

# Water Management

## Water Quality & Modelling

**KEYWORDS:** Water Quality Modeling / Best Management Practices / Indicator CECs / Antibiotic Resistant Bacteria and Genes

**Modeling tools for water quality management in river basins, enabling the prediction of allowable pollution loads and predicting impacts on water uses and ecosystems. Methodologies for selecting indicator contaminants of emerging concern in the case of reuse of reclaimed water for irrigation.**

### Introduction

Since the implementation of the Water Framework Directive (WFD), river basin management plans have been adopted to achieve the protection, improvement, and sustainable use of the water, aiming at reaching a good ecological status.

Watershed models provide easy water quality assessments by simulating the hydrologic process affected by different climate conditions, land use change, and best management practices. While a comprehensive monitoring system may not be cost-effective to implement, modeling alternative scenarios will reduce costs associated with developing and implementing water quality management plans. The hydrological model, Hydrologic Simulation Program FORTRAN (HSPF), is a comprehensive river basin model that provides an integrated framework for modeling various hydrological and quality processes.

The reuse of reclaimed water is a timely and current topic of worldwide discussion. In force and ongoing regulations and recommendations at national, European, and international levels require that wastewater treatment plants (WWTPs) produce resources and not waste: reclaimed water, nutrients, bioenergy, and biosolids. In addition, increasingly frequent scenarios of drought and water scarcity strongly support the application of water reuse concepts. In Europe, the main reasons limiting this practice are the high investment and operation costs of direct reuse of reclaimed water. At the same time, the occurrence of contaminants of emerging concern (CECs) in the water, including organic CECs and microbial CECs, such as antibiotic resistant bacteria (ARB) and antibiotic resistance genes (ARGs), may increase the concerns about reclaimed water reuse because of CEC accumulation in the environment.

### Current Development

The impact of best management practices on the water quality of Ave River was evaluated to mitigate the effects of both point and nonpoint pollution sources. The strategy adopted in this work included the following activities: (i) calibration and validation of the hydrological behavior of the Ave River basin; (ii) calibration and validation of the water quality for the existing monitoring stations, taking into account the different types of information, such as in-stream water quality data (fecal coliforms, dissolved oxygen, nitrates, orthophosphates, biochemical oxygen demand and chlorophyll-a), point sources, nonpoint sources and land use and; (iii) assessment of best management impacts on agricultural land use on water quality in Ave River basin.

Ave River Basin (Fig 1a) covers an area of approximately 1388 km<sup>2</sup> and is located in the northern region of Portugal. With a streamline of 90.9 km and two main tributaries, Este River (247 km<sup>2</sup>) and Vizela River (342 km<sup>2</sup>), it has an annual average precipitation of 1522 mm, an average temperature of 13.9 °C and an average annual flow rate of 30.6 m<sup>3</sup> s<sup>-1</sup>.

The land use occupation of the basin comprises 46.6% of forest land, 42.6% of agricultural land, 10.7% of urban land, and 0.2% of wetland (Fig 1b).

The measurement network comprises five meteorological stations spread over the catchment and two gauges, 15E03 (Ave River) and 15E01 (Este River), located 5.3 km upstream of the river mouth. Since sufficient data was available, the Ave watershed was segmented according to the meteorological stations. Once segmented, it is possible to assign a separate meteorological station to each model segment (Fig 1c) to improve the accuracy of the model output. The watershed was delineated to characterize the stations where observed data was available: station 15E03 (Ave River segment) and station 15E01 (Este River segment). The river basin receives several point discharges from industries and wastewater treatment plants (Fig 1d).

The water quantity and quality of the Ave River segment were calibrated for the period between 1990-1994 and validated for 1995-2000, while the Este River tributary was calibrated for the period between 1994-1997 and validated for 1998-2000 (where complete series of observed data was available). For each station concerning in-stream water quality data, the following parameters were assessed: water temperature, dissolved oxygen, biochemical oxygen demand (BOD<sub>5</sub>), nitrate, orthophosphate, and fecal coliforms.

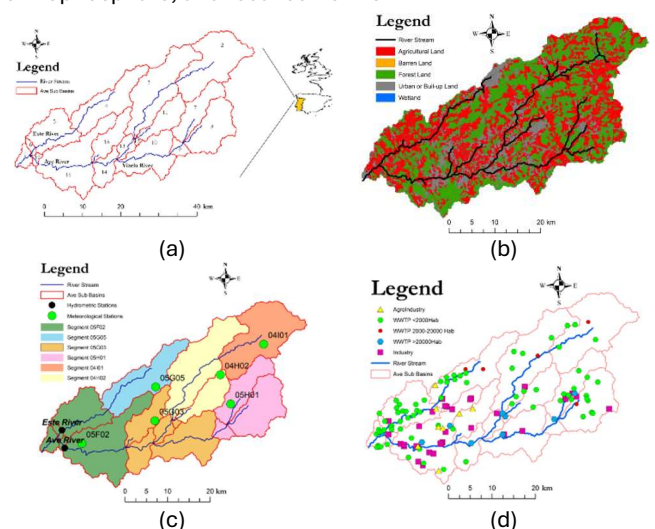


Fig 1. Characterization of Ave River basin; a) Ave watershed delineation; b) land use distribution; c) meteorological segmentation; d) point sources location.

The highest nutrient loads for total nitrogen and total phosphorous per unit of area were observed at the Este River tributary (Fig 2).

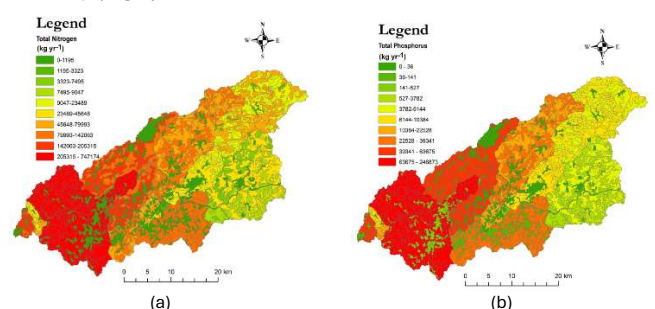


Fig 2. Nutrient load distribution in Ave Basin (kg yr<sup>-1</sup>): a) total nitrogen; b) total phosphorous.

Best management practices (infiltration basin) were applied to agricultural land (for 3%, 6%, 9%, 12%, and 15% area) with removal efficiencies of 50% for fecal coliforms and 30% for nitrogen, phosphorus, and BOD<sub>5</sub>. The inflow of water quality constituents was reduced for all scenarios, with fecal coliforms achieving the highest reduction between 5.8% and 28.9%, and nutrients and BOD<sub>5</sub> between 2% and 13%. BOD<sub>5</sub> and orthophosphate concentrations achieved a good water quality status according to the European legislation for scenarios of best management practices applied to 3% and 12% of agricultural areas, respectively. Fecal coliform levels in the Ave River basin require further treatment to fall below the established value in the abovementioned legislation. This study shows that agricultural watersheds such as Ave basins demand special attention regarding the effects of nonpoint pollution sources on water quality and nutrient loads.

Even though not yet regulated, organic and microbial CECs are of great concern in reclaimed water reuse projects. Due to the large number of CECs and their different characteristics, it is useful to include only a limited number of them in monitoring programs. Selecting the most representative CECs is still a current and open question. Therefore, it is required to develop a methodology to identify relevant indicator CECs for the evaluation of the performance of the new end-of-pipe technology in a reuse project for irrigation purposes, for the assessment of the risk for the soil and the crops in the case of reuse of reclaimed water, as well as for the surface and groundwater which may be in contact with CECs via surface runoff or percolation due to their mobility once in the soil.

As to organic CECs, the methodology developed is based on four criteria (occurrence, persistence, bioaccumulation, and toxicity) (OPBT) expressed in terms of surrogates (respectively, concentrations in the secondary effluent, removal achieved in conventional activated sludge systems, Log *K*<sub>ow</sub> and predicted-no-effect concentration). It consists of: (i) the development of a dataset including the CECs found in the secondary effluent, together with the corresponding values of surrogates found in the literature or by in-field investigations; (ii) normalization step with the assignment of a score between 1 (low environmental impact) and 5 (high environmental impact) to the different criteria based on threshold values set according to the literature and experts' judgment; (iii) CEC ranking according to their final score obtained as the sum of the specific scores; and (iv) selection of the representative CECs for the different needs.

Fig 3 shows their corresponding final OPBT score and the contribution of the different criteria. It emerges that the maximum score of 5 is assigned to most of the organic CECs for their occurrence, to erythromycin, bisoprolol, and venlafaxine for their persistence, to nonylphenol, irbesartan, PFOS, and valsartan for their bioaccumulation, and to diclofenac, ibuprofen, azithromycin, amoxicillin, ciprofloxacin, PFOS and tetracycline for their toxicity.

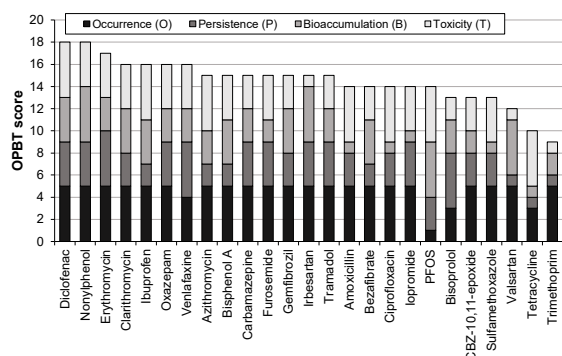


Fig 3. Final OPBT for the indicator organic CECs and contributions by the different criteria.

The selection of the indicators ARB is carried out based on the following criteria: (i) ARB is clinically relevant and it is identified as a carrier of acquired antibiotic resistance in the aquatic environments; (ii) ARB is used as an indicator of fecal contamination in the aquatic environments; (iii) analytical methods are available for its detection and quantification; (iv) recommendations by World Health Organization and by the European Regulation on minimum requirements for water reuse; (v) suggestions from specific networks or hubs, such as the Nereus COST action and Water JPI Knowledge Hub on Contaminants of Emerging Concern.

Based on those criteria, under the SERPIC project, it was selected a list of 30 indicator organic and microbial CECs (Table 1).

Table 1. Complete list of 30 indicator organic and microbial CECs.

Class	CEC
ARB	<i>Escherichia coli</i>
ARB	<i>Fecal coliforms</i>
ARG	16S rRNA
ARG	<i>sul1</i>
ARG	<i>sul2</i>
Antibiotics	Amoxicillin
Antibiotics	Azithromycin
Lipid regulators	Bezafibrate
Beta-blockers	Bisoprolol
Plastic additives	Bisphenol A
Psychiatric drug	Carbamazepine
Psychiatric drug	Carbamazepine 10,11 epoxide (metabolite)
Antibiotics	Ciprofloxacin
Antibiotics	Clarithromycin
Analgesics	Diclofenac
Antibiotics	Erythromycin
Diuretics	Furosemide
Lipid regulators	Gemfibrozil
Analgesics	Ibuprofen
X-Ray contrast media	Iopromide
Antihypertensives	Irbesartan
Surfactants	Nonylphenol
Psychiatric drug	Oxazepam
Surfactants	Perfluorooctane sulfonic acid (PFOS)
Antibiotics	Sulfamethoxazole
Antibiotics	Tetracycline
Analgesics	Tramadol
Antibiotics	Trimethoprim
Antihypertensives	Valsartan
Psychiatric drug	Venlafaxine

### Future Perspectives

Development of a decision support tool to predict the fate and transport of contaminants of emerging concern for water management in river basins.

### Related Sustainable Development Goals



### Outputs

#### Master Dissertations

[1] Mariana Filomena Teixeira Sá, Estudo sobre o impacto dos contaminantes industriais na ETAR do Ave, MIEA, FEUP, 2019

#### Selected Publications

[1] A. Fonseca et al., *Enviro. Sci. & Pollution Res.* 25, 1585 (2018)  
 [2] P. Verlicchi et al. *Sci. Total Environ.* 873, 162359 (2023)

#### Team

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