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Research Article

Optimization of the Process of Metal NanoCalcium Oxide Based Biodiesel Production through Simulation Using SuperPro Designer

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This study evaluates improvements made to a biodiesel production process from Chlorella sp. micro algae in a locomotive pilot plant using simulation. Energy and the main variables of the operation such as temperature, reaction time, alcohol molar concentration, vegetable oil, and use of homogeneous and heterogeneous catalysts and their concentration, mixing intensity, and moisture control were collected from operational data, and mass balances were tested in the SuperPro Designer retail package v.9.5. The result was an increase in the efficiency of the process of obtaining company biodiesel from 86% to 92% by volume, the same that were scaled taking into account the species' production locality, and the results obtained showed that 26% was met by obtaining 10 MM (millions) of liters of biodiesel from the scaled plant.

1. Introduction

In recent years, the world's population growth has prompted a search for alternatives to meet the rising demand for energy consumption. Even now, fossil fuels have been the primary source of energy in most daily processes, and they have been directly responsible for environmental damage, such as climate change. The recent research has shifted its focus away from adaptation to circumstances and strategies for mitigating the problems that society faces due to environmental factors, such as the United Nations Conference on Climate Change. Around 78% of energy comes from fossil fuels, while the remaining 24% comes from various sources. Biodiesel is promoted as a viable alternative to fossil fuels and is touted as a valuable energy source because it can be made from agricultural, forestry, or municipal waste. Animal, vegetable, or recycled fats can be converted into biodiesel via a transesterification process, which has better environmental characteristics than petroleum-based diesel. Vegetable oils are used to make 84% of biodiesel, and using various raw materials such as pinion, biomass, cooking oil, and animal fat is expected to decrease. If sustainability criteria are met, biodiesel should replace fossil fuels shortly. However, no appropriate technological development has occurred. The progress is dependent on various investor resolutions and research spending to meet regional goals. The market price of biodiesel today cannot compete with crude oil prices. Still, it is expected that the price of petroleum derivatives, particularly fuels, will rise by 8% from the date, resulting in a 52% increase in biodiesel demand for automotive consumption, creating job opportunities and growing the local economy. Biodiesel stimulates agricultural activity which also provides environmental benefits such as reduced greenhouse gas emissions such as CO, CO_2, and NOx, and because it contains almost no sulfur, no SO2 is produced. However, using fuels with a composition of 96% conventional diesel and 6% biodiesel results in a reduction in greenhouse gas emissions [1].

The transesterification reaction of oils or fats (which is a reaction between your triglycerides) and methanol, which produces glycerin and methyl esters, can be used to make biodiesel. In the presence of a catalyst, triglycerides are found in Chlorella sp. micro algae oil reacts with low molecular weight alcohol (methanol, ethanol, etc.) to form glycerin, a mixture of fatty esters. The catalyst's performance and the control of optimal reaction conditions are essential considerations in reaction transesterification. The reaction represented in Figure 1 is a reversible reaction in which the ROH serves as a catalyst. The strings of fatty acids associated with the oil or fat used in the reaction, usually acid palmitic, stearic, oleic, and linoleic, are represented by R', R', and R''. The transesterification of fatty acids SuperPro Designer was used to simulate Chlorella sp. micro algae Biodiesel. The proportion, chain length of carbons, and degree of unsaturation of biodiesel are all determined by fatty acid methyl esters. Viscosity kinematics, density, cetane number, iodine number, acid number, and enthalpy of combustion are some of the physicochemical characteristics used to determine biodiesel quality, as defined by ASTM D6751 in the United States and EN 14214 in Europe. Biodiesel from oils rich in fatty acids unsaturated like oleic and linoleic provides characteristics suitable for internal combustion engines' correct performance since their density and viscosity are similar to diesel. It has been discovered that the presence of monounsaturated fatty acid esters improves biodiesel ignition quality and engine flow. The genus Chlorella sp. micro algae belongs to the Euphorbiaceous family, and Latin America is a hotbed of diversity and endemism, with roughly 22% of its species found there. The Chlorella sp. micro algae species, also known as pinion or piloncillo, have toxic and nontoxic varieties. Due to its oil content of 32% to 42% and the composition chemistry, which is close to 22% saturated fatty acids and 78% unsaturated fatty acids, several studies characterize it as a species with a large capacity for the production of biodiesel [2]. Based on biomass yield, lipid content, as well as quality of lipids, Chlorella Vulgaris is considered an ideal candidate for biodiesel production. For mass cultivation of microalgae on low-cost substrates, there is a need to develop more work so that the price of biomass output can be decreased.

2. Materials and Methods

The current process of producing biodiesel from Chlorella sp. micro algae oil. The plant has an 84% production capacity and a daily output of 4 L. Table 1 shows the detail of the plant stream flows pilot used for the base simulation [3]. Figure 2 shows the photo view of Chlorella sp. micro algae. The pilot plant and simulation consist of four processes: a reactor R-101, two centrifuges DC-101 and DC 102, and a mixer of M-101, which are the same as those in the biodiesel production process shown in Figure 3 and are briefly explained below. The catalysis stream, which contains a 74% solution of methanol with 26% sodium hydroxide, forming the compound sodium methoxide (NaOCH3), is mixed with the methanol stream, forming the stream C-101, which feeds the reactor R-101 through the cap, while Chlorella sp. micro algae oil feeds the reactor through the middle part. Methanol reacts with Chlorella sp. micro algae oil in the transesterification reaction is shown in Figure 4, yielding stream C-102, which contains biodiesel, glycerol, and traces of reactants. The reactor has a one-hour residence time, resulting in a conversion rate of 83 to 86%. The C-102 stream is passed through the DC-101 centrifuge, which separates fats and oils from glycerol to produce as much as crude biodiesel (C-103) as possible (C-104). To achieve biodiesel separation from glycerol, the centrifugation processes used properties suggested by the SuperPro Designer software V9.5 for this type of equipment, such as the solvent type and separator particle size, while only changing the percentages in the mass balance [4]. The crude biodiesel stream C-103 is washed with acidified water (C-105) with a pH of 4.5 in the mixer M-101, with HCl in a 1 percent w/w ratio to oil neutralize catalysis to prevent soap formation. After that, the mixture (C-106) is sent to the second centrifuge (DC 102) to separate the aqueous phase and extract the biodiesel and glycerol residues [5]. Temperature, reaction time, alcohol: oil molar ratio plant, type of alcohol, humidity, and catalyst concentration are all factors that can influence the transesterification process. The biodiesel stream product should not contain more than 0.05% water by weight. High water content can slow down the reaction rate because water reacts with catalysts to form soaps [6]. The stoichiometric ratio for transesterification is 3 : 1 alcohol: oil, but an excess of methanol up to a 6 : 1 ratio is usually chosen for higher conversion. However, a higher alcohol ratio at 6 : 1 may affect glycerine separation by an increased solubility, which causes the reaction to revert to the left, reducing the esters' yield. [7].

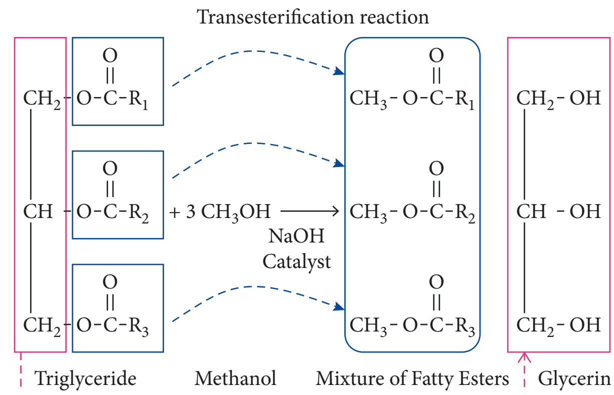

Figure 1: Transesterification reaction of Chlorella sp. micro algae Biodiesel.

Table 1: Details of plant stream flow pilot used for the base simulation.

Current	Components flow	(kg/ day)
	Reactor 1/R-101	
C-101	Methanol catalysis	0.43
Chlorella sp. microalgae oil	Chlorella sp. microalgae oil	4.00
	Centrifuge 2/DC-102	
C-102	Biodiesel	3,8000
	Glycerol	0.4038
	Chlorella sp. microalgae oil	0.1171
	Sodium methoxide	0.0125
	Water	0.0160
C-103	Biodiesel	3,8100
	Chlorella sp. microalgae oil	0.1116
	Sodium methoxide	0.0125
	Water	0.0160
C-104	Glycerol	0.4038
	Mixer/R-103	
C-105	HCl- water	0.1570
C-106	Biodiesel	3.8306
	Glycerol 0.0403	0.0403
	HCl	0.0152
	Chlorella sp. microalgae oil	0.1171
	Methanol	0.0055
	Sodium methoxide	0.0031
	Sodium chloride	0.0101
	Water	0.0160
	Centrifuge 2/DC-104	
Biodiesel	Biodiesel	3,8508
C-107	Glycerol	0.0400

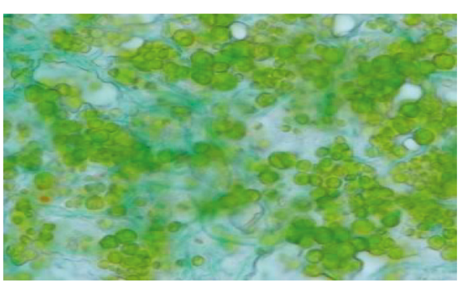

Figure 2: The photo view of Chlorella sp. micro algae.

3. Results

SuperPro Designer Software v.9.5 data was used to generate the various physical properties of compounds used in this simulation. The Production of biological products is analyzed and assessed by using the SuperPro Designer. This analysis looks at the production of citric acid, an organic acid used heavily in the beverage industry. The first commercial product of modern biotechnology is recombinant human insulin, which is manufactured by bacteria. The following operating conditions are recommended in biodiesel pilot plants: a continuously stirred reactor with a reaction temperature of 60°C and a pressure of 1 atm, with a residence time of 60 minutes. Because of the oil of Chlorella sp. Micro Algae oil from Ecuador contains only 1.27% free fatty acids,

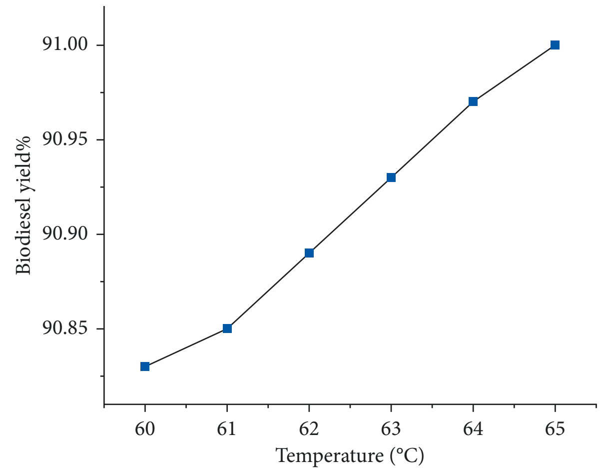

Figure 3: Biodiesel yield as a function of temperature variation.

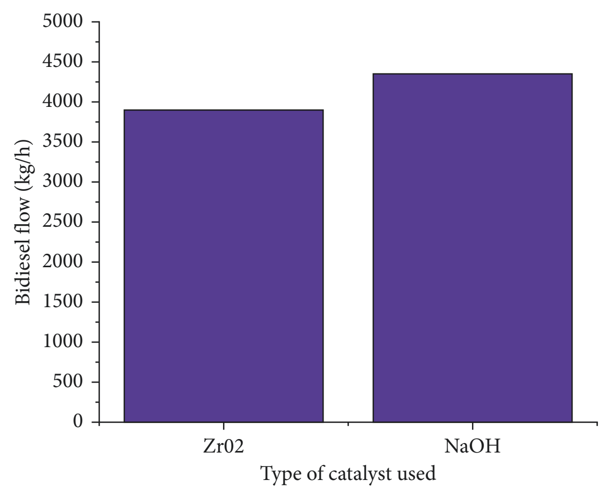

Figure 4: Biodiesel production concerning the type of catalyst used for the transesterification.

the transesterification stage. Because of its advantages, such as cost and reaction speed, NaOH was used as a catalyst; the catalyst concentration was 1%, and the alcohol: oil molar ratio was 3 : 1. The results obtained in the biodiesel pilot plant of the locomotive company studied before the realization of the simulation were 84%, based only on the volume of the product at the end of the process, which represents approximately 2.5 kg/day of biodiesel [8]. When analyzing the different operating variables mentioned in the methodology and ensuring maximum conversions, a time of 90 minutes residence in the reactor, time with the that is being worked on in some plants to obtain biodiesel in India, yielding results of 3.9 kg of biodiesel, corresponding to 92% conversion to the previous process in the base simulation, which was 86% obtaining results of 3.8 kg of biodiesel, corresponding to 92% conversion to the previous process in the base [9].

3.1. Proposal. Deescalation of 10 MM of *L*/year When analyzing the current situation in Ecuador and before the

Table 2: Identified variables and specific operation values.

Variables	Values bibliographic of operation
Reaction temperature	60°C
Molar alcohol ratio : vegetable oil	3 : 1
Alcohol type	Methanol
Catalyst type	NaOH
Concentration of catalyst	1% w/w
Reaction time	90 min
Mixing intensity	450 rpm
Humidity	0.05%

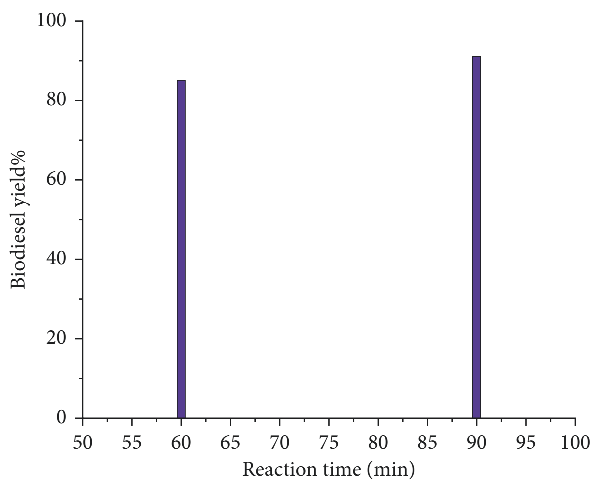

Figure 5: Biodiesel yield as a function of reaction time.

Table 3: Flash distiller/V-101 results.

	Components	kg/h	% Time
Vapour	Biodiesel	0.0019	0.0022
	Glycerol	0.0963	0.1092
	Chlorella sp. microalgae oil	0.0963	0.1092
	Methanol	0.8014	0.9078
	NaOCH3	0.1573	0.1782
	Water	87.1017	98.6934
Biodiesel	Biodiesel	4269.958	98,5342
	Glycerol	40.4833	0,9342
	Chlorella sp. microalgae oil	6.0642	0,1399
	Methanol	0.3895	0,0090
	NaOCH3	0.1874	0,0043
	Water	15.4422	0,0356

Table 4: Flash/V-101 distiller result.

		kg/hr	Time
Vapour	Biodiesel	0.0059	0.0064
	Glycerol	0.1058	0.1141
	Chlorella sp. microalgae oil	0.1472	0.1588
	Methanol	1.5813	1.7059
	Oxide zirconium	0.2798	0.3018
	Water	90.5761	97.7130
Biodiesel	Biodiesel	3742.099	98,0683
	Glycerol	45.1496	1,1832
	Chlorella sp. microalgae oil	7.1045	0,1862
	Methanol	0.8423	0,0221
	Oxide zirconium	10.1584	0,2662
	Water	10.4569	0,2740

requirement of the change of the energy matrix, arranged to design by simulation, of a plant of greater capacity. For the simulation of the new plant, the information collected from various studies on the variables involved in the biodiesel process and the inclusion of a process for treating the glycerin produced using the software, as shown in Table 2. The proposed scaling of the biodiesel production process is depicted in Figure 3. The proposal's principles are based on the simulation used in the company's biodiesel procurement process [10]. Figure 5 describes the two stages of the simulation: reaction and two additional steps for glycerin purification. They are described in the following paragraphs.

The proposed scaling of the biodiesel production process is depicted in Figure 4. The principles of the proposal are based on the simulation used in the company's biodiesel acquisition process. Figure 5 describes the two stages of the simulation: reaction and two additional steps for glycerin purification. They are described in the following paragraphs: Although transesterification of Chlorella sp. micro algae can occur at temperatures as low as 25°C, it is recommended that temperatures be kept between 60 and 65°C, due to the alcohol. Oil concentration ratio of 3 : 1. Table 3 shows that the water content in the steam stream is 98.5%, while the water content in the stream by the part lower than biodiesel is 98.5%, indicating that water and biodiesel have been separated [11]. The streams from the three centrifuges enter the mixer M-201 to be acidified with HCl 38% to separate the soaps and neutralize the NaOH residue contained in them in the glycerin purification process. Although increasing the temperature to 60°C improves performance and reduces reaction time, the operating variables used in the scaling proposal from Table 3 should be considered. It is recommended that the temperature not exceed 64.7°C, the boiling point of methanol, because it will vaporize, forming bubbles that will limit the reaction in the alcohol/oil/biodiesel phases. To achieve the goal of 10 MM L/year, the operating time of the locomotive pilot plant is used as a guide, which is 9-hours per day for 240 days. Consider the various inputs to the process over a year, which equals 10279 tons/year, and the output at the end of the process, which equals 9354 tons/year, for a yield of 91% w/w. The prices of the materials were calculated using a bibliography and marketing studies conducted in Ecuador [12].

The type of catalyst used to make biodiesel is one of the modified variables. The following are the results of a scaling plant simulation using a heterogeneous catalyst such as oxide zirconium (ZrO_2) and the values of the variables in Table 3: The rate of raw material input into the process is 4759 kg per hour [13]. In comparison, the process output is 3909 kg/h, resulting from the steam currents and biodiesel from Table 4, with an 83% w/w conversion using ZrO_2. These figures are supported by experimental results using ZrO_2 as a catalyst, in which yields of 87to 90% conversion were obtained, with a conversion of 92%, or 4334 kg/h, at the scaling plant in the Flash V-101 still using NaOH as a catalyst, as shown in Figure 3. Homogeneous catalysts, such as NaOH outperform heterogeneous catalysts in terms of price and performance. As shown in Figure 5, maintaining a 60°C range is advantageous to reaction rate, and studies conducted in India suggest that the reaction temperature is directly related to the alcohol: oil molar ratio and reaction time variables. Although it is specified that excess alcohol can be used up to a 6 : 1 concentration to ensure high conversions, this specification prevents the simulation from being developed in the SuperPro Designer v.9.5 programs because of the transesterification reaction in its database is designed to operate with alcohol: oil. When working on the scaled plant simulation with a 60-minute residence time in reactors, a product output of 4045 was obtained, corresponding to an 86% conversion; however, when using a residence time of 90 minutes in both reactors, a parameter with which we work in different plants in India, a value of 4759 kg was obtained. There was no evidence of a performance improvement, which would have resulted in a cost increase [14]. Following the acquisition of biodiesel, it must be characterized to ensure that it meets international standards such as ASTM D6751 in the United States. Biodiesel must be characterized after it is obtained to ensure that it meets international standards such as ASTM D6751 in the United States and EN 14214 in Europe. Biodiesel must be characterized after it is obtained to ensure that it meets the requirements of international standards [15, 16].

4. Conclusions

Using the oil of Chlorella sp. micro algae as a raw material, the opportunities for improvement found with the implementation of production processes allowed determining appropriate raw material quantities to achieve a 92% efficiency. The proposed design, with the values of the variables of 65°C temperature, alcohol methanol molar ratio: 3 : 1 oil, 1% catalyst concentration (NaOH) w/w, reaction time 90 min, and an intensity of 450 rpm mixing, resulted in a production of 10248 tons of lit biodiesel obtained from oil of Chlorella sp. micro algae. According to the economic analysis, the project results are profitable because of the internal rate of return (7.42%) is higher than that of the interest rate paid by a national bank (5%). Similarly, it was demonstrated that achieving a positive NPV should take at least 5 years, representing the investment's payback time, when working at a 9-hour per-day rate for 242 Table days.

Data Availability

The data used to support the findings of this study are included in the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest regarding the publication of this paper.

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