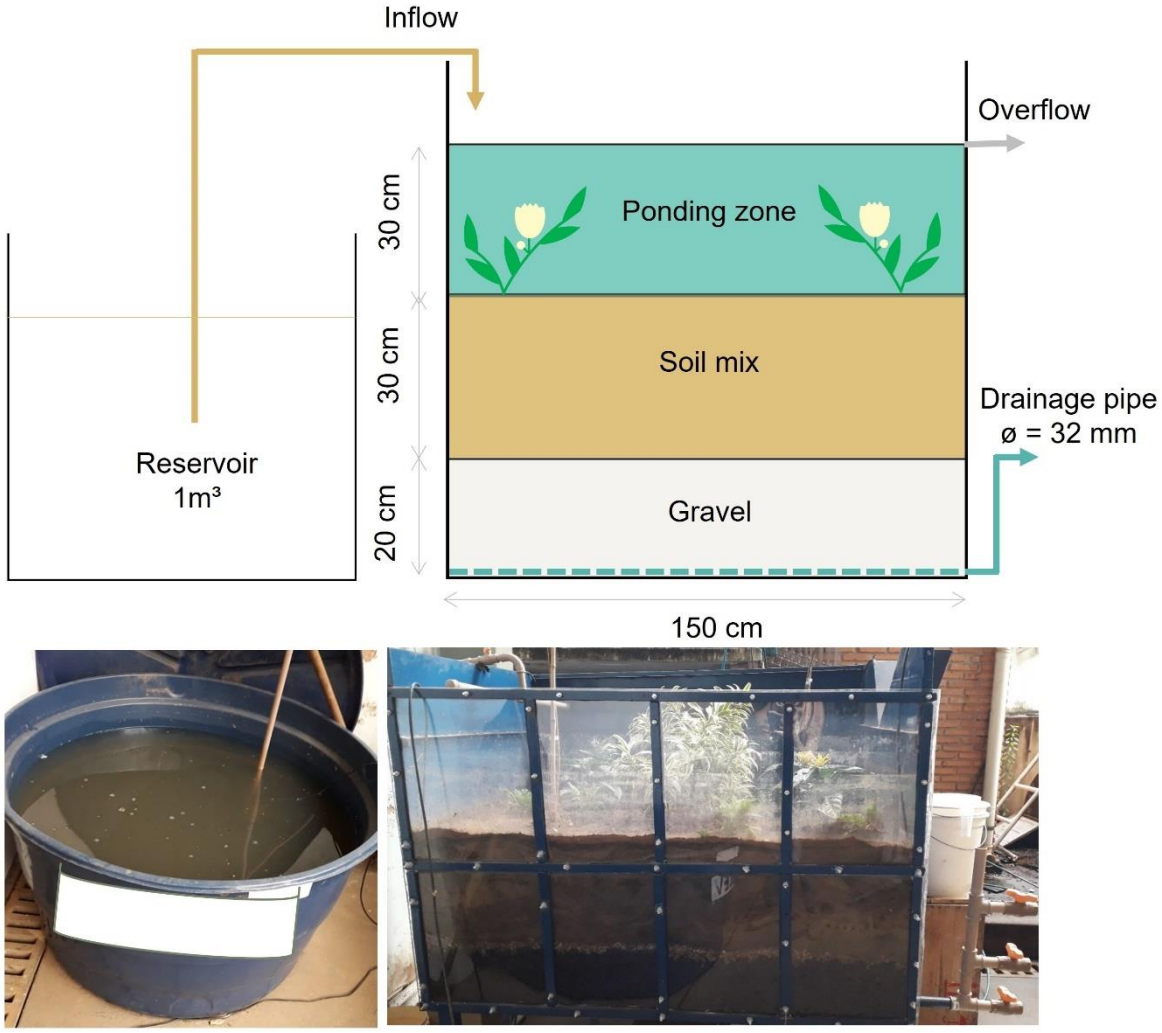
3.2 METODOLOGY

The methodology of this study follows two main modules: (1) Maintenance and updating of a mathematical model for microbiological removal in biofilters for urban waters; (2) Calibration and validation of the model based on observed data.

3.2.1 Bioretention box and synthetic monitored events

For data collection, synthetic precipitation events were monitored on a laboratory-scale bioretention system, located at the University of São Paulo (USP), in São Carlos – SP, Brazil. The bioretention prototype was built to represent a field-scale bioretention, therefore, the prototype aims to guarantee physical similarities (the dimensions of the prototype are at a 1:2 scale with the field system) and dynamic and hydraulic similarities by using the same type of building materials and filtering media. The field system receives precipitation from a roof covering 94 m^2, thus, to simulate events in the laboratory, reduced equivalent precipitation was calculated for the dimensions of the prototype, defined by Macedo et al., (2021). Figure 3.1 shows the schematic representation of the bioretention prototype.

Figure 3.1 - Schematic design of the bioretention box



The prototype consists of three main layers: the Ponding Zone (PZ); filtering media; and drainage layer. The PZ is the vegetated area designated to receive runoff, it is 30 cm high, and it is possible to store runoff to this water level height before there is flow through the spillway. The filtering media consists of a mixture of 80% sand for filtering pollutants and 20% of the region's native soil to improve plant root fixation. The drainage layer is formed by gravel with a porosity of 0.408. At the bottom, there is a perforated drain with 32 mm of diameter to outflow.

Synthetic events were monitored, evaluating quantitative (flow and water level in PZ) and qualitative (*E. coli* and Total Coliforms by the Colilert method) aspects. The events were simulated with approximately 30 minutes duration, a return period equivalent to 5 years, and constant inflow at 0.4 L/s. The inflow was prepared by the sweeping method (Maglionico, 1998), in which the pollution is swept and collected to later be added to the experiment inlet water, simulating the water quality of the local surface runoff. During the experiments, 2

samples of the inlet water were collected to verify the uniformity of the pollutant concentration at the beginning and at the end of the event; and 10 samples of the bioretention effluent were collected to monitor the behavior of the pollutant over time, one in every 5 minutes. Thus, the event pollutograph with the behavior of the pollutant over time was obtained. For the sake of comparison with other studies, the event mean concentration for the inflow and outflow were also calculated from Equation 1.

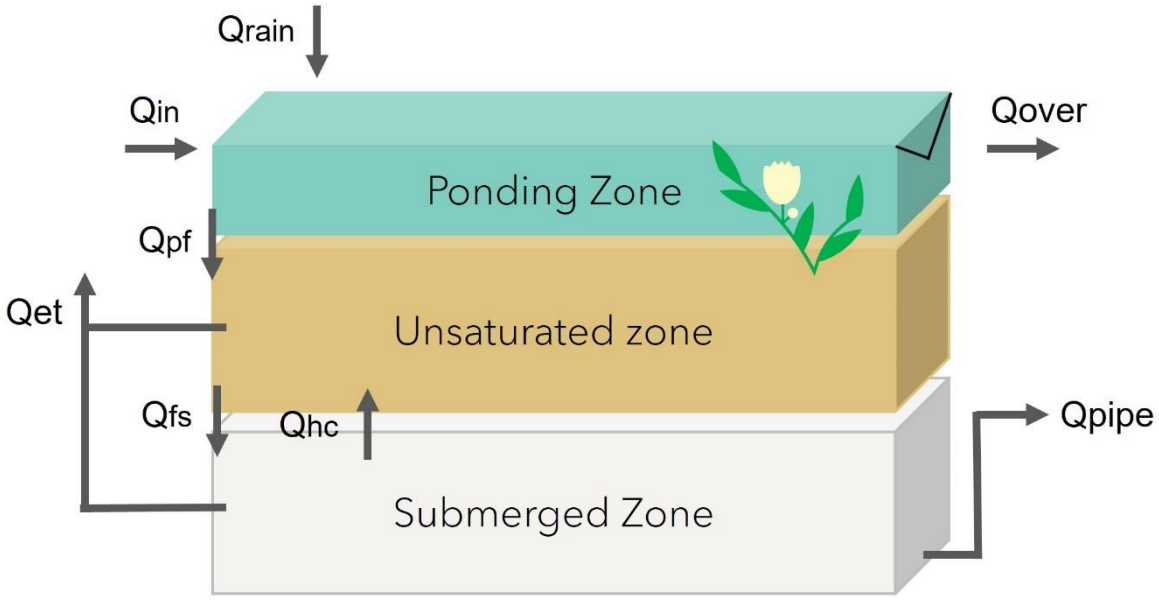
$$EMC = \frac{\sum_0^t (C^t * Q^t * \Delta t)}{\sum_0^t (Q^t * \Delta t)} \quad (1)$$

Where: $EMC =$ Event Mean Concentration [MPN/100ml]; C^t = *E. coli* concentration, in time t [MPN/100ml]; Q^t = Flow, in time t [L/min]; Δt = Time interval [min].

3.2.2 Quantitative module

Quantitative modeling is based on the equations of Randelovic et al. (2016) and Shen et al. (2018) with adaptations. Appendix A contains more details of the quantitative module equations. The model is based on the approach of "three buckets" that represent the layers of the bioretention system: Ponding Zone (PZ), Unsaturated Zone (USZ) and Submerged Zone (SZ). The water balance with inputs and outputs at each time interval was performed in all layers. The inlets and outlets of each layer were presented in Figure 3.2. The model includes as an outlet, in all layers, the flow infiltrated around the soil in case of a system unlined on the lower base and side faces, however this flow was considered null because the prototype system on a laboratory scale is lined and, therefore, it has no contact with the ground. Thus, the water balance of the PZ is defined by Equation 2. Q_{in} and Q_{rain} are input variables imported into the model. Q_{over} occurs if the height of the ponding zone exceeds 30 cm, and it is calculated by the triangular weir equation.

Figure 3.2 - Schematic representation of the layers of the bioretention system in the model from the approach of the three modules and main variables of the quantity model.



In the USZ layer, the mass balance is given by Equation 3, in which the input variables are: Flow infiltrated by the PZ (Q_{pf}) and the Flow rate of capillary rise (Q_{hc}) referring to the capillary effect of the SZ on the USZ. The outputs of this balance are the Infiltrated Flow in the SZ (Q_{fs}) and the Evapotranspiration Flow (Q_{et_usz}). The process of infiltration into the system, from PZ to USZ and from USZ to SZ, is governed by Darcy's Law. The evapotranspiration is described by the equation of the studies by Shen et al., (2018), Standard FAO-56, in which the reference daily evapotranspiration (ET_0) for the study area was used [21°57'42" S, 47°50'28" W, 860m], imported as an input variable for the model and obtained through an automatic weather station operated by EMBRAPA since 2010. An evapotranspiration coefficient for plants is also considered, which can influence the result depending on the physiology of the leaves and the plant's evapotranspiration capacity.

In the SZ, the mass balance is governed by Equation 4. The SZ occurs only when there is Internal Water Storage (IWS). In experiments that are operated with the higher outlet valve, there is an occurrence of a continuous submerged zone. The input variable is the Infiltrated flow from USZ to SZ (Q_{fs}), while the outputs are Flow by capillary rise (Q_{hc}), Evapotranspiration flow (Q_{et_sz}) and Outflow (Q_{pipe}). The significant water outlet occurs by (Q_{pipe}) defined by the filter's infiltration capacity or by the size of the exit pipe diameter. The model also considers the possibility of no submerged zone, in this case, the lower register is

used and the USZ mass balance is corrected considering the Q_{pipe} output, and disregarding Q_{hc}, Q_{fs} and Q_{et_sz}.

$$\frac{\partial S_{pz}}{\partial t} = Q_{in}{}^{t} + Q_{rain}{}^{t} - Q_{pf}{}^{t} - Q_{over}{}^{t} \quad (2)$$

$$\frac{\partial S_{usz}}{\partial t} = Q_{pf}{}^{t} + Q_{hc}{}^{t} - Q_{fs}{}^{t} - Q_{et\_usz}{}^{t} \quad (3)$$

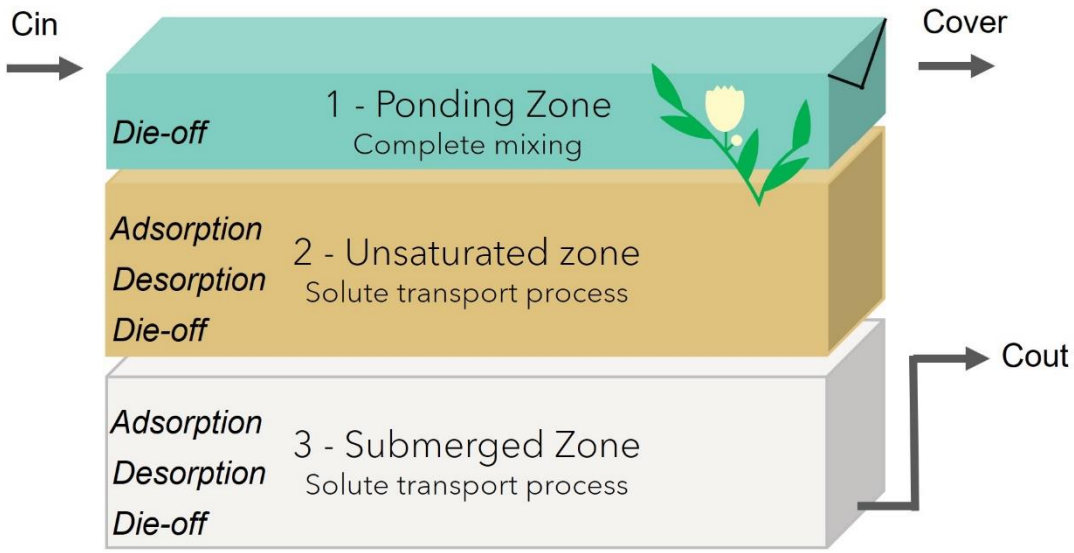
$$\frac{\partial S_{sz}}{\partial t} = Q_{fs}{}^{t} - Q_{hc}{}^{t} - Q_{et\_sz}{}^{t} - Q_{pipe}{}^{t} \quad (4)$$

Where: S_{pz} = Storage in Ponding Zone, in time t [m^3]; Q_{in} = Inflow, in time t [m^3/s]; Q_{rain} = Flow from precipitation, in time t [m^3/s]; Q_{over} = Overflow, in time t [m^3/s]; Q_{pf} = Infiltration flow to USZ, in time t [m^3/s]; S_{usz} = Storage in Unsaturated Zone, in time t [m^3]; Q_{hc} = Capillary rise flow, in time t [m^3/s]; Q_{fs} = Infiltration flow to SZ, in time t [m^3/s]; Q_{et_usz} = Total evapotranspiration flow in USZ, in time t [m^3/s]; Q_{et_sz} = Total evapotranspiration flow in SZ, in time t [m^3/s]; Q_{pipe} = Drainage pipe flow, in time t [m^3/s]; dt = Time interval [s].

3.2.3 *E. Coli* qualitative module

Figure 3.3 presents the schematic inputs and outputs of the qualitative model, as well as the governing processes of each layer. Appendix B contains more details of the *E. Coli* module equations. The qualitative model is described by the complete mixing equation of the concentration over time in the PZ (Eq. 5) and by the one-dimensional solute transport advection-dispersion equation in the filter extension, in the USZ and SZ (Eq. 6).

Figure 3.3 - Schematic representation of the layers of the bioretention system in the quality model with the main variables and microorganism removal reactions.



In the model, three governing processes occur in the removal of microorganisms: adsorption, desorption and die-off rate (Shen et al., 2018; Chandrasena et al., 2014). As considered by Shen et al., (2018), the adsorption and desorption processes were represented by different parameters, instead of the usual equilibrium approach between the two processes. Following the methodology of qualitative models of microorganisms (Shen et al., 2018; Chandrasena et al., 2014; Zhang et al., 2012), the governing processes of the model are presented by first-order kinetic equations Eq. (7), applied to USZ and SZ. Die-off is estimated in the three layers of the system since in the PZ, under saturated soil conditions when the water level may take a long time to fully infiltrate; such as along the filter, in which microorganisms can be trapped for days between the occurrence of one event and the next.

The transport equations along the filter are considered only in the z direction (downflow) and are solved by a numerical solution by the progressive difference method for the derivative in time and by the central difference method for the first order derivative in space. Thus, from a point of known value ($z = 0$), the value of the function is determined to a close value ($z + \Delta z$), where precision occurs the smaller the Δz spacing. Figure 3.4 shows the flow within the bioretention system, at the beginning of an event, over time with the schematic Δz spacings. The unit flux (q) (Eq.8), used to calculate the advection, takes the auxiliary parameters for boundary conditions α and β, whose sum will always be equal to 1, for inclusion of the influence of fluxes according to the position of the layer along the filter, (e.g., the flow in the upper layers has more influence of the flow that infiltrates from PZ to USZ

(Q_{pf}) than the capillary rise flow (Q_{hc}) present in the layers close to the SZ, thus in the upper layers α ≈ 1 and β ≈ 0 while in the lower layers α ≈ 0 and β ≈ 1).

The reactions of adsorption and desorption are incorporated in Eq. 7. The die-off rate, which represents the reduction of microorganisms by die-off, predation, and competition, is represented by Eq. 9.

$$\frac{\partial(C_{pz}^{t+1}\, h_{pz}^{t+1}\, A)}{\partial t} = C_{in}^{t} Q_{in}^{t} - C_{pz}^{t-1} * \left(Q_{pf}^{t} + Q_{over}^{t}\right) + R_{pz}^{t} \tag{5}$$

$$\frac{\partial \theta^{t+1}\, C^{t+1}}{\partial t} + \rho \frac{\partial C_{soil}^{t+1}}{\partial t} = \frac{\partial}{\partial z}\left(D * \theta^{t} \frac{\partial C^{t}}{\partial z}\right) - \frac{\partial q^{t}\, C^{t}}{\partial z} + R^{t} \tag{6}$$

$$\rho \frac{\partial C_{soil}^{t+1}}{\partial t} = \theta^{t+1} * k_{ads} * C^{t} - \rho * k_{des} * C_{soil}^{t} + R_{soil}^{t} \tag{7}$$

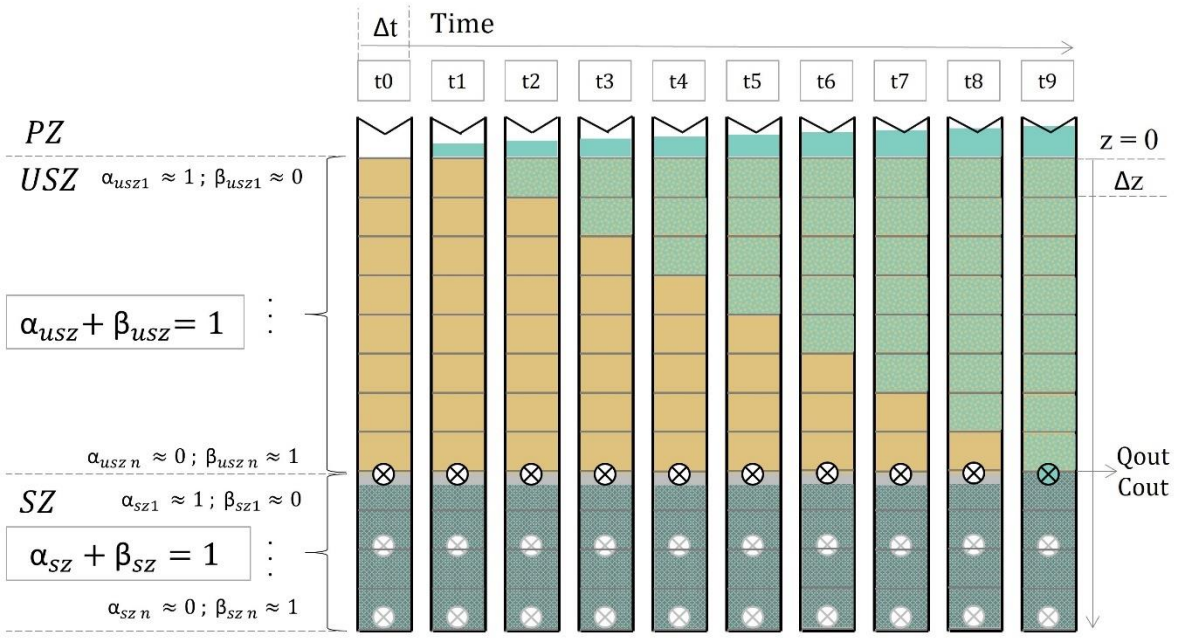
$$q_{usz}^{t} = \frac{\alpha_{usz} * \left(Q_{pf}^{t} - Q_{et_{usz}}^{t}\right) + \beta_{usz} * \left(Q_{fs}^{t} - Q_{hc}^{t}\right)}{A}$$

$$q_{sz}^{t} = \frac{\alpha_{sz} * \left(Q_{fs}^{t} - Q_{hc}^{t} - Q_{et_{sz}}^{t}\right) + \beta_{sz} * \left(Q_{pipe}^{t}\right)}{A} \tag{8}$$

$$\mu = -\mu_0 * \emptyset^{(T^t - 20)} \tag{9}$$

Where: C_{pz} = PZ concentration, in time t [MPN/100ml]; h_{pz} = Water level in PZ, in time t [m]; A = Bioretention surface area [m^2]; C_{in} = Inflow concentration, in time t [MPN/100ml]; Q_{in} = Inflow, in time t [m^3/s]; Q_{pf} =Infiltration flow from PZ to USZ, in time t [m^3/s] Q_{over} = Overflow, in time t [m^3/s]; R_{pz} = PZ reactions, in time t [MPN/100ml]; θ = Soil water fraction by volume in USZ or SZ, in time t [-]; C = Concentration in USZ or SZ, in time t [MPN/100ml]; ρ = Soil bulk density [kg/L]; C_{soil} = Soil concentration in USZ or SZ, in time t [MPN/100ml]; D = Diffusion coefficient [-]; R = Reactions in USZ or SZ, in time t [MPN/100ml]; k_{ads} = Adsorption rate [/s]; k_{des} = Desorption rate [/s]; R_{soil} = Soil reactions, in time t [MPN/100ml]; q_{usz} = Average unity flow in USZ, in time t [-]; α_{usz} = Boundary conditions parameter in USZ [-]; β_{usz} = Boundary conditions parameter in USZ [-]; $Q_{et_{usz}}$ = Evapotranspiration flow in USZ [m^3/s]; Q_{fs} = Infiltration flow from USZ to SZ, in time t [m^3/s]; Q_{hc} = Capillary rise flow, in time t [m^3/s]; q_{sz} = Average unity flow in SZ, in time t [-]; α_{sz} = Boundary conditions parameter in SZ [-]; β_{sz} = Boundary conditions parameter in SZ [-]; $Q_{et_{sz}}$ = Evapotranspiration flow in SZ, in time t [m^3/s]; Q_{pipe} = Drainage pipe flow, in time t [m^3/s]

Figure 3.4 - Representation of flow displacement within the bioretention system over time from the division of Δz spacings.



3.2.4 Calibration and validation

For calibration, an automatic calibrator was used with the Distributed Evolutionary Algorithms (DEAP) library in Python, developed by Macedo (2020). For the quantitative module, the maximization of the Nash Sutcliff Efficiency (NSE) (Eq. 10) was used, comprising the average of the outflow and the water level in PZ. The parameters and ranges used are described in Table 3.1.

$$NSE = 1 - \frac{\sum_{i=1}^{n}(Y_i^{obs} - Y_i^{sim})^2}{\sum_{i=1}^{n}(Y_i^{obs} - Y_i^{mean})^2} \quad (10)$$

Where: Y_i^{obs}= Observed value; Y_i^{sim} = Simulated value; Y_i^{mean} = Mean of observed data; n = Total number of observations.

Table 3.1 - Quantity parameter information for calibration

Symbol	Meaning	Dimensions	Min	Max
Kc	Evapotranspiration constant for plants	-	0	0.5
Ks	Saturated hydraulic conductivity	cm/s	$1.0x10^{-3}$	$1.0x10^{-1}$
Sh	Hygroscopic point moisture	-	0.02	0.08
Sw	Wilting point moisture	-	0.03	0.15
Sfc	Field capacity	-	0.1	0.7
Ss	Plant stress moisture	-	0.1	0.6
Cd	Discharge coefficient for the pipe	-	0.05	0.7

For the qualitative module, the objective function of this calibrator varies according to the presentation of *E. coli* data, for example, with the pollutograph data throughout time, the objective function was used to maximize NSE; with the EMC data, the objective function was used to minimize the Root Mean Square Error (RMSE) (Eq. 11). The quality parameters are described in Table 3.2. The limits of the parameters were initially defined by the range chosen by Shen et al. (2018) and afterwards adjusted so there was no instability in the model. The parameters were considered the same for the USZ and SZ. As it is a sensitive indicator, the input and output *E. coli* concentration values were log-transformed before using the calibration module. This step becomes necessary, therefore the peaks are not emphasized in the model, avoiding any bias. Due to the number of events available, each event was used for calibration individually and in different combinations of grouping two events at a time.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(Y_i^{obs} - Y_i^{sim})^2}{n}} \quad (11)$$

Where: n = Total number of observations.

Table 3.2 - Quality parameter information for calibration

Symbol	Meaning	Dimensions	Min	Max
k_{ads}	Adsorption rate	/s	$1.0x10^{-4}$	$9.0x10^{-4}$
k_{des}	Desorption rate	/s	$1.0x10^{-4}$	$5.0x10^{-2}$
μ_0	Die-off rate	/s	$1.0x10^{-7}$	$1.0x10^{-3}$
$\emptyset$	Temperature correction coefficient	-	$1.0x10^{-8}$	$1.0x10^{-3}$

3.3 RESULTS AND DISCUSSION

3.3.1 Description of monitored events

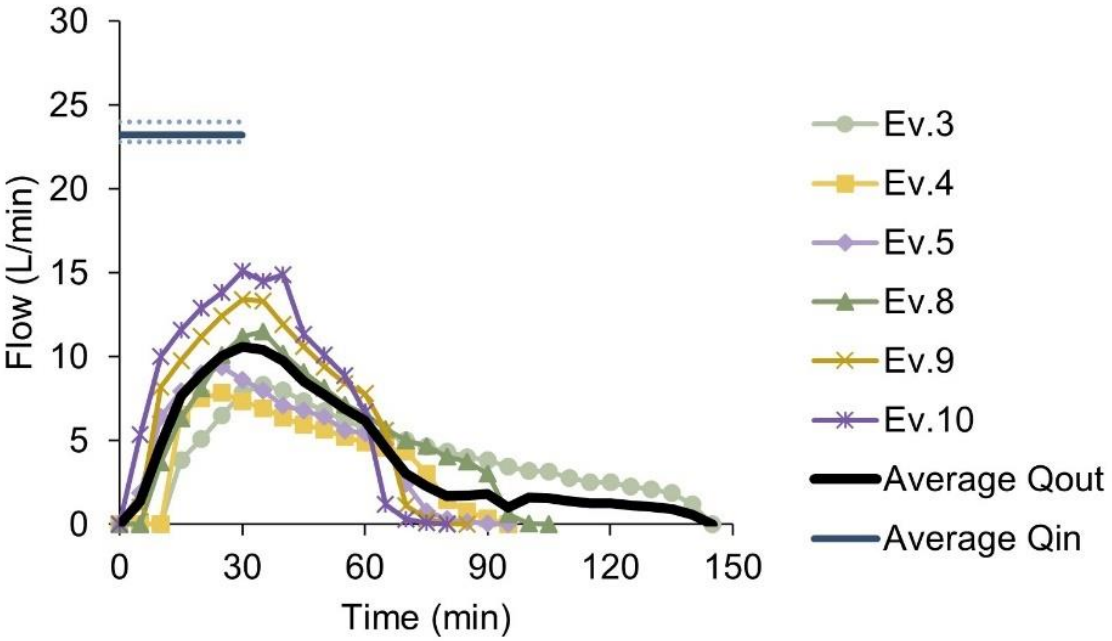
A total of 10 synthetic events were performed with the prototype configured with the presence of a submerged zone within the system. For qualitative monitoring, six events were carried out. Among these qualitative monitored events, half occurred in the winter (Ev.3, Ev.4 and Ev.5) and the other half in the summer (Ev.8, Ev.9 and Ev.10). Thus, respecting the location's climatic characteristics, the events monitored in winter have more previous dry days as it is the dry season in São Carlos, diverging from the experiments monitored in the summer, which have more regularity of rainy events. These criteria are important to ensure similarities with real events, as variables such as temperature and evapotranspiration differ according to the time of year. The main characteristics of each event are shown in Table 3.3.

Table 3.3 - Characteristics of monitored synthetic events

Event	Date	Antecedent dry days (days)	Reference Evapotranspiration (mm/d)	Average temperature (ºC)	Duration / Return Period	Type of Analysis
Ev.1	04/02/2019	3	3.4	21.5	30 minute / 5 year	Quantitative calibration
Ev.2	19/03/2019	5	4.9	24.3	30 minute / 50 year	Quantitative validation
Ev.3	26/06/2019	16	2.8	21.7	31 minute / 5 year	Qualitative
Ev.4	06/08/2019	41	2.3	17.3	29 minute / 5 year	Qualitative
Ev.5	02/09/2019	14	3.4	20.4	20.5 minute / 5 year	Qualitative
Ev.6	28/01/2020	7	3.8	22.8	30 minute / 5 year	Quantitative calibration
Ev.7	11/02/2020	14	1.9	19.2	30 minute / 5 year	Quantitative calibration
Ev.8	25/01/2021	7	4.6	24.1	30 minute / 5 year	Qualitative / Quantitative validation
Ev.9	02/02/2021	8	4.0	23.3	30 minute / 5 year	Qualitative / Quantitative validation
Ev.10	09/02/2021	7	4.1	21.5	30 minute / 5 year	Qualitative

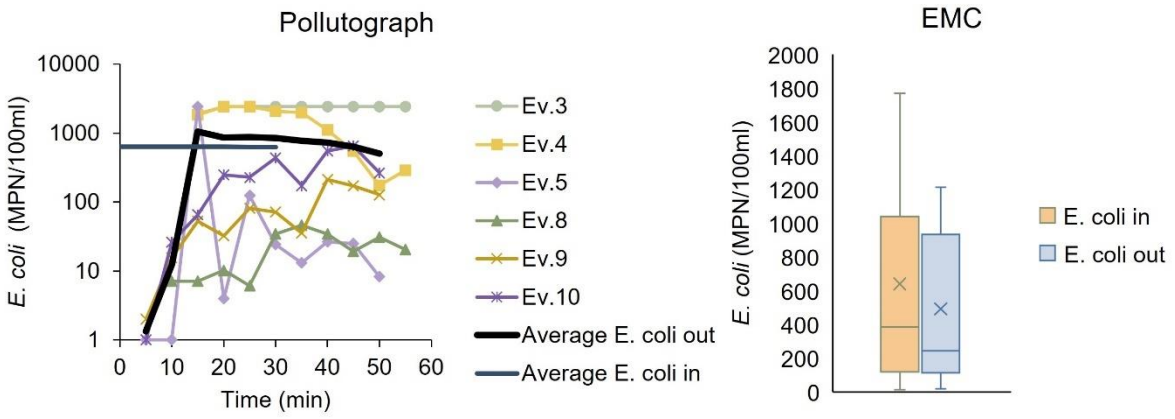
Figure 3.5 presents the hydrographs of the monitored qualitative events. It can be observed that events monitored in the summer, with fewer antecedent dry days, have a higher peak flow than events monitored in winter. This occurs because in events after a dry period, the water is initially retained as soil moisture, therefore with more regular events, the soil moisture is already high, increasing the outflow peak. Despite this, the system showed good average peak flow reduction efficiency of 52.9% ± 12.3%.

Figure 3.5 - Hydrographs of each event with qualitative monitoring.



Regarding qualitative monitoring, Figure 3.6 shows the pollutograph with the *E. coli* concentration over time of all monitored events, along with the EMC bloxplot of the input and output concentration. Thus, the input EMC was 639.8 MPN/100ml and the output was 491.5 MPN/100ml, resulting in an average system efficiency in the removal of *E. coli* of 23%. Except for Ev.4, all experiments showed a positive removal efficiency, ranging from 31% to 82%.

Figure 3.6 - *E. coli* concentration over time and average input and output *E. coli* concentration.



3.3.2 Calibration and validation results

For the calibration of the quantitative module, 7 events were used, in which the events Ev.1, Ev. 6 and Ev.7 were for calibration and events Ev.2, Ev.8 and Ev.9 for validation. In the calibration, an NSE of 0.85 was obtained, and in the validation the average NSE was 0.79. Figure 3.7 shows the graphics of the events used in the validation for comparison with the observed data. The values of the parameters obtained in the calibration are described in Table 3.4.

Figure 3.7 - Event validation with quantitative monitoring

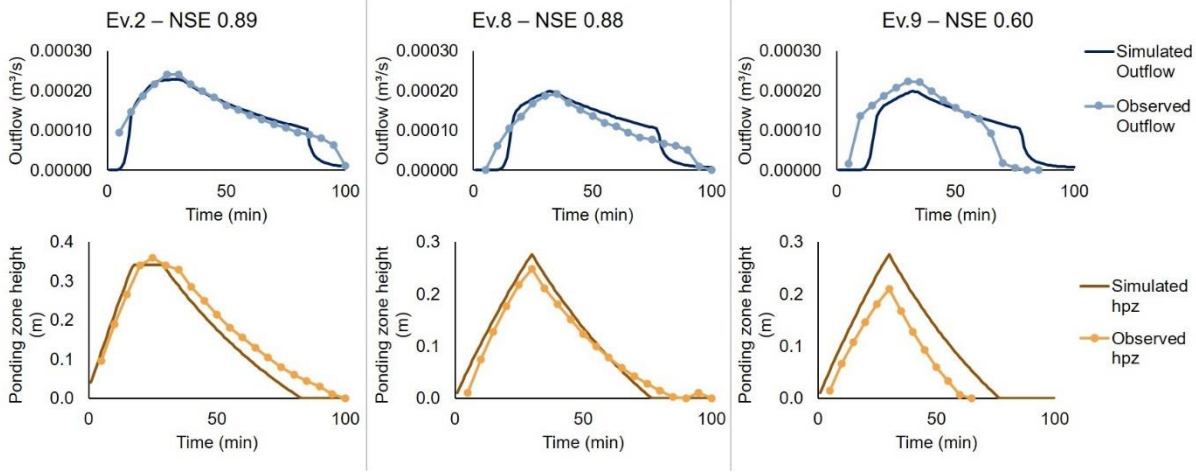


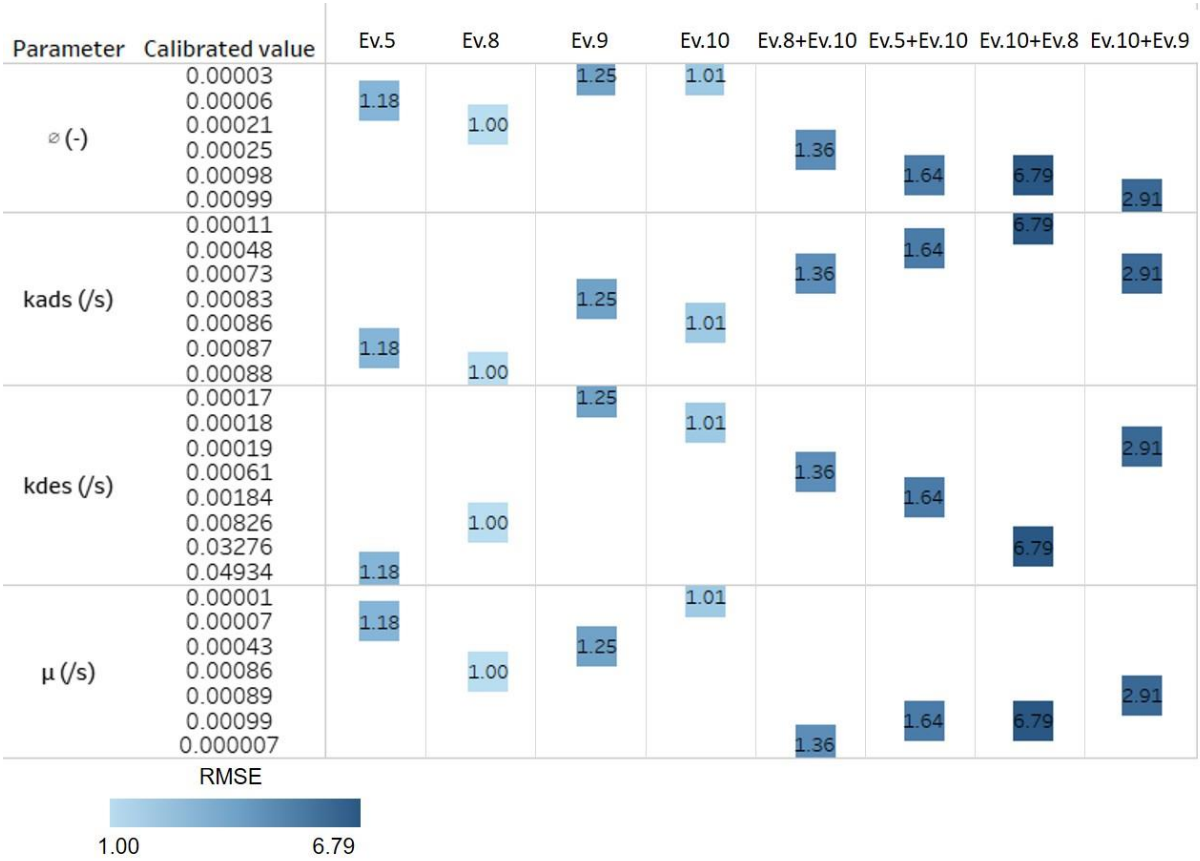
Table 3.4 - Result of calibrated parameter values

Parameter	Calibrated value	Unit
Kc	0.03	-
Ks	0.00007	m/s
Sh	0.03	-
Sw	0.1	-
Sfc	0.12	-
Ss	0.29	-
Cd	0.33	-
NSE	0.85	

Regarding the qualitative module, some samples showed a concentration above the maximum limit detected by the Colilert method of laboratory analysis (>2419.6 MPN/100ml), due to this, the Ev.3 and Ev.4 events (which presented 09 and 02 samples, respectively, above the maximum measured limit) were discarded for the modeling, due to the lack of identification of the peak concentration throughout the event. Two forms of calibration were tested: 1) EMC calibration, minimizing the RMSE; and 2) pollutograph calibration, maximizing NSE. Since the small number of events, the individual calibration was tested with each event, and then the calibration with two different events together, randomly selected.

Regarding the EMC calibration, as the analyzed events had an average concentration of *E. coli* above 400 MPN/100ml, the RMSE values achieved in all tested calibrations were considered low (1.0 to 6.8 MPN/100ml). The individual event calibrations presented lower RMSE values than the calibrations performed with 2 different events together, as shown in Figure 3.8. It can be observed that the calibration with isolated events generated higher values of the adsorption parameter (k_{ads}), indicating that pathogenic organisms tend to be retained in the system, which is confirmed because the average input concentration is higher than the output one. Moreover, in the calibrations with isolated events, the die-off rate parameters (μ_0) and temperature correction coefficient ($\emptyset$) resulted in lower values, indicating that the number of antecedent dry days to the analyzed events was not sufficient for significant die-off reactions. A relationship between the values obtained in the calibrations on the desorption parameter was not observed (k_{des}).

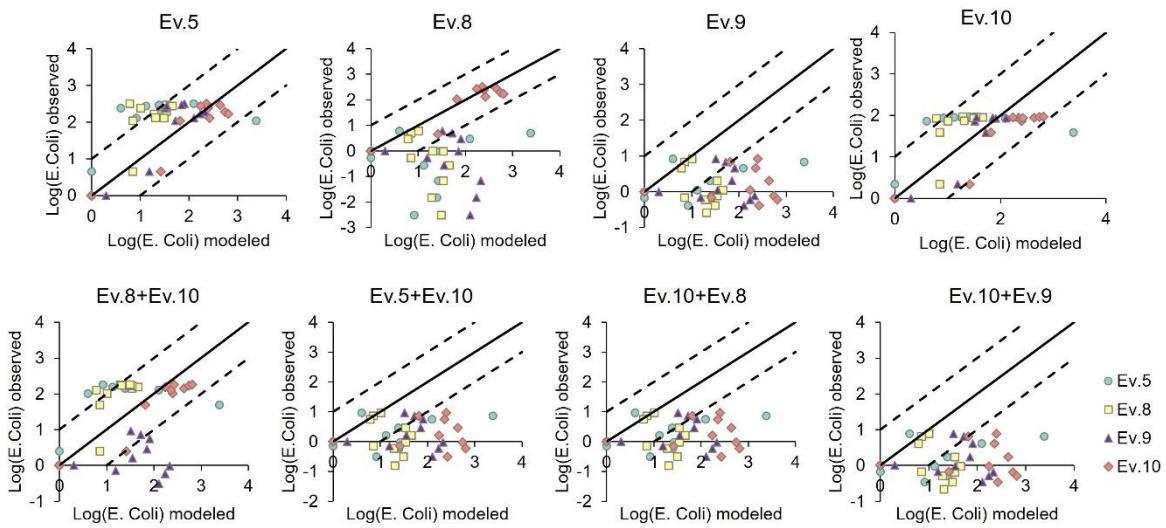
Figure 3.8 - Results of calibrated parameters for different events. RMSE calibration in MPN/100ml



Among the evaluated calibration options, the Ev.5 and Ev.10 events, when calibrated separately, presented a better relationship between the modeled values versus the observed values (Figure 3.9), that is, a graphic distribution close to the 45º line. Thus, the values obtained from these calibrations may be more suitable for this bioretention system. However, the joint calibration of Ev.5 and Ev. 10 did not show a good relationship. This can happen if the model does not represent well the behavior of the microbial concentration in the dry period between events, resulting in a worsening in the final calibration result. Regarding similarities and/or divergences between the results obtained with Ev.5 and Ev.10, both presented similar results for the values of all parameters, except for desorption, where Ev.5 presented the high value (0.049/s), close to the maximum limit (0.05/s), while Ev.10 resulted in 0.00018/s closer to the minimum limit (0.0001/s). This can be explained by the difference in the number of antecedent dry days between the two events (14 days in Ev.5 and 7 days in Ev.10), in which Ev.5, as it has more antecedent dry days, it has particles of soil that detach more easily due to the lack of moisture and in the event of precipitation, these particles are carried away, contributing to increased desorption. Events Ev.8 and Ev.10 presented the smallest and closest

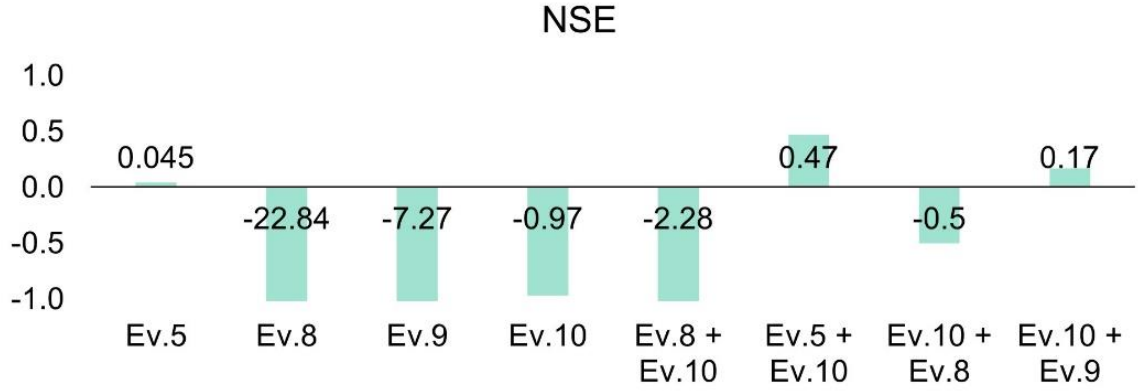
RMSE values (1.00 and 1.01, respectively), however, Ev.10 obtained a better linear relationship between the observed and modeled values than Ev.8. The similarities between these events were the number of previous dry days (7 days) and the duration of the event (30 minutes), which may have contributed to the low RMSE result; however, the biggest difference between these events was in relation to the average temperature, approximately 3 degrees of difference. Chandrasena et al., (2014) showed that temperature is a key factor in microbial behavior in bioretention systems, more specifically in the die-off rate.

Figure 3.9 - Graphical comparison between modeled vs. observed output results. Modeled results were generated from the calibration using the events indicated in the graph titles.



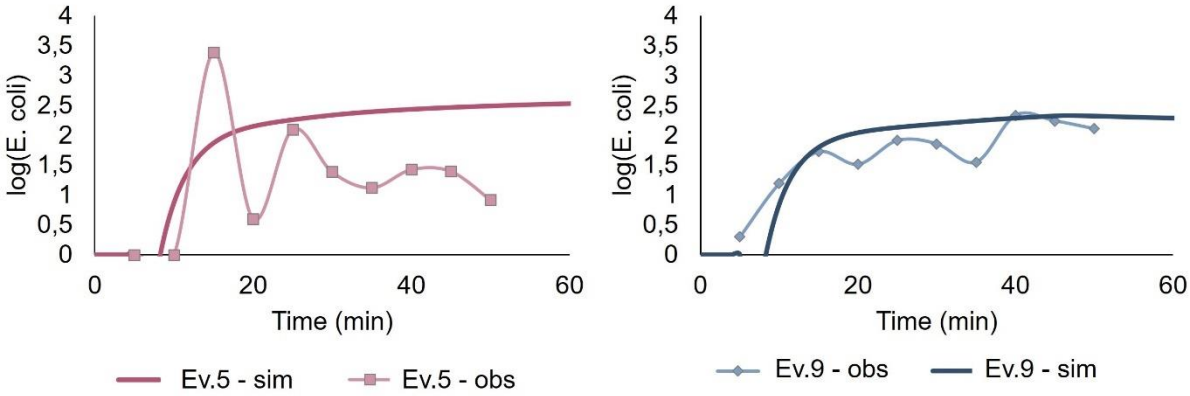
Pollutograph calibration (Figure 3.10), aiming to maximize NSE, resulted in most of the scenarios tested with negative NSE, except for Ev.5 (NSE=0.045) calibrated individually, and combinations of Ev.5+Ev.10 events (NSE=0.47) and Ev.10+Ev.9 (NSE=0.17). However, it was not possible to obtain a good fit to the model.This can be explained by the model's response not having a defined peak, and this can generate negative NSE values since this metric is used to check whether the time and magnitude of simulated peaks match the observed values (Criss & Winston, 2008). Therefore, validation was continued with only the first type of calibration with RMSE minimization.

Figure 3.10 - NSE results of the calibration of the tested events



Thus, among the options tested, the calibration scenario was selected using the lowest RMSE value and with the best approximation of the plotted values observed x modeled to 45 degrees line (Figure 3.9) for validation. Thus, the calibration chosen for validation was with Ev.8 + Ev.10, with RMSE equal to 1.36. Figure 3.11 shows a comparison of observed and modeled data for the validation of Ev.5 and Ev.9 with the calibrated parameters. The validation with the Ev.9 event presented better results than with the Ev.5 (RMSE of the Ev.5 = 0.98; RMSE of the Ev.9 = 0.15). This can be explained by the proximity that Ev.9 has to the events used in the calibration (Ev.8+Ev.10) since Ev.5 was performed much earlier than Ev.9 that was performed in sequence with the events of the calibration.

Figure 3.11 - Comparison of the modeled and observed result for validation



3.4 CONCLUSIONS

The use of the microbiological model proposed by Shen et al. (2018) proved to be adequate for the quantitative module, with NSE for calibration equal to 0.85 and 0.79 for validation. Thus, in the quantitative module, this model is representative of outflow

simulations of the bioretention box in this study. However, regarding the qualitative module, the calibration and validation were complex due to the variability of the calibrated parameters according to the conditions prior to each event. The calibration of Ev.5 and Ev.9 events had low RMSE values, however, the calibration of these two events together did not obtain a good relationship between observed and modeled data, indicating, in this case, an adversity of the model in the continuous simulation between events. Thus, it is recommended for future studies the expansion of monitored events for understanding behavior patterns of each parameter, for example: events monitored on days with similar antecedent temperature, evapotranspiration, and dry days. Thus, it may be possible to obtain different parameter values, with more accurate calibration and validation, according to previously defined conditions. Furthermore, it is recommended to test the incorporation of other reactions in the model, such as straining in all layers and sedimentation in the ponding zone that were not considered.

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4 GENERAL CONCLUSIONS

This chapter of general conclusions will be subdivided into (1) Conclusions and (2) Future Recommendations. In part (1) the conclusions of the proposed objectives are discussed. Part (2) proposes improvements for future studies and questions that are not yet fully answered.

4.1 CONCLUSIONS

This dissertation had as general purpose "To improve scientific knowledge of bioretention systems applications with multi-purposes such as reducing the risk of floods and using a new water source alternative to meet the demand for water for non-potable purposes and to evaluate the behavior of key pollutant for stormwater harvesting". Thus, the general purpose was met through the results obtained with laboratory experiments with the bioretention box in different configurations and application of modeling the behavior of the specific pollutant (*E. coli*), additionally the discussion of results.

The first specific purpose of this research was "To assess the quality of the inflow and outflow of a bioretention box targeting pollutants for non-potable uses in accordance with ABNT NBR 15527/2019". This objective was achieved by evaluating the results considering the limits of pollutants defined by NBR 15527/2019 in chapter two. Complementarily, the reference limits of CONAMA resolution 357 were also used to identify the water quality level for other parameters, common in urban waters, which are not listed in NBR 15527/2019. This analysis is important for a water quality assessment, not restricting only to the *E. coli*, pH and turbidity parameters contained in the NBR. Thus, pH values within the limits were obtained in all experiments, between 6 and 7, the E. coli parameter varied according to the presence or absence of the submerged zone and there were no values within the limit with respect to turbidity. This bioretention system promotes fine particles leaching, probably due to the type of soil native to the region, which contains clay, increasing the turbidity values in the outflow. Thus, the system in the current configuration is not sufficient to reach values within the Brazilian Standard for Rainwater Usage. Regarding the additional pollutants that were compared with the CONAMA 357, the nitrogen series met the River class I limit (NO_2 concentration < 1mg/L; NO_3 concentration < 10mg/L; NH3 concentration < 3.7 mg/L), despite the export of NO_3. TP only met the River class II category (TP concentration < 0.05mg/L) and the estimated COD did not fully reach the limit for River class II (COD concentration < 5mg/L).

The second specific objective evaluated was “Analyze water quality with unsaturated zone and saturated zone in a bioretention box in a subtropical climate”. This specific purpose was also assessed in chapter two. In this chapter, an initial exploratory analysis of the main differences in water quality in bioretention systems without and with the submerged zone was performed, focusing on reuse with a comparison of the results with the limits of NBR 15527/2019. In the observed data, the main differences were the NH_3 removal in SZ systems and NH_3 leaching in USZ; COD removal occurs in both systems, but in USZ systems the removal was greater. Regarding the parameters of NBR 15527/2019, the average turbidity of the SZ systems was lower, probably due to the height of the output valve, in which the fine particles are deposited at the base of the system. Regarding *E. coli* parameter, the experiments in the SZ configuration had high output concentration values, however, the average input concentration was also much higher than the USZ system configuration.

The third specific purpose investigated was “To apply the mathematical model to investigate the behavior of *E. coli* within the bioretention system”. In this chapter, it was chosen one of the biggest urban water pollutants that put in risk stormwater harvesting, the pathogenic microorganism *E. coli*, discussed in chapter three. From the collection of experimental data, data analysis was performed to select the observed events that could be used to carry out the modeling. The chosen model was the microbiological model proposed by Shen et al. (2018). Of the analyzed events, a part was used for the calibration and validation of the quantitative module, in which it was possible to obtain NSE for calibration equal to 0.85 and 0.79 for validation. Thus, this model is representative for outflow simulations of the bioretention box in this study. However, regarding the qualitative module, the calibration and validation proved to be complex due to the variability of the events observed, thus, it is estimated that for a good calibration and validation of the quality module it is necessary to carry out more monitored events to establish standards.

4.2 RECOMMENDATION FOR FUTURE STUDIES

For recommendations for future studies, this section aims to highlight some limitations and improvements that can be answered regarding this issue:

- Monitoring more events with both configurations (USZ and SZ) to assess pollutant output concentrations.
- Monitoring of events with different rainfall (changes in duration and inflow), as well as carrying out events with previously defined input concentrations, so that both

experiments (USZ and SZ experiments) have the same input concentrations to facilitate data comparison.

- Test different types of bio-retention systems, adding a carbon source or changing the filter media material itself to remove specific pollutants.
- Test the calibration of the code developed by Shen et al. (2018) with events with more similar antecedent conditions to increase the chances of better NSE results.
- Evaluate the representativeness of the bioretention box in relation to the field system.

APPENDIX A - Description of the equations used to the quantity model

1. Parameters and variables

Table 1 – Variables

Symbol	Meaning	Dimensions
Qin	Inflow	m³/s
Qover	Overflow	m³/s
Qpf	Infiltration from pond to the filter material	m³/s
Qfs	Infiltration from USZ to SZ	m³/s
Qhc	Capillary rise USZ	m³/s
Qet	Total evapotranspiration	m³/s
Qpipe	Underdrain flow	m³/s
Spz	Storage in PZ	m³
Susz	Storage in USZ	m³
hpz	Ponding zone height	m
husz	USZ height	m
hsz	SZ height	m
nusz	Porosity in USZ	-
nsz	Porosity in SZ	-
θ_{usz}/teta_usz	Soil water fraction in USZ	-
θ_{sz}/teta_sz	Soil water fraction in SZ	-

- ***Evapotranspiration:***

$$Q_{et}{}^{i} = \begin{cases} 0\,, & if\ S_t{}^{i} \leq S_w \\ A_b K_c ET_0 \frac{S_t{}^{i} - S_w}{S_s - S_w}\,, & if\ S_w < S_t{}^{i} \leq S_s \\ A_b K_c ET_0\,, & if\ S_s < S_t{}^{i} \leq 1 \end{cases} \text{ (mm/min)}$$

$$Q_{et}{}^{i} = Q_{et}{}^{i} / (1000 * 60) \text{ (m}^3\text{/s)}$$

$$S_t{}^{i} = \frac{S^i\, n_{usz}{}^{i}\, h_{usz}{}^{i} + n_{sz}{}^{i}\, h_{sz}{}^{i}}{n_{usz}{}^{i}\, h_{usz}{}^{i} + n_{sz}{}^{i}\, h_{sz}{}^{i}}$$

* ETo = Penman-Monteith Method (FAO - 1998)

Evapotranspiration values were used from the website: http://www.cppse.embrapa.br/meteorologia/index.php?pg=automatica

2. Water mass balance to ponding zone (PZ)

$$\frac{\partial S_{pz}}{\partial t} = Q_{in}{}^{i} + Q_{rain}{}^{i} - Q_{pf}{}^{i} - Q_{over}{}^{i} - Q_{inf,p}{}^{i}$$

- **State variables equations:**

Storage in pz:

$$S_{pz}{}^{i} = h_{pz}{}^{i} . A_b$$

Infiltration from pond to the filter material:

$$Q_{pf}{}^{i} = \min\left(\frac{k_s A_p\left(h_{pz}{}^{i} + h_{usz}{}^{i}\right)}{h_{usz}{}^{i}}, \frac{h_{pz}{}^{i} A_b}{dt} - Q_{inf,p}{}^{i}, \frac{(1 - S^i)\, n_{usz}{}^{i}\, h_{usz}{}^{i}\, A_p}{dt}\right)$$

Overflow through weir:

$$Q_{over}{}^{i} = \begin{cases} 0 & , \ if\ h_{pz}{}^{i} \leq P_v \\ \min\left(\frac{A_p\left(h_{pz}{}^{i} - P_v\right)}{dt}, \ kweir\ (2 * g)^{0.5}\left(h_{pz}{}^{i} - P_v\right)^{kexp}\right) & , \ if\ h_{pz}{}^{i} > P_v \end{cases}$$

Infiltration to bottom surrounding soil:

$$Q_{inf,pz}{}^{i} = K_f\left[\left(A_b - A_p\right) + C_s P_p h_{pz}{}^{i}\right]$$

$$h_{pz}{}^{i} = h_{pz}{}^{i-1} + \frac{\left(Q_{in}{}^{i} + Q_{rain}{}^{i} - Q_{pf}{}^{i} - Q_{over}{}^{i} - Q_{inf,p}{}^{i}\right)dt}{A_b}$$

3. Water mass balance to unsaturated zone (USZ)

$$\frac{\partial S_{usz}}{\partial t} = Q_{pf}{}^{i} + Q_{hc}{}^{i} - Q_{fs}{}^{i} - Q_{et,usz}{}^{i}$$

- **State variables equations:**

Total evapotranspiration flow in usz:

$$Q_{et,usz}{}^{i} = Q_{et}{}^{i} \frac{S_{usz}{}^{i}\, n_{usz}{}^{i}\, h_{usz}{}^{i}}{n_{usz}{}^{i}\, h_{usz}{}^{i} + n_{sz}{}^{i}\, h_{sz}{}^{i}}$$

Capillary rise flow:

$$Q_{hc}{}^{i} = \begin{cases} A_p Cr\left(S_{usz}{}^{i} - S_s\right)\left(S_{fc} - S_{usz}{}^{i}\right), & if\ S_s \le S_{usz}{}^{i} \le S_{fc} \\ 0 \end{cases}$$

$$Cr = \frac{4K_c ET_0}{2.5\left(S_{fc} - S_s\right)^2}$$

Infiltration from usz to sz:

$$Q_{fs}{}^{i} = \begin{cases} min\left(\frac{k_s A_p\left(h_{pz}{}^{i} + h_{usz}{}^{i}\right)}{h_{usz}{}^{i}} S^{i\gamma}, \frac{\left(S_{usz}{}^{i} - S_{fc}\right) A_p h_{usz}{}^{i} n_{usz}{}^{i}}{dt}\right), & if\ S_{usz}{}^{i} \ge S_{fc} \\ 0 \quad , if\ \ S_{usz}{}^{i} < S_{fc} \end{cases}$$

Depth, porosity, and soil water fraction of the unsaturated zone:

$$h_{usz}{}^{i} = L - h_{sz}{}^{i-1}$$

$$n_{usz}{}^{i} = \begin{cases} \frac{n_f D_f + n_g\left(D_g - h_{sz}{}^{i-1}\right)}{h_{usz}{}^{i}} = \ , & if\ h_{sz}{}^{i-1} < D_g \\ n_f\ , \quad if\ h_{sz}{}^{i-1} \ge D_g \end{cases}$$

$$\theta_{usz}{}^{i} = S_{usz}{}^{i} n_{usz}{}^{i}$$

$$S_{usz}{}^{i} = max\left[min\left(1,\ S_{usz}{}^{i-1} h_{usz}{}^{i-1} n_{usz}{}^{i-1} + \frac{\left(Q_{pf}{}^{i} + Q_{hc}{}^{i} - Q_{fs}{}^{i} - Q_{et,usz}{}^{i}\right) dt}{A_p h_{usz}{}^{i} n_{usz}{}^{i}}\right), S_h\right]$$

3. Water mass balance to saturated zone (SZ)

$$\frac{\partial S_{sz}}{\partial t} = Q_{fs}{}^{i} - Q_{hc}{}^{i} - Q_{et,sz}{}^{i} - Q_{pipe}{}^{i} - Q_{inf,sz}{}^{i}$$

$S_{sz} = 1$ (constant)

- **State variables equations:**

Total evapotranspiration flow in sz:

$$Q_{et,sz}{}^{i} = Q_{et}{}^{i} - Q_{et,usz}{}^{i}$$

Drainage pipe flow:

$$Q_{pipe}{}^{i} = \begin{cases} min\left(\frac{\left(h_{sz}{}^{i} - h_{pipe}\right) A_p n_{sz}{}^{i}}{dt} - Q_{inf,sz}{}^{i},\ C_d A_{pipe}\left[\left(h_{sz}{}^{i} - h_{pipe}\right) 2g\right]^{1/2}\right), & if\ h_{sz}{}^{i} \ge h_{pipe} \\ 0 \quad , if\ \ h_{sz}{}^{i} < h_{pipe} \end{cases}$$

Infiltration to bottom surrounding soil:

$$Q_{inf,sz}{}^{i} = K_f\left(A_p + C_s P_p h_{sz}{}^{i}\right)$$

Depth, porosity, and soil water fraction of the saturated zone:

$$h_{sz}{}^{i} = h_{sz}{}^{i-1} + \frac{\left(Q_{fs}{}^{i} - Q_{hc}{}^{i} - Q_{et,sz}{}^{i} - Q_{pipe}{}^{i} - Q_{inf,sz}{}^{i}\right)dt}{A_p\, n_{sz}{}^{i-1}}$$

$$n_{sz}{}^{i} = \begin{cases} \dfrac{n_g D_g + n_t D_t + n_f\left(h_{sz}{}^{i} - D_g - D_t\right)}{h_{sz}{}^{i}}, \ if\ D_t + D_g < h_{sz}{}^{i} \leq L \\ \dfrac{n_g D_g + n_t\left(h_{sz}{}^{i} - D_g\right)}{h_{sz}{}^{i}}, \ if\ D_g < h_{sz}{}^{i} \leq D_t + D_g \\ n_g\ ,\ if\ \ h_{sz}{}^{i} \leq D_g \end{cases}$$

$$\theta_{sz}{}^{i} = n_{sz}{}^{i}$$

APPENDIX B- Description of the equations used to the *E. Coli* model

1. Parameters and variables

Table 1 – Parameters and variables

Símbolo	Significado	Valor adotado	Dimensão
ρ / ro_pd	bulk soil density	2650	kg/m3
nusz	porosidade do solo inicial	0.32	-
lamta1	dispersivity in soil of USZ	0.00531	m
lamta2	dispersivity in soil of SZ	0.00531	m
d50	median grain size of the porous medium	0.00028	m
kads1	adsorption rate in USZ	*calibrated*	/s
kdes1	desorption rate in USZ	*calibrated*	/s
kads2	adsorption rate in SZ	*calibrated*	/s
kdes2	desorption rate in SZ	*calibrated*	/s
ø	temperature correction coefficient for die-off	*calibrated*	-
μ1	standard die-of rate at standard temperature in USZ	*calibrated*	/s
μ2	standard die-of rate at standard temperature in SZ	*calibrated*	/s
kstr	straining coefficient	1	-
etta	straining adjustment in coefficient	0.00001914	-
b1	straining coefficient	1	-

2. Input variables

- **Concentração ao longo do tempo de E. Coli (NMP/100ml)**

cin_file = pd.read_csv('Cinflow_ecoli.csv')

- **Temperatura (ºC)**

Temp_file = pd.read_csv('Temperature.csv')

- **Vazão de entrada (m3/s)**

Qin_file = pd.read_csv('Qin_file.csv')

3. Definitions of the equations

Informations:

USZ and SZ – method used: Adapted forward time central differences in space

n = 11 # number of cells

dz = L / n

m_usz= round((L-hpipe)/dz)

m_sz= n-m_usz

ro = (1-nusz_ini)*ro_pd

3.1. Unitary flow to transport equations

- ***Boundary conditions*:**

  α + β = 1

  upper boundary: α = 1

  lower boundary: β = 1

  $$alfa1 = \frac{(m\_usz - 1 - l)}{(m\_usz - 1)}, beta1 = \frac{l}{(m\_usz - 1)}$$

  $$alfa2 = \frac{(m\_sz - 1 - j)}{(m\_sz - 1)}, beta2 = \frac{j}{(m\_sz - 1)}$$

- ***V – usz:***

  if hpipe > 0:

  $$V\_usz = \frac{alfa1 * (Qpf - Qet1) + beta1 * (Qfs - Qhc)}{Ab * teta\_i\_usz}$$

  else:

  $$V\_usz = \frac{alfa1 * (Qpf - Qet1) + beta1 * (Qpipe + Qinf\_sz - Qhc)}{Ab * teta\_i\_usz}$$

- ***V-sz:***

  $$V\_sz = \frac{alfa2 * (Qfs - Qhc - Qet2) + beta2 * (Qpipe + Qinf\_sz)}{(Ab * teta\_i\_sz)}$$

- ***Diffusion:***

  $$D\_x = lamta1 * V\_x$$

- ***Peclet number - SZ:***

if D_usz > 0:

$$Pe\_usz = \frac{V\_usz * dz}{D\_usz}$$

else:

$$Pe\_usz = 100$$

- ***Peclet number -USZ:***

$$D\_sz = lamta2 * V\_sz$$

if D_sz > 0:

$$Pe\_sz = \frac{V\_sz * dz}{D\_sz}$$

else:

$$Pe\_sz = 100$$

4. Water mass balance to ponding zone

- ***Concentration in ponding zone – Complete mixing:***

$$Cpz = \frac{(Cpz\_a * hp\_a * Ab + (Cin * Qin - Cpz\_a * (Qpf + Qv) + Rxi * hp * Ab) * dt)}{(hp * Ab)}$$

5. Transport equations

- ***Solute transport equation:***

$$\Delta C_{i+1} = \left(\left(\frac{dt}{\theta_{i+1}}\right) * (-\theta_i * k_{ads} * c_i + \rho * k_{des} * csoil_i + \theta_i * (D_x * \left(\frac{dc}{dz^2}\right) - V_x * dc\_dz) + R_x)\right)$$

$$C_{i+1}{}^{*} = C_i + \Delta C_{i+1}$$

- ***Soil concentration:***

$$Csoil_{\,i+1} = Csoil_i + \left(\frac{\theta_x}{\rho} * k_{ads} * C_i - k_{des} * Csoil_i - Rxs\right) * dt$$

6. Definition of reactions

- ***Ponding zone:***

$$\mu_l = \mu_1 * sita^{(temp_i - 20)}$$
$$Rx_{pz} = -\mu_l * C_{pz}$$

- ***USZ reactions:***

Die-off – water:

$$dieoff_l = -\theta_i * \mu_{l1} * C_{usz,i}$$

Die-off – soil:

$$dieoff_s = -\mu_{s1} * Csoil_{usz,i}$$

Straining:

$$Str = -\theta_i * C_{usz,i} * k_{str} * etta$$

- ***SZ reactions:***

Die-off – water:

$$dieoff_l = -\theta_i * \mu_{l2} * C_{sz,i}$$

Die-off – soil:

$$dieoff_s = -\mu_{s2} * Csoil_{sz,i}$$

7. Model output data:

- Cpz list with values from the ponding zone, for each time t will have a concentration of cp [LINE]
- C_usz temporal concentration in USZ, for each time there is the layer [MATRIX]
- C_sz concentration in SZ [MATRIX]
- Csoil_usz soil concentration in USZ [MATRIX]
- Csoil_sz soil concentration in SZ [MATRIX]
- Rx_usz USZ reactions [MATRIX]
- Rx_sz SZ reactions [MATRIX]