

Simulation of Biodiesel from Waste Cooking Oil(WCO) in Aspen HYSYS and its Optimization Study

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Abstract:

This study outlines a process simulation for producing biodiesel from waste cooking oil (WCO) using Aspen HYSYS V11. A two-stage Continuous Stirred-Tank Reactor (CSTR) system was designed to operate at 65 °C and 1 atm, with a methanol-to-oil molar ratio of 6:1 and 2 wt% KOH as a catalyst. The simulation achieved a triglyceride conversion of approximately 99%, yielding biodiesel with over 99% purity. Methanol recovery from the distillation column reached ~98%, minimizing losses. The process integrates glycerol decantation and a two-stage hot-water washing unit for final purification. This setup demonstrates a practical and eco-friendly method for synthesizing biodiesel from waste-derived feedstock.

Keywords — Waste Cooking Oil, Transesterification, Aspen HYSYS, Process Simulation.

I. Introduction

The increased global demand for sustainable energy, along with various factors such as environmental concerns over fossil fuels, fuel depletion, and greenhouse gas emissions, has driven significant research into renewable sources for alternatives such as biodiesel [1]. Biodiesel, a monoalkyl ester derived from renewable liquid feedstocks, offers a valuable substitute for petroleum diesel due to its similar properties and reduced environmental impact [2,3]. Globally, the energy sector remains heavily dependent on fossil fuels, which accounted for approximately 41% of the total energy consumption (9,940 Mt) in 2018, exacerbating air pollution and climate change [4]. Therefore, there is a pressing need for sustainable alternatives like biodiesel, which not only provides a renewable energy source but also addresses waste management challenges through the utilization of waste cooking oil and other non-edible oils, along with other low-cost feedstocks.

Biodiesel is primarily produced by transesterification of various sources, which include vegetable oils, animal fats, and waste cooking oil, using alcohols like methanol and

ethanol with the help of various catalysts [1,3]. The efficiency of this process depends on several factors, including the methanol-to-oil ratio, the type and concentration of the catalyst, the reaction temperature, and the content of free fatty acids (FFAs) in the feedstock [4]. Homogeneous catalysts such as sodium hydroxide and potassium hydroxide are widely preferred in industrial applications because of their cost-effectiveness, higher conversion rates, and ability to operate under mild conditions [1]. Recent studies, however, have shown advancements in heterogeneous catalyst development, which are easier to recover and reuse, and offer high productivity that improves the economic viability of biodiesel production [4]. Various simulation tools like Aspen HYSYS have been used to model reaction conditions, analyze mass and energy balances, and optimize reactor design parameters, thereby improving process feasibility [2]. These innovations are critical, given the projected global WCO production of at least 16.54 million tonnes annually, with the EU27 alone contributing 3.55 million tonnes—49% of which originates from domestic households [4].

For biodiesel commercialization, challenges arise such as high feedstock costs, especially when edible oils are used. Thus, it is important to explore alternative sources such as non-edible oils (e.g., *Jatropha curcas*), waste cooking oil, waste vegetable oil, and animal fats [3–5]. The use of waste cooking oil not only reduces feedstock cost but also addresses waste disposal issues, making it a sustainable solution [4,6].

Biodiesel is biodegradable and safer to handle. From an environmental perspective, it reduces emissions of harmful gases such as carbon monoxide, sulfur dioxide, and particulate matter compared to diesel [4,5]. Biodiesel also has a higher flash point, making it safer for storage and transportation. However, it has a lower calorific value—approximately 9% lower than petroleum diesel—which may slightly impact fuel efficiency [6]. Despite these advantages, limitations such as higher nitrogen oxide (NO) emissions and engine compatibility concerns (e.g., B100 usage) require further investigation [4,5].

Economic barriers also persist, as biodiesel production costs remain sensitive to geopolitical factors, subsidies, and regional policies [6].

In the global scenario, Europe dominates biodiesel production, with Germany leading in rapeseed-based biodiesel supported by policy incentives [4,5]. Meanwhile, countries like Nigeria are leveraging underutilized resources such as waste vegetable oil, cassava, and sugarcane to address their food-to-fuel conflicts [2]. A wide diversity of feedstocks—from soybean to palm oil and waste cooking oil—demonstrates the adaptability of biodiesel production to local resource availability [4,6].

In alignment with global efforts, this work focuses on the simulation and design of biodiesel production from waste cooking oil using Aspen HYSYS. The objective of this study is to develop a simple, efficient, and scalable process model that ensures maximum biodiesel yield with minimal complexity and resource consumption. This study aims to model the biodiesel production process from WCO using Aspen HYSYS. It also evaluates the best operating parameters, including reaction temperature, catalyst concentration, and methanol-

to-oil molar ratio, that enhance the conversion efficiency of the transesterification reaction.

II. Methodology

A. Feedstock and Reactants

The production process for biodiesel was simulated using Aspen HYSYS V11. The system was set up as a continuous, steady-state process operating near atmospheric pressure. The flowsheet included four sequential sections:

1. Storage
2. Reaction
3. Separation
4. Purification

This setup represents a practical industrial configuration for biodiesel production from waste cooking oil (WCO) [7].

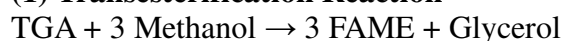
Due to the chemical variability of WCO, the simulation used three pseudo-components based on literature data [7]:

- TGA: Triglycerides
- FFA: Free fatty acids
- FAME: Fatty acid methyl esters (biodiesel product)

B. Reaction Chemistry

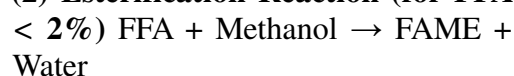
Biodiesel production primarily occurs via transesterification, with potassium hydroxide (KOH) as the catalyst:

(1) Transesterification Reaction



- Catalyst: KOH
- Glycerol: Valuable byproduct [1,4,14]

(2) Esterification Reaction (for FFA



- Assumption: Low FFA content minimizes soap formation [4,7,14].

1) *Kinetic Modelling*: Reaction kinetics followed Arrhenius-type equations [3,11,19]:

Table 2: Reaction Kinetics Parameters

Reaction	Rate Constant (K)	Activation Energy (Ea)	Units
Transesterification	0.01	47.07	kJ/mol
Esterification	0.01	29.78	kJ/mol

C. Process Flow Diagram and Simulation Setup

The flow sheet for simulation of biodiesel production from waste cooking oil (WCO) was developed with Aspen Hysys V11. The four primary units are:

1. Storage Unit: WCO tanks, methanol tank, KOH tank, and recycled methanol tank.
2. Reaction Unit: Two CSTRs for methoxide preparation and transesterification.
3. Separation Unit: Decantation of glycerol and methanol recovery via distillation.
4. Purification Unit: Water washing and elimination of moisture.

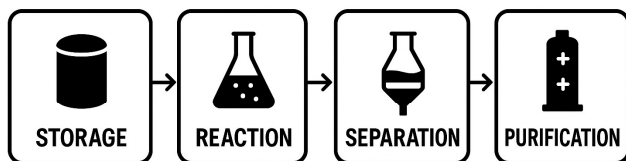


Figure 1: Process flow diagram of biodiesel production

D. Reactor Design and Parameters

The biodiesel production simulation uses two Continuous StirredTank Reactors (CSTRs), modeled with Aspen Hysys V11. The system operates at 1 atm for energy efficiency and safety. The model was simulated to produce nearly 10 tonnes/day of biodiesel from WCO.

Table 1: PSEUDO-COMPONENT PROPERTIES OF WCO

Component	Boiling Point (°C)	Molecular Weight (g/mol)	Density (kg/m³)	Critical Temp (K)	Critical Pressure (kPa)	Critical Volume (m³/kmol)
FAME	311.75	290.90	906.56	493.00	1369.18	1.5037
TGA	500.15	873.35	923.00	636.85	515.32	2.8008
FFA	347.07	276.11	876.21	503.09	1384.16	0.9882

1) CSTR Configuration: CSTR-1 (200 L) prepares methoxide; CSTR-2 (400 L) handles transesterification with 75% - 80% liquid holdup [18].

Table 3: Reactor Design Parameters (Calculated)

Parameter	Value	Unit
Batch time	0.25	hr
Residence time	0.5	hr
Volume flow of reactants	0.55917	m³/hr
Liquid volume in reactor	0.279585	m³
Total reactor volume	0.37278	m³

Reactor Design Equations

(1) Reactor Volume

$$V = Q \times \tau \quad (1)$$

Where:

- V = Reactor volume (m³)
- Q = Volumetric flow rate (m³/hr)
- τ = Residence time (hr)

(2) Total Volume from Liquid Holdup

$$V_{total} = V_{liquid} / \phi \quad (2)$$

Where:

- V_{total} = Total reactor volume (m³)
- V_{liquid} = Liquid volume (m³)
- ϕ = Liquid holdup fraction (typically 0.75–0.80)

E. Representation of Process Flow Sheets

The biodiesel production process was simulated with Aspen HYSYS V11 and designed as a continuous flow process, which runs under steady-state conditions and close to atmospheric pressure.

The resulting flowsheet consists of four consecutive blocks: Storage, Reaction, Separation, and Purification. These blocks constitute an industrially viable setup for the production of biodiesel from waste cooking oil (WCO).

Storage Facility:

The process starts with three separate storage tanks for the primary feedstocks: waste cooking oil (WCO), methanol, and potassium hydroxide (KOH). Methanol is stored in an anhydrous liquid state, and KOH is assumed to be in a liquid state as it favours the simulation environment. There is one tank reserved for the recovery of residue methanol, which is recovered in the later process.

Reaction Unit:

The feed streams are sent to two Continuous Stirred-Tank

Reactors (CSTRs) in series. Methanol and KOH react in the first CSTR and form methoxide, which is the working catalytic agent.

The methoxide is sent to the second CSTR. There, it reacts with

WCO via transesterification. This forms fatty acid methyl esters

(FAME, the biodiesel) and glycerol as a byproduct.

An overhead condenser is attached to the second CSTR. This condenses and recycles any released methanol vapor during the reaction, which improves efficiency and material utilization.

Separation Unit:

The lighter biodiesel-methanol mixture goes through a methanol recovery system, designed as a distillation column. The column separates methanol from the biodiesel stream with 98% purity, according to the simulation results. The recovered methanol is condensed and combined with the recycled methanol reservoir. Recycling improves sustainability and economic efficiency by reducing the need for fresh methanol.

Purification Unit:

The partially washed biodiesel stream with residual KOH, soaps, glycerol, and methanol is introduced into a water-washing section where the stream is washed using two stages of hot water (60-70°C) to wash away water-soluble impurities such as residual catalyst and soap by-products. The washed biodiesel is moved to a drying unit where it is heated to 100-120°C. This is the final step for

removal of all the water, and the clean, dry biodiesel stream of 99% purity is produced and now ready for fuel use and storage. Cleaned biodiesel is then stored in the product storage tank.

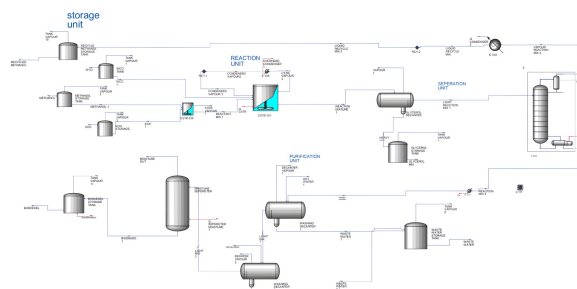


Figure 2: Simulation process flow diagram (PFD)

III. Results and Discussion

A. Description of the Process Simulation and Results In this simulation, the process was modeled for a production rate of 10 tonnes per day of biodiesel, or approximately 416 kg/hour. Methanol and potassium hydroxide (KOH) were first added to a continuous stirred-tank reactor (CSTR-1) to form a methoxide solution. This solution was then transferred to CSTR-2, where it was mixed with waste cooking oil (WCO) for transesterification. The reaction was carried out at 65 °C to achieve maximum conversion efficiency.

The simulation indicated a conversion of approximately 99% under these conditions [11, 17]. A condenser connected to CSTR-2 captured any vaporized methanol and returned it to the reactor to keep the methanol balance. The reaction mixture was sent into a glycerol decanter, which separated it into two clear phases. The heavy phase contained glycerol, KOH, and water. The light phase included biodiesel, methanol, and small amounts of impurities like KOH, water, and free fatty acids (FFAs). The light phase moved to a distillation column to recover methanol. The simulation indicated a recovery efficiency of 98%. The bottom residue from the distillation column had around 92% biodiesel, 6.8% methanol, 0.9% glycerol, 0.04% FFAs, and minimal catalyst. The stream temperature stayed at about 70 °C to prevent flash evaporation during later processing.

This pre-washed biodiesel stream was subjected to a twostage water-washing process using hot

water at 60–70 °C, which effectively removed residual impurities. The resulting biodiesel stream reached 99% purity, with only trace amounts of water and FFAs remaining. These were eliminated in a final moistureremoval step, where the biodiesel was heated to evaporate any residual water, making it suitable for storage and fuel use. The purified biodiesel was stored in a designated tank for blending, distribution, or direct use in compression ignition (CI) engines.

The mass balance from the simulation revealed that out of 416 kg/h of WCO feed, approximately 415 kg/h of biodiesel was produced. This corresponds to an overall conversion efficiency of approximately 99%, validating the effectiveness of the selected parameters and unit configurations.

Several properties affect the performance and compatibility of biodiesel in engine applications. These include density, API gravity, viscosity, flash point, acid number, cetane number, sulfur content, and ash content [16].

To evaluate the simulated biodiesel quality, its properties were compared with reported values for petroleum diesel (B0), neat biodiesel (B100), and blends (B6, B10, B20), as shown in Table IV. The simulation results closely aligned with literature values, demonstrating the model's reliability.

The simulated flash point was slightly lower than the standard value for B100, while the cetane number was also at the lower end of the expected range. A lower cetane number may be associated with higher thermal stability and a higher fire point, offering safer storage [16]. Since the simulation did not include any sulfur compounds, the sulfur content was noted as zero. While real sulfur levels depend on the feedstock, the lack of sulfur in the simulation shows a cleaner combustion profile. Ash content and acid number were also recorded as negligible, following standard simulation assumptions. Overall, the simulation validated that the biodiesel produced exhibits properties consistent with industry standards, confirming its practical applicability.

B. Process Parameter Study

1) *Influence of Temperature on Conversion:* Temperature plays an important role in the

transesterification process. It affects both the reaction rate and equilibrium. In this study, the temperature is varied from 50 °C to 80 °C under steady-state conditions to see how it impacted the conversion of triglycerides to fatty acid methyl esters (FAME).

As shown in Fig. 3, conversion stayed fairly stable between 50 °C and 65 °C.

The highest simulated conversion, about 98.5%, happened between 55 °C and 65 °C. This finding aligns with research suggesting that this range is optimal for biodiesel production [2,3,12].

Above 65 °C, conversion dropped due to methanol evaporation since methanol boils at around 64.7 °C. This vaporization lowered its concentration in the liquid phase, shifting the equilibrium negatively. It shows the need to operate below methanol's boiling point or use a reflux condenser, like the one in the simulation, to recover the vaporized methanol.

These results confirm the model and emphasize the need to keep an optimal temperature range to maximize biodiesel yield under base-catalyzed conditions.

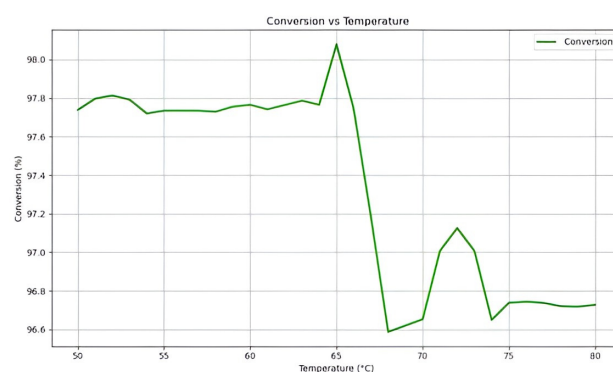


Figure 3: Conversion vs Temperature

2) *Influence of Catalyst Concentration on Conversion:* Catalyst concentration has a significant impact on transesterification efficiency. In this simulation, KOH was chosen as a homogeneous base catalyst because it reacts well with triglycerides and methanol [1,3]. The catalyst concentration ranged from 0% to 5% (w/w relative to WCO), while keeping other parameters constant: a 6:1 methanol-to-oil molar ratio and a temperature of 65 °C.

Table 4: COMPARISON OF PHYSICAL AND CHEMICAL PROPERTIES OF DIESEL (B0), BIODIESEL (B100), BLENDS (B6, B10, B20), AND SIMULATION OUTPUT

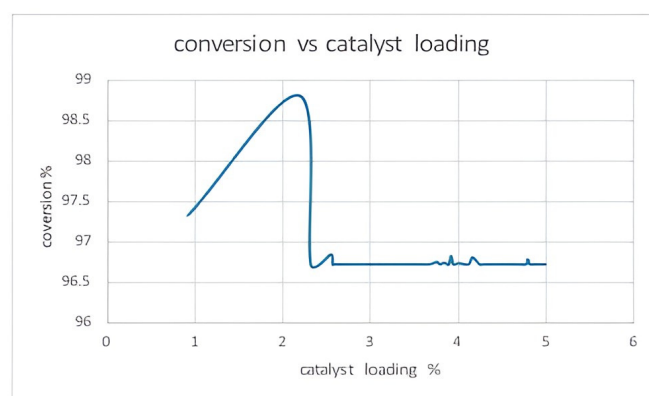
Property	B0	B6	B10	B20	B100	Simulation Result
Density at 15°C (kg/m ³)	834.0	834.0	835.0	840.0	890.3	907.01
Density API	38.16	38.16	37.96	36.96	27.49	24.48
Viscosity at 40°C (mm ² /s)	2.00	2.00	2.20	2.50	3.50	7.42
Flash point (°C)	51.0	55.2	60.5	67.0	132.0	108.34
Acid number (mg KOH/g)	0.0048	0.0048	0.0048	0.005	0.35	–
Cetane number	50.0	51.6	52.2	54.0	67.0	28.73
Sulfur content (mg/kg)	10.0	8.0	3.8	2.5	–	0
Ash content (%)	0.016	0.016	0.016	0.018	0.022	–

Table 5: MASS BALANCE WORKSHEET FROM THE SIMULATION

Stream Name	Temp (°C)	Press. (kPa)	Mass Flow (kg/h)	Molar Flow (kgmol/h)	Vap Frac	Heat Flow (kJ/h)	MeOH	KOH	FAME*	TGA*	FFA*	Glyc.	H2O
WCO	25	101.3	416.6	0.498	0	-81300	0	0	0	0.939	0.061	0	0
WOO	25	101.3	416.6	0.498	0	-81300	0	0	0	0.939	0.061	0	0
METHANOL	25	101.3	91.7	2.862	0	-692236	1	0	0	0	0	0	0
METHANOL-1	25	101.3	91.7	2.862	0	-692236	1	0	0	0	0	0	0
KOH	25	101.3	8	0.143	0	-102949	0	1	0	0	0	0	0
KOH-1	25	101.3	8	0.143	0	-102949	0	1	0	0	0	0	0
REACTANT MIX 1	25	101.3	99.7	3.005	0	-735186	0.953	0.048	0	0	0	0	0
REACTION MIX 1	65	101.4	516.3	3.526	0	-1603635	0.406	0.040	0.041	0.0001	0.0002	0.139	0.008
LIGHT RXN MIX 1	65	101.4	464.2	2.897	0	-1177547	0	0	0.493	0.494	0.0003	0.005	0.008
HEAVY MIX	65	101.4	52.2	0.629	0	-426087	0	0	0.004	0.227	0	0.758	0.012
HOT WATER 1	70	101.4	200	11.10	0	-313866	0	0	0	0	0	0	1
LIGHT MIX 1	71.1	101.4	416.9	1.440	0	-833995	0.002	0	0.995	0	0.0004	0	0.003
WASTE WATER 1	71.1	101.4	204.6	11.21	0	-3171741	0.009	0	0	0	0	0.001	0.990
LIGHT MIX 2	70.5	101.4	416.8	1.437	0	-833871	0	0	0.996	0	0.0004	0	0.003
WASTE WATER 2	70.5	101.4	200.1	11.10	0	-3138788	0.0002	0	0	0	0	0	1.000
BIODIESEL 1	120	101.3	416.8	1.437	0	-794581	0	0	0.996	0	0.0004	0	0.003
WASTE WATER	70	101.3	404.6	22.32	0.8	-6310528	0.005	0	0	0	0	0	0.995
REACTED MIX 3	49.3	101.3	421.4	1.552	0	-800334	0.068	0	0.922	0.092	0.0004	0	0
RESIDUE	70	101.3	421.4	1.552	0	-867072	0.068	0	0.922	0.092	0.0004	0	0

As shown in Fig. 4, conversion increased with catalyst loading up to 2%, reaching a maximum conversion of 98.49%. After this, conversion plateaued and slightly decreased, probably due to saponification, which is an unwanted side reaction caused by too much catalyst and leftover FFAs.

Although soap formation was not explicitly modeled in the simulation, this trend aligns with experimental literature [1]. Overall, the results affirm that 2% KOH is the optimal loading for high conversion while minimizing downstream processing issues.

**Figure 4:** Conversion vs Temperature

3) Influence of Methanol-to-Oil Molar Ratio on Conversion:

The methanol-to-oil molar ratio is an important factor that affects the reaction balance and conversion. Adding more methanol drives the

reaction to completion, leading to the production of FAME and glycerol.

In this simulation, we changed the ratio from 2:1 to 20:1 while keeping the temperature constant at 65 °C and using a 2% KOH catalyst. As Fig. 5 shows, conversion rose quickly from 2:1 to 6:1, with the largest increase happening between 2:1 and 4:1. After a 6:1 ratio, the conversion curve leveled off, showing little improvement.

This suggests that a 6:1 molar ratio is the best choice, which matches previous studies [2,3,12]. Though higher methanol ratios might slightly boost conversion, they also make separation and recovery more difficult, which raises process costs.

The close agreement between simulation and experimental trends confirms the model and supports the chosen operating conditions.

IV. Conclusion

This work presents a detailed simulation-based design for producing biodiesel from wastecooking oil (WCO) using Aspen HYSYS. The operation was simulated to generate 10 tonnes per day at ambient pressure (1 atm) and an optimal temperature of 65 °C. The transesterification reaction used methanol in a 6:1 molar ratio (methanol to oil) and potassium hydroxide (KOH) as a homogeneous catalyst at a 2 wt% concentration compared to WCO.

Simulation results showed a high conversion efficiency of about 99% and a biodiesel purity of around 99%. There was very little unreacted TGA, FFA, and methanol in the product stream. The downstream separation units that supported the reaction system included a decanter for glycerol separation, a distillation column for methanol recovery, and a two-stage water-washing unit to purify the

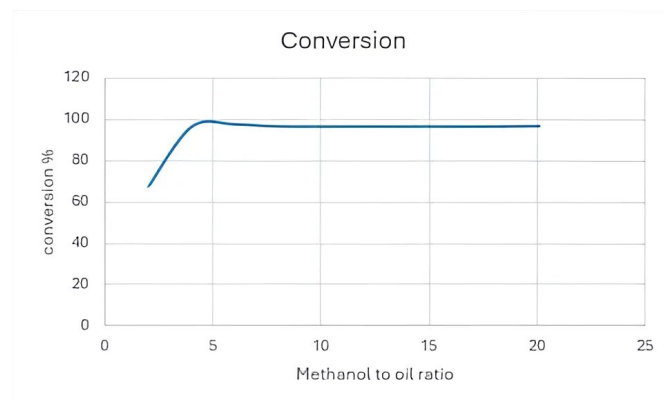


Figure 5: Conversion vs Temperature biodiesel.

A parametric sensitivity analysis revealed the following:

- Peak conversion occurs between 60-65 °C. Conversion decreases below or above this range due to methanol loss from vaporization.
- Increasing the catalyst loading above 2% does not provide significant benefits and can lead to saponification.
- Molar ratios greater than 6:1 offer only marginal improvements in conversion, indicating a point of saturation.

The simulation results confirm experimental findings published in the literature, demonstrating the model's validity and its assumptions. The outcomes support the technical feasibility of the developed process and highlight its potential for industrial-scale operation using low-cost, waste-derived feedstock.

Conflict of Interest:

The authors declare no conflicts of interest regarding this article.

Data Availability Statement

The data used in this study were obtained from publicly available sources and have been appropriately cited in the manuscript. Most of the additional data reported in this study were generated through simulation using Aspen HYSYS and Aspen Plus environments.

Future work

Future updates to this simulation model might include adding heat exchangers at key points for effective heat recovery. This change could greatly improve the system's overall energy efficiency. Additionally, we could make the simulation better

by including a closed-loop methanol recycling system, which would help reduce resource use.

Expanding the process to a dynamic simulation environment would allow for better management of changing conditions and provide real-time operational flexibility. Also, including detailed equipment sizing, piping layout, and control plans will make the model more relevant to real-world industrial applications, improving its use for pilot or commercial-scale projects.

Acknowledgment

I would like to sincerely thank my guide, Dr. Ritesh Malani, for his invaluable guidance and for providing me the opportunity to work under his mentorship throughout this project.

I am also grateful to Punyatoya Subudhi and Adarsh Verma for their constant support and encouragement.

Special thanks to the Department of Chemical Engineering, ICT-IOCB, for providing the facilities and opportunity to conduct this research.

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