

## Supporting Information

### **An integrated techno-economic-environmental-policy assessment of supercritical biodiesel production: Pathway to competitiveness**

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**Table S1.** Cost factors used for CAPEX estimation. *Source:* Peters, M. S.; Timmerhaus, K. D.; West, R. E. *Plant Design and Economics for Chemical Engineers*, 5th ed.; McGraw-Hill, 2003.

<b>Cost Component</b>	<b>Factor (fraction of bare equipment cost)</b>
Equipment erection	0.3
Piping	0.8
Instrumentation & control	0.3
Electrical	0.2
Civil works	0.2
Structures and buildings	0.2
Insulation (lagging) and painting	0.1
Offsites (OSBL)	0.3
Design and engineering	0.3
Contingency	0.1
Working capital (fraction of FCI)	0.1

**Table S2.** Financial parameters and raw material costs for base case TEA.

<b>Financial parameters</b>	<b>Value</b>	<b>Ref</b>
Discount rate/Interest rate (%)	10.7%	1, 2
Taxes (%)	30.0%	1
Indirect costs (% of direct costs)	30%	3
Design and engineering costs (% of direct and indirect costs)	30%	3
Contingency (% of direct and indirect costs)	10%	4, 5
Working/startup capital (% of fixed capital investment)	10%	4, 5
<b>Utility prices</b>		
Electricity price (\$/kWh)	0.07	6-8
Raw water price (\$/m <sup>3</sup> )	1.5	9
Natural gas price (\$/GJ)	5.5	9
<b>Raw materials and product prices</b>		
Methanol (\$/t)	339	9, 10
WCO (\$/t)	826	11, 12
Glycerol (\$/t)	1300	13

**Table S3.** ANOVA for the response surface quadratic model

Source	SoS*	Df*	Mean square	F-value	p-value	Significance
Model	3376.89	10	337.69	11.19	<0.0001	Significant
A (Temperature)	164.08	1	164.08	5.44	0.0331	
B (Pressure)	61.82	1	61.82	2.05	0.1717	
C (Time)	51.67	1	51.67	1.71	0.2092	
D (M:O ratio)	1060.32	1	1060.32	35.13	<0.0001	
AC	674.98	1	674.98	22.36	0.0002	
AD	19.50	1	19.50	0.6460	0.4333	
BD	143.11	1	143.11	4.74	0.0448	
CD	28.35	1	28.35	0.9391	0.3469	
A <sup>2</sup>	1138.18	1	1138.18	37.71	<0.0001	
D <sup>2</sup>	157.08	1	157.08	5.20	0.0366	
Residual	482.97	16	30.19			
Lack of fit	331.82	14	23.70	0.3136	0.9277	Not significant

\*SoS, sum of squares; Df, degrees of freedom.

The model's fit was further evaluated using the coefficient of determination ( $R^2$ ), predicted  $R^2$ , adjusted  $R^2$ , and adequate precision (Table S2).  $R^2$  showed that 87.5% of the variation in biodiesel yield was explained by the model. The predicted  $R^2$  closely matched the adjusted  $R^2$  (difference <0.2), indicating strong predictive ability for new data. Additionally, the adequate precision, which measures the signal-to-noise ratio, exceeded the threshold of 4, confirming a reliable signal across the tests. Moreover, the coefficient of variation (CV) of 6.90% indicates minimal relative dispersion around the mean, demonstrating high precision in the predicted biodiesel yields. These metrics emphasize the model's reliability, precision, and consistency in predicting biodiesel yield.

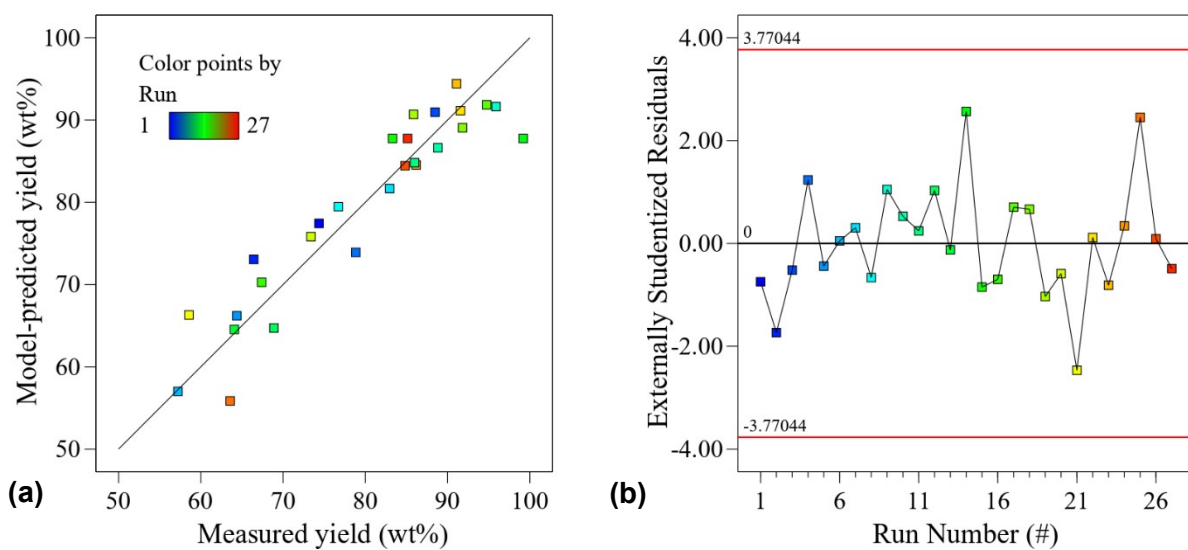
**Table S4.** Summary of model fit statistics

Metric	Value
Std. dev.	5.49
Mean	79.62
CV %	6.90
$R^2$	0.8749
Adjusted $R^2$	0.7967
Predicted $R^2$	0.6141
Adequate precision	10.9989

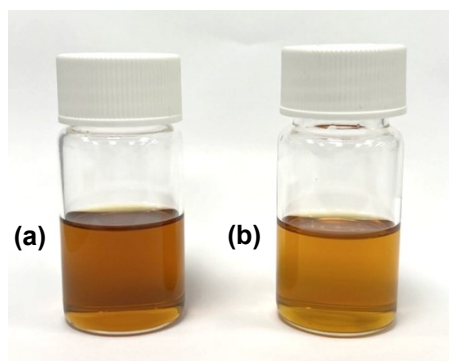
**Table S5.** Validation table with 95% confidence interval

Predicted mean	Predicted median	Std dev	n*	SE Pred	95% PI low	Data mean	95% PI high
95.9241	95.9241	5.49415	4	4.00401	87.436	92.2775	104.412

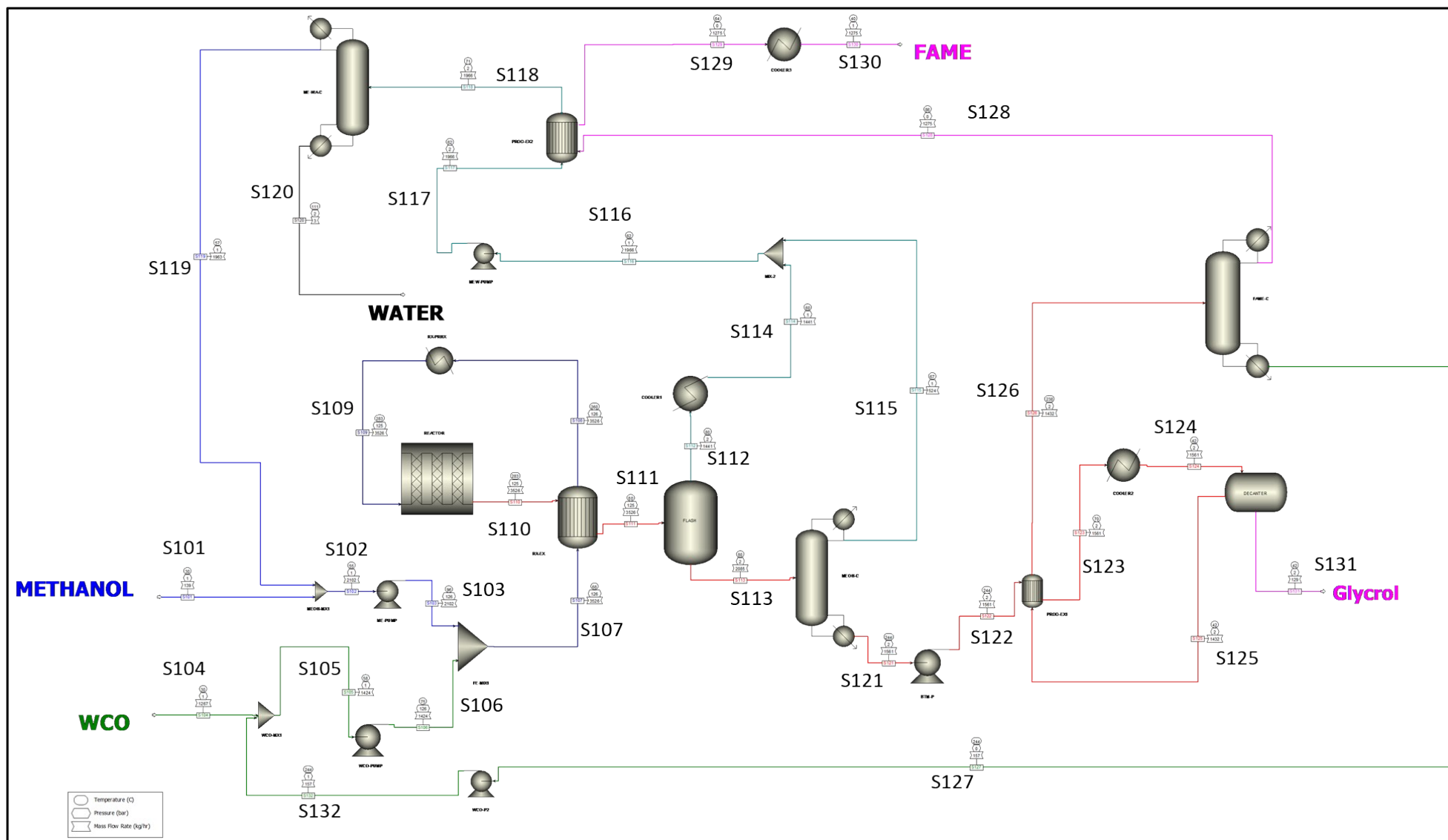
\*n, number of experiments.



**Fig. S1.** Comparison of model-predicted versus experimentally observed biodiesel yield (a) and plot of residuals versus experimental run (b).



**Fig. S2.** Samples of (a) untreated WCO and (b) supercritical biodiesel after centrifugation.



**Fig. S3.** Process flow diagram of biodiesel production via the SCM process including stream numbers.

**Table S6.** Material and energy balances for various process streams

	Units	S101	S102	S103	S104	S105	S106	S107	S108	S109	S110	S111	S112	S113	S114	S115	S116
Description		Fresh Methanol from BL	Methanol to Pump	Methanol to Mix	Fresh WCO from BL	WCO to Pump	WCO to Mix	Combined feed to Feed/Effluent RX Exchanger	Combined feed to pre-heater	Combined feed to Reactor	Raw product from Reactor	Raw product to flash drum	Flashed vapor	Raw product to MEOH Column	Recovered MEOH from Flash	Recovered MEOH from MEOH Column	Recovered MEOH from Mix
From		From BL	MEOH-MX1	ME-PUMP	From BL	WCO-MX1	WCO-PUMP	FE-MIX1	RX-EX	RX-PRHX	REACTOR	RX-EX	FLASH	FLASH	COOLER1	MEOH-C	MIX-2
To		MEOH-MX1	ME-PUMP	FE-MIX1	WCO-MX1	WCO-PUMP	FE-MIX1	RX-EX	RX-PRHX	REACTOR	RX-EX	FLASH	COOLER1	MEOH-C	MIX-2	MIX-2	MEW-PUMP
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	30.0	55.0	96.6	30.0	57.7	74.8	67.6	260.5	282.8	282.8	80.0	80.0	80.0	60.0	66.7	61.8
Pressure	bar	1.01325	1.01325	126	1.01325	1.01325	126	126	126	125	125	125	1.5	1.5	1.1	1.1	1.1
Mass Liquid Fraction		1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0
Molar Enthalpy	ca/mol	-56831.4	-56238.1	-55775.9	-471840.8	-441663.6	-431337.1	-65841.6	-55868.3	-55353.4	-55763.2	-65735.1	-47412.7	-86507.0	-56136.3	-55968.8	-56091.8
Mass Enthalpy	cal/gm	-1773.6	-1755.1	-1740.7	-573.1	-560.3	-547.2	-1258.6	-1068.0	-1058.3	-1066.1	-1256.7	-1480.9	-927.4	-1753.4	-1748.9	-1752.2
Molar Density	mol/cc	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Density	gm/cc	0.8	0.8	0.7	0.8	0.8	0.8	0.5	0.3	0.3	0.3	0.7	0.0	0.7	0.8	0.7	0.7
Enthalpy Flow	cal/sec	-68485.6	-1024907.7	-1016484.8	-201761.0	-221670.9	-216488.0	-1232972.7	-1046209.8	-1036709.9	-1044385.0	-1231147.9	-593908.0	-536566.1	-703181.8	-253625.7	-956807.6
Average MW		32.0	32.0	32.0	823.3	788.3	788.3	52.3	52.3	52.3	52.3	52.3	32.0	93.3	32.0	32.0	32.0
Mole Flows	kmol/hr	4.3	65.6	65.6	1.5	1.8	1.8	67.4	67.4	67.4	67.4	67.4	45.1	22.3	45.1	16.3	61.4
Mass Flows	kg/hr	139.0	2102.2	2102.2	1267.3	1424.4	1424.4	3526.6	3526.6	3526.7	3526.7	3526.7	1443.8	2082.9	1443.8	522.1	1965.8
TRIPA-01	kg/hr	0.0	0.0	0.0	108.7	119.1	119.1	119.1	119.1	119.1	10.4	10.4	0.0	10.4	0.0	0.0	0.0
TRIOI-01	kg/hr	0.0	0.0	0.0	1118.6	1225.8	1225.8	1225.8	1225.8	1225.6	107.1	107.1	0.0	107.1	0.0	0.0	0.0
OLEIC-01	kg/hr	0.0	0.0	0.0	39.9	40.0	40.0	40.0	40.0	40.0	1.1	1.1	0.0	1.1	0.0	0.0	0.0
METHA-01	kg/hr	139.0	2102.2	2102.2	0.0	0.0	0.0	2102.2	2102.2	2102.5	1963.7	1963.7	1442.0	521.7	1442.0	521.7	1963.2
WATER	kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	2.5	1.6	0.9	1.6	0.9	2.5
GLYCE-01	kg/hr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	128.7	128.7	0.1	128.6	0.1	0.0	0.1
METHY-01	kg/hr	0.0	0.0	0.0	0.0	0.8	0.8	0.8	0.8	0.8	110.0	110.0	0.0	110.0	0.0	0.0	0.0
METHY-02	kg/hr	0.0	0.0	0.0	0.0	38.6	38.6	38.6	38.6	38.6	1203.2	1203.2	0.0	1203.1	0.0	0.0	0.0
Mass Fractions																	
TRIPA-01		0.0	0.0	0.0	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TRIOI-01		0.0	0.0	0.0	0.9	0.9	0.9	0.3	0.3	0.3	0.0	0.0	0.0	0.1	0.0	0.0	0.0
OLEIC-01		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METHA-01		1.0	1.0	1.0	0.0	0.0	0.0	0.6	0.6	0.6	0.6	0.6	1.0	0.3	1.0	1.0	1.0
WATER		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLYCE-01		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0
METHY-01		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0
METHY-02		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.3	0.0	0.6	0.0	0.0	0.0
Volume Flow	l/min	2.9	46.3	50.4	25.6	31.1	31.5	120.4	190.6	223.8	171.4	81.3	14712.0	46.6	32.1	11.7	43.8

**Table S6.** Material and energy balances for various process streams (Cont.)

	S117	S118	S119	S120	S121	S122	S123	S124	S125	S126	S127	S128	S129	S130	S131	S132
Description	Recovered MEOH from MEW-PUMP	Recovered MEOH from PROD-EX2	Recycled MEOH from ME-WA-C	Waste Water from ME-WA-C	Raw product to BTM-P	Raw product to BPROD-EX1	Raw product to BPROD-COOLER2	Raw product to DECANTER	Raw FAME to PROD-EX1	Raw FAME to FAME-C	Recycle WCO to WCO-P2	Purified FAME from FAME-C	Purified FAME to COOLER3	Purified FAME to BL	Glycerol	Recycle WCO
From	MEW-PUMP	PROD-EX2	ME-WA-C	ME-WA-C	MEOH-C	BTM-P	PROD-EX1	COOLER2	DECANTER	PROD-EX1	FAME-C	FAME-C	PROD-EX2	COOLER3	DECANTER	WCO-P2
To	PROD-EX2	ME-WA-C	MEOH-MX1		BTM-P	PROD-EX1	COOLER2	DECANTER	PROD-EX1	FAME-C	WCO-P2	PROD-EX2	COOLER3	BL	BL	WCO-MX1
Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	61.9	70.8	56.6	88.4	244.2	244.2	70.0	42.0	42.0	238.2	244.1	85.9	64.0	40.0	42	244.3694391
Pressure	2	2	1.1	1.5	1.8	1.5	1.5	1.5	1.5	1.5	0.028	0.013332237	0.013332237	1.1	1.5	1.01325
Mass Liquid Fraction	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Molar Enthalpy	-56088.7	-55850.5	-56196.1	-67995.5	-146183.3	-146184.2	-172484.6	-176246.1	-182508.3	-148232.7	-268071.7	-166690.6	-170053.1	-173651.0	-158092.4	-267981.0
Mass Enthalpy	-1752.1	-1744.6	-1753.8	-3576.1	-563.4	-563.4	-664.8	-679.3	-588.0	-477.6	-456.5	-568.2	-579.6	-591.9	-1722.1	-456.4
Molar Density	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass Density	0.7	0.7	0.8	0.9	0.6	0.6	0.8	0.8	0.8	0.6	0.5	0.8	0.8	0.9	1.3	0.5
Enthalpy Flow	-956754.5	-952692.9	-956422.1	-2619.0	-244275.3	-244276.7	-288225.3	-294510.8	-234014.3	-190065.7	-19916.6	-201348.3	-205409.9	-209755.9	-61553.3	-19909.9
Average MW	32.0	32.0	32.0	19.0	259.5	259.5	259.5	259.5	310.4	310.4	587.2	293.4	293.4	293.4	91.8	587.2
Mole Flows	61.4	61.4	61.3	0.1	6.0	6.0	6.0	6.0	4.6	4.6	0.3	4.3	4.3	4.3	1.4	0.3
Mass Flows	1965.8	1965.8	1963.2	2.6	1560.9	1560.9	1560.9	1560.9	1432.8	1432.8	157.1	1275.7	1275.7	1275.7	128.7	157.1
TRIPA-01	0.0	0.0	0.0	0.0	10.4	10.4	10.4	10.4	10.4	10.4	10.4	0.0	0.0	0.0	0.0	10.4
TRIOI-01	0.0	0.0	0.0	0.0	107.1	107.1	107.1	107.1	107.1	107.1	107.1	0.0	0.0	0.0	0.0	107.1
OLEIC-01	0.0	0.0	0.0	0.0	1.1	1.1	1.1	1.1	1.1	1.1	0.1	1.0	1.0	1.0	0.0	0.1
METHA-01	1963.2	1963.2	1963.2	0.0	0.5	0.5	0.5	0.5	0.3	0.3	0.0	0.3	0.3	0.3	0.2	0.0
WATER	2.5	2.5	0.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLYCE-01	0.1	0.1	0.0	0.1	128.6	128.6	128.6	128.6	0.2	0.2	0.0	0.2	0.2	0.2	128.4	0.0
METHY-01	0.0	0.0	0.0	0.0	110.0	110.0	110.0	110.0	110.1	110.1	0.8	109.3	109.3	109.3	0.0	0.8
METHY-02	0.0	0.0	0.0	0.0	1203.1	1203.1	1203.1	1203.1	1203.6	1203.6	38.6	1165.0	1165.0	1165.0	0.0	38.6
Mass Fractions																
TRIPA-01	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.1
TRIOI-01	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.7	0.0	0.0	0.0	0.0	0.7
OLEIC-01	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
METHA-01	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER	0.0	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GLYCE-01	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
METHY-01	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.0	0.1	0.1	0.1	0.0	0.0
METHY-02	0.0	0.0	0.0	0.0	0.8	0.8	0.8	0.8	0.8	0.8	0.2	0.9	0.9	0.9	0.0	0.2
Volume Flow	43.8	44.5	43.4	0.0	40.8	40.8	34.3	33.6	30.8	37.1	5.1	25.7	25.2	24.8	1.7	5.1

- (1) Kumar, D.; Long, S. P.; Arora, A.; Singh, V. Techno-economic feasibility analysis of engineered energycane-based biorefinery co-producing biodiesel and ethanol. *GCB Bioenergy* **2021**, *13* (9), 1498–1514.
- (2) Sukor, N. R.; Shamsuddin, A. H.; Mahlia, T. M. I.; Mat Isa, M. F. Techno-economic analysis of CO<sub>2</sub> capture technologies in offshore natural gas field: Implications to carbon capture and storage in Malaysia. *Processes* **2020**, *8* (3), 350.
- (3) Apostolakou, A.; Kookos, I.; Marazioti, C.; Angelopoulos, K. Techno-economic analysis of a biodiesel production process from vegetable oils. *Fuel Processing Technology* **2009**, *90* (7-8), 1023–1031.
- (4) Turton, R.; Bailie, R. C.; Whiting, W. B.; Shaeiwitz, J. A. *Analysis, synthesis and design of chemical processes*; Pearson education, 2008.
- (5) Al-Sakkari, E. G.; Mohammed, M. G.; Elozeiri, A. A.; Abdeldayem, O. M.; Habashy, M. M.; Ong, E. S.; Rene, E. R.; Ismail, I.; Ashour, I. Comparative technoeconomic analysis of using waste and virgin cooking oils for biodiesel production. *Frontiers in Energy Research* **2020**, *8*, 583357.
- (6) Haas, M. J.; McAloon, A. J.; Yee, W. C.; Foglia, T. A. A process model to estimate biodiesel production costs. *Bioresource technology* **2006**, *97* (4), 671–678.
- (7) Khan, M.; Nabil, S. K.; Al-Attas, T.; Yasri, N. G.; Roy, S.; Rahman, M.; Larter, S.; Ajayan, P. M.; Hu, J.; Kibria, M. G. Zero-crossover electrochemical CO<sub>2</sub> reduction to ethylene with co-production of valuable chemicals. *Chem Catalysis* **2022**, *2* (8), 2077–2095.
- (8) [https://www.eia.gov/electricity/monthly/epm\\_table\\_grapher.php?t=table\\_5\\_03](https://www.eia.gov/electricity/monthly/epm_table_grapher.php?t=table_5_03).
- (9) Nagapurkar, P.; Smith, J. D. Techno-economic and life cycle analyses for a supercritical biodiesel production process from waste cooking oil for a plant located in the Midwest United States: P. Nagapurkar et al. *Environment, Development and Sustainability* **2025**, *27* (9), 22749–22773.
- (10) <https://methanol.org/methanol-price-supply-demand/>.
- (11) <https://www.rti-inc.com/blog/how-much-is-used-cooking-oil-worth/>.
- (12) <https://www.commodity3.com/instrument/TLW1MNF1/yellow-grease>.
- (13) Pandit, K.; Jeffrey, C.; Keogh, J.; Tiwari, M. S.; Artioli, N.; Manyar, H. G. Techno-economic assessment and sensitivity analysis of glycerol valorization to biofuel additives via esterification. *Industrial & Engineering Chemistry Research* **2023**, *62* (23), 9201–9210.