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Process Simulation and Optimization of Biodiesel Production from Algae Biomass

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ABSTRACT: There is need to further examine optimization of biodiesel production from renewable sources. In this study, we report the optimization of biodiesel produced from microalgae biomass using the CHEMCAD process simulator. Results show that the overall molar flow and energy was calculated to be 7.010kmoles/h and -4936.5MJ/h respectively. And also the liquid viscosity of the microalgae oil is greater than that of the biodiesel produced.

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Micro algae are seaweed or kelp - aquatic plants that are cultivated either directly in the sea, attached to solid structures like poles and rafts, or, in some cases, as small individual plants, kept in suspension in agitated ponds (Zhang et al 2018). Presently there is also interest in seaweeds as a feedstock for production of biofuels (Jiang et al 2016; Maneein *et al* 2018; Pablo *et al* 2020). Consequently, studies have reported the role of optimization and simulation in enhancing biodiesel production from different species of algal biomass. Optimization of process parameters presents models and optimal yield conditions of the production processes. To illustrate, Vinoth-Arul-Raj and co-workers (Vinoth-Arul-Raj *et al* 2019) examined the optimal biodiesel production process from *Nannochloropsis Salina*, a marine microalgae.

The process was optimized via the artificial neural network (ANN) model, with over 85% biodiesel yield. This yield was obtained at reaction conditions of 60degree Celsius, 55 minutes, 3% nano catalyst amount and 1:6 oil to methanol ratio. Similarly, Ching *et al* (2021) alternatively utilized *Chlorococcum infusionum* algal to produce biodiesel through an optimized vacuum drying process. They used artificial intelligence to model the drying process, as it could optimize the drying efficiency and energy utilization processes for industrial applications. Building on the work of Vinotharul-Raj *et al*, Garg *et al (2*020) utilized artificial neural network (ANN) and the response surface methodology (RSM) to optimize production of biodiesel from the algae oil of *Chlorella vulgaris.* Furthermore, more findings have considered the use of computer-aided simulations as alternative approaches for optimization.

For example, Adnan and Hossain (2018) gasified microalgae biomass of *Nannochloropsis oculata*, *Fucus serratus*, and *Scenedesmus almeriensis.* This process and the biomass pyrolysis were simulated using Aspen Hysys software. From the study, press increase retarded the gasification performance as indicated by the syngas composition, gasification system and cold gas efficiency. Also, a different study performed computer-aided simulation via metaheuristic multi-objective optimization approaches of optimized biodiesel production from *Chlorella vulgaris* (Hernandez - Perez *et al* 2019).

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More recently, the production of hydrogen-based synthetic gas from algal waste, *Chlorella vulgaris*, *Rhizoclonium species*, and *Spirogyra* have been reported (Ruiz-Marin *et al* 2020). The gasification process and biomass pyrolysis were simulated through Aspen Plus software for the steady-state equilibrium. Maximum syngas was produced at conditions of 600 degree Celsius, 1atm and 0.01metre cube per hour airflow rate.

Unfortunately, the use of CHEMCAD process simulator have not been reported, to the best of our knowledge. This is important because the software can bypass the need for rigorous analysis in order to design the process flow sheet for the production of biodiesel from microalgae oil. Herein, we report the process simulation and optimization of biodiesel production from algae biomass, using CHEMCAD simulator.

MATERIALS AND METHODS

Materials used in the simulation of biodiesel using the Chemical Computer Aided Design include data on microalgae oil, Biodiesel data gotten from literature, and software simulator. While the equipment used for the simulation include equilibrium reactor, Mixer, Pumps, Fire heater, Heat exchanger, Separators and Tower and tower plus.

Simulation Components: The selected stimulation components are presented in Table 1.

Table 1: Overview of Selected Simulation Components

Components	CAS
Fatty Acid Methyl Ester	112-02-9
Glycerol	56-81-5
Methanol	67-56-1
Calcium Oxide	1305-7
Calcium Sulphate	7778-1
Phosphoric Acid	7664-3
TiNa Phosphate	7601-5
Oil	122-32-7
Sulphuric Acid	7664-9
Water	7732-1
Sodium Hydroxide	1310-7

Process Description: The major feedstock used in the process is microalgae oil, and other feed materials in the process includes; methanol, sodium hydroxide (NaOH) as catalyst, water, phosphoric acid and triNa phosphate. The methanol is mixed with NaOH (catalyst) in the mixer (1) and pumped (2) through to mixer (3) which also has a recycle stream connected to it, the oil is pumped (10) and heated by heat exchanger (11) through stream (6) to the mixer (13) also the methanol and NaOH (catalyst) meets at the mixer (13). Hence, the component mixture from mixer (13) is sent to the transesterification reactor (12) where the base catalysed transesterification of the microalgae oil with alcohol occurs, hence stream (7) contains the following product properties; FAME (fatty acid methyl esters) (78.19%), Glycerol (8.10%), Methanol (8.83%), Unconverted Microalgae oil (4.10%) and NaOH (0.78%). At a flow rate of 1281.5441kg/hr. After the transesterification, the mixture is brought into a distillation column with total condenser (4) from stream (7) in order to separate the methanol from other components. The distillate that contains almost pure methanol is recycled at the reactor inlet through stream (13) whereas the residue is pumped (6), is cooled to 600c by heat exchanger (7) and its pressure is set to 110kpa. It is then washed with water in an extraction column (8) from stream (11).

The washing separates the biofuel from methanol, glycerol and catalyst. The overhead flow stream (19) is sent to a gravity splitter that allows recovering NaOH at the bottom stream (20) and the FAME oil and a fraction of water and methanol at the head stream (18). The FAME, oil, water and methanol recovery ratios in the organic phase of the splitter (8) is set to 1. These components are then separated by a distillation column with partial condenser. This additional separation is required to obtain a biodiesel purity of 99.66% that meets the ASTM (American Society for Testing and Materials) specifications and that has to exceed 99.6%. The partial condenser facilitates the FAME and water-methanol separation at the top of the column.it should be noted that the vacuum operating conditions are required in order to keep the temperature low enough to avoid the biodiesel degradation. The extraction column (14) and the splitter bottom streams are sent to a reactor in order to neutralize NaOH by adding pure phosphoric acid (H3PO4). The product Na3PO4 is separated from other components in a components splitter. After recovery of Na3PO4 stream (24), the stream contains more than 99.68% mass of glycerol. However, glycerol is considered as a secondary product that must have about 92% purity. Consequently, an additional separation is required and head stream is sent to a distillation column with total condenser. The products from (14) that is stream (21) are; FAME (99.66%), Methanol (0.033%), Microalgae oil (0.262%) and Water (0.042%). Is further distilled given vent, FAME (biodiesel) both containing a large percentage of biodiesel and the bottom product of these column is the unconverted oil.

Specifications: The main specification imposed on the process are; the primary feed (microalgae oil) was sent into the reactor at a temperature and pressure of 250c and 100kpa and flow rate 1050kg/hr (25tons/day). The secondary feeds (methanol, NaOH, water, phosphoric acid) to the process simulation have the following specification temperature and pressure (250c all through but 500c for phosphoric acid) and (100kpa all through but 200kpa for water) while their flow rates are (117.2kg/hr, 10kg/hr,100kg/hr and 15kg/hr) respectively.

Simulation Procedure: Hit the start icon, Go to the programs menu, Go to the ChemCAD for windows menu, Select ChemCAD for windows menu, Ignore the prompt that instructs you, to insert the ChemCAD installation disk. Hit cancel, ignore the job accounting information box prompt. Hit cancel, Go to the control menu, Go to new job, Named your job and Start simulating.

Create a job name and file

Establish the engineering units' system

Add unit operations to the flow sheet

Connect the unit operations with streams

i. Build the chemical component list

ii. Select K-value and enthalpy thermodynamic models

iii. Specify feeds properties

iv Specify equipment parameters

v. Run the simulator

vi. View the output

vii. Make sure the output is sound and logical

viii. Save the simulation.

RESULTS AND DISCUSSION

The overall mass balance, overall energy balance and equipment sizing obtained from the simulation carried out on the production of the biodiesel from micro algae oil are presented in Tables 1, 2 and 3 respectively. From the simulation it was determined that the optimum transesterification temperature was at 60oc. The viscosity of the microalgae oil reduced from 1.82346*10-2 Ns/m2 to biodiesel of viscosity of 2.61420*10-3Ns/m2. At 60o c the viscosity of the microalgae oil reduced geometrically.

The effective operation of an engine depends in the proper viscosity of the liquid fuel. The viscosity of fuel is important for its flow through pipelines, injector nozzles and for atomization of the fuel in cylinders. The liquid viscosity meets ASTM standard D445. The finish product, biodiesel, is an environmental friendly renewable fuel with little or no noxious gas release during the process of combustion. There is a great energy loss of 4936.5MJ/h (i.e. -4936.5MJ/h) in the transesterification process. From the result gotten above, the biodiesel purity of 99.66% was gotten, that meets the ASTM (American Society for Testing and Materials) specification.

Table 1: Overall mass balance

Overall mass Balance	K mole/h	K mole/h	kg/h	kg/h
	Input	Output	Input	Output
FAME	0.000	3.380	0.000	1002.082
Glycerol	0.000	1.127	0.000	103.753
Methanol	3.658	0.278	117.200	8.905
Calcium Oxide	0.000	0.000	0.000	0.000
Calcium sulphate	0.000	0.000	0.000	0.000
Phosphoric Acid	1.306	1.223	128.000	119.833
TriNa Phosphate	0.000	0.083	0.000	13.663
OIL	1.186	0.059	1050.000	52.480
Sulphuric Acid	0.000	0.000	0.000	0.000
Water	0.611	0.861	11.000	15.504
Sodium Hydroxide	0.250	0.000	10.000	0.000
Total	7.010	7.010	1316.200	1316.200

From the simulation above it was determined that the optimum transesterification temperature was at 60^{o}c. The viscosity of the microalgae oil reduced from $1.82346*10^{-2}$ Ns/m^2 to biodiesel of viscosity of $2.61420*10^{-3} Ns/m^2$.

Table 2: Overall Energy Balance

Overall Energy Balance	MJ/h Input	MJ/h Output
Feed Streams	-5948.44	0
Product Streams	0	-4936.5
Total Heating	2135.18	0
Total Cooling	-1123.79	0
Power Added	0.556145	0
Power Generated	0	0
Total	-4936.5	-4936.5

At 60^{o} c the viscosity of the microalgae oil reduced geometrically. The liquid viscosity meets ASTM standard D445. The finish product, biodiesel, is an environmental friendly renewable fuel with little or no noxious gas release during the process of combustion. There is a great energy loss of 4936.5MJ/h (i.e. -4936.5MJ/h) in the transesterification process. Total mass input was calculated to be 1316.220kg/h, are presented in Tables 4 and 5 respectively.

Conclusion: The study examines effects of the simulation on several process parameters, involved in the biodiesel production. Among the investigated parameters, liquid viscosity of the oil was reportedly higher than that of biodiesel. Nonetheless, the biodiesel yield increased with reducing temperature. The viscosity is important because **t**he effective operation of an engine depends in the proper viscosity of the liquid fuel.

Table 3: Equipment Sizing

Number of trays	10
Tray area	0.657m^2
Active tray area	0.598m^2
Valve materials	Stainless steel
Joint efficiency	0.85
Corrosion allowance	0.001m
Allowable stress	94,458.211kpa
Tray spacing	0.610m
Tray pressure loss	0.539kpa
Clearance	0.044m
Hole area	0.114m^2
Flooding	63.851%
Valve thickness gauge	12
Desk thickness gauge	14
Tower internal diameter	0.914m
velocity	0.045m/s

Table 4: Total mass input was calculated to be 1316.220kg/h

Microalgae oil extracted	1050kg/h
NaOH	10kg/h
Water for washing	11kg/h
Phosphoric acid	128kg/h

Table 5: Total mass output was calculated to be 1316.220kg/h

Biodiesel produced	1002.082kg/h
Glycerol	103.753kg/h
Methanol	8.905kg/h
Phosphoric acid	119.832kg/h
TriNa phosphate	13.663kg/h
Unconverted microalgae oil	52.480kg/h
Water left after washing	15.504kg/h

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