A TERM PAPER ON

MODELLING AND OPTIMISATION OF BIODIESEL PRODUCTION FROM CAPER SPURGE (*Euphorbia lathyris*) USING ASPEN HYSYS

ChE 306: Chemical Engineering Laboratory IV

Submitted By

Group: 08

Group members:

Pujan Ashish Mohanta	Student ID: 1702043
Nishat Tasnim Nimmu	Student ID: 1702044
Tanvir Ahmed	Student ID: 1702045
Mehnaj Tabassum	Student ID: 1702046
Tasfia Ferdoush	Student ID: 1702047
B.M. Hasanuzzaman Rafin	Student ID: 1702048

Submitted To

Dr. Md. Tanvir Sowgath

Associate Professor

Ahaduzzaman Nahid

Assistant Professor

Nishat Tabassum

Lecturer

Swarit Ahmed Shadman

Lecturer

Md. Burhan Kabir Suhan

Lecturer

Date of Submission: 25.02.2022

Abstract

Biodiesel can be produced from *Euphorbia lathyris* using methanol and NaOH catalyst on an in-silico platform. The objective of this work was to simulate the conversion process of Caper spurge (*E. laythris)* into biodiesel. This simulation process along with the optimization of its economic aspects was modeled using Aspen HYSYS v10. Methanol, triolein and NaOH (as catalyst) were used as reactants and the reaction was conducted into a CSTR. Biodiesel was obtained as the desired product along with glycerol as by-product. Initially, a yield of 2.056 kgmole/h biodiesel with 84% mole fraction and 0.96 kgmole/h glycerol was obtained from 1 kgmole/h fresh feed. After modeling the process, taking the cost of raw materials, products and power input into consideration, the triolein stream (caper spurge oil) was optimized to gain maximum profit. The optimization for highest profit showed that, from 0.93 kgmole/h oil, 1.781 kgmole/h biodiesel with 100% mole fraction and 0.81 kgmole/h glycerol can be obtained and the profit gained from the process is 888.4 USD. The optimized value represents a fine yielding process with a decent amount of profit for biodiesel production.

Introduction

Caper spurge oil has high percentage of mono-unsaturation in fatty acid, which can be used to produce biodiesel with high yield. As sources of fossil fuels are decreasing day by day, this kind of weed can be used as a source of biofuel production. Biodiesel, a renewable, biodegradable and non-toxic biofuel, is produced by trans-esterification of virtually any triglyceride feedstock. Caper spurge (*Euphorbia lathyris*) oil reacts with small chain alcohols, like methanol, to produce biodiesel in presence of an alkaline catalyst. Glycerol is a by-product in this reaction. The reaction is-

Tri-glyceride of Fatty acid + 3×Methanol → 3×Fatty acid methyl esters + Glycerol

To produce biodiesel from this oil, a model has been developed using Aspen HYSYS v10. In this model, triolein (triglyceride of Oleic acid) is assumed a component of capur spurge oil and after reaction, it produces Methyl oleate, which is biodiesel, and glycerol in presence of alkaline catalyst like NaOH. This biodiesel can be used as substitute of diesel or can be blended with diesel to use in diesel engines.

Methodology

A steady state simulation model was prepared in this project using the ASPEN Hysys version 10. The premise of this project was the oil composition which got processed in the model considered as triglyceride of oleic acid or Triolein. The component list also includes methanol to proceed with the esterification and glycerol as a by-product; Sodium hydroxide was also included as a catalyst and pure water was used to heat exchange and to store unconverted methanol. The fluid package used for the simulation was general NRTL as it provides good representation of experimental equilibrium data for non-ideal mixtures and partially immiscible systems. It was suited best for highly polar compounds like methanol and glycerol in the simulation. The kinetic reaction was set adding the specification of the forward reaction. In the flowsheet, NaOH and methanol stream at 25°C and 1 atm was mixed with a recycled methanol stream from a flash separator. This mixed stream was again fused with the oil stream. And this final stream was brought to a heat exchanger's tube side to increase the temperature close to 65°C; in the shell side of the heat exchanger, a saturated stream of 100°C was used to heat the mixed stream. This heated stream was carried to CSTR and the temperature was kept to 65°C and the yield was almost 69.58%. The liquid stream from the CSTR was entered into a flash separator which was operated into 70°C. The vapor stream from the separator contained pure methanol which was recycled back and mixed with fresh feed and the liquid stream was inserted into a component splitter. Methanol, water, NaOH and triolein was splitted into the overhead stream of a component splitter adding the outlet condensed water from the heat exchanger; if needed this stream can be separated using liquid-liquid extractor with Chloroform as solvent but it was not precedence in this project and not discussed further. M-oleate and glycerol was splitted to the bottom stream; the whole split process was operated at STP. Then this stream was heated with a heater to 350°C to convert into a vapor phase and fed into a distillation column of 10 stages. The overhead stream of the column contained the highest fraction of glycerol and the bottom head stream contained the pure biodiesel. The recovery of the biodiesel i.e. M-oleate was approximately 92%. The whole process was conducted under the atmospheric pressure and without any pressure drop in various equipment.

Taking the cost of raw materials, products and essential energy inputs the optimization was performed to maximize the profit of this model

Results and Discussion

The amount of feed oil was almost 824.1 kg/h and the biodiesel production rate was 528 kg/h and the valuable glycerol as by-product was also being produced at a rate of 107.6 kg/h. As the model was simulated at atmospheric pressure unlike the reference article, the use of the valves and pumps could be cut down easily and the required energy streams got lower as well. The optimal conversion was predicted slightly higher than the reference model which is 92% at the methanol-oil ratio of 25mol/mol, the catalyst of 1.12 mol% and at 65°C temperature. The use of heat exchanger reduced the cost of heater duty and also the necessity of water at component splitter could be managed efficiently. Power required for reactor, flash separator, component splitter and the heater were 35.82 KW, 242.3 KW, 38.02 KW and 189.4 KW respectively. The comparison of the feed and production amount is shown in Table 09 from where it is visible that though the biodiesel production rate got slightly lower but 100% purity could be achieved. Moreover, profit optimization was done to attain a profit of 888.4 USD per hour which makes this simulation of processing mono-unsaturated tri-glyceride fatty acid oil to a biodiesel very achievable.

Conclusion

The results of this model showed a good result with maximum profit of 888.4 USD/h in simulation. Biodiesel was obtained as pure product and a good amount of glycerol was also obtained as by product. Energy requirements were also moderate. Around 69.58% conversion was achieved in CSTR which was favorable for producing a moderate amount of biodiesel. The overall process was held at steady sate condition.

Process Flow Diagram

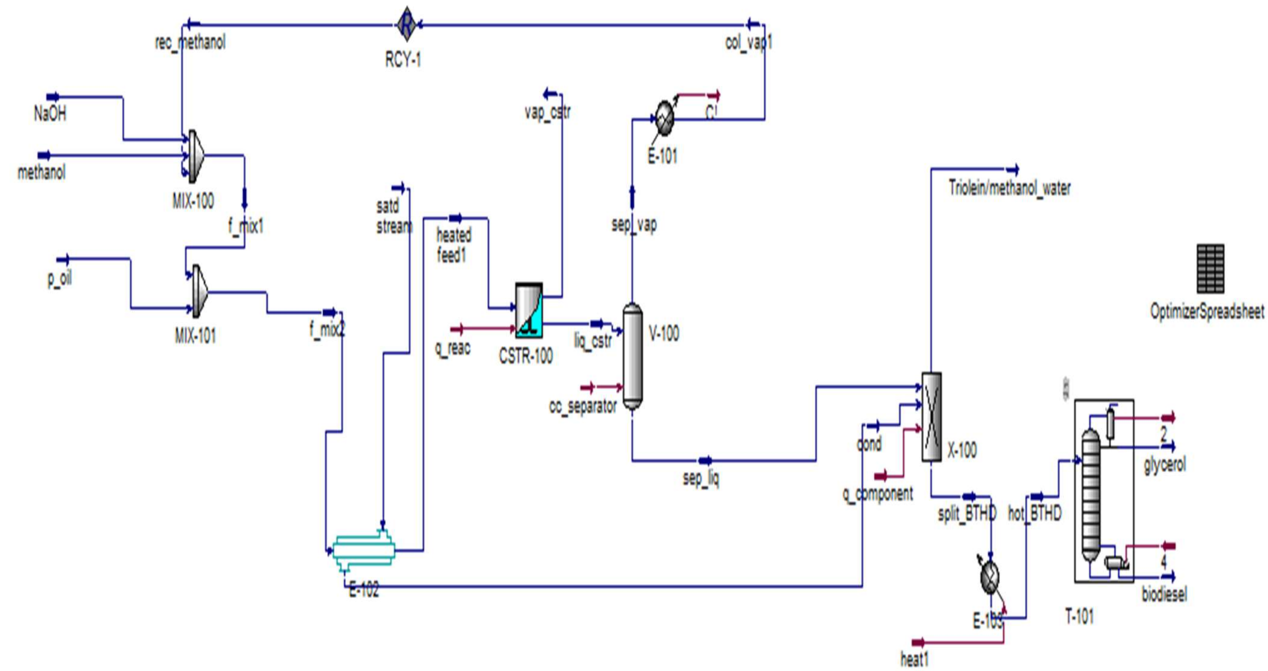

Figure 01: Process flow diagram of Biodiesel production

Feed specifications

Caper Spurge (*Euphorbia lathyris*) oil

Table 01: Fresh stream composition and conditions for Caper Spurge oil

Component	Triolein
Composition (Mole fraction)	1
Vapor / Phase Fraction	0
Temperature	25 ℃
Pressure	101.3 kPa
Molar Flow	0.9307 kgmole/h
Mass Flow	824.1 kg/h
Std Ideal Liquid Volume Flow	0.8997 m^3/h
Molar Enthalpy	-1.938×10^6 kJ/kgmole
Molar Entropy	8245 kJ/kgmole ℃
Heat Flow	-1.803×10^6 kJ/h
Liquid Vol Flow @Std Cond	0.9009 m^3/h

Methanol

Table 02: Fresh stream composition and conditions for methanol

Component	Methanol
Composition (Mole fraction)	1
Vapor / Phase Fraction	0
Temperature	25 ℃
Pressure	101.3 kPa
Molar Flow	7.61 kgmole/h
Mass Flow	243.8 kg/h
Std Ideal Liquid Volume Flow	0.3064 m^3/h
Molar Enthalpy	-2.394×10^5 kJ/kgmole
Molar Entropy	46.69 kJ/kgmole ℃
Heat Flow	-1.822×10^6 kJ/h
Liquid Vol Flow @Std Cond	0.3062 m^3/h

NaOH

Table 03: Fresh stream composition and conditions for NaOH

Component	NaOH
Composition (Mole fraction)	1
Vapor / Phase Fraction	0
Temperature	25 ℃
Pressure	101.3 kPa
Molar Flow	0.298 kgmole/h
Mass Flow	11.92 kg/h
Std Ideal Liquid Volume Flow	6.687×10^{-3} m^3/h
Molar Enthalpy	-8.342×10^{4} kJ/kgmole
Molar Entropy	-105.8 kJ/kgmole ℃
Heat Flow	-2.486×10^{4} kJ/h
Liquid Vol Flow @Std Cond	7.917×10^{-3} m^3/h

Saturated steam

Table 04: Fresh stream composition and conditions for saturated steam

Component	Water
Composition (Mole fraction)	1
Vapor / Phase Fraction	1
Temperature	100 ℃
Pressure	101.3 kPa
Molar Flow	5 kgmole/h
Mass Flow	90.08 kg/h
Std Ideal Liquid Volume Flow	9.026×10^{-2} m^3/h
Molar Enthalpy	-2.386×10^{5} kJ/kgmole
Molar Entropy	132.5 kJ/kgmole ℃
Heat Flow	-1.193×10^{6} kJ/h
Liquid Vol Flow @Std Cond	8.876×10^{-2} m^3/h

Recycle stream specification

Table 05: Recycle stream (rec_f) composition and conditions

Component	Methanol
Composition (Mole fraction)	1
Vapor / Phase Fraction	0
Temperature	25 ℃
Pressure	101.3 kPa
Molar Flow	17.71 kgmole/h
Mass Flow	567.4 kg/h
Std Ideal Liquid Volume Flow	0.7131 m^3/h
Molar Enthalpy	-2.394×10^5 kJ/kgmole
Molar Entropy	46.69 kJ/kgmole ℃
Heat Flow	-4.24×10^6 kJ/h
Liquid Vol Flow @Std Cond	0.7125 m^3/h

Product specifications

Biodiesel

Table 06: Composition and conditions for biodiesel stream

Component	Methyl oleate
Composition (Mole fraction)	1
Vapor / Phase Fraction	0
Temperature	343.7 ℃
Pressure	100 kPa
Molar Flow	1.781 kgmole/h
Mass Flow	528 kg/h
Std Ideal Liquid Volume Flow	0.6022 m^3/h
Molar Enthalpy	-4.937×10^5 kJ/kgmole
Molar Entropy	912.4 kJ/kgmole ℃
Heat Flow	-8.792×10^5 kJ/h
Liquid Vol Flow @Std Cond	0.6018 m^3/h

Glycerol

Table 07: Composition and conditions for glycerol stream

Components	Glycerol, Methyl oleate
Composition (Mole fraction)	Glycerol-0.8, Methyl oleate-0.2
Vapor / Phase Fraction	0.0592
Temperature	262℃
Pressure	100 kPa
Molar Flow	0.8095 kgmole/h
Mass Flow	107.6 kg/h
Std Ideal Liquid Volume Flow	0.102 m^3/h
Molar Enthalpy	-6.011×10^5 kJ/kgmole
Molar Entropy	343.7 kJ/kgmole ℃
Heat Flow	-4.866×10^5 kJ/h
Liquid Vol Flow @Std Cond	8.608×10^{-2} m^3/h

CSTR reactor Specification

Table 08: Pre-exponential factor A and activation energy E for CSTR

Parameter	**In (Pre-exponential Factor)**	**Activation energy (Kcal mol^{-1})**
Kinetic constant (K_C)	12.93	14
Equilibrium constant (K_E)	4.17	2.68

Optimization information

Table 09: Prices assumed for feeds, products and power

Name	Price
Caper spurge oil	0.90 USD/kg
Methanol	0.30 USD/kg
NaOH	0.40 USD/kg
Saturated steam	0.006 USD/kg
Biodiesel	3.00 USD/kg
Glycerol	1.94 USD/kg
Power	0.10 USD/kWh

Table 10: Table of revenue, cost and profit after optimization

Name	Price
Total Revenue	1793 USD/h
Total cost	904.5 USD/h
Profit	888.4 USD/h

Comparison between values before and after optimization

Table 11: Table for comparison of before and after optimization

Object stream	Variable name	Before optimization	After optimization
Oil	Molar flow	1.00 kgmole/h	0.9307 kgmole/h
Biodiesel	Molar flow	2.056 kgmole/h	1.781 kgmole/h
	Mole fraction	0.84	1.00
Glycerol	Molar flow	0.96 kgmole/h	0.81 kgmole/h
	Mole fraction	0.80	0.80

References

1. “Biodiesel prices (SME & FAME) | Neste.” https://www.neste.com/investors/market-data/biodiesel-prices-sme-fame?fbclid=IwAR1GhS0RSaVLK9sTQZQCQSzllb6Ak_UyHxx6eAH08jUt8XeZ2z1sMXIwgY0#77ee8d9f (accessed Feb. 25, 2022).
2. “Glycerol Price and Market Analysis - ECHEMI.” https://www.echemi.com/productsInformation/pid_Seven41077-glycerol.html?fbclid=IwAR03iWN-Ttn_gI8mrQTpDaRRubhS4X6fuMoSG6rcGsOvwjmV-OfBlu0hpCo (accessed Feb. 25, 2022).
3. G. Adeniyi, J. O. Ighalo, A. S. Adeoye, and D. V. Onifade, “Modelling and optimisation of biodiesel production from Euphorbia lathyris using ASPEN Hysys,” *SN Appl. Sci.*, vol. 1, no. 11, 2019, doi: 10.1007/s42452-019-1522-0.
4. For CSTR reactor- “42452_2019_1522_MOESM1_ESM.”
5. “Oleochemical’s Market Price” http://www.hbint.com/datas/media/5b7d6eb55e3e88fa6677fa28/two-weekly-oleochimicals.pdf