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Optimization and Simulation of Bioethanol Production from Different Grades of Molasses

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Abstract:

The country has been grappling with a significant rise in pollution in recent years, primarily caused by vehicle emissions and the improper disposal of agricultural and industrial waste. To address this issue, the Indian government has launched a campaign to foster innovative ideas for managing agricultural waste, particularly biomass. One such idea involves the production of biofuel from biomass sources such as sugarcane bagasse, sugarcane molasses, corn, rice husk, and wheat straw.

This paper focuses on a study that investigates the production of biofuel, specifically bioethanol, using sugarcane molasses as the raw material. The study explores different categories of sugarcane molasses, classifying them based on their sucrose content. The research methodology involves pre-treating the sugarcane through crushing and hydrolysis, followed by fermentation using Saccharomyces Cerevisiae. The process then proceeds to distillation and analysis of the resulting bioethanol. Additionally, the study includes a simulation of the production process using Aspen Plus, based on the obtained analysis results.

Overall, this paper delves into the production of biofuel, mainly focusing on bioethanol derived from sugarcane molasses. It examines various aspects of the process, from molasses classification to pre-treatment, fermentation, distillation, analysis, and simulation using Aspen Plus.

Keywords **—Pollution, Agricultural Waste, Biomass, Sugarcane Molasses, Biofuels, Fermentation, Distillation, Analysis, Simulation, Aspen Plus.**

1. INTRODUCTION:

The energy demand in our country is rising due to an expanding economy, exponential growth in population, tremendous increment in urbanization, and evolving lifestyles. As per current scenario about 98% of the fuel requirement in the road transportation sector is currently fulfilled by the burning of fossil fuels and the remaining 2% by biofuels [1].

As India is agricultural state; nearly about 65% of families are included directly in this agriculture economy. Whereas sugarcane plays a vital role in this agricultural economy. According to study an area of 5 million hectares, sugarcane production in India carried out on about 2.57% of the total cropped area. It provides employment to nearly 60 lakh sugarcane growers and indirect employment to many people in the association[2]. Also, the increase in production of sugarcane leads to increase in agricultural waste (biomass) and industrial waste in the form of sugarcane molasses, sugarcane bagasse, etc.

As a solution to reuse and reduce this waste in recent years, growing attention has been given for the study of conversion of biomass to biofuel. This conversion additionally helps to decrease the problem of pollution due to the flue gasses from vehicle. This is basically done by blending the biofuel in estimated amount with fuels used for ignition (e.g. petrol, diesel, etc.) in vehicle.

1.1 Biofuels

Biofuel is a type of renewable energy source derived from agricultural, animal or human waste. Examples of biofuels are bio-ethanol (mainly made from starch in United States and from glucose in Asia), bio-diesel (often made from vegetable oils and liquid animal fats), green-diesel (derived from algae and other plant sources), and bio-gas (methane derived from animal manure and other digested organic material).

1.2 Classification of Biofuels

Generally, biofuels are classified into three generation based on the raw materials available [5].

TABLE I
CLASSIFICATION OF BIOFUELS

Acronym	Abbreviation	Source	Example
1G	First Generation	Edible Feedstock	Rice, Wheat, Sugarcane molasses, Corn
2G	Second Generation	Non-Edible Feedstock	Rice Husk, Wheat Husk, Sugarcane Bagasse
3G	Third Generation	Oleaginous Feedstock	Microalgae, Waste animal fat, Waste cooking oil

1.3 Production in India

The global ethanol production was nearly 110 billion liters in 2019 which is been continuously growing with the rate of 4% year per year compared to last decade. At the time the Unites States of America and Brazil contributes upto 92 billion liters (nearly 84% of global production) followed byEuropean Union, China, India, Canada and Thailand [1].

For calendar year 2022 India's average ethanol blending rate with petroleum is up to 9.3%. India's position as a structural surplus sugar producer and gradual utilization of alternative feedstock's will drive supply, while a 35% increase in off takes by parasternal oil marketing companies for ethanol blending will drive demand [3].

At current scenario according to report the ethanol production capacity in India is of 426 cr. liters derived from molasses-based distilleries, and 258 cr. liters from grain based distilleries is proposed to be expanded to 760 cr. liters and 740 cr. liters respectively. This would be sufficient to produce 1016 cr. liters of ethanol required for ethanol blended program and 334 cr. liters for other uses [1].

As initiative by Government of India the National Policy on Biofuels - 2018 is been introduced to accelerate the biofuel production with the target of 20% ethanol blending under the Ethanol Blended Petrol Programme by 2030 [4].

2.LITERATURE SURVEY:

As the production of bioethanol is encouraged so many studies have been performed to analyze the production of bioethanol from different raw materials. Mainly the raw materials used are wheat straw, rice straw, rice husk, corn, sugarcane bagasse, sugarcane molasses, etc. The following is a summary of the process for producing first-generation bioethanol using sugarcane molasses as a primary source.

Kartini et al. (2018) investigated bioethanol production from sugarcane molasses. The study aimed to improve production rate through a process involving pre-treatment, hydrolysis, saccharification, fermentation, and GC analysis. The highest bioethanol concentration achieved was 14.38% (v/v) with a 20% substrate usage after 72 hours [6].

Raharja et al. (2019) studied bioethanol production from sugarcane molasses. The study revealed that sugarcane molasses typically contain 50-60% sugar, with potassium levels ranging from 300-12000 mg/l, calcium levels from 150-2000 mg/l, and magnesium levels from 80-3900 mg/l. By comparing sugar concentrations (20%, 25%, and 30% brix) and employing H_2SO_4 pre-treatment, fermentation, and distillation, the study aimed to enhance production rate. Notably, the ethanol yield achieved was 71.52 per cent[7].

Ribs Huang et al. (2020) examined bioethanol production from sugarcane molasses. The study highlighted that sugarcane molasses typically contain approximately 50% sugar content. To enhance production rate, the study employed a four-step process involving pre-treatment, fermentation with PHO4 generation, distillation, and data analysis using liquid chromatography. Notably, the study concluded with ethanol purity ranging from 79.25 g/l to 96.29 g/l[8].

Wang Song et al. (2021) investigated bioethanol production from sugarcane molasses. Sugarcane molasses typically contain 50-60% sugar, with potassium levels ranging from 300-12000 mg/l, calcium levels from 150-2000 mg/l, and magnesium levels from 80-3900 mg/l. The study aimed to enhance production rate through a five-stage procedure involving pre-treatment, hydrolysis, fermentation using Saccharomyces Cerevisiae, and distillation with dehydration. The analysis showed a remarkable production rate of 99.7% wt. anhydrous ethanol [9].

Oludolapo O. (2022) proposed a study on bioethanol production from sugarcane molasses. Sugarcane molasses typically contain 30-36% sucrose, 10-17% fructose and glucose mixture, and 10-16% ash. The study aimed to enhance production rate through pre-treatment, yeast propagation, pre-fermentation, fermentation, and analysis. Results showed production of nearly 95% v/v ethanol. Additionally, the study concluded that adding benzene and performing ternary distillation can achieve 100% bioethanol [10].

3.MATERIALS AND METHODS OF ANALYSIS:

Materials were selected based on required purity for the production process, varying among different manufacturers. Sugarcane was pre-treated using chemicals, resulting in molasses of different grades based on sucrose content. Ethanol (99% purity) was obtained from Sigma-Aldrich Chemical Pvt. Ltd. with molecular formula C_2H_6O. Iso Propyl Alcohol (99.8% purity, C_3H_8O) was sourced from SRL Pvt. Ltd. Saccharomyces Cerevisiae (Baker's Yeast) and Calcium Hydroxide (96% purity, $Ca(OH)_2$) were acquired from Sigma-Aldrich and SRL Pvt. Ltd. respectively. Sodium Chloride (99.9% purity, NaCl) was obtained from SRL Pvt. Ltd.

Gas chromatography with a NUCON gas chromatograph (thermal conductivity detector) was employed to confirm chemical purity. Liquid samples were prepared by dissolving them with a known amount of isopropyl alcohol, which served as the internal standard. Weighed samples (0.5 µL) were injected into a stainless steel porapack-Q packed column (1.82 m length, 1/8 inch outer diameter) using a syringe. The analysis was conducted at an oven temperature program starting at 150°C for 1 minute, followed by a ramp of 5°C/min until reaching 230°C. The total run time was 20 minutes, with injector and detector temperatures maintained at 240°C (using the Nucon Nuchrom software). Integrated areas obtained from the analysis were converted to weight percentages for each component present in the samples, utilizing standard calibration curves.

4.PRODUCTION PROCESS:

The production of bioethanol from molasses involves several key steps: molasses preparation, pre-fermentation, fermentation, distillation, and analysis. Molasses is prepared and adjusted for optimal fermentation conditions. During pre-fermentation, it is mixed with water and additives to create an ideal environment for yeast activity. The fermentation step utilizes selected yeast strains to convert sugars into ethanol. Distillation separates ethanol from other components in the fermented mixture, and purification further refines the ethanol to obtain a high-purity product. These steps ensure the efficient conversion of molasses into high-quality bioethanol, a renewable and sustainable energy source.

4.1 Molasses Preparation

The purity of bioethanol is significantly influenced by the selection of the grade of molasses. Molasses, being the primary raw material, undergoes classification into three distinct grades: Grade A, Grade B, and Grade C (Table II). This classification is based on the sucrose content present in the molasses sample.

TABLE II
CLASSIFICATION OF MOLASSES

Grade	Sucrose Content	Physical Properties
A	65% (W/W)	Light in Colour
B	60% (W/W)	Dark in Colour
C	55% (W/W)	Extremely Dark (Black Tar)

4.2 Pre-Fermentation

The pre-fermentation process in bioethanol production from sugarcane molasses is an important step that prepares the molasses for fermentation. Sugarcane molasses, a by-product of sugar production, contains a significant amount of fermentable sugars that can be converted into ethanol. The pre-fermentation process aims to optimize the conditions for yeast growth andethanol production. It ensures that the molasses is well-prepared for fermentation, maximizing the yield and quality of bioethanol produced from sugarcane molasses.

4.3 Fermentation

The fermentation process is a crucial step in bioethanol production from sugarcane molasses. During fermentation, the sugars present in the molasses are converted into ethanol and carbon dioxide by yeast through the process of anaerobic respiration.

In fermentation process following steps are followed:-

i) Prepare a conical flask with a volume of 250 ml.
ii) Measure 70 ml of molasses.
iii) Add 70 ml of tap water to the molasses.
iv) Introduce 25 ml of Pasteur's Salt Solution.
v) Incorporate 0.5 gm. of Saccharomyces Cerevisiae (Baker's Yeast).
vi) Thoroughly shake the flask to ensure proper mixing of all components.
vii) Seal the flask with a one-hole rubber stopper that contains a bent glass tube.
viii) Insert the bent glass tube into a large test tube containing 2/3 of lime water.
ix) Allow the solution to ferment for approximately 2 weeks.

4.4 Distillation

The distillation process is a crucial and fundamental step in the production of bioethanol from fermented solutions, particularly those derived from sugarcane molasses. Distillation serves the purpose of separating ethanol from the other components present in the fermented broth, thereby purifying it to obtain a high concentration of ethanol.

It's important to note that the specific temperature of 92°C must be maintained which indicates an upper limit to avoid excessive evaporation of ethanol, which would lead to lower ethanol yields. Temperature control is a critical aspect of the distillation process to ensure efficient separation and optimize the ethanol concentration in the distillate.This method is suitable for separating ethanol from substances that have significantly higher boiling points, like water.

All three samples underwent the distillation process under the same conditions regardless of their grades. The distillation conditions remained consistent throughout the process, ensuring uniformity and standardization across the samples.

TABLE III
AMOUNT OF ETHANOL OBTAINED AFTER DISTILLATION

Grade	Amount
A	10 ml
B	5 ml
C	5 ml

TABLE IV
RESULTS FROM GAS CHROMATOGRAPHY

Grade	Sample weight	Mass of water	Mass of ethanol	w/w% of ethanol
A	2.0069	1.840778749	0.213924699	10.09746349
B	2.0114	1.41677823	0.208645002	12.5383492
C	2.0175	1.296460941	0.228632211	**14.67026042**

4.5 Result

The method employed for calibration and analysis in this study was gas chromatography (GC). The results obtained from the gas chromatography analysis (Table IV) revealed the specific composition and concentrations of the target compounds in the samples. These results were typically reported as peak areas or peak heights, which were proportional to the quantity of each compound present.

4.6 Conclusion

Based on the results obtained through gas chromatography (GC) analysis (Table IV), it was observed that the C grade of molasses exhibited a higher w/w% concentration, specifically 14.6702%, compared to Grades A and B. This suggests that the C grade of molasses contained a greater proportion of the target compounds of interest.
In line with this, a study conducted in 2018 reported that the highest ethanol yield, approximately 14.38 v/v%, was achieved after a fermentation period of 72 hours. The observed finding suggests that the fermentation conditions, including yeast amount and the selection of the molasses grade, were suitable and effective[6].
Based on this promising data, which provides a solid foundation, the obtained data and values can be taken as a baseline for further pursuit of higher ethanol percentages. The Aspen Plus simulation will play a crucial role in exploring different scenarios, particularly in optimizing fermentation conditions and identifying strategies to enhance the overall ethanol production process.

5. SIMULATION

5.1 Aspen Plus

Aspen Plus is a highly regarded and user-friendly process simulator that has gained significant popularity in both industrial and educational settings. Its widespread adoption is a result of its ability to simulate and predict the behaviour of complex chemical processes accurately. By employing fundamental principles such as material balance, energy balance, reaction kinetics, and equilibrium data, Aspen Plus enables engineers and researchers to analyze and optimize processes under specified operating conditions.
The software offers a comprehensive platform for modelling and simulating various chemical systems, ranging from simple unit operations to intricate, integrated process flowsheet. It allows users to construct detailed process models, define input parameters, and simulate the behaviour of the system.
Aspen Plus employs material balances to track the flow of mass throughout the process, ensuring that the quantities of different components are properly accounted for at every stage. Energy balances are used to analyze and optimize the energy requirements and heat transfer within the system.

5.2 Simulation of Production Process using Aspen Plus

Aspen Plus is initialized by launching the software and creating a blank simulation. In the component specifications section, the key components including glucose, ethanol, carbon dioxide, and water are added one by one in a sequential manner as shown in fig. 4. The appropriate thermodynamic model for the system is then selected as the fundamental method for the entire process as NRTL. In the blank sheet, a process flowsheet is designed using library of unit operation modules, these modules (blocks) are selected accordingly to the requirement as detailed in Table V. First, a mixer is selected and named appropriately. Thereafter, input feed stream and output product streams are specified from the mixer. Then a heat exchanger is selected and output mixer stream is connected to input heat exchanger stream. Rstoic is selected as a fermenter for our process of interest. Similarly, a flash2 column is selected as a separator and all streams are connected andappropriately labelled to complete the process flowsheet drawing as shown in fig. 5. Operating conditions for streams and unit modules are specified to accurately reflect the bioethanol production process in Aspen Plus.

The mixer is set to a temperature of 298.15 K and a pressure of 1 atm, with a total flow rate of 1 kg/hr. The compositions of glucose and water are 0.55 w/w and 0.45 w/w, respectively. The heater operates at 358.15 K and 1 atm, limited to the liquid phase. The fermenter column is maintained at 303.15 K and 1 atm, while the flash vaporizer column is set to 328.15 K and 1 bar.The liquid phase for fermenter and vapour-liquid phase for flash vaporizer are selected as respective valid phases[11].

After the removal of CO_2 using a flash vaporizer, the bioethanol mixture underwent distillation using two columns, namely Dist1 and Dist2. Dist1 consisted of 15 stages, while Dist2 had 10 stages. The feed was introduced at the 14th stage for Dist1 and at the 9th stage for Dist2. The reflux ratio and distillate to feed mole ratio for Dist1 were set to 1.8 and 0.02, respectively, while for Dist2, they were 1.8 and 0.98. A partial condenser was selected for Dist1, while Dist2 utilized a total condenser.

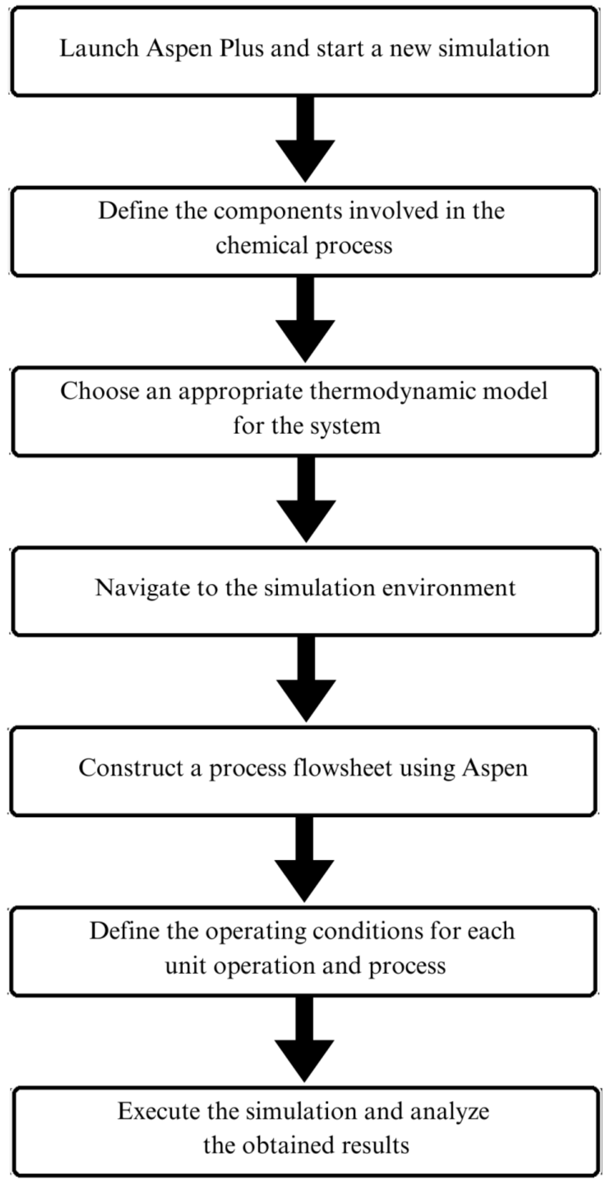

Fig. 4 Algorithm for Aspen plus Simulation Process

5.3 Result

The simulation results reveal that the outlet stream of Dist2 obtained the highest mass fraction (i.e. 0.997316223) of ethanol compared to other streams (Table VI). This signifies an exceptional level of purity and concentration of ethanol achieved through the distillation process. The high mass fraction indicates that nearly 99.73% of the outlet stream consists of the ethanol, showcasing the effectiveness of Dist2 in separating and purifying the ethanol. These findings hold great promise for producing high-quality and concentrated substances in various industries, offering valuable insights for process optimization and meeting stringent specifications.

6. CONCLUSION

In conclusion, this project on the production of bioethanol from sugarcane molasses has yielded significant insights and promising results. The analysis and simulation of the production process have demonstrated the effectiveness of the selected fermentation conditions and molasses grade. The pre-fermentation process has successfully prepared the molasses for efficient fermentation, leading to the conversion of sugars into ethanol. The distillation process has exhibited exceptional levels of purity and concentration, with the outlet stream of Dist2 obtaining the highest mass fraction, indicating a high concentration of the desired ethanol. These findings hold great promise for the production of high-quality and concentrated substances in various industries. The obtained data and values serve as a solid foundation for further pursuit of higher ethanol percentages. The Aspen Plus simulation has played a crucial role in exploring different scenarios, optimizing fermentation conditions, and identifying strategies to enhance the overall ethanol production process.
Overall, this project highlights the potential of bioethanol production from sugarcane molasses as a viable solution for addressing pollution issues and promoting sustainable energy sources. The success of this project contributes to the advancement of efficient and environmentally friendly biofuel production processes, ultimately leading towards a greener and more sustainable future.

TABLE V
BLOCK DESCRIPTION FOR BIOETHANOL PRODUCTION USING ASPEN SIMULATION

Name	Equipment	Description
Mixer	Mixer	To mix water with the raw material (glucose)
Heater	Heater	To heat the main stream
Ferment	Rstoic	To convert raw material into ethanol and CO_2
Sep-CO2	Flash2	To separate CO_2 from mixture
Dist1	Distl	To separate vinasses and ethanol water
Dist2	Distl	To separate bioethanol and emissions

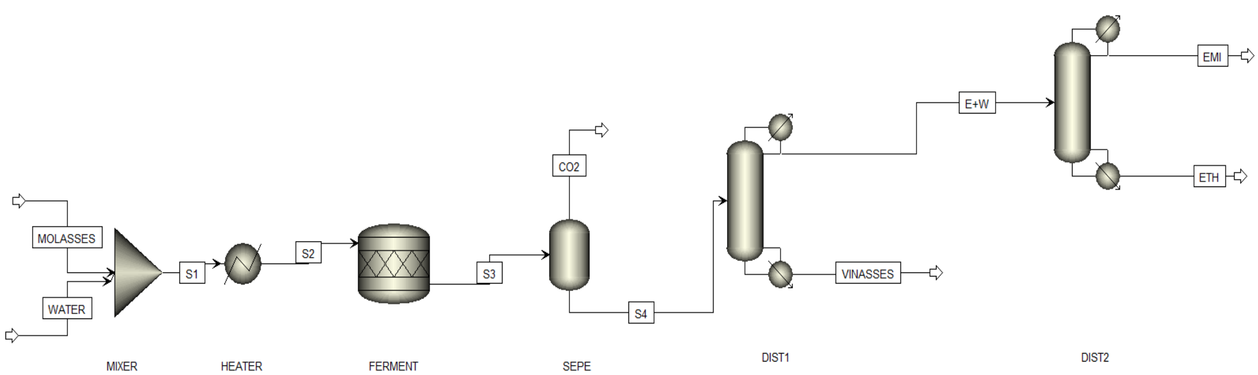

Fig. 5 Aspen plus simulation flowsheet

TABLE VI
RESULTS OBTAINED FROM OUTLET STREAMS

Mass Fractions					
Streams → / Components ↓	ETH	CO2	EMI	VINASSES	E+W
DEXTR-01	0	0	0	0	0
ETHAN-01	**0.9973162**	0.173591	0.61108326	0.32472241	0.61894388
WATER	0.00267942	0.061285	0.00265895	0.67502883	0.00265936
CARBO-01	4.22E-06	0.765125	0.3862578	0.00024876	0.37839676

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