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SIMULATION IN DWSIM OF A MINING EFFLUENT WASTEWATER TREATMENT PROCESS

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Abstract: In Ecuador, mining responsibility includes social and environmental aspects. Wastewater generated by mining industry operations is the main problem. Medium and large-scale mining drives the country's economic growth. Gold mining uses cyanide (NaCN and KCN) in an environmentally damaging process that causes heavy contamination of soil and water resources due to its high toxicity and ability to accumulate in organisms. In the province of El Oro, mining activity uses metallurgical methods to extract non-renewable minerals, which has led to significant contamination of rivers with highly toxic substances. They have the potential to generate negative impacts and even destroy habitats. Various minerals are received at the beneficiation plant, including iron, nickel, gold, arsenic and hydrogen cyanide in minor proportions. A solids separator was used in the simulation of the mine effluent wastewater treatment plant to separate the minerals from the mine wastewater. Hydrogen peroxide dosing is applied in the CSTR reactor to promote cyanide oxidation and reduce contamination. A high agreement with reality will be observed when comparing the results obtained with scientific sources. To achieve 99.97% oxidation of CN-, two reactors were used: a continuous stirred tank reactor (CSTR) and a conversion reactor. A statistical analysis of percentage error was performed, which confirmed the results of the simulation and the literature review. The simulation performed in the software agrees positively with the experimental data, with a mean absolute percentage error of 0.17%.

Keywords: mining; cyanide; water treatment; DWSIM simulator; mining; cyanide; water treatment.

INTRODUCTION

In Ecuador, responsibility in the mining sector refers to compliance with both social and environmental standards. In 2012 in Ecuador, large-scale artisanal mining began, where SENPLADES planned 5 strategic projects for mining with some Ecuadorian companies, where they should sign a contract indicating their commitment to mining activity, in order to reduce environmental impacts, either directly or indirectly to the environment produced by large mining industries. (HERRERA; TORRES, 2022).

Humans use various natural minerals to satisfy their needs, which impacts water resources due to the various mineral extraction methods used. Obtaining mineral resources is considered a fundamental tool for achieving a better quality of life and greater economic development, two aspects of great relevance in today's society (DUTTA; ARYA; KUMAR, 2021).

In the 1900s, wastewater treatment began with the removal of suspended particles, which led to physical treatment. Oxidative treatment is based on the removal of dissolved and colloidal organic matter through biochemical oxidation processes (MASINDI; FOTEINIS; CHATZISYMEON, 2022). In these treatments aerobic and anaerobic processes are involved, it is important to know. In an aerobic process, bubbling is applied in the storage tanks to work in the presence of oxygen. Applying a simulation of a wastewater treatment plant is fundamental to the development and behavior of a pilot plant. This can decrease the production costs without the need for experiments (MENG et al., 2022).

Performing the simulation of a wastewater treatment plant for mining effluents using the freely available simulation software DWSIM presents significant benefits (TANGSRIWONG et al., 2020). This is because it enables the creation of a model of the real system and the understanding of its performance under various situations. It also allows the evaluation of the optimal results within the plant (BAHRUN et al. (BAHRUN et al., 2022). It is important to consider that the cost of implementing this tool is less than 1% of the total cost of large-scale production.

Within the framework of this technological research, we intend to approach the search for a solution from an engineering perspective. The development of a simulation of a wastewater treatment process for mining effluents, using primary and secondary treatments, will be carried out. (ANDREASEN, 2022). The objective is to find a solution to reduce the concentration of cyanide in these effluents, so that the results obtained can be considered as a possible alternative for the municipalities located in the highlands of the province of El Oro.

METHODOLOGY

The present research study consists of a technological proposal that focuses on the simulation of a wastewater treatment process in mining effluents. This proposal is based on the review of a database of specialized scientific articles in the canton of Portovelo, located in the province of El Oro. The methodology to simulate a wastewater treatment plant using conversion reactors, a solid separator, a mixer, and other functions of the DWSIM simulator (HASSAN; MANJI, 2023).

A systematic approach will be used to analyze and verify the behavior and reaction rate in the physical and chemical process. This will allow addressing and improving the possible problems that may arise during the development of the process through the corresponding simulation (NAVARRO PÉREZ; MORENO DÍAZ; SIMEONE BARRIENTOS, 2022).

COLLECTION AND ANALYSIS OF DATA FOR PROCESS SIMULATION

To initiate the simulation, a review of the scientific literature related to wastewater treatment by primary (physical) and oxidative treatment methods was conducted (HUANG et al., 2020a). These methods contribute to the reduction of the concentration of cyanide and other components present in the water. Special attention is paid to the flow rate of the mining effluent and the composition of the pollutants present in it. A statistical analysis will also be carried out to enable the interpretation and study of the various data obtained in the simulation (ISSA, 2019).

ESTABLISHMENT OF PARAMETERS

For the simulation of the mining effluent wastewater treatment process, information from a thesis entitled “Cyanide reduction in wastewater from a metallurgical company by oxidative treatment with hydrogen peroxide”, prepared by Luis Mario Auquilla Arévalo and Clara Inés Damián, was used. The data related to the concentration of pollutants entering the plant were extracted from this document and were subsequently introduced into the freely available simulation software DWSIM (HAN et al., 2020).

Parameters	Values	Units
Temperature	25	°C
Pressure	101.325	KPa
Mass Flow	0,0112795	Kg/s
Molar Flow	0,428974	mol/s
Total volumetric flow	0,00166667	m^3/s

Table 1 Parameters for the input current in the simulator.

SIMULATION IN DWSIM

The simulation of a wastewater treatment plant, including primary and secondary processes, was carried out. In this study, the PENG-ROBINSON thermodynamic model was used, which provides more accurate predictions for liquid densities and is especially suitable for nonpolar or low-polar substances (HUANG et al., 2020b). Figure 1 presents, through a block diagram, the input and output parameters associated with each of the devices used in the process of wastewater treatment from mining effluents (BASHAR; KARTHIKEYAN; NOGUERA, 2021).

A block diagram illustrating a wastewater treatment process according to previously established specifications for the equipment is presented (ASAMI; GOLABI; ALBAJI, 2021). This process includes a solids separator with 100% efficiency. It also incorporates a mixer where two streams are combined: one of liquid coming from the solids separator and another of H_2O_2 concentration destined to degrade the cyanide (LIN; HANYUE; BIN, 2022). As a result of this mixing, a combined stream is obtained in which four different concentrations are identified: H_2 O, CN-, OCN- and H_2O_2.

Subsequently, it will be connected to the CSTR reactor, which operates with a volume of 5m3, and finally it will be connected to a conversion reactor that achieves an efficiency of 88.9%.

PARAMETERS TO BE SIMULATED

Parameters were established to obtain input and output data, as well as to identify the components present in the mining effluent. The parameters used at the beginning of the simulation using the Peng Robinson thermodynamic model are presented, and consequently the components that will later be combined to reduce the amount of HCN.

Parameters	Variables
Components	HCN, H_2 O, H_2O_2 , CON
General thermodynamic model	Peng-Robinson
System of units	YES

Table 2. General parameters of the simulation.

Hydrogen peroxide enters the mixer with a mole fraction of 0.185762, as presented in the thesis entitled "Study of the chemical oxidation reaction of cyanide for the treatment of wastewater from a mining company". This input is carried out together with the liquid stream coming from the solids separator, and subsequently comes out as a mixture stream with respective mole fractions of H_2O, H_2O_2, HCN and CON, which will be introduced into the CSTR reactor (HERRERA; TORRES, 2022).

Parameters		**C1 (liquids)**	**Units**
Food composition (F)	H_2O	0,751	
	H_2O_2	0	
	HCN	0,097	
	CNO	0	
	As	0,083	
	Au	0,009	
	Faith	0,044	
	Ni	0,016	
Volumetric flow rate		0,00166667	m^3/s
Mass flow rate		0,0112795	Kg/s
Molar flow rate		0,428974	Mol/s
Specific Enthalpy		-1534,72	KJ/(Kg.K)
Molar Entropy		-108,524	KJ/(Kmol.K)
Density		9,3432	Kg/m^3

Table 3 Conditions of C1

Table 3 shows the values obtained from the literature review on the oxidation of CN, where the mole fraction of each compound introduced in the C1 stream is presented. A volumetric flow rate of 100 L/min was used, which is equivalent to a velocity of 0.001667 m3/s when entering the simulator. In addition, a pressure of 1 atmosphere and a temperature of 25 °C were set.

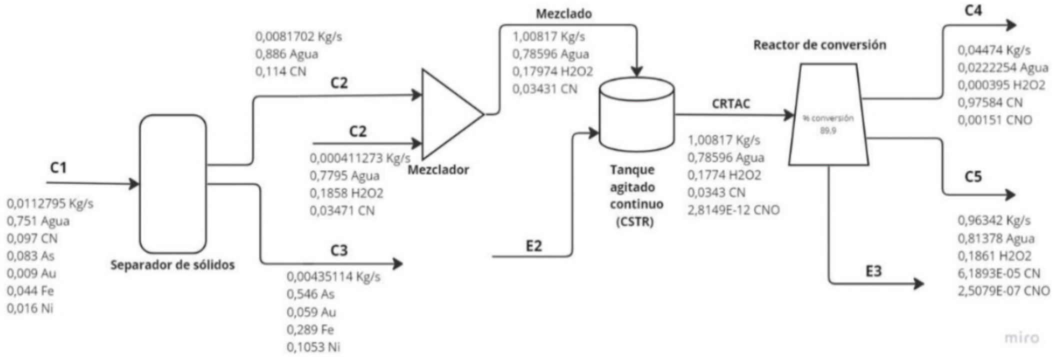


Chart 1 Block diagram of wastewater treatment for mining effluents.

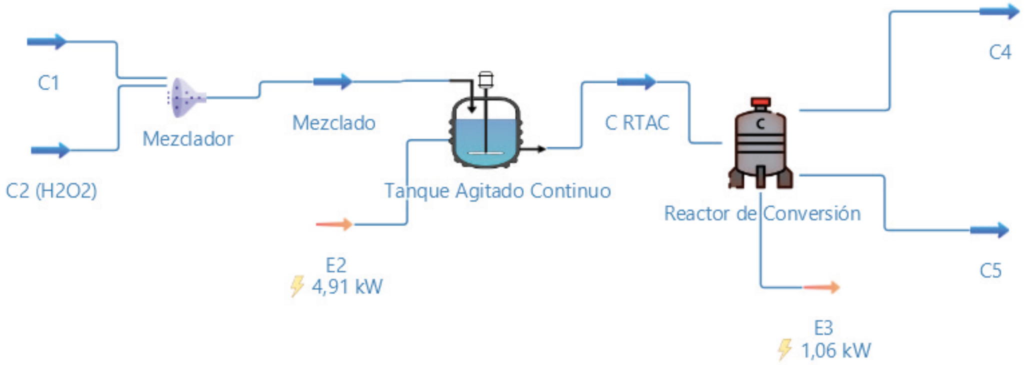


Chart 2 Simulation flow process diagram.

CSTR REACTOR

Table 4 shows the parameters that are introduced in the CSTR reactor, together with their corresponding units.

Parameters	Values	Units
Calculation mode	Adiabatic	
Reactor volume	5	m^3
Headspace	3	m^3
Reactor drop pressure	0	Pa

Table 4 Simulation characteristics of the CSTR Reactor.

CONVERSION REACTOR

In the simulation, the parameters used in the conversion reactor for its operability are presented in Table 5.

Parameters	Values	Units
Calculation mode	Adiabatic	
Reactor drop pressure	0	Pa
Conversion Rate	88,9	%

Table 5. Simulation characteristics of the conversion reactor.

RESULTS AND DISCUSSION

Based on the database collected from scientific sources, Excel statistical software was used to analyze the data collected.

The data presented below were extracted from a thesis entitled “Cyanide reduction in wastewater from a metallurgical company by oxidative treatment with hydrogen peroxide”, details of which can be found in the methodology section, together with the results of the simulation carried out in the DWSIM program. Graph 2 shows the process diagram of the simulation.

The result of cyanide oxidation and subsequent reduction was derived from the above process diagram.

SOLIDS SEPARATOR RESULTS

Table 6 presents the results obtained by the solids separator after the simulation. This equipment was used as primary treatment with the objective of eliminating suspended solids present in the mining effluent. It was observed that the separator achieved 100% efficiency in the separation between solids and liquids. As a consequence, the separation of liquids was achieved in stream 2, being this the stream of main interest.

Parameters		**C2 (liquids)**	**C3 (solids)**	**Units**
Food composition (F)	H_2O	0,88561323	0	
	H_2O_2	0	0	
	HCN	0,11438677	0	
	CNO	0	0	
	As	0	0,54605263	
	Au	0	0,059210526	
	Faith	0	0,28947368	
	Ni	0	0,105263164	
Volumetric flow rate		0,00120724	0	m^3/s
Mass flow rate		0,0081702	0,00435114	Kg/s
Molar flow rate		0,428974	0,065204	Mol/s
Specific Enthalpy		-2118,78	0	KJ/Kg
Density		6,76768	0	Kg/ m^3

Table 6 Simulation results in DWSIM for the solids separator.

However, the stream of interest is C2 (liquids) due to the absence of solids, as it represents the concentration of cyanide in the effluent with a mole fraction of 0.11438677.

CONTINUOUS STIRRED TANK REACTOR RESULTS

The results of the continuous stirred tank reactor (CSTR) are presented in Table 7. The purpose of the reactor is to decrease the concentration of CN- by the addition of hydrogen peroxide at a dosage of 0.18656643. A CN- mole fraction of 0.013829944 was achieved, in contrast to the initial mole fraction of 0.097 present in the inlet stream to the plant.

Parameters		CSTR Reactor	Units
Food composition (F)	H_2O	0,78595651	
	H_2O_2	0,179736	
	HCN	0,03430715	
	CNO	2,814860E-12	
	As	0	
	Au	0	
	Faith	0	
	Ni	0	
Volumetric flow rate		0,0405887	m^3/s
Mass flow rate		1,00817	Kg/s
Molar flow rate		47,555	Mol/s
Specific Enthalpy		-2153,11	KJ/Kg
Density		1052,99	Kg/m^3

Table 7. Simulation results of the Continuous Stirred Tank Reactor.

CONVERSION REACTOR RESULTS

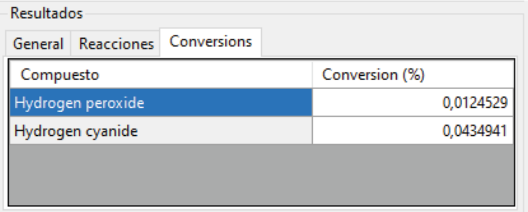
Table 8 shows the simulation results corresponding to the C4 and C5 output current of the conversion reactor.

Parameters		**C4**	**C5 (NC reduction)**	**Units**
Food composition (F)	H_2O	0,022225	0,81377665	
	H_2O_2	0,000395298	0,186161	
	HCN	0,97584242	6,189312E-05	
	CNO	0,0015073	2,507908E-07	
	As	0	0	
	Au	0	0	
	Faith	0	0	
	Ni	0	0	
Volumetric flow rate		0,000791579	0,000919273	m^3/s
Mass flow rate		0,0447423	0,963428	Kg/s
Molar flow rate		1,66637	45,8899	Mol/s
Specific Enthalpy		-1090,44	-2251,73	KJ/Kg
Density		56,5228	1048,03	Kg/m^3

Table 8 Simulation results in DWSIM for the Conversion Reactor.

By means of the conversion reactor, the amount of cyanide present in the mining effluent was reduced using an 88.9% conversion rate, showing in the C5 stream (CN reduction) a concentration of 6.189312E -05, achieving an oxidation of cyanide compared to the initial amount entering the plant with a mole fraction of 0.097.

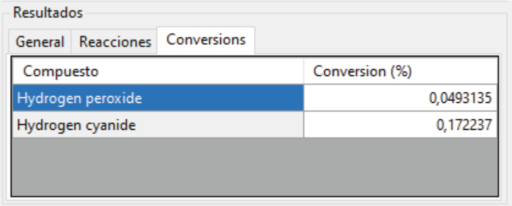
However, a lower or higher conversion than the one proposed by the author, which indicated 88.9%, can be applied to observe if it affects or benefits the reduction of cyanide. Graphs 3 and 4 show the values obtained from the conversion reactor where the conversion between hydrogen peroxide and cyanide is observed with respect to the conversion percentage applied.



Compuesto	Conversion (%)
Hydrogen peroxide	0,0124529
Hydrogen cyanide	0,0434941

Chart 3 Result obtained from the conversion reactor with 25%.

Graph 3 shows the conversion data for cyanide and hydrogen peroxide in a reactor with a conversion efficiency of 25%.



Compuesto	Conversion (%)
Hydrogen peroxide	0,0493135
Hydrogen cyanide	0,172237

Chart 4 Result obtained from the conversion reactor simulator with 99%.

The fourth graph shows the conversion of cyanide and hydrogen peroxide in a reactor with a conversion efficiency of 99%.

Parameters		Conversion 25% Conversion	99% conversion
Compounds	H_2O_2	0,0124529	0,0493135
	HCN	0,0434941	0,172237

Table 9 Comparison of the change in conversion value.

The values obtained by the conversion reactor are presented in Table 9. When a conversion of 25% is reached, the initial cyanide concentration of 0.097 experiences a conversion of 0.0434941%. On the other hand, when increasing the conversion to 99%, the conversion reaches 0.172237%.

STATISTICAL ANALYSIS

First, the performance efficiency of the samples collected in the cyanide oxidation process was evaluated. For this purpose, a thesis database was analyzed, the results of which are presented in Table 10.

Table 10 presents the correlation between the authors' nitrogen fraction and the nitrogen fraction obtained by the DWSIM simulation. The percentage removal in the simulation was calculated by multiplying the final nitrogen mole fraction by 100 and dividing the result by the initial nitrogen mole fraction.

According to equation 1 for the calculation of the percentage error, the percentage error was determined using the removal percentage data provided by various authors and the removal percentage obtained in the simulation. This calculation yielded both negative and positive values. However, when the absolute value function is applied, the negative values are converted into positive values.

$$E\% = \frac{|V_t - V_e|}{V_t} * 100 \qquad (1)$$

Where:

- V_t is the theoretical value
- V_e is the experimental value

Equation 2 was used to determine the mean absolute percentage error, using the percentage error previously obtained through this equation. The total sum of the percentage errors is divided by the total number of data.

$$MAPE = \frac{\sum_{t=1}^{n} \frac{|V_t - V_e|}{V_t}}{n} \qquad (2)$$

Where:

- $\sum_{t=1}^{n} \frac{|V_t - V_e|}{V_t}$ is the sum total of the percentage error
- n is the total number of data

Authors	Concentration of authors' NCs	Fraction of CN obtained from the simulator	Percentage of simulation removal	Percentage removal of cited authors
(ESTRADA MONTOYA, 2019)	102 mg/L	6,1891E-05	94,03%	99,99%
(SAA CARDONA; GUARNIZO RUÍZ, 2022)	105 mg/L	6,9542E-06	99,33%	99,6%
(GARAY PABLO; LLATAS LEGOAS, 2019)	100 mg/L	6,0845E-06	99,39%	99,90%
(AUQUILLA ARÉVALO; DAMIÁN VELEZ, 2019)	97 mg/L	6,1893E-05	93,62%	99,70%

Table 10 Results obtained with each of the authors.

Authors	Percentage removal of cited authors	Percentage of simulation removal	Relative error	Percentage error (%)	Absolute error
(ESTRADA MONTOYA, 2019)	99,99%	94,03%	0,063384026	6,338402637	6,33840264
(SAA CARDONA; GUARNIZO RUÍZ, 2022)	99,6%	99,33%	0,002718212	0,271821202	0,2718212
(GARAY PABLO; LLATAS LEGOAS, 2019)	99,90%	99,39%	0,005131301	0,513130094	0,51313009
(AUQUILLA ARÉVALO; DAMIÁN VELEZ, 2019)	99,70%	93,62%	0,064943388	6,494338816	6,49433882

Table 11 Percentage error between authors and simulation.

Table 11 presents the mean absolute percentage error, which amounts to 3.404423187%, evidencing that the simulation performed in this software agrees positively with the experimental data. The author Saa & Guarnizo (2022) presents the lowest percentage error, with 0.00272%, while the author Estrada (2019) exhibits the highest error, reaching 6.3384%. It is highlighted that the discrepancy in the removal percentages between the author and the simulation is 99.6% and 99.33%, respectively.

CONCLUSION

In order to carry out this simulation within the DWSIM software, we used a database compiled from various academic theses, which allowed us to collect the required data, such as the composition of the inlet stream, volumetric flow rate, mass flow rate, density, as well as other fundamental parameters to start the simulation properly.

For the detailed simulation of this mining wastewater treatment plant, an efficient solids separator was implemented, which facilitated the adequate separation of the various minerals present in the wastewater generated by the mining activity. In addition, two very important reactors were incorporated: a continuous stirred tank reactor (CSTR) and a conversion reactor, which played a fundamental role in the cyanide ion (CN-) oxidation process, achieving an efficiency of 93.62%.

An exhaustive statistical analysis was carried out in which the data obtained from the simulation were compared in detail with the data provided by the authors. In this analysis, a rigorous study of the percentage error was applied, taking into account in detail the results obtained both from the simulation and also the results acquired from the bibliographic compilation. It was determined that the mean absolute percentage error was 3.41%, which indicates that the simulation performed in this software is positively aligned with the experimental data.

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