Environmental sustainability evaluation of glycerol and propylene-based pathways to acrylic acid via different intermediates

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1. Reaction kinetics for the catalysts used in simulations

1.1. Glycerol to acrylic acid via allyl alcohol process

The kinetic constant was calculated as following:

$$k = k_0 e^{-\frac{E}{RT}}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant (8.314 J/K-mol) and T is the temperature. The reaction rate is calculated in kmol/ kg.sec, the rate is based on catalyst weight and all reactions occur in vapour phase.

1.1.1. Kinetics for allyl alcohol to acrylic acid

Table S1. Kinetics for allyl alcohol to acrylic acid[1].

Sr. no.	Reaction	k_0	E (kJ/mol)	Reaction order	Kinetics rate type
1	$C_3H_6O + O_2 \rightarrow C_3H_4O_2 + H_2O$	0.1663	20.04	$C_3H_6O = 1$	Power law
2	$2C_3H_6O + O_2 \rightarrow C_3H_4O + 2H_2O$	0.2886	32.25	$C_3H_6O = 1$	
3	$C_3H_6O + O_2 \rightarrow C_2H_4O_2$	1.5513	40.52	$C_3H_6O = 1$	
4	$C_3H_6O + 4O_2 \rightarrow 3CO_2 + 3H_2O$	0.03349	27.47	$C_3H_6O = 1$	
5	$C_3H_6O + 2.5O_2 \rightarrow 3CO_2 + 3H_2O$	0.0917	33.84	$C_3H_6O = 1$	

1.2. Glycerol to acrylic acid via lactic acid process

1.2.1. Kinetics for glycerol to dihydroxyacetone

The kinetic constant was calculated as following:

$$k = k_0 e^{-\frac{E}{RT}}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant (8.314 J/K-mol) and T is the temperature. The reaction rate is calculated in kmol/ m^3.sec, the rate is based on reactor volume and all reactions occur in liquid phase.

Table S2. Kinetics for glycerol to dihydroxyacetone[2].

Sr. no.	Reaction	k_0	E (kJ/mol)	Reaction equation	Kinetics rate type
1	$Glycerol + \frac{1}{2}O_2 \rightarrow DH$	157.675	35	$\frac{k[Glycerol]}{(K1[Glycerol] + K2[DHA] + K3[Glyceraldehyde] + K4)^2}$ where $k = k_0 e^{-\frac{E_i}{RT}}$, $K1 = 2.6 \times 10^{-4} e^{-\frac{2092.85}{T}}$, $K2 = 6.8 \times 10^{-3}$, $K3 = 3.9 \times 10^{-3}$, $K4 = 1$	LHHW
2	$Glycerol + \frac{1}{2}O_2 \rightarrow Gl$	26.36	35.3		

1.2.2. Kinetics for dihydroxyacetone to methyl lactate

The kinetic constant was calculated as following:

$$k = k_0 e^{-\frac{E}{RT}}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant (8.314 J/K-mol) and T is the temperature. The reaction rate is calculated in kmol/kg.sec, the rate is based on catalyst weight and all reactions occur in liquid phase.

Table S3. Kinetics for dihydroxyacetone to methyl lactate[3].

Sr. no.	Reaction	k_0	E (kJ/mol)	Reaction equation	Kinetics rate type
1	$DHA \rightarrow Pyruvaldehyde + H_2O$	3.604×10^7	53	$DHA = 1$	Power law
2	$Pyruvaldehyde + CH_3OH \rightarrow Me$	4.851×10^8	61	$Pyruvaldehyd = 1,$ $CH_3OH = 1$	
3	$Pyruvaldehyde + H_2O \rightarrow Glyce$	1.857×10^{11}	89	$Pyruvaldehyde = 1$	

1.2.3. Kinetics for reactive distillation of methyl lactate to lactic acid

The kinetic constant was calculated as following:

$$k = k_0 e^{-\frac{E}{RT}}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant (8.314 J/K-mol) and T is the temperature. The reaction rate is calculated in kmol/ kg.sec, the rate is based on catalyst weight and all reactions occur in liquid phase.

Table S4. Kinetics for reactive distillation of methyl lactate to lactic acid[4].

Sr. no.	Reaction	k_0	E_i (kJ/mol)	Reaction equation	Kinetics rate type
1	$Methyllactate + H_2O$	600.52	45.84	$k[Methyllactate][H_2O]$ where $k = (k_0 + w.k_w)\, e^{-\frac{E_i}{RT}}$, $w = 78.65$, $k_w = 44.34$	Power law
2	$Lacticacid + CH_3OH$	600.52	45.84	$\frac{k[Lacticacid][CH_3OH]}{K_e}$ where $k = (k_0 + w.k_w)\, e^{-\frac{E_i}{RT}}$, $w = 78.65, k_w = 44.34, K_e = 12.86\, e^{-\frac{1291.4}{T}}$	

1.2.4. Kinetics for lactic acid to acrylic acid

The kinetic constant was calculated as following:

$$k = k_0 e^{-\frac{E}{RT}}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant (8.314 J/K-mol) and T is the temperature. The reaction rate is calculated in kmol/ kg.sec, the rate is based on catalyst weight and all reactions occur in vapour phase.

Table S5. Kinetics for lactic acid to acrylic acid[5].

Sr. no.	Reaction	k_0	E (kJ/mol)	Reaction equation	Kinetics rate type
1	$Lactic\ acid \rightarrow Acrylic$	5.24×10	152.7	$Lactic\ acid = 0.19, H_2O = 0.36$	Power law
2	$Lactic\ acid \rightarrow Acetald$	9.30×10	165.3	$Lactic\ acid = 0.52, H_2O = 0.86$	

1.3. Glycerol to acrylic acid via acrolein process

The kinetic constant was calculated as following:

$$k = k_0 e^{-\frac{E}{RT}}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant (8.314 J/K-mol) and T is the temperature. The reaction rate is calculated in kmol/ kg.sec, the rate is based on catalyst weight and all reactions occur in vapour phase.

1.3.1. Kinetics for glycerol to acrolein

Table S6. Kinetics for glycerol to acrolein[6].

Sr. no.	Reaction	k_0	E (kJ/mol)	Reaction order	Kinetics rate type
1	$C_3H_8O_3 \rightarrow C_3H_4O + 2H_2O$	20.7	46	$C_3H_8O_3 = 1$	Power law
2	$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O$	12.1	53.3	$C_3H_8O_3 = 1$	
3	$C_3H_8O_3 \rightarrow C_2H_4O + CO + H_2O + H_2$	6.3×10^{-5}	5	$C_3H_8O_3 = 1$	
4	$C_3H_4O + H_2O \rightarrow C_3H_6O_2$	1.8×10^{-4}	6.1	$C_3H_4O = 1$, $H_2O = 0$	
5	$C_3H_6O_2 \rightarrow C_3H_6O + \frac{1}{2}O_2$	2.6	46.6	$C_3H_6O_2 = 1$	

1.3.2. Kinetics for acrolein to acrylic acid

Table S7. Kinetics for acrolein to acrylic acid[7].

Sr. no.	Reaction	k_0	E (kJ/mol)	Reaction order	Kinetics rate type
1	$Acrolein + \frac{1}{2}O_2 \rightarrow Acrylicaci$	8×10^{12}	108	$Acrolein$ =1, O_{2}= 1	Power law
2	$Acrolein + \frac{7}{2}O_2 \rightarrow 3CO_2 + 2H$	5×10^{15}	153	$Acrolein$=1, O_{2}= 1	
3	$Acrolein + 2O_2 \rightarrow 3CO + 2H_2$	8.95×10^{15}	158	$Acrolein$=1, O_{2}= 1	

1.4. Propylene to acrylic acid via acrolein process

The kinetic constant was calculated as following:

$$k = k_0 e^{-\frac{E}{RT}}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant (8.314 J/K-mol) and T is the temperature. The reaction rate is calculated in kmol/ kg.sec, the rate is based on catalyst weight and all reactions occur in vapour phase.

1.4.1. Kinetics for propylene to acrolein

Table S8. Kinetics for propylene to acrolein[8].

Sr. no.	Reaction	k_0	E (kJ/mol)	Reaction order	Kinetics rate type
1	$C_3H_6 + O_2 \rightarrow C_3H_4O + H_2O$	0.0628	39.6	C_3H_6= 1, $O_2 = 0$	Power law
2	$C_3H_4O + \frac{1}{2}O_2 \rightarrow C_3H_4O_2$	2.32	72.5	C_3H_4O = 0.86, O_2 = 0.3	
3	$C_3H_4O_2 + 3O_2 \rightarrow 3CO_2 + 2H_2O$	1.19×10^{-4}	82.9	$C_3H_4O_2$ = 0, O_2 = 1	
4	$2C_3H_6 + 9O_2 \rightarrow 6CO_2 + 6H_2O$	8.484×10^{-7}	38.1	C_3H_6 = 1, O_2 = 0	
5	$C_3H_6 + O_2 \rightarrow C_2H_4O + CH_2O$	0.015	52.4	C_3H_6 = 0, O_2 = 1	
6	$2C_2H_4O + O_2 \rightarrow 2C_2H_4O_2$	1.47	86.7	C_2H_4O = 0, O_2 = 0.73	
7	$C_3H_6 + 3O_2 \rightarrow 3CO + 3H_2O$	9.058×10^{-5}	60.9	C_3H_6 = 0, O_2 = 1	
8	$2C_3H_4O + 3O_2 \rightarrow 4CH_2O + 2CO_2$	2.03	78.8	C_3H_4O = 0.58, O_2 = 0.8	

9	$C_2H_4O_2 + 2O_2 \rightarrow 2CO_2 + 2H_2O$	4.75×10^9	178.7	$C_2H_4O_2 = 1,$ $O_2 = 0$	
10	$C_2H_4O + \frac{5}{2}O_2 \rightarrow 2CO_2 + 2H_2O$	3.8×10^{-4}	14.9	$C_2H_4O = 1,$ $O_2 = 0$	

1.4.2. Kinetics for acrolein to acrylic acid

Table S9. Kinetics for acrolein to acrylic acid[7].

Sr. no.	**Reaction**	k_0	E **(kJ/mol)**	**Reaction order**	**Kinetics rate type**
1	$Acrolein + \frac{1}{2}O_2 \rightarrow Acrylicaci$	8×10^{12}	108	$Acrolein = 1,$ $O_2 = 1$	Power law
2	$Acrolein + \frac{7}{2}O_2 \rightarrow 3CO_2 + 2H$	5×10^{15}	153	$Acrolein = 1,$ $O_2 = 1$	
3	$Acrolein + 2O_2 \rightarrow 3CO + 2H$	8.95×10^{15}	158	$Acrolein = 1,$ $O_2 = 1$	

2. Mass balance

Table S10. Mass balance results for G-AA (via ALY) process.

G-AA (via ALY)																				
Stream Name	**ACRYLIC**	**AIR-1**	**AIR-2**	**ALLYL-AL**	**DIPE1**	**FLUEGAS**	**FORMIC**	**GLYCEROL**	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**	**S12**
From	COOLER-2			DISTIL-2		INCINERA			MIXER-1	HEATER-1	REACT-1	COOLER-1	FLASH-1	FLASH-1	ABSORB-1	ABSORB-1	MIXER-2	DISTIL-1	DISTIL-1	LL-EXTRC
To		MIXER-3	INCINERA	MIXER-3	MIXER-5		MIXER-1	MIXER-1	HEATER-1	REACT-1	COOLER-1	FLASH-1	ABSORB-1	MIXER-2	INCINERA	MIXER-2	DISTIL-1	LL-EXTRC	MIXER-1	DISTIL-2
Temperature (°C)	25.0	320.0	25.0	93.7	25.0	100.0	25.0	25.0	78.9	25.0	235.0	25.0	25.0	25.0	25.9	23.7	25.0	90.8	105.0	162.8
Pressure (bar)	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	1.0	1.0	1.0	1.0
Mole Flows (kmol/hr)	146.6	902.9	2580.0	204.7	31.6	3721.3	188.3	358.1	2021.1	2021.1	2397.6	2397.6	139.0	2258.6	138.5	20.6	2279.2	804.6	1474.6	1392.5
Mole Fractions																				
GLYCEROL	-	-	-	-	-	-	-	0.5257	0.0941	0.0941	0.0008	0.0008	-	0.0008	-	-	0.0008	-	0.0013	-
ALLYL-AL	-	-	-	0.9185	-	-	-	-	-	-	0.0785	0.0785	0.0085	0.0828	0.0017	0.0462	0.0825	0.2337	-	0.1354
ACROLEIN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FORMIC	-	-	-	-	-	-	1.0000	-	0.3190	0.3190	0.1903	0.1903	0.0029	0.2019	-	0.0194	0.2002	-	0.3095	-
ACETIC	0.0449	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	-	0.2100	0.2100	-	-	0.0619	-	-	-	-	-	-	-	-	-	-	-	-	-	-
N2	-	0.7900	0.7900	-	-	0.7365	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2O	0.0001	-	-	-	-	0.0910	-	0.4743	0.5869	0.5869	0.6518	0.6518	0.0228	0.6905	0.0329	0.9088	0.6925	0.6985	0.6892	0.2256
CO2	-	-	-	-	-	0.1106	-	-	-	-	0.0785	0.0785	0.9658	0.0239	0.9655	0.0256	0.0239	0.0678	-	0.0565
CO	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETALDE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
DIPE	-	-	-	0.0815	1.0000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.5825
ACRYLIC	0.9550	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
TOLUENE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S10 continued…

Stream Name	**S13**	**S14**	**S15**	**S16**	**S17**	**S18**	**S19**	**S20**	**S21**	**S22**	**S23**	**S24**	**S25**	**S26**	**S28**	**S30**	**S31**	**S32**	**WATER**	**WATER2**

From	LL-EXTRC	DISTIL-2	MIXER-3	HEATER-2	COMP-1	REACT-2	FLASH-2	FLASH-2	ABSORB-2	ABSORB-2	MIXER-4	DISTIL-3	DISTIL-3	PUMP	B3	MIXER-5	FLASH-3	FLASH-3		
To		FLASH-3	HEATER-2	COMP-1	REACT-2	FLASH-2	ABSORB-2	MIXER-4	B3	MIXER-4	DISTIL-3		PUMP	COOLER-2	INCINERA	LL-EXTRC	INCINERA	MIXER-5	ABSORB-1	ABSORB-2
Temperature (°C)	30.8	57.9	55.1	220.0	360.2	230.0	85.0	85.0	77.0	81.1	84.4	57.4	94.7	94.7	45.7	29.8	30.0	30.0	25.0	25.0
Pressure (bar)	1.0	1.0	1.0	1.0	3.1	3.1	3.1	3.1	3.1	3.1	3.1	0.2	0.2	1.0	1.0	1.0	1.0	1.0	1.0	3.1
Mole Flows (kmol/hr)	580.3	1187.8	1107.6	1107.6	1107.6	1127.8	870.5	257.3	867.1	54.8	312.0	165.5	146.6	146.6	867.1	1168.2	51.2	1136.6	20.1	51.3
Mole Fractions																				
GLYCEROL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ALLYL-AL	0.0001	0.0004	0.1697	0.1697	0.1697	0.0034	0.0021	0.0081	0.0016	0.0068	0.0078	0.0148	-	-	0.0016	0.0004	-	0.0005	-	-
ACROLEIN	-	-	-	-	-	0.0233	0.0238	0.0218	0.0228	0.0168	0.0210	0.0395	-	-	0.0228	-	-	-	-	-
FORMIC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETIC	-	-	-	-	-	0.0130	0.0036	0.0449	0.0006	0.0486	0.0455	0.0461	0.0449	0.0449	0.0006	-	-	-	-	-
O2	-	-	0.1712	0.1712	0.1712	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
N2	-	-	0.6440	0.6440	0.6440	0.6324	0.8095	0.0334	0.8102	0.0396	0.0345	0.0651	-	-	0.8102	-	-	-	-	-
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2O	0.9631	0.2644	-	-	-	0.1682	0.0995	0.4005	0.1228	0.5747	0.4311	0.8128	0.0001	0.0001	0.1228	0.2662	0.0606	0.2736	1.0000	1.0000
CO2	0.0319	0.0663	-	-	-	0.0127	0.0163	0.0008	0.0163	0.0009	0.0008	0.0016	-	-	0.0163	0.0366	0.7036	0.0376	-	-
CO	-	-	-	-	-	0.0076	0.0098	0.0001	0.0099	0.0001	0.0001	0.0002	-	-	0.0099	-	-	-	-	-
ACETALDE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
DIPE	0.0049	0.6688	0.0151	0.0151	0.0151	0.0148	0.0158	0.0113	0.0154	0.0074	0.0106	0.0199	-	-	0.0154	0.6968	0.2358	0.6883	-	-
ACRYLIC	-	-	-	-	-	0.1245	0.0197	0.4791	0.0005	0.3051	0.4485	-	0.9550	0.9550	0.0005	-	-	-	-	-
TOLUENE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S11. Mass balance results for G-AA (via-LAC) process.

G-AA (via LAC)

Stream Name	ACETONE	ACRYLIC	AIR	AIR2	DHA	DIPE	FLUEGAS	GLYCER	M-LACTAT	METHANOL	N2	S1	S2	S3	S4	S5	S6	S7	S8	S9
From		COOLER-6			S-DRYER		INCINERA		DISTIL-2			REACT-1	COOLER-1	FLASH-1	FLASH-1	DISTIL-1	DISTIL-1	S-CRYSTL	S-FILTER	S-FILTER
To	MIXER-1		REACT-1	COMP-1	MIXER	MIXER-4		REACT-1	MIXER-2	MIXER	MIXER-3	COOLER-1	FLASH-1	INCINERA	DISTIL-1		S-CRYSTL	S-FILTER	S-WASHER	
Temperature (°C)	5.0	25.0	50.0	25.0	50.0	25.0	100.0	50.0	113.0	25.0	25.0	50.0	25.0	25.0	25.0	16.8	224.9	40.0	40.0	40.0
Pressure (bar)	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	1.0	1.0	1.0	1.0
Mole Flows (kmol/hr)	7.3	139.4	3129.0	120.0	158.1	6.3	4281.4	1011.0	316.1	158.0	800.0	4231.0	4231.0	3117.5	1113.4	935.3	178.1	178.1	158.1	20.1
Mole Fractions																				
GLYCEROL	-	-	-	-	-	-	-	0.1800	-	-	-	-	-	-	-	-	0.0002	0.0002	-	0.0018
DHA	-	-	-	-	-	-	-	-	-	-	-	0.0374	0.0374	-	0.1421	-	0.8882	-	-	-
GLYCALDE	-	0.0027	-	-	-	-	-	-	0.0132	-	-	0.0056	0.0056	-	0.0212	0.0042	0.1106	0.1106	0.0001	0.9811
O2	-	-	0.2100	0.2100	-	-	0.1190	-	-	-	-	0.1338	0.1338	0.1812	0.0010	0.0012	-	-	-	-
H2O	-	0.0025	-	-	-	-	0.1055	0.8200	0.4869	-	-	0.2389	0.2389	0.0264	0.8339	0.9926	0.0010	0.0010	-	0.0092
N2	-	-	0.7900	0.7900	-	-	0.7637	-	-	-	1.0000	0.5842	0.5842	0.7923	0.0017	0.0020	-	-	-	-
DHA(S)	-	-	-	-	1.0000	-	-	-	-	-	-	-	-	-	-	-	-	0.8882	0.9999	0.0079
ACETONE	1.0000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
LACTIC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
M-LACTIC	-	-	-	-	-	-	-	-	0.4869	-	-	-	-	-	-	-	-	-	-	-
METHANOL	-	-	-	-	-	-	-	-	0.0130	1.0000	-	-	-	-	-	-	-	-	-	-
PYRUVALD	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
CO2	-	-	-	-	-	-	0.0118	-	-	-	-	-	-	-	-	-	-	-	-	-
ACRYLIC	-	0.9948	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETALDE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
DIPE	-	-	-	-	-	1.0000	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S11 continued…

Stream Name	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27	S28	S29
From	S-WASHER	S-WASHER	S-DRYER	FLASH-4	FLASH-2	FLASH-4	MIXER-1	PUMP-2	COMP-1	FLASH-2	MIXER-4	MIXER	REACT-2	DISTIL-2	COOLER-2	MIXER-2	REACT-D	REACT-D	MIXER-3	HEATER-1
To	S-DRYER	FLASH-2		INCINERA	MIXER-1	PUMP-2	S-WASHER	MIXER-4	S-DRYER	INCINERA	LL-EXTRC	REACT-2	DISTIL-2	COOLER-2	MIXER	REACT-D	MIXER-3		HEATER-1	REACT-3
Temperature (°C)	48.0	48.0	50.0	32.0	50.0	32.0	48.7	32.0	111.6	50.0	31.8	120.0	120.0	64.6	25.0	51.1	102.8	66.5	57.3	360.0
Pressure (bar)	1.0	1.0	1.0	0.3	1.0	0.3	1.0	1.0	2.0	1.0	1.0	1.0	2.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mole Flows (kmol/hr)	165.4	238.5	127.3	2.1	238.5	205.8	245.8	205.8	120.0	0.0	212.1	571.6	571.6	255.5	255.5	1744.9	1570.3	174.5	2370.3	2370.3
Mole Fractions																				
GLYCEROL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
DHA	-	-	-	-	-	-	-	-	-	-	-	0.2766	-	-	-	-	-	-	-	-
GLYCALDE	0.0001	0.0027	0.0002	-	0.0027	-	0.0026	-	-	-	-	-	0.0073	-	-	0.0024	0.0027	-	0.0018	0.0018
O2	-	-	0.1979	-	-	-	-	-	0.2100	-	-	-	-	-	-	-	-	-	-	-
H2O	-	-	-	0.0084	-	0.0529	-	0.0529	-	-	0.0513	0.0001	0.2694	0.0003	0.0003	0.9070	0.8993	0.0948	0.5958	0.5958
N2	-	-	0.7444	0.1263	-	0.0001	-	0.0001	0.7900	-	0.0001	-	-	-	-	-	-	-	0.3375	0.3375
DHA(S)	0.9556	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETONE	0.0443	0.9973	0.0575	-	0.9973	-	0.9974	-	-	0.0001	-	-	-	-	-	-	-	-	-	-
LACTIC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.0980	-	0.0649	0.0649
M-LACTIC	-	-	-	-	-	-	-	-	-	-	-	-	0.2693	-	-	0.0882	-	-	-	-
METHANOL	-	-	-	-	-	-	-	-	-	-	-	0.7233	0.4540	0.9997	0.9997	0.0023	-	0.9052	-	-
PYRUVALD	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
CO2	-	-	-	0.0103	-	0.0001	-	0.0001	-	-	0.0001	-	-	-	-	-	-	-	-	-
ACRYLIC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETALDE	-	-	-	0.0274	-	0.0056	-	0.0056	-	-	0.0054	-	-	-	-	-	-	-	-	-
DIPE	-	-	-	0.8275	-	0.9414	-	0.9414	-	-	0.9431	-	-	-	-	-	-	-	-	-

Table S11 continued…

Stream Name	S30	S31	S32	S33	S34	S35	S36	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	WATER	WATER-3
From	REACT-3	COOLER-4	ABSORBER	ABSORBER	LL-EXTRC	LL-EXTRC	DISTIL-3	DISTIL-3	COOLER-5	FLASH-3	DECANTER	DECANTER	FLASH-3	DISTIL-4	DISTIL-4	DISTIL-5	DISTIL-5	PUMP-1		
To	COOLER-4	ABSORBER	LL-EXTRC	INCINERA		DISTIL-3	DISTIL-4	COOLER-5	FLASH-3	DECANTER	DISTIL-3	FLASH-4	INCINERA	DISTIL-5			PUMP-1	COOLER-6	MIXER-2	ABSORBER
Temperature (°C)	359.8	70.0	68.9	68.1	48.1	71.9	75.2	61.1	5.0	5.0	75.0	75.0	5.0	75.1	128.7	69.2	105.7	105.7	25.0	25.0
Pressure (bar)	1.0	1.0	1.0	1.0	1.0	1.0	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	1.0	1.0	1.0
Mole Flows (kmol/hr)	2531.7	2531.7	1481.6	1150.1	991.6	702.0	493.8	480.0	480.0	479.7	271.8	207.9	0.3	490.8	3.0	351.4	139.4	139.4	1428.8	100.0
Mole Fractions																				
GLYCEROL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
DHA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GLYCALDE	0.0017	0.0017	0.0028	-	0.0012	0.0043	0.0062	-	-	-	-	-	-	0.0008	0.8780	-	0.0027	0.0027	-	-
O2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2O	0.6157	0.6157	0.9015	0.2809	0.9940	0.5140	0.7087	0.5857	0.5857	0.5861	0.9943	0.0524	0.0170	0.7130	0.0001	0.9949	0.0025	0.0025	1.0000	1.0000
N2	0.3160	0.3160	0.0005	0.6950	0.0002	0.0008	-	0.0014	0.0014	0.0008	0.0004	0.0014	0.8597	-	-	-	-	-	-	-
DHA(S)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETONE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
LACTIC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
M-LACTIC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
METHANOL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
PYRUVALD	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H2	0.0029	0.0029	-	0.0065	-	-	-	-	-	-	-	-	0.0024	-	-	-	-	-	-	-
CO2	0.0029	0.0029	-	0.0064	-	0.0001	-	0.0001	0.0001	0.0001	0.0001	0.0002	0.0103	-	-	-	-	-	-	-
ACRYLIC	0.0578	0.0578	0.0948	0.0053	-	0.2000	0.2843	-	-	-	-	-	-	0.2853	0.1219	0.0039	0.9948	0.9948	-	-
ACETALDE	0.0029	0.0029	0.0004	0.0059	0.0006	0.0017	-	0.0029	0.0029	0.0029	0.0007	0.0058	0.0050	-	-	-	-	-	-	-
DIPE	-	-	-	-	0.0041	0.2791	0.0009	0.4098	0.4098	0.4100	0.0045	0.9402	0.1055	0.0009	-	0.0012	-	-	-	-

Table S12. Mass balance results for G-AA (via ACR) process.

G-AA (via ACR)																				
Stream Name	**ACRYLIC**	**AIR-1**	**AIR-2**	**FLUEGAS**	**GLYCEROL**	**LP.secTEAM**	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**	**S12**	**S13**	**S14**
From	COOLER-4			INCINERA			COMP-1	HEATER-1	HEATER-2	HEATER-3	MIXER-1	REACT-1	COOLER-1	DISTIL-1	DISTIL-1	COMP-2	MIXER-2	COMP-3	HEATER-4	REACT-2
To		COMP-1	COMP-2		HEATER-1	HEATER-2	HEATER-3	MIXER-1	MIXER-1	MIXER-1	REACT-1	COOLER-1	DISTIL-1	MIXER-2		MIXER-2	COMP-3	HEATER-4	REACT-2	COOLER-2
Stream Class	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Temperature (°C)	25.0	25.0	25.0	100.0	25.0	160.0	201.3	307.0	500.0	500.0	400.9	374.0	112.0	42.2	100.0	241.9	174.8	433.6	375.0	375.0
Pressure (bar)	1.0	1.0	1.0	1.0	1.0	6.0	3.9	1.0	6.0	6.0	4.0	4.0	4.0	1.0	1.0	5.0	1.0	5.0	5.0	5.0
Mole Flows (kmol/hr)	139.1	90.7	1875.0	1930.9	414.1	1112.9	90.7	414.1	1112.9	90.7	1617.7	2021.4	2021.4	309.5	1711.9	1875.0	2184.5	2184.5	2184.5	2153.4
Mole Fractions																				
GLYCEROL	-	-	-	-	0.5300	-	-	0.5300	-	-	0.1357	0.0008	0.0008	-	0.0009	-	-	-	-	-
ACROLEIN	-	-	-	-	-	-	-	-	-	-	-	0.0887	0.0887	0.5793	-	-	0.0821	0.0821	0.0821	-
ACETOL	-	-	-	-	-	-	-	-	-	-	-	0.0099	0.0099	-	0.0117	-	-	-	-	-
ACETALDE	-	-	-	-	-	-	-	-	-	-	-	0.0005	0.0005	0.0032	-	-	0.0005	0.0005	0.0005	0.0005
CO	-	-	-	-	-	-	-	-	-	-	-	0.0005	0.0005	0.0032	-	-	0.0005	0.0005	0.0005	0.0213
PROPIONI	-	-	-	-	-	-	-	-	-	-	-	0.0042	0.0042	-	0.0050	-	-	-	-	-
ACETONE	-	-	-	-	-	-	-	-	-	-	-	0.0045	0.0045	0.0293	-	-	0.0041	0.0041	0.0041	0.0042
CO2	-	-	-	0.0945	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.0295
ACRYLIC	0.9969	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.0665
WATER	-	-	-	0.0406	0.4700	1.0000	-	0.4700	1.0000	-	0.8083	0.8433	0.8433	0.0742	0.9824	-	0.0105	0.0105	0.0105	0.0442
OXYGEN	-	0.2100	0.2100	0.0640	-	-	0.2100	-	-	0.2100	0.0118	0.0117	0.0117	0.0762	-	0.2100	0.1910	0.1910	0.1910	0.1123
NITROGEN	-	0.7900	0.7900	0.8009	-	-	0.7900	-	-	0.7900	0.0443	0.0354	0.0354	0.2315	-	0.7900	0.7109	0.7109	0.7109	0.7211
H2	-	-	-	-	-	-	-	-	-	-	-	0.0005	0.0005	0.0032	-	-	0.0005	0.0005	0.0005	0.0005
TOLUENE	0.0031	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S12 continued…

Stream Name	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27	S28	S29	S30	S31	S32	S33	TOLUENE	WATER
From	COOLER-2	FLASH-1	FLASH-1	PUMP-1	MIXER-4	ABSORBER	ABSORBER	MIXER-3	DISTIL-2	DISTIL-2	COOLER-3	FLASH-2	FLASH-2	DECANTER	DECANTER	COMP-4	DISTIL-3	DISTIL-3	PUMP-2		
To	FLASH-1	ABSORBER	MIXER-3	ABSORBER	DISTIL-2	COMP-4	MIXER-3	DISTIL-2	COOLER-3	DISTIL-3	FLASH-2	COMP-4	DECANTER	MIXER-4		INCINERA	DECANTER	PUMP-2	COOLER-4	MIXER-4	PUMP-1
Stream Class	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Temperature (°C)	40.0	40.0	40.0	25.0	15.7	36.6	36.4	40.0	40.8	98.2	15.0	15.0	15.0	15.0	15.0	131.9	52.2	88.1	88.1	25.0	25.0
Pressure (bar)	5.0	5.0	5.0	5.0	0.3	5.0	5.0	5.0	0.3	0.3	0.3	0.3	0.3	0.3	0.3	1.0	0.2	0.2	1.0	0.3	1.0
Mole Flows (kmol/hr)	2153.4	1892.8	260.7	27.8	104.3	1896.0	24.6	285.2	202.6	187.0	202.6	44.2	158.3	96.0	110.2	1940.2	47.9	139.1	139.1	8.3	27.8
Mole Fractions																					
GLYCEROL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACROLEIN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETOL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETALDE	0.0005	0.0004	0.0007	-	0.0037	0.0004	0.0004	0.0007	0.0029	-	0.0029	0.0035	0.0027	0.0040	0.0004	0.0005	-	-	-	-	-
CO	0.0213	0.0242	0.0004	-	-	0.0241	0.0005	0.0004	0.0006	-	0.0006	0.0027	-	-	-	0.0236	-	-	-	-	-
PROPIONI	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACETONE	0.0042	0.0027	0.0154	-	0.0455	0.0025	0.0090	0.0149	0.0443	-	0.0443	0.0267	0.0493	0.0494	0.0277	0.0031	-	-	-	-	-
CO2	0.0295	0.0331	0.0032	-	0.0005	0.0330	0.0035	0.0032	0.0048	-	0.0048	0.0192	0.0007	0.0005	0.0006	0.0327	-	-	-	-	-
ACRYLIC	0.0665	0.0016	0.5375	-	0.1146	-	0.1254	0.5020	0.0021	0.8273	0.0021	-	0.0027	0.1245	0.0406	-	0.3343	0.9969	0.9969	-	-
WATER	0.0442	0.0071	0.3135	1.0000	0.0184	0.0126	0.7080	0.3475	0.4919	0.0073	0.4919	0.0749	0.6084	0.0200	0.8692	0.0140	0.0286	-	-	-	1.0000
OXYGEN	0.1123	0.1273	0.0030	-	0.0001	0.1271	0.0034	0.0030	0.0043	-	0.0043	0.0193	0.0002	0.0001	0.0001	0.1246	-	-	-	-	-
NITROGEN	0.7211	0.8030	0.1263	-	0.0506	0.7997	0.1498	0.1283	0.2068	-	0.2068	0.6817	0.0741	0.0550	0.0585	0.7970	-	-	-	-	-
H2	0.0005	0.0005	-	-	-	0.0005	-	-	-	-	-	-	-	-	-	0.0005	-	-	-	-	-
TOLUENE	-	-	-	-	0.7667	-	-	-	0.2423	0.1654	0.2423	0.1719	0.2619	0.7464	0.0028	0.0039	0.6371	0.0031	0.0031	1.0000	-

Table S13. Mass balance results for P-AA (via ACR) process.

P-AA (via ACR)																				
Stream Name	**ACRYLIC**	**AIR-1**	**AIR-2**	**DIPE**	**FEED**	**FLUEGAS**	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**	**S12**	**S13**	**S14**	**S15**
From	COOLER-3					INCINERA	COMP-1	MIXER-1	HEATER-1	REACT-1	HEATER-2	COMP-2	REACT-2	COOLER-1	ABSORBER	ABSORBER	FLASH-1	FLASH-1	MIXER-2	LL-EXTRC	LL-EXTRC
To		COMP-1	INCINERA	MIXER-4	MIXER-1		MIXER-1	HEATER-1	REACT-1	HEATER-2	COMP-2	REACT-2	COOLER-1	ABSORBER	FLASH-1	MIXER-2	COMP-3	MIXER-2	LL-EXTRC	DISTIL-1	DISTIL-2
Temperature (°C)	20.0	25.0	25.0	25.0	25.0	100.0	201.8	165.7	366.0	360.0	375.0	500.1	375.0	25.0	119.5	122.8	60.0	60.0	95.8	91.8	27.1
Pressure (bar)	1.0	1.0	1.0	6.9	11.5	1.0	3.7	3.7	3.7	3.7	3.7	6.9	6.9	6.9	6.9	6.9	6.9	6.9	6.9	6.9	6.9
Mole Flows (kmol/hr)	139.5	2488.6	3380.0	32.1	233.6	5867.6	2488.6	3652.5	3652.5	3650.0	3650.0	3650.0	3623.0	3623.0	3183.8	929.2	2342.1	841.7	1770.9	874.9	1355.6
Mole Fractions																					
PROPENE	-	-	-	-	0.9400	-	-	0.0601	0.0601	0.0062	0.0062	0.0062	0.0063	0.0063	0.0070	0.0004	0.0091	0.0010	0.0007	0.0018	0.0006
PROPANE	-	-	-	-	0.0300	-	-	0.0019	0.0019	0.0019	0.0019	0.0019	0.0019	0.0019	0.0022	0.0002	0.0028	0.0004	0.0003	0.0007	0.0003
ETHANE	-	-	-	-	0.0300	-	-	0.0019	0.0019	0.0019	0.0019	0.0019	0.0019	0.0019	0.0022	0.0001	0.0029	0.0001	0.0001	0.0002	-
GLYCEROL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NITROGEN	-	0.7900	0.7900	-	-	0.7901	0.7900	0.5383	0.5383	0.5386	0.5386	0.5386	0.5426	0.5426	0.6169	0.0022	0.8374	0.0033	0.0027	0.0051	0.0002
OXYGEN	-	0.2100	0.2100	-	-	0.0593	0.2100	0.1431	0.1431	0.0784	0.0784	0.0784	0.0368	0.0368	0.0418	0.0002	0.0568	0.0003	0.0002	0.0004	-
DIPE	-	-	-	1.0000	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.4798	0.0039
WATER	-	-	-	-	-	0.0754	-	0.2547	0.2547	0.3079	0.3079	0.3079	0.3275	0.3275	0.2776	0.8534	0.0282	0.9715	0.9095	0.3333	0.9902
ACROLEIN	-	-	-	-	-	-	-	-	-	0.0428	0.0428	0.0428	-	-	-	-	-	-	-	-	-
ACRYLIC	0.9953	-	-	-	-	-	-	-	-	0.0043	0.0043	0.0043	0.0387	0.0387	0.0051	0.1335	0.0004	0.0183	0.0787	0.1595	-
ACETIC	0.0047	-	-	-	-	-	-	-	-	0.0013	0.0013	0.0013	0.0013	0.0013	-	0.0050	-	-	0.0026	0.0039	0.0009
CO2	-	-	-	-	-	0.0752	-	-	-	0.0059	0.0059	0.0059	0.0212	0.0212	0.0240	0.0004	0.0323	0.0010	0.0007	0.0014	0.0001
ACETALDE	-	-	-	-	-	-	-	-	-	0.0014	0.0014	0.0014	0.0014	0.0014	0.0006	0.0034	0.0007	0.0002	0.0019	0.0077	0.0016
FORMALDE	-	-	-	-	-	-	-	-	-	0.0094	0.0094	0.0094	0.0094	0.0094	0.0104	0.0013	0.0127	0.0039	0.0025	0.0061	0.0023
CO	-	-	-	-	-	-	-	-	-	-	-	-	0.0108	0.0108	0.0123	-	0.0167	0.0001	0.0001	0.0001	-

Table S13 continued…

Stream Name	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27	S28	S29	S30	S31	S32	S33	S34	S35	STEAM
From	DISTIL-2	DISTIL-2	DISTIL-1	COOLER-2	FLASH-2	FLASH-2	DECANTER	DECANTER	DISTIL-1	DISTIL-3	DISTIL-3	PUMP-1	MIXER-3	FLASH-3	FLASH-3	MIXER-4	COOLER-4	PUMP-2	COMP-3	COMP-4	
To	MIXER-3		COOLER-2	FLASH-2	COMP-4	DECANTER	DISTIL-1	PUMP-1	DISTIL-3		COOLER-3	MIXER-3	FLASH-3	INCINERA	MIXER-4	COOLER-4	PUMP-2	LL-EXTRC	INCINERA	INCINERA	MIXER-1
Temperature (°C)	52.7	82.1	47.5	10.0	23.0	23.0	75.0	75.0	72.4	24.8	78.7	75.1	59.5	56.0	56.0	53.9	10.0	10.6	-43.4	59.7	160.0
Pressure (bar)	1.0	1.0	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.1	0.1	1.0	1.0	1.0	1.0	1.0	1.0	6.9	1.0	1.0	6.0
Mole Flows (kmol/hr)	6.9	1348.6	693.7	693.7	38.8	654.9	223.1	431.8	404.3	264.8	139.5	431.8	438.7	11.3	427.4	459.5	459.5	459.5	2342.1	38.8	930.3
Mole Fractions																					
PROPENE	0.0925	0.0001	0.0025	0.0025	0.0175	0.0016	0.0005	0.0021	-	-	-	0.0021	0.0036	0.0383	0.0026	0.0025	0.0025	0.0025	0.0091	0.0175	-
PROPANE	0.0363	0.0001	0.0010	0.0010	0.0056	0.0007	0.0002	0.0009	-	-	-	0.0009	0.0015	0.0141	0.0011	0.0011	0.0011	0.0011	0.0028	0.0056	-
ETHANE	0.0040	-	0.0002	0.0002	0.0031	0.0001	-	0.0001	-	-	-	0.0001	0.0002	0.0032	0.0001	0.0001	0.0001	0.0001	0.0029	0.0031	-
GLYCEROL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NITROGEN	0.0464	-	0.0065	0.0065	0.1137	0.0001	-	0.0001	-	-	-	0.0001	0.0009	0.0312	0.0001	-	-	-	0.8374	0.1137	-
OXYGEN	0.0050	-	0.0006	0.0006	0.0099	-	-	-	-	-	-	-	0.0001	0.0033	-	-	-	-	0.0568	0.0099	-
DIPE	0.5551	0.0011	0.6059	0.6059	0.5980	0.6064	0.0046	0.9172	0.0011	0.0017	-	0.9172	0.9115	0.6220	0.9192	0.9249	0.9249	0.9249	-	0.5980	-
WATER	0.1029	0.9947	0.3626	0.3626	0.1565	0.3748	0.9905	0.0567	0.6456	0.9857	-	0.0567	0.0574	0.1832	0.0541	0.0503	0.0503	0.0503	0.0282	0.1565	1.0000
ACROLEIN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ACRYLIC	-	-	0.0002	0.0002	-	0.0002	-	0.0004	0.3448	0.0021	0.9953	0.0004	0.0004	-	0.0004	0.0003	0.0003	0.0003	0.0004	-	-
ACETIC	-	0.0009	-	-	-	-	-	-	0.0085	0.0105	0.0047	-	-	-	-	-	-	-	-	-	-
CO2	0.0248	-	0.0018	0.0018	0.0257	0.0004	0.0001	0.0005	-	-	-	0.0005	0.0008	0.0207	0.0003	0.0003	0.0003	0.0003	0.0323	0.0257	-
ACETALDE	0.0286	0.0014	0.0103	0.0103	0.0292	0.0091	0.0016	0.0130	-	-	-	0.0130	0.0133	0.0306	0.0128	0.0119	0.0119	0.0119	0.0007	0.0292	-
FORMALDE	0.1035	0.0017	0.0084	0.0084	0.0385	0.0067	0.0023	0.0089	-	-	-	0.0089	0.0104	0.0528	0.0093	0.0086	0.0086	0.0086	0.0127	0.0385	-
CO	0.0010	-	0.0001	0.0001	0.0024	-	-	-	-	-	-	-	-	0.0007	-	-	-	-	0.0167	0.0024	-

Table S14. Transport data for raw materials and waste transport.

Process name	Material Transported	Transport Route	Transport type	Distance (km)	Mass Transported (kg)	Empty return trip?	Database section
G-AA (via ALY)	Glycerol	Raw materials to Processing plant	40t truck	100	17339.99	TRUE	CCaLC Transport
	Formic acid		40t truck	100	8666.16	TRUE	CCaLC Transport
	Diisopropyl ether		40t truck	100	3228.90	TRUE	CCaLC Transport
	Wastewater treatment - industrial,1	Processing plant to Waste management facility	40t truck	100	11177.32	TRUE	CCaLC Transport
	Wastewater treatment - industrial,3		40t truck	100	4041.72	TRUE	CCaLC Transport
G-AA (via LAC)	Glycerol	Raw materials to Processing plant	40t truck	100	26940.26	TRUE	CCaLC Transport
	Acetone		40t truck	100	425.37	TRUE	CCaLC Transport
	Methanol		40t truck	100	5062.66	TRUE	CCaLC Transport
	Nitrogen		40t truck	100	22410.78	TRUE	CCaLC Transport
	Diisopropyl ether		40t truck	100	644.72	TRUE	CCaLC Transport
	Wastewater treatment - industrial,1	Processing plant to Waste management facility	40t truck	100	17168.37	TRUE	CCaLC Transport
	Landfill - biodegradable waste		40t truck	100	1794.14	TRUE	CCaLC Transport
	Wastewater treatment - industrial,1		40t truck	100	18307.06	TRUE	CCaLC Transport
	disposal, organic remains, 0% water, to hazardous waste incineration		40t truck	100	267.40	TRUE	CCaLC Transport
	Wastewater treatment - industrial,1		40t truck	100	6440.69	TRUE	CCaLC Transport
G-AA (via ACR)	Glycerol	Raw materials to Processing plant	40t truck	100	20160.78	TRUE	CCaLC Transport
	Steam		40t truck	100	20049.21	TRUE	CCaLC Transport
	Toluene		40t truck	100	768.84	TRUE	CCaLC Transport
	Wastewater treatment - industrial,1	Processing plant to Waste management facility	40t truck	100	32558.65	TRUE	CCaLC Transport
	Wastewater treatment - industrial,3		40t truck	100	2439.89	TRUE	CCaLC Transport
P-AA (via ACR)	Propylene	Raw materials to Processing plant	40t truck	100	9758.91	TRUE	CCaLC Transport
	Steam		40t truck	100	16759.54	TRUE	CCaLC Transport
	Diisopropyl ether		40t truck	100	3283.12	TRUE	CCaLC Transport
	Wastewater treatment - industrial,1	Processing plant to Waste management facility	40t truck	100	24550.62	TRUE	CCaLC Transport

Table S15. Water footprint for the four acrylic production processes.

Process name	Stage	Data set	Water needed in the process (kg/FU)	Water needed for cooling (kg/FU)	Water footprint (m3/FU)
G-AA (via ALY)	Stage one	Process water	362.11	629619.66	248.84
	Stage two		924.18	87700.26	35.01
G-AA (via LAC)	Stage one		25740.23	149765.89	69.32
	Stage two		1801.53	286110.95	113.73
	Stage three		0.00	121674.01	48.06
G-AA (via ACR)	Stage one		0.00	212263.82	83.84
	Stage two		500.82	95217.85	37.81
P-AA (via ACR)	Stage one		8827.49	75346.37	33.25
	Stage two		0.00	96583.27	38.15

Table S16. Environmental impacts for different purifications processes of crude glycerol. [9]

Purification process	Environmental impacts	Value
Physicochemical treatment and membrane process (PMP)	Carbon footprint (kg CO2 eq./kg)	3.47E+00
	Acidification potential (kg SO2 eq./kg)	1.21E-02
	Eutrophication potential (kg PO4 eq./kg)	4.47E-03
	Ozone layer depletion potential (kg R11 eq./kg)	2.68E-07
	Photochemical smog potential (kg C2H4 eq./kg)	1.16E-03
	Human toxicity potential (kg DCB eq./kg)	5.25E-01
	Water footprint (stress weighted) (m3 eq./kg)	3.05E+01
Vacuum distillation process (VDP)	Carbon footprint (kg CO2 eq./kg)	1.75E+00
	Acidification potential (kg SO2 eq./kg)	6.17E-03
	Eutrophication potential (kg PO4 eq./kg)	2.70E-03
	Ozone layer depletion potential (kg R11 eq./kg)	1.85E-07
	Photochemical smog potential (kg C2H4 eq./kg)	3.77E-04
	Human toxicity potential (kg DCB eq./kg)	3.36E-01
	Water footprint (stress weighted) (m3 eq./kg)	1.40E+01
Ion exchange process (IEP)	Carbon footprint (kg CO2 eq./kg)	2.24E+00
	Acidification potential (kg SO2 eq./kg)	6.40E-03
	Eutrophication potential (kg PO4 eq./kg)	3.14E-03
	Ozone layer depletion potential (kg R11 eq./kg)	1.51E-07
	Photochemical smog potential (kg C2H4 eq./kg)	3.57E-04
	Human toxicity potential (kg DCB eq./kg)	6.13E-01
	Water footprint (stress weighted) (m3 eq./kg)	1.31E+01

3. Sensitivity Analysis

Table S17. Global warming for different crude glycerol purification with varied glycerol content[9].

Purification process	% glycerol in crude glycerol	Global warming (kg CO2 eq./kg)
PMP	30%	3.652
	40%	3.467
	50%	3.354
VDP	30%	1.901
	40%	1.746
	50%	1.635
IEP	30%	2.705
	40%	2.237
	50%	2.196
PMP	30%	3.652
	40%	3.467
	50%	3.354
VDP	30%	1.901
	40%	1.746
	50%	1.635
IEP	30%	2.705
	40%	2.237
	50%	2.196
PMP	30%	3.652
	40%	3.467
	50%	3.354
VDP	30%	1.901
	40%	1.746
	50%	1.635
IEP	30%	2.705
	40%	2.237
	50%	2.196

Table S18. Sensitivity analysis of global warming with respect to purification process and composition of crude glycerol for the glycerol-based acrylic acid production processes.

Process name	Source of glycerol	Global warming (kg CO_2 eq./ FU)
G-AA (via ALY)	30% Crude glycerol purified by PMP	145233.25
	40% Crude glycerol purified by PMP	142025.35
	50% Crude glycerol purified by PMP	140065.93
	30% Crude glycerol purified by VDP	114870.93
	40% Crude glycerol purified by VDP	112183.23
	50% Crude glycerol purified by VDP	110258.49
	30% Crude glycerol purified by IEP	128812.28
	40% Crude glycerol purified by IEP	120697.17
	50% Crude glycerol purified by IEP	119986.23
G-AA (via LAC)	30% Crude glycerol purified by PMP	145201.40
	40% Crude glycerol purified by PMP	140217.45
	50% Crude glycerol purified by PMP	137173.20
	30% Crude glycerol purified by VDP	98029.00
	40% Crude glycerol purified by VDP	93853.26
	50% Crude glycerol purified by VDP	90862.89
	30% Crude glycerol purified by IEP	119688.97
	40% Crude glycerol purified by IEP	107080.93
	50% Crude glycerol purified by IEP	105976.38
G-AA (via ACR)	30% Crude glycerol purified by PMP	108215.75
	40% Crude glycerol purified by PMP	104486.00
	50% Crude glycerol purified by PMP	102207.84
	30% Crude glycerol purified by VDP	72914.22
	40% Crude glycerol purified by VDP	69789.30
	50% Crude glycerol purified by VDP	67551.46
	30% Crude glycerol purified by IEP	89123.49
	40% Crude glycerol purified by IEP	79688.24
	50% Crude glycerol purified by IEP	78861.65

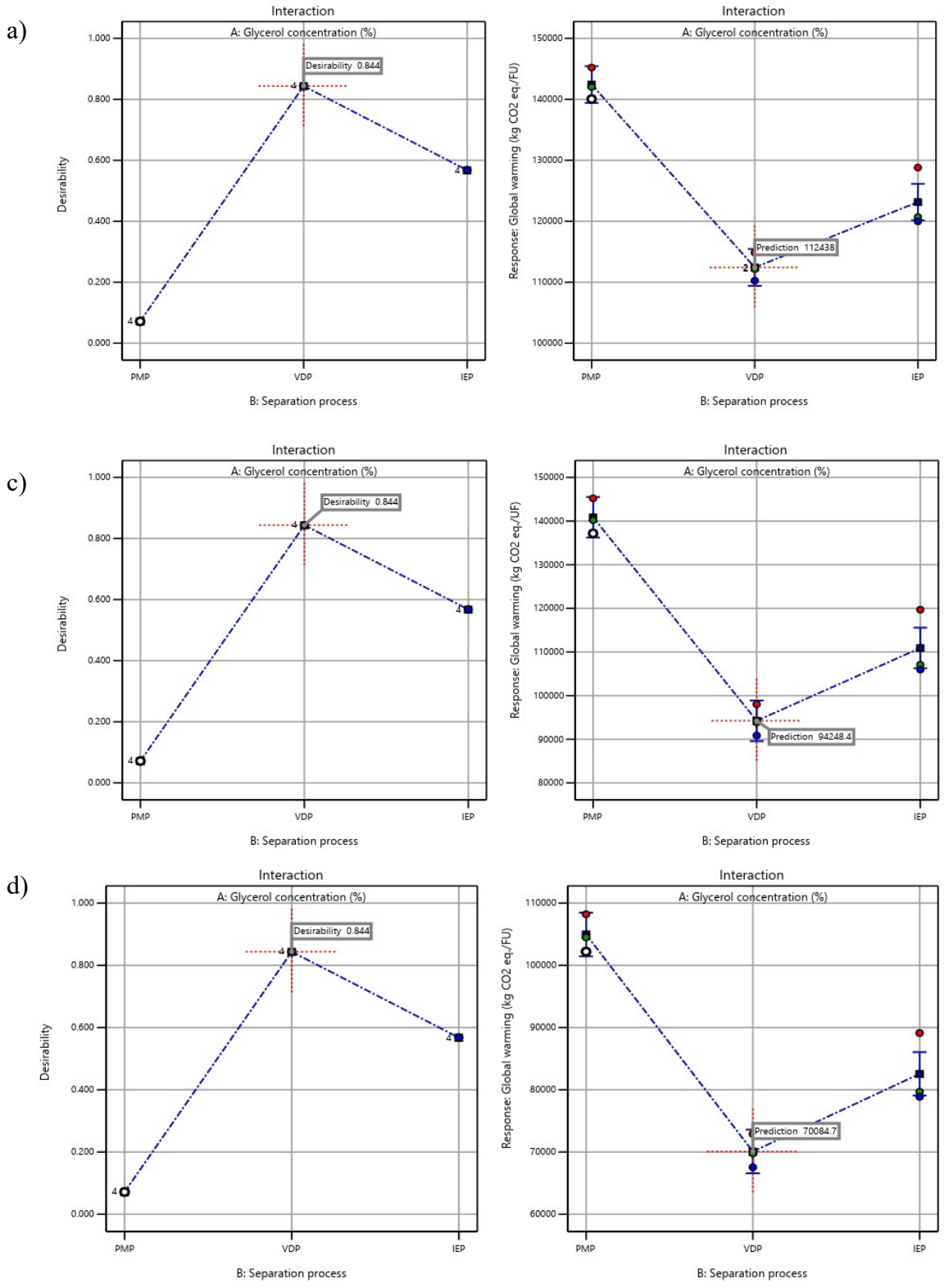

Figure S1. Desirability and prediction values calculated by 2FI model factorial method for a) G-AA (via ALY), b) G-AA (via LAC) and c) G-AA (via ACR) processes.

References

1 X. Li and Y. Zhang, *ACS Catal*, 2016, **6**, 143–150.

2 N. Wörz, A. Brandner and P. Claus, *Journal of Physical Chemistry C*, 2010, **114**, 1164–1172.

3 R. M. West, M. S. Holm, S. Saravanamurugan, J. Xiong, Z. Beversdorf, E. Taarning and C. H. Christensen, *J Catal*, 2010, **269**, 122–130.

4 L. Mo, J. Shao-Tong, P. Li-Jun, Z. Zhi and L. Shui-Zhong, *Chemical Engineering Research and Design*, 2011, **89**, 2199–2206.

5 B. Yan, Z. H. Liu, Y. Liang and B. Q. Xu, *Ind Eng Chem Res*, 2020, **59**, 17417–17428.

6 A. Talebian-Kiakalaieh and N. A. S. Amin, *Chem Eng Trans*, 2017, **56**, 655–660.

7 A. Drochner, P. Kampe, N. Menning, N. Blickhan, T. Jekewitz and H. Vogel, *Chem Eng Technol*, 2014, **37**, 398–408.

8 H. Redlingshöfer, A. Fischer, C. Weckbecker, K. Huthmacher and G. Emig, *Ind Eng Chem Res*, 2003, **42**, 5482–5488.

9 Y. Bansod, B. Crabbe, L. Forster, K. Ghasemzadeh and C. D'Agostino, *J Clean Prod*, 2024, **437**, 140485.