

SUPPLEMENTARY MATERIAL

Table Captions

Table S1. Input and output data for process of biodiesel production.

Table S2. Input and output data for alcohol recycle unit.

Table S3. Input and output data for etherification reaction using ethanol and isopropanol at 110°C and molar ratio of 1:6 (glycerol/alcohol).

Table S4. Input and output data from DWSIM for etherification reaction using ethanol and isopropanol at 110°C and molar ratio of 1:12 (glycerol/alcohol).

Table S5. Input and output data for ether purification process (etherification using glycerol/ethanol molar ratio of 1:3 at 110°C).

Table S6. Input and output data for ether purification process (etherification using glycerol/isopropanol molar ratio of 1:3 at 110°C).

Table S1

Conditions	Input	Output	
	STR-01	Biodiesel	Crude glycerol
Temperature (°C)	28.7	60.0	60.0
Pressure (bar)	1.01	1.01	1.01
Mass Flow (kg/h)	1227.12	1004.31	222.81
Volumetric Flow (m³/h)	1.347	1.178	0.260
Specific Enthalpy (kJ/kg)	-203.64	-232.52	-936.48
Component mole fraction			
Triolein	0.138	0.000	0.017
Methanol	0.830	0.436	0.728
Sodium Hydroxide	0.030	0.030	0.051
Biodiesel	0.000	0.394	0.000
Crude glycerol	0.000	0.131	0.219

STR-01: Mixture of vegetable oil, methanol and sodium hydroxide.

Table S2

Alcohol recovery / Ethanol			
Conditions	Input	Output	
	Polar comp.	STR-67	Alcohol
Temperature (°C)	79.9	-10.0	-10.0
Pressure (bar)	1.01	1.01	1.01
Mass Flow (kg/h)	117.89	51.00	66.89
Volumetric Flow (m³/h)	0.137	0.050	0.082
Spec. Enthalpy (kJ/kg)	-1162.72	-1931.98	-1012.28
Component mole fraction			
Ethanol	0.434	0.000	1.000
Glycerol	0.068	0.121	0.000
Water	0.496	0.878	0.000
Alcohol recovery / Isopropanol			
Conditions	Input	Output	
	Polar comp.	STR-67	Alcohol
Temperature (°C)	85.8	-10.0	-10.0
Pressure (bar)	1.01	1.01	1.01
Mass Flow (kg/h)	203.86	52.78	151.07
Volumetric Flow (m³/h)	26.267	0.043	0.186
Spec. Enthalpy (kJ/kg)	-527.98	-1523.60	-844.97
Component mole fraction			
Isopropanol	0.704	0.000	1.000
Glycerol	0.127	0.433	0.000
Water	0.167	0.566	0.000

STR-67: Mixture of water and glycerol.

Table S3

Etherification with ethanol (1:6 molar ratio)				
Conditions	Input		Output	
	Glycerol	Ethanol	STR-12	STR-13
Temperature (°C)	229.2	25.0	110.0	110.0
Pressure (bar)	1.01	1.01	1.01	1.01
Mass Flow (kg/h)	95.51	286.66	219.59	162.57
Volumetric Flow (m ³ /h)	0.087	0.364	166.250	0.188
Spec. Enthalpy (kJ/kg)	-475.76	-922.64	134.65	-587.50
Component mole fraction				
Ethanol	0.000	1.000	0.829	0.259
Glycerol	1.000	0.000	0.000	0.112
3-ethoxypropan-1,2-diol	0.000	0.000	0.000	0.154
1,3-diethoxypropan-2-ol	0.000	0.000	0.002	0.255
1,2,3-triethoxypropane	0.000	0.000	0.000	0.000
Water	0.000	0.000	0.169	0.220
Etherification with isopropanol (1:6 molar ratio)				
Conditions	Input		Output	
	Glycerol	Isopropanol	STR-12	STR-13
Temperature (°C)	229.2	25.0	110.0	110.0
Pressure (bar)	1.01	1.01	1.01	1.01
Mass Flow (kg/h)	95.51	373.94	313.26	156.19
Volumetric Flow (m ³ /h)	0.087	0.478	176.982	0.174
Spec. Enthalpy (kJ/kg)	-475.76	-754.44	140.72	-615.86
Component mole fraction				
Isopropanol	0.000	1.000	0.894	0.309
Glycerol	1.000	0.000	0.000	0.224
3-isopropoxypropan-1,2-diol	0.000	0.000	0.000	0.402
1,3-di-isopropoxypropan-2-ol	0.000	0.000	0.000	0.010
Water	0.000	0.000	0.106	0.055

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).

Table S4

Etherification with ethanol (1:12 molar ratio)				
Conditions	Input		Output	
	Glycerol	Ethanol	STR-12	STR-13
Temperature (°C)	229.2	25.0	110.0	110.0
Pressure (bar)	1.01	1.01	1.01	1.01
Mass Flow (kg/h)	95.51	573.32	495.01	173.82
Volumetric Flow (m ³ /h)	0.087	0.729	365.001	0.196
Spec. Enthalpy (kJ/kg)	-475.76	-922.64	134.14	-465.04
Component mole fraction				
Ethanol	0.000	1.000	0.860	0.281
Glycerol	1.000	0.000	0.000	0.092
3-ethoxypropan-1,2-diol	0.000	0.000	0.000	0.089
1,3-diethoxypropan-2-ol	0.000	0.000	0.001	0.167
1,2,3-triethoxypropane	0.000	0.000	0.002	0.185
Water	0.000	0.000	0.136	0.186
Etherification with isopropanol (1:12 molar ratio)				
Conditions	Input		Output	
	Glycerol	Isopropanol	STR-12	STR-13
Temperature (°C)	229.2	25.0	110.0	110.0
Pressure (bar)	1.01	1.01	1.01	1.01
Mass Flow (kg/h)	95.51	745.35	676.14	164.72
Volumetric Flow (m ³ /h)	0.087	0.953	371.136	0.188
Spec. Enthalpy (kJ/kg)	-475.76	-754.44	140.46	-588.77
Component mole fraction				
Isopropanol	0.000	1.000	0.933	0.335
Glycerol	1.000	0.000	0.000	0.128
3-isopropoxypropan-1,2-diol	0.000	0.000	0.000	0.494
1,3-di-isopropoxypropan-2-ol	0.000	0.000	0.000	0.011
Water	0.000	0.000	0.067	0.032

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).

Table S5

Ether purification for simulation using ethanol (1:3 molar ratio)						
Conditions	Input			Output		
	STR-12	STR-13	Solvent	Ethers	Solvent	Polar Comp.
Temperature (°C)	110.0	110.0	25.0	213.9	69.8	79.8
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01
Mass Flow (kg/h)	59.62	179.21	238.83	116.12	243.66	117.88
Molar Flow (kmol/h)	1.65	2.50	2.77	0.78	2.80	3.34
Vol. Flow (m³/h)	51.91	0.20	0.36	0.14	53.65	0.14
Spec. Enthalpy (kJ/kmol)	137.42	-614.17	-366.01	-92.81	-30.33	- 1173.78
Component mole fraction						
Ethanol	0.636	0.160	0.000	0.000	0.000	0.434
Glycerol	0.000	0.092	0.000	0.000	0.000	0.068
3-ethoxypropan-1,2-diol	0.000	0.095	0.000	0.304	0.000	0.000
1,3-dietoxipropan-2-ol	0.001	0.115	0.000	0.361	0.001	0.000
1,2,3-triethoxypropane	0.001	0.112	0.000	0.324	0.010	0.000
Water	0.361	0.425	0.000	0.000	0.000	0.496
N-hexane	0.000	0.000	1.000	0.010	0.988	0.000

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).

Table S6

Ether purification for simulation using isopropanol (1:3 molar ratio)						
Conditions	Input			Output		
	STR-12	STR-13	Hexane	Ethers	Hexane	Polar Comp.
Temperature (°C)	110.00	110.00	25.00	224.30	69.09	81.93
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01
Mass Flow (kg/h)	675.91	164.72	840.63	97.85	854.59	728.83
Molar Flow (kmol/h)	11.80	1.63	9.75	0.73	9.85	12.61
Vol. Flow (m3/h)	371.02	0.19	1.28	0.12	1.38	0.98
Spec. Enthalpy (kJ/kmol)	140.44	-587.04	- 366.01	-277.79	-261.67	-615.80
Component mole fraction						
Isopropanol	0.932	0.335	0.000	0.000	0.000	0.916
Glycerol	0.000	0.127	0.000	0.000	0.000	0.016
3-ethoxypropan-1,2-diol	0.000	0.494	0.000	0.975	0.010	0.000
1,3-dietoxipropan-2-ol	0.000	0.011	0.000	0.014	0.001	0.000
Water	0.067	0.031	0.000	0.000	0.000	0.067
N-hexane	0.000	0.000	1.000	0.010	0.989	0.000

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).