Remoción de Cr (VI) en solución utilizando *Theobroma cacao L.*: Simulación de columna empacada a escala industrial

Removal of Cr (VI) in solution using *Theobroma cacao L.*: Simulation of an industrial-scale packed column

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Resumen

Introducción: Se han desarrollado muchos estudios donde utilizan técnicas para eliminar contaminantes en cuerpos de agua. Entre estas técnicas se encuentra la adsorción, técnica de superficie que utiliza adsorbente a base de residuos agrícolas para remover dichos contaminantes, como los metales pesados pero estos estudios en su mayoría se han realizado a escala laboratorio, son pocas las investigaciones que han buscado anticipar la eficacia del adsorbente a nivel industrial.

Objetivo: Simular la remoción de Cr (VI) en solución mediante una columna empacada a escala industrial utilizando biomasa de Theobroma cacao L. como adsorbente.

Metodología: Se utilizó un método del tipo de modelado y simulación donde se empleó el instrumento informático Aspen Adsorption, para simular la columna de adsorción empleando diversas configuraciones combinadas con una evaluación paramétrica.

Resultados: Con los descubrimientos realizados se obtuvo que, usando los modelos matemáticos Langmuir y Fuerza Motriz Lineal (LDF) se presentaron eficiencias del proceso de adsorción hasta un 97% de remoción de Cr (VI). Además, los mejores valores paramétricos fueron una altura de la columna de 5m, un caudal de 100 m3/día y una concentración inicial de 3500 mg/L.

Conclusiones: Estos hallazgos permiten presentar este estudio como una forma novedosa en el campo de la ingeniería de cómo las herramientas computacionales tienen la capacidad de predecir el posible comportamiento de columnas de adsorción rellenas con biomasas basadas en residuos orgánicos.

Palabras clave: Cromo (VI), Curvas de ruptura, Parámetros, Simulación, Tratamiento de Aguas.

Abstract

Introduction: Many studies have been developed using techniques to remove pollutants in water bodies. Among these techniques is adsorption, a surface technique that uses an adsorbent based on agricultural residues to remove pollutants such as heavy metals. However, these studies have mostly been conducted at a laboratory scale, and few investigations have sought to anticipate the effectiveness of the adsorbent at an industrial scale.

Objective: To simulate the removal of Cr(VI) in solution by a packed column at industrial scale using Theobroma cacao L. biomass as adsorbent.

Method: A modeling and simulation type method was used where the computer tool Aspen Adsorption was employed to simulate the adsorption column using different configurations combined with a parametric evaluation.

Results: From the findings it was obtained that, using the Langmuir and Linear Driving Force (LDF) mathematical models, adsorption process efficiencies of up to 97% Cr (VI) removal were presented. In addition, the best parametric values were a column height of 5m, a flow rate of 100 m3/day and an initial concentration of 3500 mg/L.

Conclusions: These findings allow presenting this study as a novel way in the engineering field of how computational tools have the ability to predict the possible behavior of adsorption columns packed with organic waste-based biomasses.

Keywords: Chromium (VI), Rupture curves, Parameters, Simulation, Water treatment

INTRODUCTION

The constant progress of civilization, industrialization, and urbanization, associated with multiple anthropogenic activities, have led to the emission of harmful substances into the environment, [1], added to natural processes, such as rock erosion and climatic changes, generate negative effects that affect water quality [2]. Heavy metals in water bodies come from different pollution sources, such as mining, agricultural, industrial, and metallurgical activities. The pollution generated by these metals causes great concern, as they are toxic, non-biodegradable, and challenging to remove [3]. Chromium is a heavy metal that, in its natural form, can occur as trivalent chromium in the form of chromium oxides and hydroxides or hexavalent chromium in the form of chromate salts [4]. Chromium (VI) is characterized as poisonous, mutagenic, highly soluble, and carcinogenic, while Chromium (III) is an essential trace element for human well-being [5]. Hexavalent chromium is used in various fields, mainly in the tanning, textile, electroplating, and pigment industries, among others [6]. The World Health Organization's permitted limit for Cr in drinking water is 0.05 mg/L [7]. In Colombia, the allowable limit for chromium in drinking water, as dictated in Law 0631 of 2015, is 0.5 mg/L [8]. The adsorption process is a surface technique where adsorbates are transferred to adsorbents. This technique has been used to treat water sources and wastewater because it is an inexpensive, simple, effective, and environmentally friendly process [9]. Different types of natural residues have been used to remove heavy metals. Among these, cocoa shells have proven to be an efficient adsorbent [10]. However, adsorption experiments have mostly been kept at the laboratory scale; therefore, methods have been sought to predict the behavior and performance of adsorption processes at the industrial scale, for which specialized computational tools have been developed to perform simulations of different processes and/ or equipment, software such as Aspen Plus [11] or ChemCAD [12] where accurate results have been demonstrated in predicting the performance of a complete equipment or process. However, the parameterization of packed columns is still at an early stage. Therefore, this study seeks to model an industrial-level packed column with cocoa shell waste as an adsorbent using a computational tool and parametric evaluation to remove Cr (VI) in solution based on experimental data previously obtained by the authors [13], [14]. Demonstrating the potential of computational tools for predicting the performance of an adsorption column and contributing quantitative information regarding the scaling and parameterization of an industrial-scale column packed with *Theobroma Cacao L.*

METHODOLOGY

Physical properties of the metal ion.

In order to perform the simulations of the packed adsorption column for the removal of Cr (VI) in solution using the Aspen Adsorption V12 software, it is necessary to add the list of components to be adsorbed, in this case chromium, using the database provided by Aspen Properties®. Subsequently, it is necessary to select the physical properties package that fits the type of solution that is entering the bed. Therefore, the Electrolyte Non-Random Two-Liquid Properties (ELECNTRL) method was selected for this study because this package allows operating with aqueous solutions of liquid electrolytes with low and high concentrations, as long as there is no vapor phase in the mixture [15].

Parameters required by Aspen Adsorption.

Once the components and physical properties have been defined, the packed column configuration must be set up to simulate the adsorption process. This requires the specification of several parameters necessary for Aspen Adsorption. Therefore, similar studies of adsorption processes using packed columns at industrial level for the removal of heavy metals were taken as a basis, establishing different variables such as column diameter, column porosity, total void porosity, adsorbent bulk density and mass transfer coefficient, which are required for the packed column configuration. In turn, it is necessary to establish the values of the constants of the selected isothermal mathematical model, in this case, the Langmuir model, since the values are necessary for the simulation process. Table 1 shows the parameters used to perform the simulation and the data source.

TABLE 1. PARAMETERS USED TO SIMULATE THE COLUMN

Required parameter	Unit	Values	Source
	mg/g	227.348	[16]
	L/mg	0.0112	
Column diameter	m	1	[15]
Column porosity	m3 vacuum / m3 bedding	0.67	[17], [18]
Total void porosity	m3 vacuum / m3 bedding	0.4	
Bulk density	g/cm3	0.0365	[10]
Constant mass transfer coefficient	1/s	1.37x10-4	[19]

On the other hand, the software requires defining the conditions under which the simulations will be carried out, which includes the selection of calculation methods, operating conditions, kinetic and isothermal models, among other parameters. First, the Upwind Differencing Scheme 1 (UDS1) discretization method, a numerical scheme used to solve mass transport equations, is established. Also, a constant number of 10 nodes is set in order to ensure accuracy and stability in the simulations. Next, it is assumed that the fluid flowing through the column presents only convective transport, without axial dispersion, and that its velocity is constant. Furthermore, it is considered that the film is liquid and that the mass transfer coefficient remains constant. Subsequently, the kinetic model and the isothermal model used in the study are defined: the Linear Driving Force (LDF) model to describe the velocity of the adsorption process, and the Langmuir isothermal model, already mentioned, to represent the interactions between the adsorbate and the adsorbent. Finally, it is assumed that the process takes place under isothermal conditions.

Stipulation of the conditions for the sensitivity analysis.
To evaluate the performance of the packed adsorption column for the removal of Cr (VI), three scenarios were established to carry out the simulation process of the bed. That is, three main parameters were assessed to determine their effect on the adsorption process through a parametric evaluation. Therefore, the column height, inlet flow rate, and initial contaminant concentration were varied. The different simulations were conducted under dynamic conditions by plotting breakthrough curves over time to observe how changes in these parameters impact breakthrough time, saturation time, and overall process performance.To verify the impact of height variation on time and process performance, this parameter was varied within a range of 3, 4, and 5 m, keeping the initial concentration and inlet flow rate constant. Likewise, the impact of inlet flow rate variation on the breakthrough curve profile and process performance was studied using flow rates of 100, 150, and 200 m³/day, while keeping the column height and initial concentration fixed [20]. Finally, the effect of varying the initial concentration parameter on adsorption was analyzed using values of 1000, 2000, and 3500, keeping the column height and inlet flow rate constant [7], [21]

Mathematical fundamentals
Aspen Adsorption uses different equations embedded in its database to perform the calculations necessary for adsorption process simulation processes. This software performs the mass balance of the adsorption column using a partial difference equation (Eq.1) to express the metal ion concentration in a small control volume within the adsorbent column [22]:

$$-\varepsilon_i E_i \left(\frac{\delta^2 C_i}{\delta z^2}\right) + \frac{\delta}{\delta z}(v_i \times c_i) + \varepsilon_i \frac{\delta C_i}{\delta t} + \rho_s \frac{\delta q}{\delta t} = 0 \quad (1)$$

Where ε_i is the porosity of the bed, is the axial dispersion coefficient (m²/s), is the distance along the bed (m), is the number of metal ions adsorbed by the adsorbent (mg/g), c_i is the concentration of cadmium ions in the liquid phase, is the bulk density and is the interstitial velocity of the fluid through the adsorbent bed. The Langmuir isotherm model shows that adsorption usually occurs with numerous monolayer adsorption processes, and the desired adsorption takes place at defined active sites on the adsorbent surface [23], [24]. It is described by the following equation (2):

$$q_e = \frac{q_{max} \times b \times C_e}{1 + b \times C_e} \quad (2)$$

Therefore, its homologous used by the software presented was sought for the following expression (3):

$$w_i = \frac{IP_{1i} \times IP_2 \times c_i}{1 + IP_2 \times c_i} \quad (3)$$

Where a comparison between the equation found in the literature and the one presented by the software can be determined that , i.e. the maximum amount of solute in the solid phase (mg/g), , i.e. it is the Langmuir constant that expresses the affinity of the active sites for the pollutant (L/mg), , i.e., it is the equilibrium concentration of the contaminant present in the solution. On the other hand, the Linear Driving Force (LDF) kinetic model employed by the software describes the rate of adsorption using the global mass transfer coefficient; it assumes that the mass transfer of the components is driven by a linear expression expressed in terms of the concentration, either in the liquid or solid state [20], [25]. This model is described by equation (4):

where MTC is the global coefficient of mass transfer (m/s), and is the instantaneous equilibrium adsorbate loading on the adsorbent (mg*g).

RESULTS AND DISCUSSIONS

Data obtained from the simulation of the packed adsorption column using Aspen Adsorption Using the Aspen Adsorption computational tool, a packed column was modeled for the removal of Cr (VI), using the Langmuir isothermal model and the LDF kinetic model with different distributions of the input flow parameters, the initial concentration and the bed height, obtaining results of the Rupture Time (R.T.), which refers to the moment in which the sorbent begins to reduce its capacity to remove the contaminant, and the Saturation Time (S.T.), which is the moment when the sorbent reaches its maximum capacity to retain the contaminant. These results are presented in Table 2.

TABLE 2. DATA OBTAINED FROM SIMULATIONS

Initial concentration (mg/L)	Inlet flow rate (m3/day)	Bed height (m)	R.T. (min)	S.T. (min)
3500	200	3	143	1408
		4	195	1820
		5	247	2215
	150	3	195	1820
		4	264	2348
		5	334	2869
	100	3	299	2608
		4	403	3367
		5	507	4107
2000	200	3	157	1341
		4	214	1732
		5	271	2105
	150	3	214	1732
		4	289	2232
		5	365	2791
	100	3	327	2481
		4	441	3186
		5	553	3865

1000	200	3	179	1253
		4	242	1619
		5	306	1962
	150	3	242	1619
		4	327	079
		5	413	2516
	100	3	370	2299
		4	498	2942
		5	626	3544

Parametric sensitivity analysis

The impact of altering the parameters of column height, inlet flow rate, and initial Cr (VI) concentration on the Cr (VI) adsorption process was analyzed.

Analysis of the effect caused by bed height variation

The evaluation of the variation in bed height during the adsorption process was carried out using a height range of 3, 4, and 5 meters, while keeping the initial concentration fixed at 3500 mg/L and the inlet flow rate at 100 m³/day. Figure 1 shows the behavior of the breakthrough curves obtained after completing the bed simulation process. It was observed that decreasing the bed height leads to a reduction in breakthrough and saturation times, but an increase in efficiency. This is because, with a smaller column, the fluid will need less time to pass through the equipment, obtaining a reduction in residence time. In addition, the efficiencies obtained for each height were 92.4% for 3 meters, 90% for 4 meters, and 87.7% for 5 meters. [27], [28].
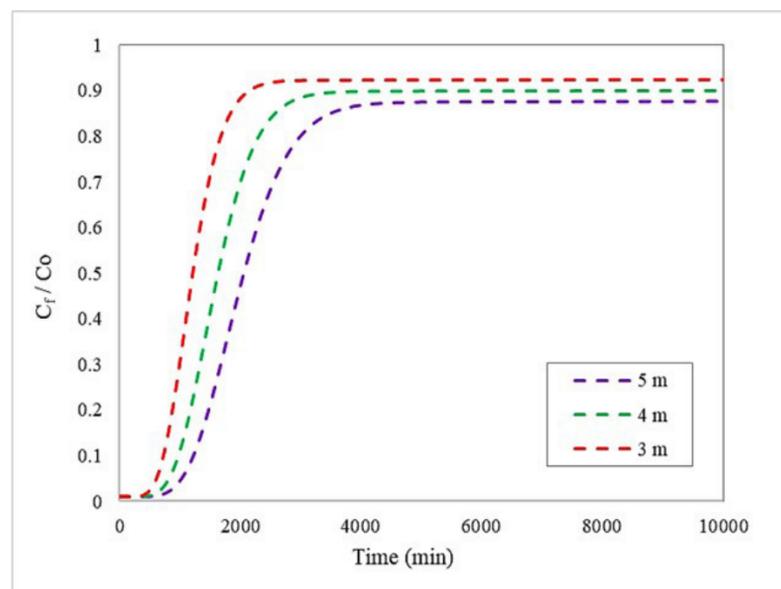

Figure 1. Breakthrough curves profiles of column height variation for the Langmuir - LDF model.

Analysis of the effect caused by the variation of the inlet flow rate

The inlet flow rate parameter was evaluated using magnitudes of 200, 150, and 100 m³/day working at a head of 5 m and an initial concentration of 3500 mg/L. Figure 2 shows the behavior of the breakthrough curves obtained after completing the bed simulation process. It was observed that, as the flow rate increased, there was an increase in the efficiency obtained but a decrease in the rupture and saturation times (Figure 2). This is because there is a positive effect on mass transfer and mass transfer resistance since there is a more significant effluent input per unit of time, causing a reduction in time and an increase in the efficiency of the adsorption process. For each flow rate, the following efficiencies were obtained: 93,7% for 200 m³/day, 91,6% for 150 m³/day, and 87,7% for 100 m³/day [29].
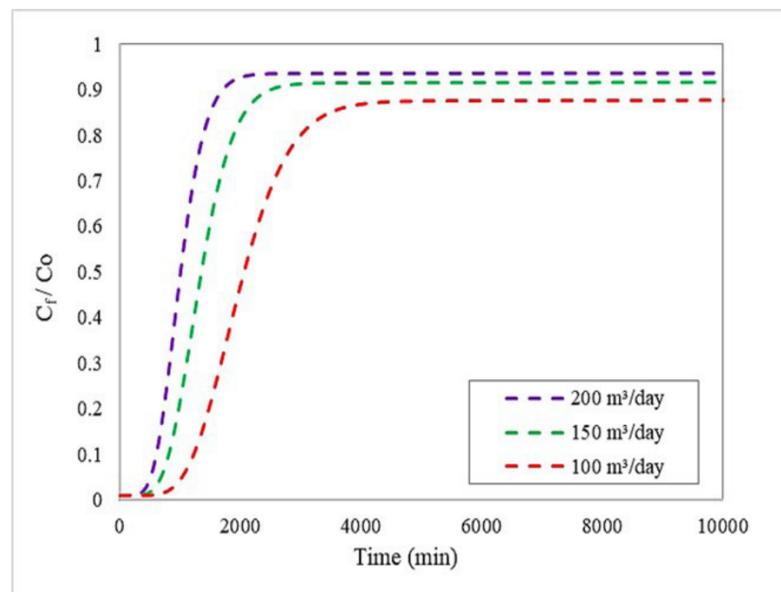
Figure 2. Breakthrough curves profiles of Inlet flow variation for the Langmuir - LDF model.

Analysis of the effect caused by the variation of the initial Cr (VI) concentration

The variation of the initial concentration parameter was analyzed with values of 3500, 2000, and 1000 mg/L, leaving fixed with a height of 5 m and an inlet flow rate of 100 m³/ day. Figure 3 shows the behavior of the breakthrough curves obtained after completing the bed simulation process, observing that decreasing or increasing the initial concentration did not significantly affect the process efficiency or the rupture and saturation times suggests that this parameter alters the adsorption process (Figure 3). This may be due to the number of active sites in the adsorbent or the adsorbent's affinity with the adsorbate, which allows a rapid adsorption equilibrium. The following efficiencies were obtained for each initial concentration: 87,7% for 3500 mg/L, 87,8% for 2000 mg/L, and 88,1% for 1000 mg/L. It was observed that this parameter does not significantly affect the adsorption process [30].
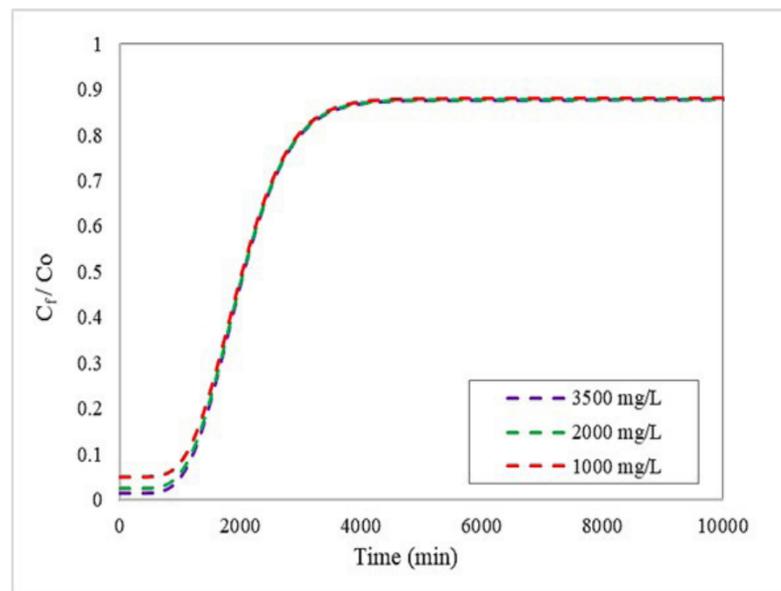

Figure 3. Breakthrough curves profiles of the variation of the initial concentration of Cr (VI) for the Langmuir - LDF model.

Comparative studies

The results obtained from the different simulations of the packed column for Cr (VI) removal were compared with data reported in scientific literature. It should be noted that this comparison is of a relative nature since the studies present differences in the operating conditions used. Table 3 shows the values compared between the results obtained in this study and those found in the literature.

TABLE 3. COMPARISON OF THE RESULTS WITH THE LITERATURE.

Contaminant	Pb (II)	Cr (VI)	Pb (II)	Cr (VI)
Adsorbent	*Eichhornia crassipes*	*Litchi chinensis sonn*	*Bambusa spp.*	*Theobroma cacao L.*
Initial concentration (mg/L)	20	20	20	3500
Inlet flow rate (m3/day)	17.28	0.0864	1.728	100
Bed height (m)	1	0.7	1	5
Rupture time (min)	558	5.583	52	507
Saturation time (min)	-	-	-	4107
Source	[30]	[31]	[32]	This study

CONCLUSION

A parametric evaluation was conducted to analyze the impact of altering the bed height, the inlet flow rate, and the initial concentration on the process's efficiency, rupture time, and saturation time. The bed height parameter was studied in magnitudes of 3 meters, 4 meters, and 5 meters. When using the highest value, the R.T. and S.T. increased, but the efficiency obtained decreased. A range of inlet flow rates of 100, 150, and 200 m3/day, where using the higher flow rate decreases rupture and saturation times but increases adsorption performance. In addition, initial concentrations of 3500, 2000, and 1000 mg/L were used, whereby by changing the concentration, the adsorption efficiency is not noticeably influenced. This study presents a novel way of predicting the behavior of adsorption columns at an industrial scale, showing a contribution to the scientific literature of relevant data for the development of modeling and simulation of packed columns to adsorb pollutants in water bodies to reduce the existing gap in the development of industrial adsorption processes using agro-industrial wastes for the removal of pollutants such as Cr (VI) using Theobroma cacao L. as adsorbent packing material. The next steps in the short term will include an economic evaluation to determine the financial viability and long-term sustainability of the adsorption column, with the objective of identifying the associated operating and investment costs, evaluating the performance of the system under different operating and economic conditions, and contributing to decision making in real-world contexts.

INTEREST CONFLICT

The authors declare that they have no conflicts of interest.

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STATEMENT OF CONTRIBUTION TO THE AUTHORSHIP OF THE CREDIT

C. Tejada-Tovar: Conceptualization, Research, Data processing, Acquisition of funds, Resources, Methodology, Visualization, Writing - Original Draft, Writing - Review and Editing. A. Villabona-Ortiz: Conceptualization, Formal analysis, Acquisition of funds, Research, Project management, Resources, Software, Supervision, Writing - proofreading and editing. A. González-Delgado: Conceptualization, Formal analysis, Research, Resources, Methodology, Software, Acquisition of funds, Writing - proofreading and editing. H. Bonilla-Mancilla: Data processing, Formal analysis, Research, Writing - proofreading and editing. J. Vergara-Villadiego: Data processing, Formal analysis, Research, Software, Writing - original draft.

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REFERENCES

[1] M. He et al., "Waste-derived biochar for water pollution control and sustainable development," *Nat Rev Earth Environ*, vol. 3, no. 7, pp. 444–460, 2022, doi: 10.1038/s43017-022-00306-8.

[2] T. Yan, S. L. Shen, and A. Zhou, "Indices and models of surface water quality assessment: Review and perspectives," *Environmental Pollution*, vol. 308, no. March, p. 119611, 2022, doi: 10.1016/j.envpol.2022.119611.

[3] M. K. Kadim and Y. Risjani, "Biomarker for monitoring heavy metal pollution in aquatic environment: An overview toward molecular perspectives," *Emerg Contam*, vol. 8, pp. 195–205, 2022, doi: 10.1016/j.emcon.2022.02.003.

[4] M. N. Georgaki et al., "Chromium in Water and Carcinogenic Human Health Risk," *Environments - MDPI*, vol. 10, no. 2, pp. 1–26, 2023, doi: 10.3390/environments10020033.

[5] M. A. Selimin, A. F. A. Latif, Y. C. Er, M. S. Muhamad, H. Basri, and T. C. Lee, "Adsorption efficiency of banana blossom peels (musa acuminata colla) adsorbent for chromium (VI) removal," Mater Today Proc, Dec. 2021, doi: 10.1016/J.MATPR.2021.10.502.

[6] R. F. Oliveira, K. G. P. Nunes, I. V. Jurado, I. C. B. Amador, D. C. Estumano, and L. A. Féris, "Cr (VI) adsorption in batch and continuous scale: A mathematical and experimental approach for operational parameters prediction," *Environ Technol Innov*, vol. 20, p. 101092, 2020, doi: 10.1016/j.eti.2020.101092.

[7] B. Gupta, A. Mishra, R. Singh, and I. S. Thakur, "Fabrication of calcite based biocomposites for catalytic removal of heavy metals from electroplating industrial effluent," *Environ Technol Innov*, vol. 21, p. 101278, 2021, doi: 10.1016/j.eti.2020.101278.

[8] Ministerio de Ambiente y Desarrollo Sostenible, "Resolucion 631 de 2015 vertimientos minambiente.pdf," 2015.

[9] J. Wang and X. Guo, "Adsorption isotherm models: Classification, physical meaning, application and solving method," *Chemosphere*, vol. 258, p. 127279, 2020, doi: 10.1016/j.chemosphere.2020.127279.

[10] J. Lara, C. Tejada, Á. Villabona, A. Arrieta, and C. Granados, "Adsorción de plomo y cadmio en sistema continuo de lecho fijo sobre residuos de cacao," *Revista ION*, vol. 29, no. 2, pp. 113–124, 2016, doi: : http://dx.doi.org/10.18273/revion.v29n2-2016009.

[11] V. Marcantonio, E. Bocci, J. P. Ouweltjes, L. Del Zotto, and D. Monarca, "Evaluation of sorbents for high temperature removal of tars, hydrogen sulphide, hydrogen chloride and ammonia from biomass-derived syngas by using Aspen Plus," *Int J Hydrogen Energy*, vol. 45, no. 11, pp. 6651–6662, 2020, doi: 10.1016/j.ijhydene.2019.12.142.

[12] A. P. Sánchez, E. J. P. Sánchez, and R. M. S. Silva, "Simulation of the acrylic acid production process through catalytic oxidation of gaseous propylene using ChemCAD® simulator," *Ingeniare*, vol. 27, no. 1, pp. 142–150, 2019, doi: 10.4067/S0718-33052019000100142.

[13] A. Villabona-Ortíz, C. Tejada-Tovar, and Á. D. González-Delgado, "Statistical Modelling of Biosorptive Removal of Hexavalent Chromium Using Dry Raw Biomasses of Dioscorea rotundata, Elaeis guineensis, Manihot esculenta, Theobroma cacao and Zea mays," *Sustainability (Switzerland)*, vol. 15, no. 12, p. 9156, Jun. 2023, doi: 10.3390/SU15129156/S1.

[14] C. Tejada-Tovar, Á. Villabona-Ortíz, V. Caballero Romero, J. Paternina Cuesta, and C. Granados Conde, "PARAMETER OPTIMIZATION FOR Cr(VI) ADSORPTION BREAKDOWN CURVES ONTO COCOA SHELL," *Revista U.D.C.A Actualidad & Divulgación Científica*, vol. 21, no. 1, pp. 167–177, Jun. 2018, doi: 10.31910/RUDCA.V21.N1.2018.675.

[15] A. Agarwal, U. Upadhyay, I. Sreedhar, and K. L. Anitha, "Simulation studies of Cu(II) removal from aqueous solution using olive stone," *Cleaner Materials*, vol. 5, p. 100128, 2022, doi: 10.1016/j.clema.2022.100128.

[16] C. T. Tovar, Á. V. Ortiz, and M. J. Villadiego, "Remoción de cromo hexavalente sobre residuos de cacao pretratados químicamente.," *Rev. U.D.C.A Act. & Div. Cient.*, vol. 20, no. 1, pp. 139–147, 2017.

[17] F. Benyahia and K. E. O'Neill, "Enhanced voidage correlations for packed beds of various particle shapes and sizes," *Particulate Science and Technology*, vol. 23, no. 2, pp. 169–177, 2005, doi: 10.1080/02726350590922242.

[18] A. G. Dixon, "Correlations for wall and particle shape effects on fixed bed bulk voidage," *Can J Chem Eng*, vol. 66, no. 5, pp. 705–708, 1988, doi: 10.1002/cjce.5450660501.

[19] B. K. Koua, P. M. E. Koffi, and P. Gbaha, "Evolution of shrinkage, real density, porosity, heat and mass transfer coefficients during indirect solar drying of cocoa beans," *Journal of the Saudi Society of Agricultural Sciences*, vol. 18, no. 1, pp. 72–82, 2019, doi: 10.1016/j.jssas.2017.01.002.

[20] U. Upadhyay, S. Gupta, A. Agarwal, I. Sreedhar, and K. L. Anitha, "Process Optimization at an Industrial Scale in the adsorptive removal of Cd2+ ions using Dolochar via Response Surface Methodology," *Environmental Science and Pollution Research*, pp. 0–27, 2021, doi: 10.1007/s11356-021-17216-9.

[21] S. Bao et al., "Amino-functionalized graphene oxide-supported networked Pd–Ag nanowires as highly efficient catalyst for reducing Cr(VI) in industrial effluent by formic acid," *Chemosphere*, vol. 257, p. 127245, 2020, doi: 10.1016/j.chemosphere.2020.127245.

[22] Á. D. González-Delgado, C. Tejada-Tovar, and A. Villabona-Ortíz, "Computer-aided Modeling and Evaluation of a Packed Bed for Chromium (vi) Removal using Residual Biomass of Theobroma Cacao L.," *Chem Eng Trans*, vol. 92, no. December 2021, pp. 517–522, 2022, doi: 10.3303/CET2292087.

[23] S. Sultana et al., "Adsorption of crystal violet dye by coconut husk powder: Isotherm, kinetics and thermodynamics perspectives," *Environ Nanotechnol Monit Manag*, vol. 17, no. May 2021, p. 100651, 2022, doi: 10.1016/j.enmm.2022.100651.

[24] P. Punia, R. K. Aggarwal, R. Kumar, R. Dhar, P. Thakur, and A. Thakur, "Adsorption of Cd and Cr ions from industrial wastewater using Ca doped Ni–Zn nanoferrites: Synthesis, characterization and isotherm analysis," *Ceram Int*, vol. 48, no. 13, pp. 18048–18056, 2022, doi: 10.1016/j.ceramint.2022.02.234.

[25] I. Durán, F. Rubiera, and C. Pevida, "Modeling a biogas upgrading PSA unit with a sustainable activated carbon derived from pine sawdust. Sensitivity analysis on the adsorption of CO2 and CH4 mixtures," *Chemical Engineering Journal*, vol. 428, 2022, doi: 10.1016/j.cej.2021.132564.

[26] Á. D. González-Delgado, C. Tejada-Tovar, and A. Villabona-Ortíz, "Parametric Sensitivity Analysis of Chromium (Vi) Adsorption using Theobroma Cacao L Biomass via Process Simulation," *Chem Eng Trans*, vol. 92, no. January, pp. 535–540, 2022, doi: 10.3303/CET2292090.

[27] R. F. Mansa, M. L. Ting, and A. O. Patrick, "Simulation of Lead Removal Using Palm Kernel Shell Activated Carbon in a Packed Bed Column," 2021.

[28] A. D. Nieva, J. C. S. Andres, and K. P. Gonzales, "Simulated biosorption of Cu2+ in aqueous solutions using Cucumis melo VAR. cantalupensis," *IOP Conf Ser Earth Environ Sci*, vol. 191, no. 1, 2018, doi: 10.1088/1755-1315/191/1/012035.

[29] H. Patel, "Batch and continuous fixed bed adsorption of heavy metals removal using activated charcoal from neem (Azadirachta indica) leaf powder," *Sci Rep*, vol. 10, no. 1, pp. 1–12, 2020, doi: 10.1038/s41598-020-72583-6.

[30] F. Mazzoni et al., "Aspen adsorption simulation on biosorption between water hyacinth (Eichhornia crassipes) and Pb (II) ions in packed bed column," *IOP Conf Ser Mater Sci Eng*, vol. 1257, no. 1, p. 012049, Oct. 2022, doi: 10.1088/1757-899X/1257/1/012049.

[31] Aileen. Nieva, R. C. Garcia, and R. M. R. Ped, "Simulated Biosorption of Cr6+ Using Peels of Litchi chinensis sonn by Aspen Adsorption® V8.4," *International Journal of Environmental Science and Development*, vol. 10, no. 10, pp. 331–337, 2019, doi: 10.18178/ijesd.2019.10.10.1195.

[32] M. L. R. M. Lubiano, C. V. L. Manacup, A. N. Soriano, and R. V. C. Rubi, "Continuous Biosorption of Pb2+ with Bamboo Shoots (Bambusa spp. using Aspen Adsorption Process Simulation Software," *ASEAN Journal of Chemical Engineering*, vol. 23, no. 2, pp. 153–166, 2023, doi: 10.22146/ajche.77314.

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