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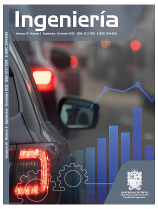

Research

Use of Computational Tools in the Modeling of Columns for Cr(VI) Adsorption in Wastewater by Means of *Theobroma cacao* L.

Uso de herramientas computacionales en el modelado de columnas para la adsorción de Cr(VI) en aguas residuales utilizando *Theobroma cacao* L.

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Abstract

Context: Industrial growth and various anthropogenic activities have generated multiple pollutants, including heavy metals such as hexavalent chromium, or Cr(VI), which pose a major threat to both humans and the environment, as their characteristics make them persistent, bioaccumulative, and non-biodegradable.
Method: In this paper, computer-aided process engineering (CAPE) was used to simulate an industrial-scale adsorption column packed with a biomass based on cocoa husk residues for the removal of Cr(VI) in solution. A parametric sensitivity analysis was conducted, using Aspen Adsorption as a simulation tool to analyze different column configurations.
Results: The Freundlich isothermal model, in combination with the linear driving force (LDF) kinetic model, yielded efficient results in removing Cr(VI) via adsorption, with values of up to 97.1 %. The best operating conditions included an initial concentration of 5000 mg/L, a bed height of 5 m, and an inlet flow rate of 100 m^3/day.
Conclusions: This study demonstrates that the use of computational assistance holds great potential for predicting the performance of an adsorption column packed with agro-industrial waste, which constitutes a safe and cost-effective alternative for the design and modeling of industrial-scale columns.

Keywords: waste biomass, adsorption column, chromium (VI), simulation, water treatment, wastewater treatment

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Resumen

Contexto: El crecimiento industrial y diversas actividades antropogénicas han generado múltiples contaminantes, entre los que se encuentran metales pesados como el cromo hexavalente, o Cr(VI), los cuales representan una amenaza significativa tanto para el medio ambiente como para el ser humano, pues sus características los hacen persistentes, bioacumulativos y no biodegradables.

Método: En este artículo se empleó la ingeniería de procesos asistida por ordenador (CAPE) para simular una columna de adsorción a escala industrial llena de biomasa a base de residuos de cáscara de cacao para la eliminación de Cr(VI) en solución. Se realizó un análisis de sensibilidad paramétrica, utilizando Aspen Adsorption como herramienta de simulación para analizar diferentes configuraciones de la columna.

Resultados: El modelo isotérmico de Freundlich, junto con el modelo cinético de fuerza motriz lineal (LDF) arrojó resultados eficientes en la remoción de Cr(VI) mediante adsorción, con valores de hasta 97.1 %. Las mejores condiciones de operación incluyeron una concentración inicial de 5000 mg/l, una altura del lecho de 5 m y un caudal de entrada de 100 m^3/día.

Conclusiones: Este estudio demuestra que el uso de la asistencia computacional tiene gran potencial para predecir el rendimiento de una columna de adsorción llena de residuos agroindustriales, constituyéndose en una alternativa segura y rentable para el diseño y modelado de columnas a escala industrial.

Palabras clave: biomasa residual, columna de adsorción, cromo (VI), simulación, tratamiento de agua, tratamiento de aguas residuales

Table of contents

Nomenclature

C_e	Pollutant concentration in solution at equilibrium (mg/L)
n	Effect of initial concentration on adsorption capacity
k_f	Freundlich's constant indicating adsorption capacity $\left(\frac{\text{mg}}{\text{g}}\right)\left(\frac{\text{Lm}}{\text{g}}\right)^n$
MTC	Global mass transfer coefficient $\left(\frac{\text{m}}{\text{s}}\right)$
$\frac{C_f}{C_o}$	Efficiency
w_k	Instantaneous equilibrium adsorbate loading on the adsorbent $\left(\frac{\text{mg}}{\text{g}}\right)$
z	Distance along the bed (m)
Q_i	Quantity of metal ions adsorbed by the adsorbent (mg/g)
C_i	Concentration of cadmium ions in the liquid phase (mg/L)
ρ_s	Bulk density (g/cm^3)
t	Time (min)
ε	Bed porosity
u_o	Fluid velocity (m/s)

1. Introduction

Water sources play an essential role in human life due to their great usefulness and versatility in different activities, *e.g.*, industrial processes, agricultural and livestock activities, hospitals, shopping centers, rural areas, and domestic households, among others (1). Using this resource generates different types of wastewater that are loaded with pollutants. A large portion of this water, which originates from industrial activity, is considered to be of great concern due to its properties, as is the case with the toxic substances it contains (2, 3). This toxicity depends on various factors such as chemical composition, which varies from sector to sector, making the elimination of these substances a challenge, as each effluent contains unique pollutants that require customized treatment (4, 5). Among the various pollutants present in industrial wastewater are heavy metals, a worldwide concern due to their high toxicity, their detrimental impact on both the environment and human health, and their high strength and non-biodegradability (6).

Despite being an essential metal, chromium is considered to be one of the 16 main toxic pollutants with adverse effects on human health. This metal, which can be ingested, inhaled, or absorbed through the skin (7), is used in various manufacturing sectors, such as the metallurgy, tanning, cement, textile, and dyeing industries. These sectors represent major sources of pollution (8). Chromium ranks second in abundance among the heavy metal pollutants, surpassed only by lead. It is naturally found in three forms: metallic, trivalent, and hexavalent, with the latter, Cr(IV), being the toxic one. This form has a variety of detrimental health effects, such as digestive, urinary, reproductive, and immune system dysfunctions. Therefore, it is necessary to treat any water sources contaminated with Cr(IV) that are discharged into the environment (9). In Colombia, the limit for chromium in drinking water, as dictated by Law 0631 of 2015, is 0.5 mg/L (10), while the World Health Organization's permitted level is 0.05 mg/L for Cr (11).

Adsorption is an effective method for removing unwanted pollutants, given its feasibility and easy scalability. This method is also able to effectively remove various inorganic chemicals that affect the adsorption system (12). This technique has several advantages that make it a very attractive method for use in water treatment. Among these advantages are its efficiency in removing various types of pollutants, including heavy metals, dyes, emerging contaminants, and other types of substances (13); its applicability at low temperature and pressure, since, compared to other water treatment processes, it does not require extreme conditions; its versatility in dealing with pollutants in both gaseous and liquid form (14); the regenerative capacity of the materials used in the adsorption process, which allows reusing biomaterials multiple times depending on the type of biomass employed and its characteristics (15); the speed at which this technique removes pollutants, allowing for effective and fast processes; and its versatility in enabling a modular and scalable design of the adsorption process in the form of columns or adsorbent beds, modeled on a small or a large scale as required (16).

This technique may involve one of two different adsorption methods: *physisorption*, wherein adsorption stems from the presence of weak attractions between the pollutant and the adsorbent material, generated by short-range electrostatic forces (*i.e.*, van der Waals forces) (17); and *chemisorption*, where adsorption takes place due to the presence of chemical bonds between the adsorbate and the adsorbent, causing a stronger and more selective interaction. This process is less reversible than physisorption and requires considerably more energy for the desorption of the adsorbed species (18). The adsorption process can be carried out in two ways: in batches or in columns (19).

This technique has been recognized as one of the simplest and most economical strategies due to its remarkable ability for heavy metal removal (20,21). Different biomaterials have been developed and used to this effect, such as *Ulva flexuosa*, a species of algae (22); babano shell (23); rapeseed (*Brassica napus*) (24); and coconut (25), among others. Cocoa (*Theobroma cacao L.*) is a widely cultivated product in Colombia, and it generates a large amount of residual biomass, comprising the husk of the cob, the husk of the bean, and the pulp. Among the different byproducts of this plant, the husk is a promising material for the production of adsorbent materials, given its abundance, low cost, and renewable nature. The cocoa husk is composed of cellulose, hemicellulose, and lignin, and it offers a high adsorption capacity, which makes it a sustainable alternative for the elimination of pollutants in aqueous media, *e.g.*, heavy metals (26). Most adsorption studies have been conducted at the laboratory level under simple conditions and on small scales. This is due to different limiting factors, such as resource, space, and time availability, among others. In light of the above, several computational tools like Aspen Plus (27) or ChemCAD (28), have been developed for modeling processes on a larger scale, but scaling to solids in adsorption towers is still in its early stages. Therefore, researchers have searched for new ways to scale their proposals under the existing limitations. Among them, the Aspen Adsorption software has proven to be a tool for adsorption columns. This tool allows modeling multi-scale adsorption columns by simulating key phenomena such as mass transfer, adsorption equilibrium, and fluid dynamics. It allows predicting performance at the laboratory, pilot, and industrial scales, optimizing system design and operation based an experimental data. Its use in treating chromium-contaminated water also demonstrates its ability to respond to various operating conditions, improving process efficiency and supporting scaling from laboratory-level to industrial applications. This tool constitutes an advantage for a broader exploration of different parameters or operating variables such as flow, bed height, and pollutant concentration, among others, facilitating the optimization of the process before designing a pilot or building industrial plant.

A study published by (29) delved into the performance of dolochar as a Cd(II) adsorbent, using Aspen Adsorption to simulate a large-scale process. The results, obtained via the response surface methodology, show that, with optimal bed height, inlet concentration, flow rate, and fixed biosorbent mass values, the CD(II) ion adsorption capacity and depletion time of the packed dolochar bed are 1.85 mg/g and 11.39 hours, respectively.

Using Aspen Adsorption V11, the study by (30) simulated the adsorption of Pb(II) on tire-based activated carbon (TAC) and commercial activated carbon (CAC) in a fixed-bed column while considering different concentration ranges, bed heights, and flow rates. The optimal conditions found in this study included a concentration of 500 mg/L, a bed height of 0.6 m, and a flow rate of 9.88×10^{-4} m^3/s, which yielded breakthrough times of 488 and 23 s for TAC and CAC, respectively, with removal capacities of 114.26 and 7.72 mg/g.

In light of the above, the objective of this study was to model an industrial column packed with *Theobroma cacao* L. for the adsorption of Cr(VI) in solution, using Aspen Adsorption to conduct a parametric sensitivity analysis and evaluate the performance of the system by altering key parameters. Our work demonstrates the potential of computational tools for predicting the performance of adsorption columns and provides a solid basis for the design and simulation of large-scale adsorption systems that employ agro-industrial materials for water treatment.

2. Materials and methods

2.1. Parameterization and modeling

In this study, we used Aspen Adsorption V12.1 to simulate an adsorption column packed with *Theobroma cacao* L. for the removal of Cr(VI) in an industrial stream. A parametric study was carried out regarding the inlet flow rate, the initial concentration, and the column height, with the aim of determining the extent to which modifying these factors affects adsorption performance. We also conducted a sensitivity analysis that considered the breakthrough profile. Different parameter ranges were used to evaluate the performance of the adsorption system. For the inlet flow rate, values of 250, 200, 150, 100, and 50 m3/day were employed; for the bed height, we established values of 3, 4, and 5 m[30]; and, finally, for the initial concentration of Cr(VI), 5000, 3500, 2000, and 1000 mg/L were considered (31,32).

To design our proposal, studies on the use of columns for the removal of heavy metals from industrial wastewater were used as a basis, considering the different parameters required to simulate the process in Aspen Adsorption. In this vein, we established a bed diameter of 1 m (33), a bulk density of 0.0365 g/cm^3 for the biomaterial (34), a bed porosity of 0.67 (m^3 of voids per m^3 of bed), a total vacuum porosity of 0.4 (35,36), and a constant mass transfer coefficient of 1.37×10^{-4} s^{-1} (37).

To understand the behavior caused by the interactions between the adsorbate and the adsorbent during the process, we employed the Freundlich isothermal model (38), while the linear driving force (LDF) kinetic model was used to determine the rate at which the adsorption occurred (39). Fig. **1** presents the simulation flowchart for the column.

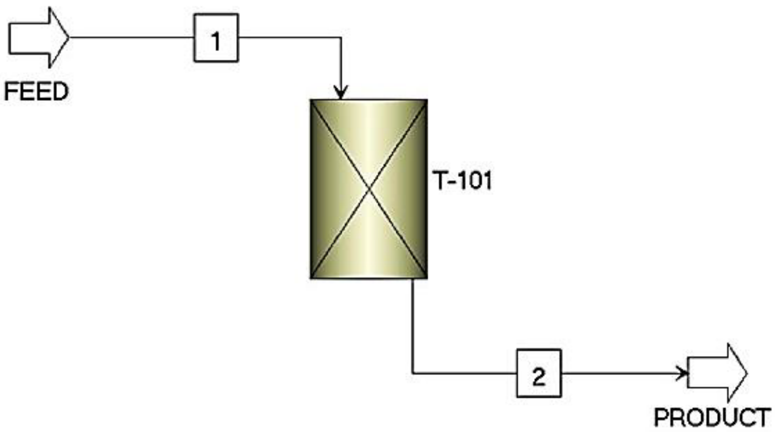

Figure 1. Simulation flowchart for the adsorption column

2.2. Mathematical fundamentals

2.2.1. Mass balance

The equation used by Aspen Adsorption for the mass balance of the adsorption column is presented below:

$$u_0\varepsilon\frac{\partial C_i}{\partial z}+\varepsilon\frac{\partial C_i}{\partial t}+\rho_s\frac{\partial Q_i}{\partial t}=0 \tag{1}$$

2.2.2. Freundlich isothermal model

The Freundlich model considers a multilayer adsorption on a heterogeneous surface, where the distribution of the components depends on the time and energy of the secured sites (40,41). This model is described by Eq. 2.

$$q_e = k_f C_e^{1/n} \tag{2}$$

2.2.3. LDF kinetic model

The LDF kinetic model implies that the driving force for the mass transfer of components is a linear function of the concentration of the component in the liquid or solid phase (42,43). This model is presented in Eq. 3.

$$\frac{\partial w_k}{\partial t} = MTC_{sk} \left(w_k^* - w_k \right) \tag{3}$$

3. Results and discussion

3.1. Evaluating the mathematical models using Aspen Adsorption

The Freundlich isothermal model and the LDF kinetic model were evaluated while considering the above-presented parameters and ranges. The results indicated that, by reducing the height of the column and increasing the flow rate, the break and saturation times can be reduced. This is due to the fact that, with a low bed height and a high flow rate, the fluid passes through the bed more quickly, which results in reduced process times. The results for the break time (TR) and the saturation time (TS) are shown in Table **II**.

3.2. Influence of the inlet flow rate

By means of a parametric sensitivity analysis, the influence of the inlet flow rate on the performance of the adsorption column was evaluated. To this effect, inlet flow rates of 250, 200, 150, 100, and 50 m^3/day were considered. Fig. **2** shows the breakthrough profiles obtained from the Freundlich-LDF model. Note that the efficiency increases with the flow rate, but the breakthrough and saturation times are reduced. This behavior is due to the fact that a high inflow rate has a positive effect on mass transfer, causing a faster accumulation of the pollutant and decreasing the number of available active sites, which leads to reduced times. This behavior is also evident in the efficiency values obtained: 95.2 % for 250 m^3/day, 94 % for 200 m^3/day, 92.1 % for 150 m^3/day, 88.4 % for 100 m^3/day, and 78.1 % for 50 m^3/day (44,45).

3.3. Influence of initial concentration

For the parametric sensitivity analysis of the initial Cr(VI) concentration, values of 5000, 3500, 2000, and 1000 mg/L were considered. Fig. **3** shows the breakthrough profiles obtained from the simulation of the Freundlich-LDF model. Note that, when this parameter is increased or decreased, the rupture times

Table II. Results obtained for the analyzed models

Freundlich -LDF		Flow rate (m^3/day)														
		250			200			150			100			50		
		Bed height (m)														
Concentration (mg/L)	**Results**	3	4	5	3	4	5	3	4	5	3	4	5	3	4	5
5000	**TR (min)**	105	144	184	135	184	233	184	250	315	282	381	480	579	778	978
	TS (min)	1194	1540	1884	1449	1884	2294	1884	2440	2978	2708	3499	4264	5014	6429	7792
3500	**TR (min)**	112	153	195	143	195	247	195	264	334	299	403	507	612	822	1032
	TS (min)	1161	1494	1820	1409	1820	2231	1820	2361	2880	2678	3394	4129	4830	6187	7475
2000	**TR (min)**	124	169	214	157	214	271	214	289	365	327	441	555	669	898	1129
	TS (min)	1100	1422	1732	1341	1732	2111	1732	2234	2731	2480	3201	3885	4545	5783	6967
1000	**TR (min)**	141	192	242	179	242	306	242	327	412	370	498	626	755	1013	1272
	TS (min)	1037	1331	1620	1254	1620	1969	1620	2081	2518	2307	2950	3555	4146	5240	6239

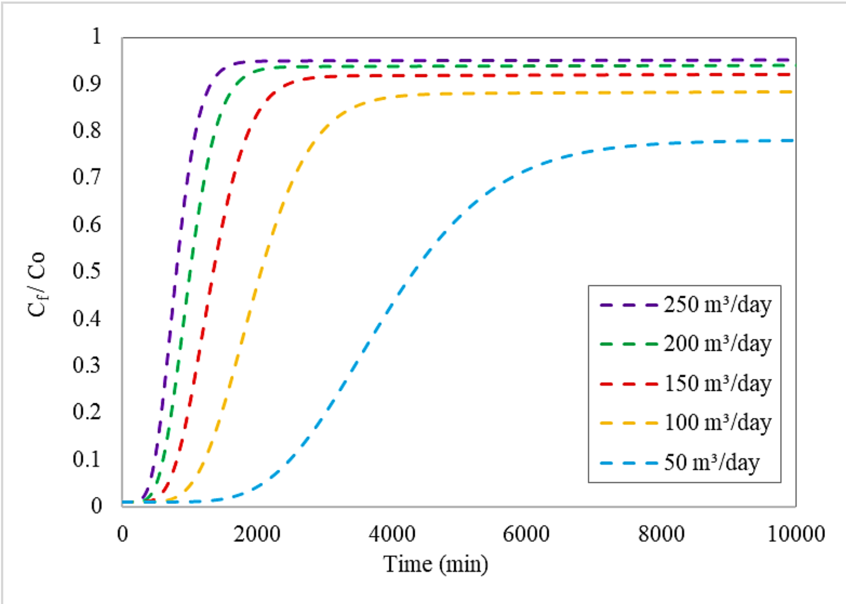

Figure 2. Breakthrough curve for a bed height of 5 m and an initial concentration of 500 mg/L at different flow rates

(TR) and saturation times (TS) obtained for each column configuration are very close to each other. Similarly, the efficiencies achieved show a similar trend, indicating that, under these conditions, the influence of concentration on the difference between TR, TS, and the overall system performance is limited. This phenomenon is due to the high presence of Cr(VI) in the flow, which causes an early break in the curve—this behavior is also observed at different times. Nevertheless, varying this parameter does not affect the adsorption performance, as the observed difference was less than 1 %. This can be attributed to different factors, such as the number of active sites available in the adsorbent, the strong affinity between the adsorbent and the adsorbate (which allows quickly reaching adsorption equilibrium), and the operating conditions considered, among others (46).

3.4. Influence of bed height

We also analyzed the influence of bed height on the performance of the adsorption column used for the removal of Cr(VI) in aqueous solution. The values considered in this analysis were 3, 4, and 5 m. Fig. 4 shows the breakthrough profiles obtained from the simulation of the Freundlich-LDF model. The breakthrough and saturation times increase with bed height, whereas efficiency is reduced. This is due to the fact that, with a larger adsorption surface, the fluid entering the column takes longer to exit. In addition, there are more active sites available, which extends the useful life of the adsorbent material, since it does not saturate as quickly, resulting in increased process times. On the other hand, the efficiency values obtained after the simulation were 92.9 % for 3 m, 90.6 % for 4 m, and 88.4 % for 5 m (47).

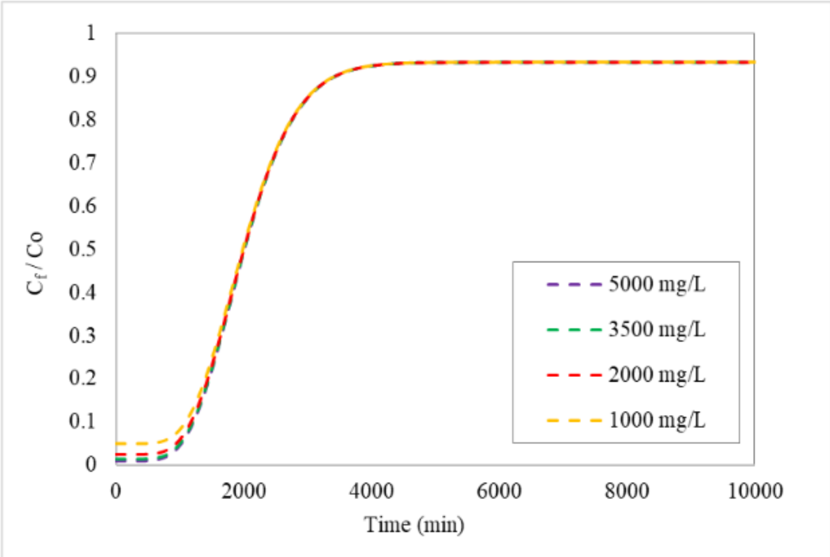

Figure 3. Breakthrough profiles for a column height of 5 m and an inlet flow rate of 100 m^3/day at various Cr(IV) concentrations

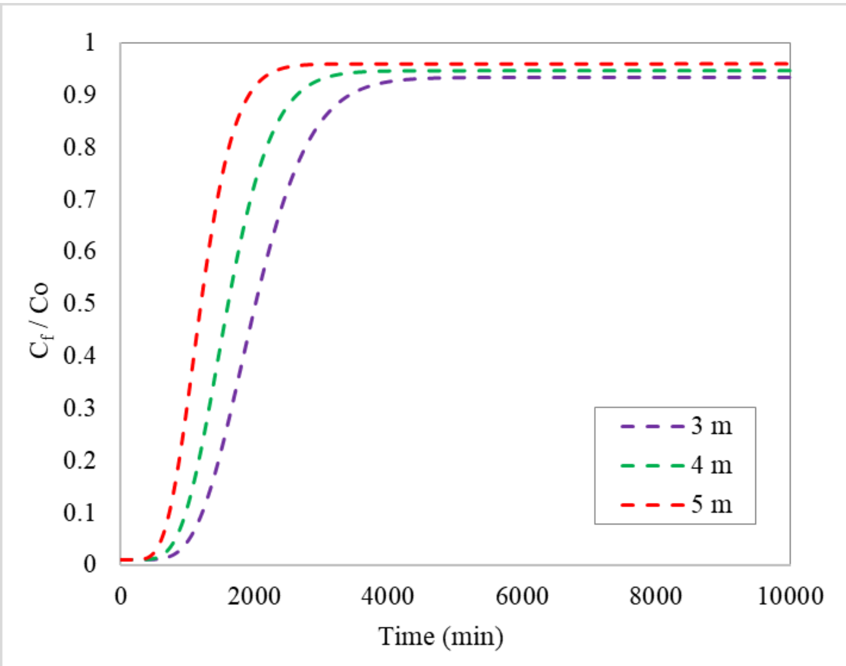

Figure 4. Breakthrough profiles for an initial concentration of 5000 mg/L and a flow rate of 100 m^3/day at different bed heights

3.5. Comparison with other results in the literature

The data obtained after conducting various simulations of the industrial cocoa-packed adsorption column were compared against the results of studies published in the specialized literature. It should be noted that this comparison has relative value, since each study was carried out under different inlet flow rate, initial concentration, bed height, and biomaterial conditions. The results of this work indicate that *Theobroma cacao* L. offers an acceptable in Cr(VI) removal. Table III shows de aforementioned comparison.

Table III. Comparison with literature-reported results

Contaminant	Adsorbent	Parameters	Results	Source
Pb(II)	Activated alumina	Initial concentration: 0.1 mg/L Inlet flow rate: 54.52 m^3/day Bed height: 1.459 m	Rupture time: 40 320 min	(48)
Pb(II)	*Bambusa* spp.	Initial concentration: 20 mg/L Inlet flow rate: 1.728 m^3/day Bed height: 1 m	Rupture time: 52 min	(49)
Cr(VI)	*Theobroma cacao* L.	Initial concentration: 5000 mg/L Inlet flow rate: 100 m^3/day Bed height: 5 m	Rupture time: 480 min Saturation time: 4264 min	This study

4. Conclusions

This study presented an innovative approach to modeling and simulating large-scale adsorption columns using agro-industrial waste (cocoa residues in this case) to remove heavy metals such as Cr(VI) from water systems. This work provides valuable quantitative data that contribute to the development and understanding of industrial adsorption processes. A parametric sensitivity analysis allowed evaluating the effect of varying the column's bed height, inlet flow rate, and initial pollutant concentration on the efficiency of the process. The results that increasing the bed height increases the break and saturation times but reduces the adsorption efficiency. On the other hand, high inlet flows improve the adsorption efficiency but decrease the biomaterial's saturation times. It is also noteworthy that the initial concentration does not have a significant effect on adsorption efficiency. These results constitute a robust technical basis for the design and optimization of industrial effluent treatment systems, as they allow anticipating the behavior of the system prior to its full-scale implementation.

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6. Author contributions

Ángel González Delgado: contextualization, software, formal analysis, writing (review and editing), visualization.
Ángel Villabona Ortiz: project administration, contextualization, methodology, software, validation, formal analysis, research, resources, data curation, writing (original draft).
Candelaria Tejada Tovar: methodology, validation, research, data curation, writing (original draft), visualization, supervision.

7. Funding

This research received no external funding.

8. Data availability

The data will be made available upon request.

9. Conflicts of interest

The authors declare no conflict of interest.

10. Use of artificial intelligence

During this work, the authors did not employ any technologies associated with artificial intelligence.

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