

TREATMENT OF PESTICIDES PRESENT IN WATER BY POWDER ACTIVATED CARBON

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ABSTRACT

In this study, we have investigated how to reduce three emerging pollutants (atrazine, simazine and linuron) in water, through the use of advanced technologies such as powder activated carbon (PAC). Tests for contaminant reduction were conducted using ASTM D3860-98 in ultra-pure water. The concentrations were analyzed by HPLC equipment with an UV detector. The results obtained within 24 h at an initial concentration of 2,000 mg m⁻³ of the contaminant show that in PAC at 20,000 mg m⁻³ atrazine achieves a reduction of 65.4%, simazine achieves a reduction of 71.8% and linuron, a reduction of 70%.

Keywords: active carbon, emerging contaminant, atrazine, simazine, linuron.

1 INTRODUCTION

Emerging pollutants (ECs) are a type of organic pollutants that are introduced into the environment, mainly the terrestrial and marine environment, in large quantities. In recent years there has been an increase in the study and concern about the presence of these pollutants due to possible consequences for the environment, people and animals. In recent years, the sources that generate this type of pollution have begun to be studied in greater depth.

Research on the behavior and effects of ECs is very numerous and is of interest to many research groups around the world and to the main organizations dedicated to the protection of public health and the environment, such as the World Health Organization, the US Environmental Protection Agency or the European Commission. These substances cause increasing social alarm due to their presence in inland waters [1], including underground waters [2], where they cause various negative effects [3]. Some of them, through research carried out in recent years [4], have been included in the list of priority substances in water in the European Union, regulating their maximum admissible concentration in inland waters, however, for other compounds such as pesticides, regulated in Directive 2013/39/EU [5]. The discovery that some metabolites present in their degradation may be as toxic or more toxic than the original compounds has renewed concern for them [6]–[8].

The activated carbon (AC) is used to remove certain organic pollutants, it is very common in wastewater treatment. Several authors have studied the efficiency, both powder activated carbon (PAC) and granular activated carbon, in the elimination of ECs in wastewater treatment.

The object of this research addresses one of the most important technical challenges for the good ecological status of inland waters, the study of the reduction of three refractory ECs present in the waters, atrazine, simazine and linuron, with PAC (Pulsorb PWX HA) in ultra-pure water, although, based on the results obtained, could be applied to real wastewater. Several authors [9]–[12] have studied similar treatments in real wastewater for diclofenac, carbamazepine, sulfamethoxazole, benzotriazole.

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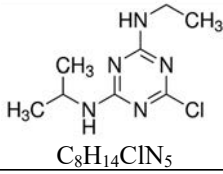
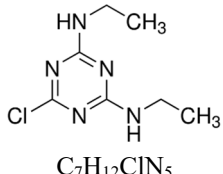
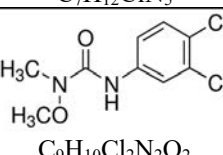
1.1 Pesticides

Simazine is a whitish crystalline compound with a characteristic odor and is not very soluble in water. It is a member of herbicides derived from triazine and was widely used as a non-selective residual herbicide but is now banned in European Union states [13]. It is absorbed by the root system and accumulates in the leaves of the plant where it interferes with the process of photosynthesis. It remains active in the soil for 2–7 months or more after application. It is found in the environment as a consequence of its use as an herbicide in agriculture. The main contaminated media are soil and groundwater.

Atrazine is an herbicide in the triazine family. It is an artificial herbicide of fundamentally systemic and residual action, used to control the growth of weeds in agriculture, inhibiting the photosynthetic process of plants. Used primarily as a herbicide in agriculture, generating leaching and pollution of surface and groundwater. It is also used as a non-selective herbicide in industrial lands. Being a substance of anthropogenic origin, there are no known natural sources of emission.

Linuron is an herbicide derived from phenylureas that is frequently used in different types of crops. Its persistence in the soil is variable depending on the characteristics of the soil and the environmental conditions under which it is applied [14]. Studies on its adsorption and mobility in soil have shown that organic matter is the parameter mainly involved in these processes [15]. Table 1 shows the physical–chemical properties of the ECs of this research [16], [17].

Table 1: Physico–chemical properties of the ECs studied.

Name	Formula	No. CAS	Molecular weight (g mol ⁻¹)	Log Kow	Solubility in water (mg L ⁻¹)	pKa
Atrazine	 C ₈ H ₁₄ ClN ₅	1912-24-9	215.685	2.61	34.7 (26 °C)	1.6
Simazine	 C ₇ H ₁₂ ClN ₅	122-34-9	210.658	2.18	6.2 (20 °C)	1.62
Linuron	 C ₉ H ₁₀ Cl ₂ N ₂ O ₂	330-55-2	249.091	3.2	75 (25 °C)	–

According to the toxicological properties of the ECs studied by the European Chemicals Agency (ECHA) [18] they are harmful and dangerous to the aquatic environment and simazine and linuron have carcinogenic properties.

2 MATERIALS AND METHODS

AC adsorption tests were performed according to ASTM D3860-98(2014) [19]. This method makes it possible to determine the adsorption capacity of activated carbon to remove undesirable components from water and wastewater. The adsorption experiment was conducted on a magnetic stirrer plate between 250–300 rpm. The test is performed at 20°C but other temperatures can be used, in this case a constant temperature of 25°C ± 1°C was maintained by means of a methacrylate vat filled with water with a thermal head that allows the temperature to be regulated. The volume of the sample solution was 500 mL of ultra-pure water in each topaz bottle. Topaz vials of 500 mL were used with a closing cap to avoid evaporation of the mixture and to avoid any interaction of direct sunlight. The samples were extracted periodically in intervals of 5, 10, 15, 30, 45, 60, 90, 120, 150, 210, 270, 330, 550 and 1,440 min during the first 24 h. In each test, the same initial concentration of the ECs was maintained in each of the 5 experiments, between 700, 1,200 and 2,000 mg m⁻³. The concentration of PAC in each experiment varied by 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ AC. It was always evaluated under the same test conditions as mentioned above.

2.1 Active carbon (AC)

ACs are porous organic materials and have covered numerous areas of research due to applications that can be achieved with them such as biodegrading and oxidizing organic materials, to eliminate or absorb some micro-contaminants as well as to improve the flavor, odor and color of water during the filtration process as for water treatment [20]–[22].

There are different types of AC due to their composition, all of them present accessible space inside their structure, that is to say, the capacity of aggregation of these small particles in the solid particles, being defined as intra-particles or textural porosity. The diameter of the textural pores is directly related to the size of the grains forming these pores.

According to the International Union of Pure and Applied Chemistry (IUPAC), it classifies them by pore size [23]. When they have a pore diameter, approximately 2 nm are micropores; when the range is between 2 and 50 nm they are mesopores; finally, when the pore diameter is in a range greater than 50 nm they are macropores [19].

The AC used is PULSORB PWX HA, an industrial type PAC from Chemivron, Belgium. It is a pulverized carbon with a size generally less than 0.177 mm, according to ASTM D5158-98(2013) [24]. It is made of bituminous carbon. The raw material and the manufacturing process develop a large internal surface area of this activated carbon. This internal structure allows maximum adsorption of organic compounds. The AC is washed with ultra-pure water and then placed in the oven at 150°C for 3 h.

Fig. 1 shows the characterization of the porous texture by means of adsorption isotherm from N₂ to 77°K, showing that the PAC studied is Type I [25], typical of a microporous solid, but which also presents quite mesoporosity, which is seen in the slope of intermediate pressures and in the hysteresis cycle.

2.2 High performance liquid chromatography (HPLC)

To determine the concentration of the studied ECs, high resolution liquid chromatography (HPLC) was used with an Agilent 1100 series commercial brand equipment, equipped with an UV detector, whose wavelength was fixed at 220 nm. An Ascentis RP-Amida column of 5 µm (dimensions: 150 mm x 4.6 mm) (Sigma-Aldrich, Supelco, Steinheim, Germany) was used as stationary phase.



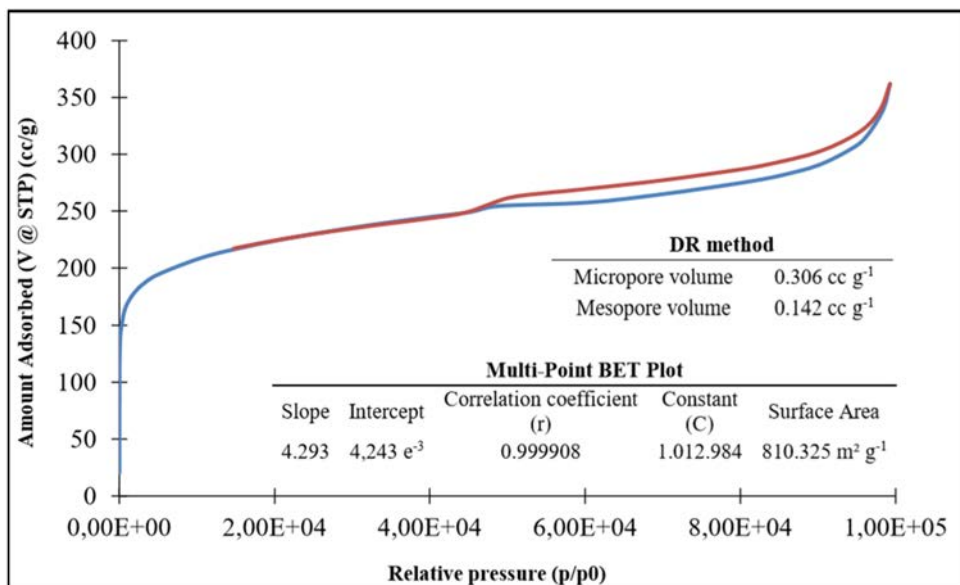


Figure 1: Characterization of the PAC.

The analyzed samples (V : 20 μL) were injected manually, previously passed through a Filter-Lab filter (material: hydrophilic PVDF; pore size: 0.22 μm ; diameter: 25 mm). The mobile phase consisted of a mixture of acetonitrile/ultra-pure water (ACN:H₂O), being for Atrazine and Simazine the same percentage (55:45, v/v) and for the different Linuron (60:40, v/v), at a flow rate for both ECs of 1.0 mL min⁻¹.

The identification of the peaks was done by comparing the retention times of the standard solutions. The matrix used for all the tests was ultra-pure water of type I [26].

3 RESULTS

Experiments were conducted for 3 initial concentrations of 700, 1,100 and 2,000 mg m⁻³ contaminants. For each initial contaminant concentration, 5 different AC adsorption experiments were performed at concentrations between 4,000 and 20,000 mg m⁻³.

3.1 Atrazine

Fig. 2 shows the results obtained for the trial with an initial concentration of 700 mg m⁻³ of atrazine at different doses of PAC for 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 38% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 77% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 94% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 95% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 95% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 6.9, 5.1, 1.2, 14.2 and 0.8% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

Fig. 3 shows the results obtained for the trial with an initial concentration of 1,200 mg m⁻³ of atrazine at different doses of PAC for 24 h.

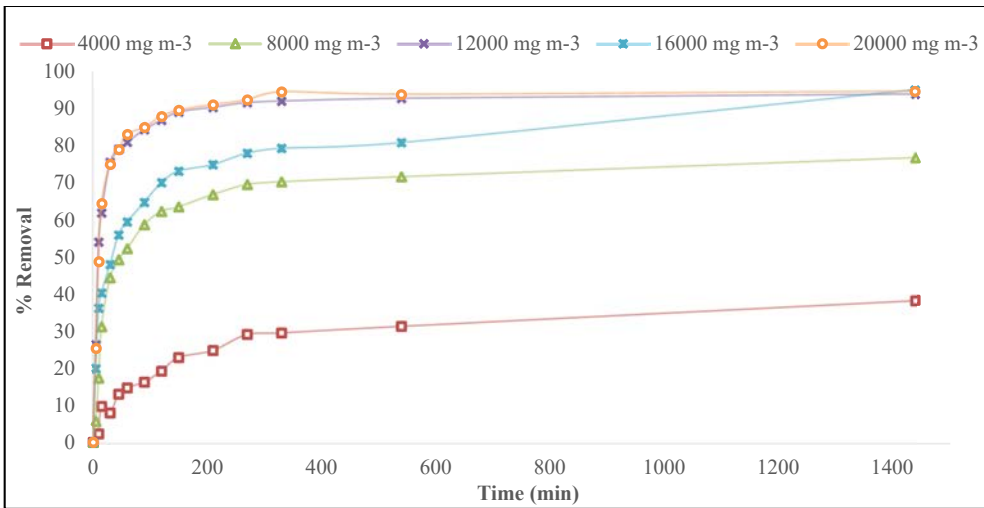


Figure 2: Reduction of atrazine (%), Co 700 mg m⁻³, 24 h.

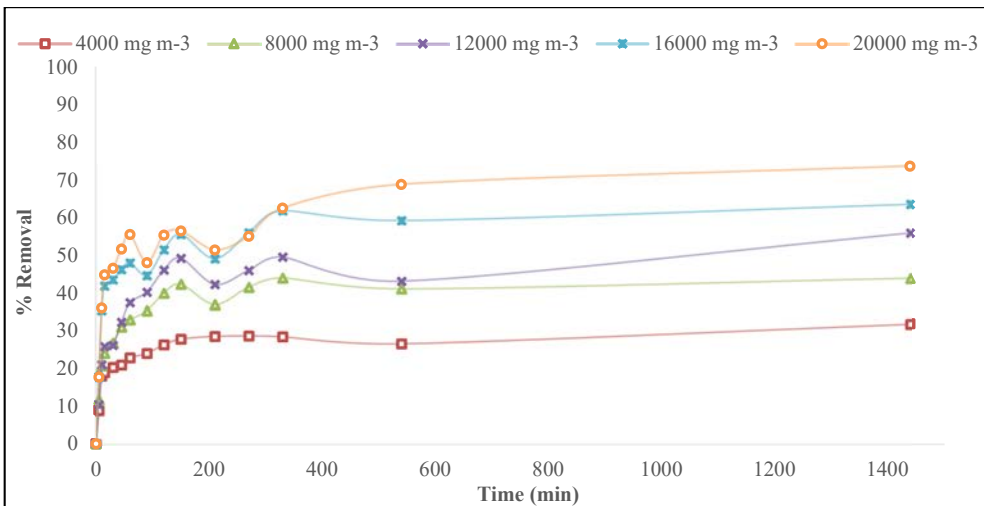


Figure 3: Reduction of atrazine (%), Co 1,200 mg m⁻³, 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 32% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 44% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 56% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 64% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 74% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 5.2, 2.8, 12.8, 4.3 and 4.9% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

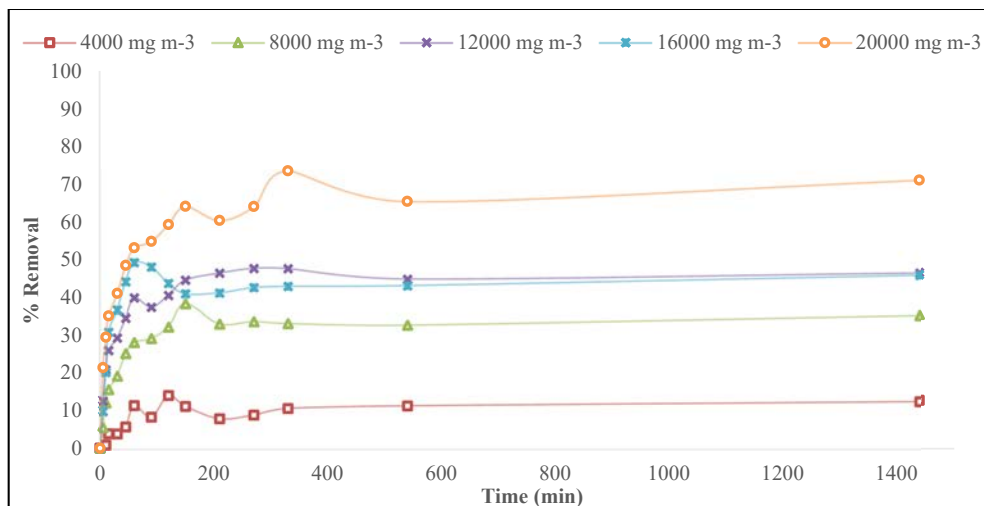


Figure 4: Reduction of atrazine (%), Co 2,000 mg m⁻³, 24 h.

Fig. 4 shows the results obtained for the trial with an initial concentration of 2,000 mg m⁻³ of atrazine at different doses of PAC for 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 13% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 35% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 47% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 46% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 71% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 1.1, 2.5, 1.6, 2.7 and 5.7% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

3.2 Simazina

Fig. 5 shows the results obtained for the trial with an initial concentration of 700 mg m⁻³ of simazine at different doses of PAC for 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 36% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 58% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 68% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 74% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 89% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 16.6, 23.2, 2.5, 5.6 and 1.9% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

Fig. 6 shows the results obtained for the trial with an initial concentration of 1,200 mg m⁻³ of simazine at different doses of PAC during 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 31% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 51% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of

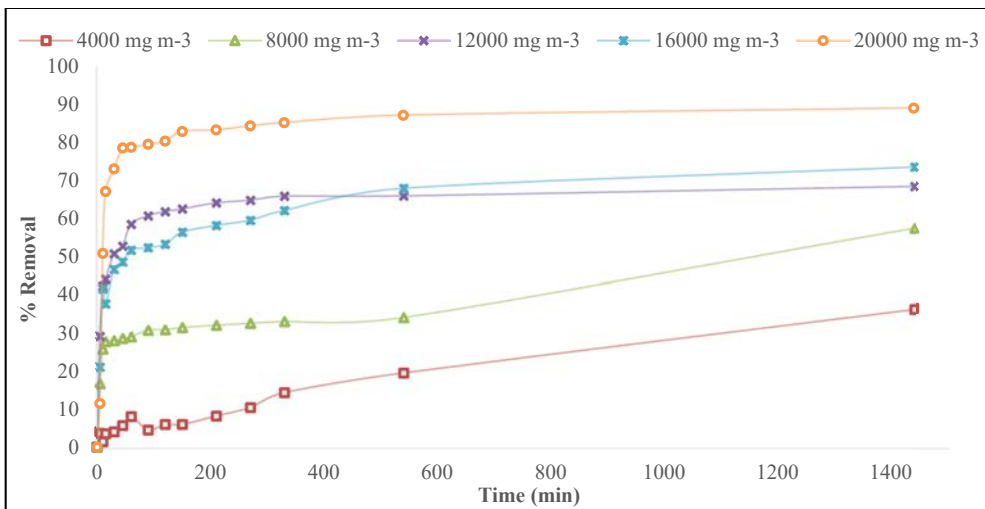


Figure 5: Reduction of simazine (%), Co 700 mg m⁻³, 24 h.

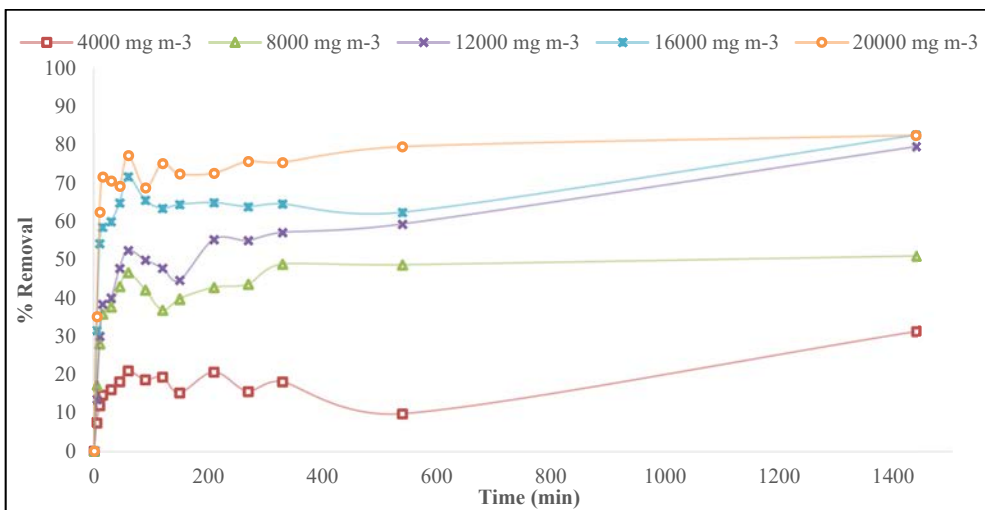


Figure 6: Simazine reduction (%), Co 1,200 mg m⁻³, 24 h.

79% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 82% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 82% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 21.5, 2.3, 20.2, 20.2 and 3% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

Fig. 7 shows the results obtained for the trial with an initial concentration of 2,000 mg m⁻³ of simazine at different doses of PAC for 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 14% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 42%

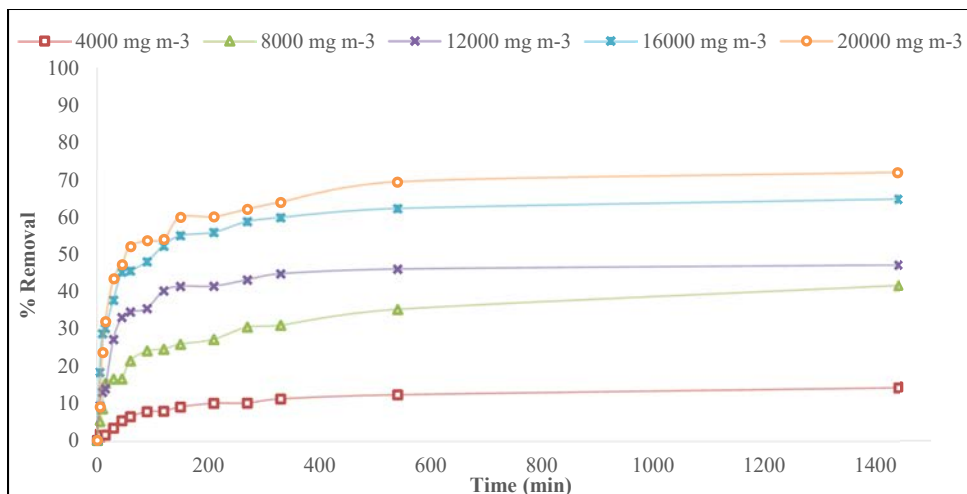


Figure 7: Reduction of simazine (%), Co 2,000 mg m⁻³, 24 h.

is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 47% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 65% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 72% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 1.9, 6.4, 1, 2.5 and 2.5% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

3.3 Linuron

Fig. 8 shows the results obtained for the trial with an initial concentration of 700 mg m⁻³ of linuron at different doses of PAC for 24 h.

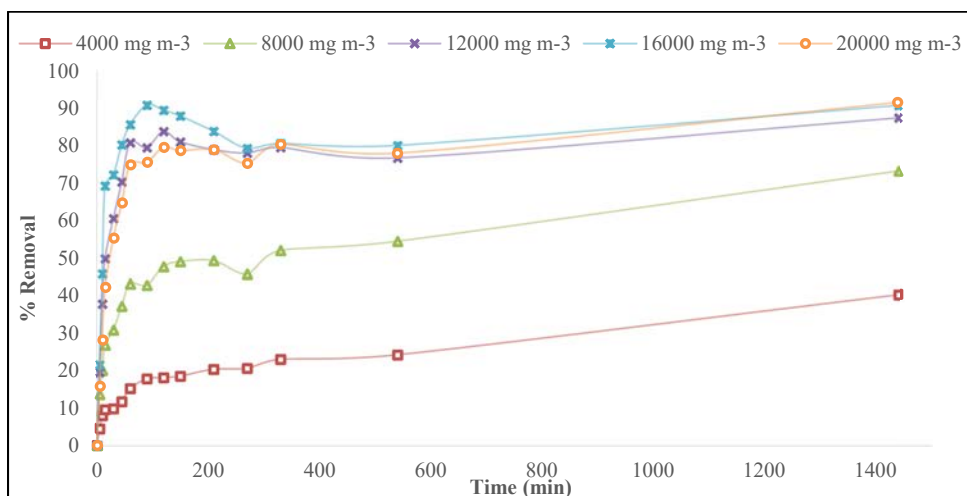


Figure 8: Reduction of linuron (%), Co 700 mg m⁻³, 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 40% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 73% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 87% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 91% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 92% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 16, 18.8, 10.7, 11, 10.5 and 13.6% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

Fig. 9 shows the results obtained for the trial with an initial concentration of 1,200 mg m⁻³ of linuron at different doses of PAC for 24 h.

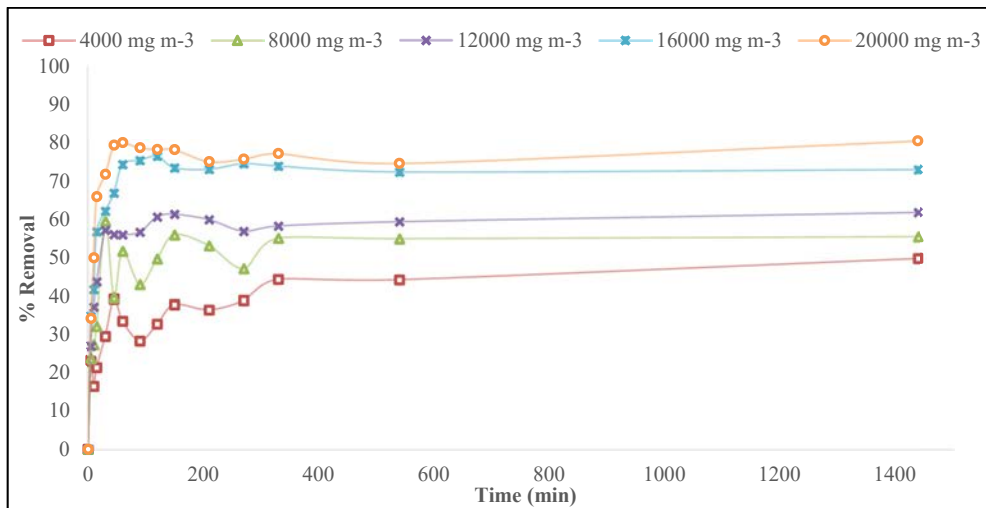


Figure 9: Reduction of linuron (%), Co 1,200 mg m⁻³, 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 49% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 56% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 62% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 70% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 80% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 5.5, 0.5, 2.4, 0.6 and 5.9% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

Fig. 10 shows the results obtained for the trial with an initial concentration of 2,000 mg m⁻³ of linuron at different doses of PAC for 24 h.

For a PAC concentration of 4,000 mg m⁻³ after 24 h a reduction percentage of 29% is obtained, for a PAC concentration of 8,000 mg m⁻³ after 24 h a reduction percentage of 41% is obtained, for a PAC concentration of 12,000 mg m⁻³ after 24 h a reduction percentage of 57% is obtained, for a PAC concentration of 16,000 mg m⁻³ after 24 h a reduction percentage of 67% is obtained and for a PAC concentration of 20,000 mg m⁻³ after 24 h a reduction percentage of 70% is obtained. From 550 min, the difference in reduction of the contaminant until the end of the assay is an increase of 0.7, 0.2, 2.8, 0.9 and 0.5% for PAC concentrations of 4,000, 8,000, 12,000, 16,000 and 20,000 mg m⁻³ respectively.

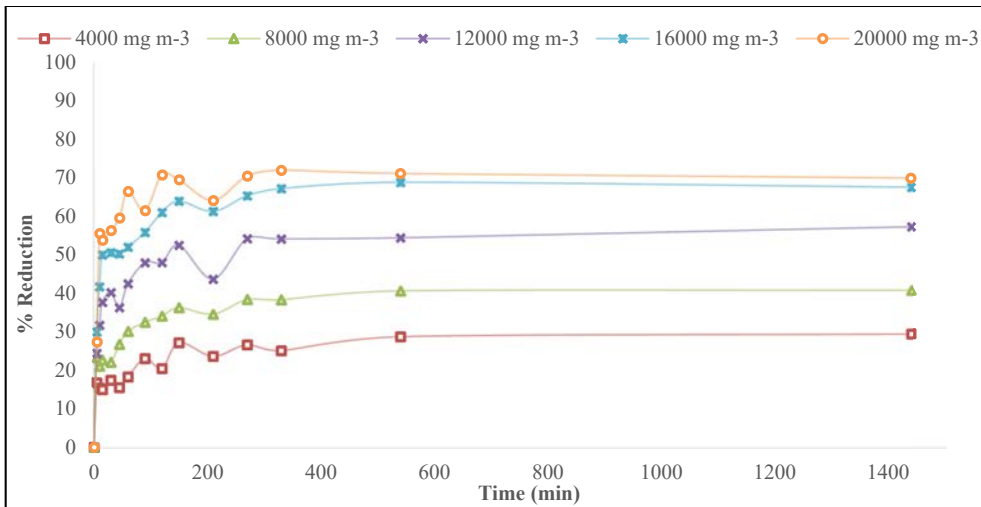


Figure 10: Reduction of linuron (%), Co 2,000 mg m⁻³, 24 h.

4 CONCLUSIONS

In view of the results presented, it can be seen that as the concentration of the PAC increases, a greater reduction in the concentration of the studied EC is achieved.

The reduction of simazine concentration when PAC is used, in general, achieves slightly better reduction percentages than those obtained for atrazine and linuron, due to its lower molecular weight 201.65 g mol⁻¹ since atrazine is 215.68 g mol⁻¹ and linuron is 249.091 g mol⁻¹ and therefore has more capacity to access the active centers of the AC. An increase of the carbon dose up to 12,000 mg m⁻³ improves the reduction percentages of pollutants. For doses of 4,000 mg m⁻³ the Linuron achieves greater reduction than for the other ECs. For higher doses of AC in certain cases an improvement in the reduction of the contaminant is not achieved, as happens to atrazine at 700 mg m⁻³ with 12,000 of PAC, increasing by 1% the reduction of the contaminant to 16,000 mg m⁻³ of PAC and 20,000 mg m⁻³ of PAC is maintained with the same reduction. In general, for PAC doses of 20,000 mg m⁻³, percentages of reduction above 70% are achieved for the three compounds. Table 2 represents the percentage reduction of each test of the 3 ECs studied with their different AC concentrations.

Table 2: Reduction of ECs (%), 24 h.

(PAC) _o	4,000 mg m ⁻³			8,000 mg m ⁻³			12,000 mg m ⁻³			16,000 mg m ⁻³			20,000 mg m ⁻³		
(EC) _o	A	S	L	A	S	L	A	S	L	A	S	L	A	S	L
700 mg m ⁻³	38	36	40	77	58	73	94	68	87	95	74	91	95	89	92
1,200 mg m ⁻³	32	31	49	44	51	56	56	79	62	64	82	70	74	82	80
2,000 mg m ⁻³	13	14	29	35	42	41	47	47	57	46	65	67	71	72	70

A = atrazine; S = simazine; L = linuron.



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MACHINE LEARNING AS A DECISION SUPPORT TOOL FOR WASTEWATER TREATMENT PLANT OPERATION

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ABSTRACT

Wastewater treatment is a significant environmental challenge. It is also an economic challenge for all operators, who face more and more demanding national and supranational regulations. Optimizing wastewater treatment processes requires physical, biological and chemical models with various degrees of complexity. From an operational perspective, programmable logic controllers are generally used. Those controllers follow strategies implemented by technicians with various degrees of expertise. This may lead to over- or under-aeration, which can be very costly. Commonly used strategies are mostly based on business rules and expert guidelines, which do not necessarily consider specific operating conditions. In this study, focused on the aeration process, a machine learning approach is applied to predict the daily operating time of aerators. Two types of models, according to the data considered, have been evaluated. The first model considers only the operation data as explanatory variables (pollutant concentrations and inflow), while the second model includes exogenous weather data (temperature, hygrometry, rainfall depth). The best model reaches a mean error less than 1%.

Keywords: machine learning, wastewater treatment, aeration process, model verification.

1 INTRODUCTION

This study is part of a project aiming to optimize wastewater treatment processes. It is based on machine learning techniques. This article covers the aeration process, which consists in bringing oxygen to micro-organisms (bacteria) while brewing water to reach homogenisation. The whole process is based on heterotrophic bacteria, which consume organic carbon for their anabolism and catabolism. This biological procedure, called nitrification, ends up producing nitrate (NO_3). A second phase in anaerobic environment reduces nitrate into dinitrogen (N_2). To optimize the process, it is recommended to go through several aerobic and anaerobic phases [1]. Aerators bring the oxygen to the pool; they are activated and deactivated several times in a day to alternate between phases. The control of this process is, in some cases, performed by technicians responsible for pump management, often without any specific guidelines. This practice leads to over-aeration or under-aeration problems, depending on the technician experience. This article aims to propose a machine learning algorithm to predict the daily aeration time. The goals are to harmonize the aerator operation, to minimize unnecessary fluctuations and to understand, through machine learning, how daily operational decisions are made. Expected benefits include, firstly, to avoid extreme aeration time and, secondly, to reduce energy consumption while meeting operational quality standards. To achieve this goal, statistic and machine learning-based approaches have been applied using both operation and weather data. The following sections describe the experimental site, the data, the modelling approaches and the preliminary results of this study.

2 DATA AND EXPERIMENTAL SITE

The data used in this investigation concern an experimental site located in the south east of France. With less than 50,000 population equivalent, it can be considered as a small or medium-size plant. For confidential reasons, the name and the exact location will not be



disclosed. Collected data are composed of a three-year historical record of operation and weather data. The list of parameters and data quantity are given in Table 1. Fig. 1 presents the observed aeration time over the period, expressed as a fraction of the observed mean time. The behaviour seems to follow some seasonal trends, but the behaviour looks otherwise quite erratic. This observation is the source of one of the objectives: to smooth the aeration process operation.

Table 1: List of variables and data quantity.

	Variable	Number of values
Operational data	Inflow (m ³ /day)	1,096
	BOD ₅ (kg/day)	72
	COD (kg/day)	156
	Nitrogen (kg/day)	70
	TSS (total suspended solid) (kg/day)	156
	Phosphorus (kg/day)	72
Weather data	Rainfall depth (mm/day)	1,096
	Temperature (°C)	1,096
	Sunshine duration (h/day)	1,096

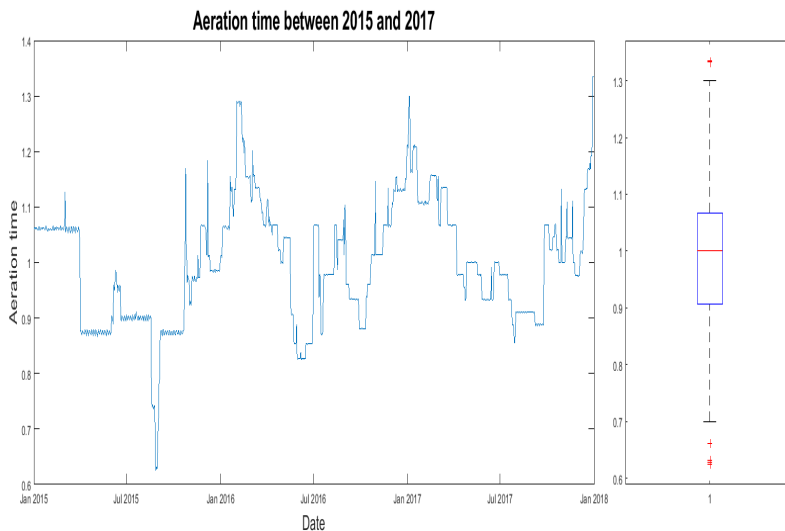


Figure 1: Observed aeration time between 1 January 2016 and 31 December 2017 (left) and data distribution (right).

Before training models, a pre-processing step was carried out. *Aquadvanced wastewater plant* is a software tool developed by Suez Smart Solution to help wastewater plant manager in their daily operations. Aquadvanced extracts data from a database supplied by several sensors or users. Some of these data were erroneous and some corrections were needed. For example, two values were set to 0 for the nitrogen inflow. Automatic outlier detection and data imputation are among our future objectives. At that time, we were not able to reconstruct these data and they were simply ignored.

3 MODELLING AND RESULTS

3.1 Modelling

Many regression models have been trained. A not exhaustive list is presented hereafter:

- Constant: the mean value of the available observations is taken as prediction value.
- Full regression: Linear regression using all the data of available variables.
- Restrained regression: Linear regression using only variables with significant p-values.
- Quadratic restrained regression: Quadratic regression using variables from the restrained regression.
- Principal component analysis (PCA) regression: Linear regression using the principal components (95% of explained variance).
- Multi-model regression: Linear regressions over separated clusters identified by using the k-means algorithm.
- Boosted trees: Aggregation of weak learners (regression trees).

These models are based on operational data. They are referred to as *operational models*.

Weather data have been used differently. An algorithm that computes a mean weighted by the similarity between observations has been implemented. The observations may be represented in a p-dimensional space (where p is the number of variables). In this space, we can compute a measure of distance between the learning set and the explicative variables. With this distance, we are then able to compute similarity. Hereafter, these models will be referred as *meteorological models*. These models could model seasonal trends but not very local behaviour. To increase robustness and solve this problem a temporal similarity was introduced. A variable representing the elapsed time between observation is added to the model to compute this similarity. The resulting new models will be identified as *historical models*.

3.2 Results and discussion

The performances of the operational models are presented in Table 2. The normalized mean errors are between 9.56% and 7.75%. These errors have been computed by cross validation [2]. For the *operational models* 5 folds were used, while, for *meteorological models* and *historical models*, a leave-one-out cross validation was applied.

Table 2: Performances of *operating models*.

Model	Observed error
Constant	9.00%
Full regression	9.14%
Restrained regression	8.48%
Quadratic restrained regression	8.09%
PCA regression	9.38%
Multi model regression	9.56%
Boosted trees	7.75%

The most efficient *operating model* was the boosted regression trees algorithm with a normalized mean error of 7.75%. The values for some functional variables were not available



daily. Thus, it led us not to include them systematically, in the most complex models. This had probably an impact on performances of the functional models. The k-means algorithm identified two classes based on the inflow. This result, which was predictable as the inflow has a large variance, do not lead to good performances. A possible reason is that the inflow might be, for a given wastewater treatment plant (WTP), nearly seen as a constant. Consequently, the variation does not have a significant effect on aeration time.

Including weather variables, we could use our similarity algorithm with different subsets of variables. The most efficient model used less than five variables. Among these variables, we find temperature, which is known to have a significant influence on plant operation [3], [4]. These *meteorological models* reached a cross-validation error of 6.69%. Fig. 2 presents the results over the year 2017. In this paper, the aeration time is expressed as a fraction of the mean time.

Finally, addition of a time component variable allows us to further increase the model's performances to a mean error of 0.96% (Fig. 3). The maximal error of 17% was obtained for a day where the observed aeration time was 40% under the mean. This anomaly could not be imputed to a failure of the aerators, nor to a high variation in other variables at our disposal. We have for sure no explanation about this very particular observation. Thus, in nominal operation, the performances of this model can be considered as satisfactory.

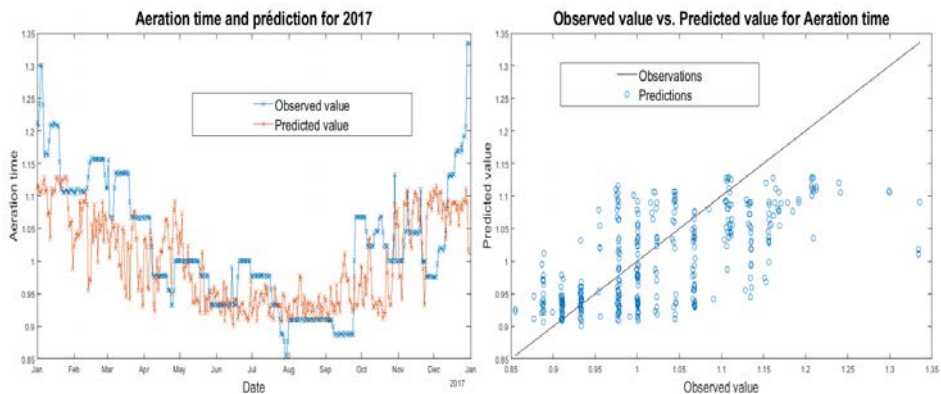


Figure 2: Result of a *meteorological model* for 2017.

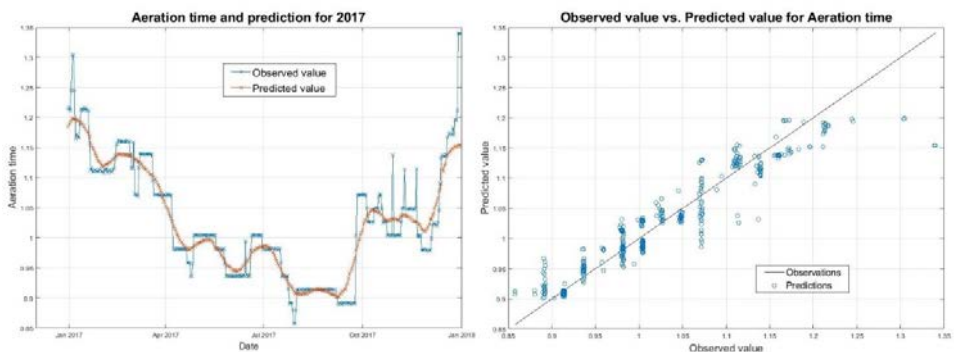


Figure 3: Results of a *historical model* for 2017.



4 CONCLUSION AND PERSPECTIVES

During this study, several statistical and machine learning approaches have been assessed. We could evaluate three different kinds of models (operational, meteorological and historical) based on various variables. The best model uses weather data, in addition to the operational data, to predict the daily aeration time. The achieved prediction error is less than 1%, which is acceptable for this application. Furthermore, we achieved two other objectives, which were: to smooth aeration daily time and to learn how choices are made by operators. Indeed, after asking them how they made operational decisions, they answered that they were based mainly on weather parameters. This methodology must be experimented on each wastewater treatment plant as each plant's behaviour might not be based on the same variable.

We may expect that the plant operation is (highly) dependent of non-numeric considerations such as distinction between working day or holiday. This assumption will lead us to add categorical data in future models. We will, then, must determine a way to compute similarities [5], [6] on categorical data, and how to weight this similarity with numerical similarity as computed in this study.

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