Simulation of Anaerobic Treatment of Vinasse Generated from the Ethanol Production Process

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***Abstract*— Vinasse is a primary byproduct of the sugarcane distillation process used in ethanol production. It is characterized by high concentrations of nitrogen, phosphorus, and sulfates, along with elevated levels of chemical oxygen demand (COD) and biochemical oxygen demand (BOD). If not managed properly, vinasse can have detrimental environmental effects, particularly on soil quality. Therefore, its treatment is essential not only to mitigate environmental risks but also to capitalize on potential energy and economic opportunities, such as bioenergy production and the generation of valuable byproducts. This study aimed to develop a virtual model using ASPEN PLUS® software for the treatment of vinasse generated in an ethanol biorefinery. The simulation achieved a theoretical organic matter removal efficiency of 100%, with biogas compositions consisting of 59 mol% methane, 32 mol% carbon dioxide, 5.5 mol% water, and 3 mol% nitrogen. Furthermore, this research contributes to the limited body of literature on vinasse treatment simulations, underscoring its potential as an eco-friendly and cost-effective waste management solution.**

***Keywords*— anaerobic treatment, Aspen Plus® software, simulation, vinasse.**

I. Introduction

The Brazilian sugar and alcohol industry stands as a robust and well-integrated biorefinery model, producing essential products such as sugar, ethanol, and thermoelectric energy from bagasse [1], [2]. Globally, Brazil is the second-largest ethanol producer, with a recorded output of 8.3 billion gallons in 2023 [3]. The country leads in ethanol production from sugarcane, contributing 18% of the total renewable energy resources in Brazil's energy matrix [4].

Sugarcane mills generate various by-products and residues, including bagasse, straw, leaves, grasses, molasses, vinasse, and carbon dioxide [5]. Among these, vinasse, a major by-product of ethanol production, consists of approximately 10% organic matter and 90% water [6]. Its organic load is rich in phenolic compounds, glycerol, ethanol, melanoidins, sugars, volatile fatty acids, and other compounds. Furthermore, vinasse contains valuable nutrients such as organic nitrogen, potassium, and phosphorus [7], [8]. For every liter of ethanol produced, between 10 to 15 liters of vinasse are generated, depending on the distillation equipment used [6], [9].

In Brazil, vinasse is predominantly used in fertigation due to its high organic content and large volume. However, direct application to soil poses several challenges. Its low pH and high concentrations of sulfate and organic matter can disrupt soil structure, contaminate nearby water bodies, and reduce crop yields [10]. To address these issues, anaerobic digestion provides an alternative solution for vinasse management.

Anaerobic digestion is a well-established renewable technology that involves the biological degradation of organic waste in the absence of oxygen. This process not only treats and recycles biodegradable materials but also produces an energy-rich gas known as biogas. Biogas can be used in various applications, including cooking, heating, vehicle fuel (after upgrading), and electricity generation [11].

Despite its widespread application, the potential of anaerobic digestion in addressing specific industrial waste streams, such as vinasse from ethanol production, remains underexplored. Process simulation tools like ASPEN PLUS® offer opportunities to model and optimize anaerobic digestion processes, including the treatment of vinasse. Developing a virtual model tailored to the unique characteristics of vinasse could help bridge this gap.

This study aimed to develop a virtual model using ASPEN PLUS® software for the treatment of vinasse generated in an ethanol biorefinery. Through the use of process simulation, the study provides insights into improving the efficiency and sustainability of ethanol biorefineries, contributing to both waste management and renewable energy generation. The model can also serve as a tool for evaluating different operating conditions, enabling a more effective integration of biorefinery processes within the framework of a circular bioeconomy.

II. Methodology

The simulation of the anaerobic treatment of vinasse was carried out using Aspen Plus® software. The RGIBBS module in Aspen Plus® was used to simulate the UASB reactor, and the FLASH module was used to separate the gaseous and liquid fractions of the reactor's product. The RGIBBS module is designed for simulating chemical equilibrium by minimizing Gibbs free energy. It focuses on single-phase systems and eliminates the need for kinetic parameters, allowing users to determine equilibrium compositions based on specified temperature and pressure conditions. The module can also calculate phase equilibria without requiring detailed reaction specifications. It is particularly useful in scenarios where the reaction conditions are known, but the exact product distribution is not readily available [12], [13]. The FLASH module is designed for performing liquid-vapor equilibrium calculations, enabling the separation of a liquid feed into vapor and liquid phases based on thermodynamic principles. Fig. 1 represents the reaction and separation flowsheet for vinasse treatment.

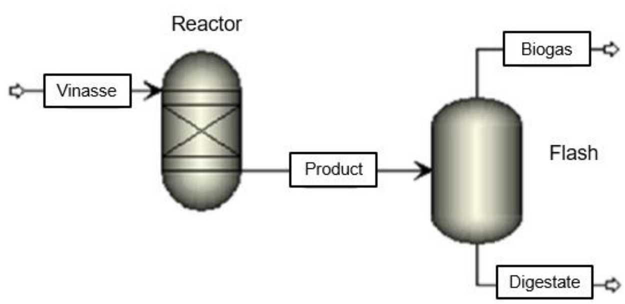

Fig. 1. Reaction and separation flowsheet for vinasse treatment.

The main reactions that occur in the anaerobic digestion process are:

Hydrolysis:

$$C_{12}H_{22}O_{11} + H_2O \rightarrow 2C_6H_{12}O_6 \quad (1)$$

Acidogenesis:

$$C_6H_{12}O_6 + 2H_2O \rightarrow 2CH_3COO^- + 2CO_2 + 2H^+ + 4H_2 \quad (2)$$

$$C_6H_{12}O_6 + 2H_2 \rightarrow 2CH_3CH_2COO^- + 2H_2O + 2H^+ \quad (3)$$

$$C_6H_{12}O_6 \rightarrow CH_3CH_2CH_2COO^- + 2CO_2 + H^+ + 2H_2 \quad (4)$$

Acetogenetic:

$$CH_3CH_2COO^- + 3H_2O \rightarrow CH_3COO^- + HCO_3^- + H^+ + 3H_2 \quad (5)$$

$$CH_3CH_2COO^- + 2HCO_3^- \rightarrow CH_3COO^- + H^+ + 3HCOO^- \quad (6)$$

$$CH_3CH_2CH_2COO^- + 2H_2O \rightarrow 2CH_3COO^- + H^+ + 2H_2 \quad (7)$$

Methanogenesis:

$$CH_3COO^- + H_2O \rightarrow CH_4 + HCO_3^- + 2H_2 \quad (8)$$

$$H_2 + 1/4HCO_3^- + 1/4H^+ \rightarrow 1/4CH_4 + 3/4H_2O \quad (9)$$

$$HCOO^- + 1/4H_2O + 1/4H^+ \rightarrow 1/4CH_4 + 3/4HCO_3^- \quad (10)$$

Vinasse, a byproduct of ethanol manufacturing, is fed into the reactor where it undergoes treatment, likely through anaerobic digestion. This process breaks down the organic components in the vinasse, yielding outputs that move to the flash separator. In the separator, the mixture is divided into two streams: biogas and digestate. The biogas, containing gases such as methane and carbon dioxide, is extracted and can be used as a source of renewable energy. The digestate, which is either a solid or liquid byproduct, exits through another outlet and can be repurposed as a fertilizer or soil amendment.

The vinasse feed used in the simulation of anaerobic treatment is not present in the software's database. Therefore, the inputs need to be defined in terms of chemical components. The composition of vinasse is variable and can be influenced by several factors, including the type of sugarcane used, the method of ethanol production, the processing conditions, and the geographic location of the ethanol plants. For this study, the average composition of the main components of vinasse, derived from a survey conducted at 28 ethanol plants in São Paulo, Brazil, was utilized, as shown in Table 1.

TABLE 1: VINASSE COMPOSITION [14, ADAPTED].

Component	Concentration (mg/L)
Biochemical Oxygen Demand (BOD)	16949.76
Potassium	2034.89
Sulfate	1537.66
Chloride	1218.91
Calcium	515.25
Nitrogen	356.63
Magnesium	225.64

The organic matter, which is the main component of vinasse, was represented in the simulation by the component sucrose, selected for its structural and functional similarity to chemical oxygen demand (COD) [6]. Concerning the composition of the input stream, Gomes et al. [15] noted that vinasse consists of approximately 97% water, despite its significant organic matter content. This ratio was applied in defining the input stream composition. Furthermore, the components and their concentrations, as shown in Table 1, are presented in Table 2 as mass fractions for the simulation.

TABLE 2: VINASSE COMPOSITION USED IN SIMULATION.

Compounds	Mass fraction
Sucrose	0.02226
Potassium	0.00267
Sulfate	0.00202
Chloride	0.00160
Calcium	0.00068
Nitrogen	0.00047
Magnesium	0.00030
Water	0.97

To calculate the feed volume for the simulation, data from the Brazilian National Agency of Petroleum, Natural Gas and Biofuels (ANP) was used. In 2020, Brazil's total ethanol production reached 32,803,190.55 m³, averaging approximately 89,871.75 m³ per day. With a total of 360 authorized ethanol plants in operation, this results in an estimated daily production of about 250 m³ for each plant [16]. Additionally, considering that vinasse is produced at an average rate of 14 liters for each liter of ethanol generated, the estimated daily vinasse output per plant is around 3,500 m³, equating to roughly 146 m³ per hour. This value of 146 m³ of vinasse per hour was subsequently adopted as the input stream volume for the simulation.

Regarding the thermodynamic model utilized, the NRTL model is considered the most appropriate for the simulation due to its accuracy in predicting the behavior of non-ideal solutions, particularly in systems involving organic compounds [17]. The temperature adopted was a mesophilic range of 35°C, which is typically used for anaerobic digestion processes [18]. The operational conditions for the reactor and the flash are detailed in Table 3.

TABLE 3: PARAMETERS DEFINED FOR SIMULATION [6].

Parameters adopted in simulations	
Feed rate (m^3/h)	146
Feed temperature (°C)	25
Feed pressure (atm)	1
Reactor temperature (°C)	35
Reactor pressure (atm)	1
Flash temperature (°C)	35
Flash pressure (atm)	1
Thermodynamic model	NRTL

III. RESULTS AND DISCUSSION

The simulation of the vinasse treatment process through anaerobic digestion was conducted using Aspen Plus® software, utilizing the data from Tables 2 and 3. The results of the product streams, including biogas and digestate compositions, are shown in Table 4.

TABLE 4: RESULTS OF THE SIMULATION.

Compounds	Product	Biogas	Digestate
Sucrose	0.000000	0.000000	0.000000
Potassium	0.001215	8.04E-14	0.001227
Sulfate	0.000304	0.000000	0.000307
Chloride	0,000500	0.000000	0.000505
Calcium	0.000319	0.000000	0.000322
Nitrogen	0.000326	0.030695	2.91E-05
Magnesium	0.000226	0.000000	0.000228
Water	0.982804	0.055116	0.99188
Methane	0.007139	0.589512	0.001441
Carbon dioxide	0.007148	0.322778	0.00406
Hydrogen	1.85E-05	0.0019	1.33E-07

As demonstrated in Table 4, the simulation achieved a theoretical removal rate of 100% for the component representing organic matter. This result indicates that, under the simulated conditions, the organic matter was fully converted into biogas components, aligning with the goal of maximizing biogas production in anaerobic digestion processes. Similarly, Moreira et al. [6] conducted a simulation study and, like in this work, observed complete conversion of the component used to represent COD into biogas. Carniato et al. [19] modeled biogas production using a more concentrated vinasse feed with 33.33% water. They also achieved total removal of organic matter, with methane concentrations of 50.36% and carbon dioxide concentrations of 29.8%. This reinforces the idea that simulations, when properly calibrated with experimental data, can bridge the gap between theoretical predictions and practical applications, effectively modeling the anaerobic digestion process and offering valuable insights into optimal operating conditions.

In contrast, Tunes [20], using a bench-scale UASB reactor, observed a COD removal rate of 71%, which, while significant, reflects the challenges of achieving complete removal in experimental settings. This difference can be attributed to various factors inherent to physical experiments, such as reactor design, microbial activity, and operational limitations, which can influence the efficiency of organic matter breakdown.

Achieving 100% removal of organic matter in real-world conditions is recognized as a significant challenge due to various operational and environmental factors that can impact the efficiency of treatment processes. However, in this study, the vinasse treatment was evaluated through theoretical simulations, which necessarily involve certain simplifications to model the process within a controlled environment. These simplifications are aimed at providing an idealized version of the treatment, free from many of the constraints faced in practical applications, such as microbial variability or mechanical inefficiencies. Despite these theoretical adjustments, the model offers valuable insights into optimizing the anaerobic digestion process for vinasse treatment.

In addition to the reduction of organic matter present in vinasse, the anaerobic digestion process is also associated with biogas production. Unrefined biogas generally contains a mixture of methane, which makes up about 50% to 75%, along with carbon dioxide comprising approximately 25% to 50%. Additionally, it has smaller quantities of nitrogen, typically ranging from 2% to 8%. Additionally, biogas may contain trace amounts of other gases, such as hydrogen sulfide, ammonia, hydrogen, and various volatile organic compounds, all of which can vary based on the type of feedstock used in the anaerobic digestion process [21]. Table 5 presents a comparison of biogas composition data obtained from the literature, the regulatory standards set by the Brazilian National Agency of Petroleum, Natural Gas and Biofuels (ANP), and the results from this study.

TABLE 5: BIOGAS COMPOSITION OF LITERATURE, THIS STUDY, AND REGULATORY STANDARDS.

Compounds	Literature (% mol)	Regulatory standards (% mol)	This study (% mol)
Methane	50-75	90	59
Carbon dioxide	25-50	3	32
Water	< 5	-	5.5
Nitrogen	2-8	-	3

From Table 5, it is evident that methane is the predominant component in biogas. The concentration of methane observed in this study aligns with values reported in the literature; however, it falls short of the regulatory requirement established by the Brazilian National Agency of Petroleum, Natural Gas and Biofuels (ANP), which mandates a minimum methane content of 90%. This study recorded a lower concentration of 59%, indicating that while the biogas produced here meets certain benchmarks, there is significant potential for enhancing methane production efficiency.

Carbon dioxide levels are also a crucial factor in assessing biogas quality. The regulatory standard stipulates a much lower permissible concentration of only 3%. In contrast, this study found a carbon dioxide concentration of 32%, which significantly surpasses the regulatory limit. Elevated levels of carbon dioxide can negatively impact the overall efficiency of biogas as a renewable energy source, highlighting an area where process optimization may be necessary. Reducing carbon dioxide concentration could enhance the energy yield of the biogas and improve its competitiveness as a sustainable energy option.

The presence of water is also noted in the table 5. While the literature suggests trace amounts (less than 5%), this study recorded a higher concentration of 5.5%. The water content in biogas can impact the efficiency of gas utilization in energy generation and should be monitored closely.

Lastly, nitrogen was found to be present in this study at 3%, with no regulatory standard provided. The literature reports nitrogen levels between 2% and 8%. Nitrogen can dilute the energy content of biogas and may contribute to the overall composition variability.

The analysis of the digestate composition presented in the table 4 reveals valuable insights into the byproducts of the anaerobic digestion process. The digestate, the liquid residue left after biogas extraction, contains a range of compounds that suggest its potential use as a soil amendment and in fertilizer production. Notably, the digestate contains essential nutrients such as nitrogen (0.030695%), potassium (0.001227%), and magnesium (0.000228%), which makes it a potential fertilizer. The nitrogen content, in particular, is significant as it is a key nutrient for plant growth. Moreover, the high water content of approximately 99.88% indicates that the digestate could be utilized in liquid form or processed further to concentrate its nutrient profile.

Overall, the simulated data from this study are generally consistent with values reported in the literature, although they do not meet regulatory standards. This indicates that biogas refinement is necessary to enhance quality. Furthermore, the findings suggest that the simulation serves as a dependable predictive tool for estimating real-world outcomes, which could facilitate optimization before conducting physical trials. While actual applications may yield different results due to the complexities of real-world processes, this model provides a robust framework for understanding the essential parameters and conditions required to maximize organic matter reduction and biogas production in industrial contexts.

IV. Conclusion

Vinasse is the primary residue resulting from the sugarcane distillation process for ethanol production. Due to its chemical composition, proper treatment is essential and can be linked to bioenergy production, offering both energy and economic benefits. This study aimed to develop a virtual plant model for the treatment of vinasse produced by an ethanol biorefinery. Through the proposed model, anaerobic digestion of the vinasse was simulated. As a result, 100% of the organic matter present in the compound was removed. Despite the simplifications involved, this demonstrates the promising potential of the model, successfully achieving the goal of organic load reduction. Additionally, the model was able to produce biogas with compositions similar to the range reported in the literature. This indicates that, beyond organic load reduction, the model also yields positive results in terms of biogas generation, which can be economically beneficial since the biogas could be reused by the plant. In conclusion, this study contributes to the growing field of research on vinasse treatment simulations, paving the way for future investigations that could lead to optimized processes and improved efficiencies.

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