

**Supplementary Information for “Biochemical Production of Short-Chain Alcohols
from Glycerol: Process Simulation and Economic Evaluation”**

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Table S.1. Process streams for ethanol production.

Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	25.0	25.0	25.0	24.9	37.0	37.0	37.0	37.0	100.0	78.2	154.0	154.0	154.0	35.1
Pressure (atm)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	3.8	3.8	3.8	1.0
Vapor mass fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000	0.0000
Liquid mass fraction	1.0000	1.0000	0.0000	0.9996	0.9996	0.9996	0.7059	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	1.0000
Solid mass fraction	0.0000	0.0000	1.0000	0.0004	0.0004	0.0004	0.2941	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Mass enthalpy (kJ/kg)	-7,246.9	-15,864.4	-11,859.1	-15,776.3	-15,726.6	-15,727.5	-14,590.8	-15,729.0	-15,509.1	-5,436.4	-5,309.3	-6,507.8	-4,939.4	-6,048.4
Molar flow (kmol/h)	11.3	5,701.8	1.7	5,714.8	5,714.8	5,726.1	7.2	5,718.9	5,706.0	12.9	12.9	3.7	9.2	9.2
Volume flow (m ³ /h)	0.8	103.3	0.0	104.1	105.4	105.9	0.1	105.8	112.4	366.9	116.7	33.4	83.2	0.5
Mass flow (kg/h)	1,042.0	102,720.0	41.7	103,803.7	103,803.7	103,803.7	141.7	103,662.0	103,109.4	552.6	552.6	130.3	422.2	422.2
Comp. Mass fraction														
Water	0.0000	1.0000	0.0000	0.9896	0.9896	0.9896	0.6988	0.9900	0.9950	0.0498	0.0498	0.1944	0.0052	0.0052
Glycerol	1.0000	0.0000	0.0000	0.0100	0.0100	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<i>E. coli</i>	0.0000	0.0000	1.0000	0.0004	0.0004	0.0004	0.2941	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Formic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0047	0.0033	0.0047	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000
Ethanol	0.0000	0.0000	0.0000	0.0000	0.0000	0.0053	0.0038	0.0053	0.0003	0.9502	0.9502	0.8056	0.9948	0.9948

Table S.2. Process streams for propanol production.

Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	25.0	25.0	25.0	24.6	31.0	31.0	31.0	31.0	100.1	89.8	110.7	110.7	110.7	35.1
Pressure (atm)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.3	1.3	1.3	1.0
Vapor mass fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000	0.0000
Liquid mass fraction	1.0000	1.0000	0.0000	0.9928	0.9928	0.9928	0.6970	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000	1.0000
Solid mass fraction	0.0000	0.0000	1.0000	0.0072	0.0072	0.0072	0.3030	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Mass enthalpy (kJ/kg)	-7,246.9	-15,864.4	-11,859.1	-15,494.2	-15,468.7	-15,400.3	-14,345.1	-15,426.0	-15,438.3	-7,574.4	-7,538.0	-11,945.3	-4,128.3	-5,034.6
Molar flow (kmol/h)	11.3	1,392.1	7.7	1,411.1	1,411.1	1,416.2	31.2	1,385.0	1,348.1	36.9	36.9	25.7	11.2	11.2
Volume flow (m ³ /h)	0.8	25.2	0.0	26.0	26.2	26.6	0.4	26.2	26.7	1.087.5	861.6	603.0	258.0	0.8
Mass flow (kg/h)	1,042.0	25,079.0	189.5	26,310.5	26,310.5	26,310.5	625.4	25,685.1	24,502.0	1,183.2	1,183.2	516.1	667.1	667.1
Comp. Mass fraction														
Water	0.0000	1.0000	0.0000	0.9532	0.9532	0.9532	0.6692	0.9601	0.9884	0.3747	0.3747	0.8556	0.0027	0.0027
Glycerol	1.0000	0.0000	0.0000	0.0396	0.0396	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<i>E. coli</i>	0.0000	0.0000	1.0000	0.0072	0.0072	0.0072	0.3030	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propionic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0110	0.0077	0.0111	0.0116	0.0005	0.0005	0.0012	0.0000	0.0000
Propanol	0.0000	0.0000	0.0000	0.0000	0.0000	0.0286	0.0201	0.0288	0.0000	0.6248	0.6248	0.1432	0.9973	0.9973

Table S.3. Process streams for butanol production.

Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	25.0	25.0	25.0	24.9	37.0	37.0	37.0	37.0	112.0	100.0	94.2	99.4	100.0	91.9
Pressure (atm)	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
Vapor mass fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9998	0.0000	0.0000	0.6967	0.0000	1.0000
Liquid mass fraction	1.0000	1.0000	0.0000	0.9977	0.9977	0.9977	0.6970	1.0000	0.0002	1.0000	1.0000	0.3033	1.0000	0.0000
Solid mass fraction	0.0000	0.0000	1.0000	0.0023	0.0023	0.0023	0.3030	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Mass enthalpy (kJ/kg)	-7,246.9	-15,864.4	-11,859.1	-15,739.7	-15,690.0	-15,659.6	-14,514.0	-15,668.3	-13,138.5	-15,529.0	-14,890.6	-13,385.7	-15,520.0	-7,592.1
Molar flow (kmol/h)	11.3	4,245.2	7.2	4,263.6	4,263.6	4,266.7	29.6	4,237.2	4,237.2	3,435.3	801.9	801.9	755.6	46.3
Volume flow (m ³ /h)	0.8	76.9	0.0	77.7	78.7	79.1	0.4	78.7	133,018.6	67.5	16.6	16,636.8	14.9	1,371.1
Mass flow (kg/h)	1,042.0	76,477.7	177.1	77,696.8	77,696.8	77,696.8	584.6	77,112.3	77,112.3	61,973.2	15,139.1	15,139.1	13,638.5	1,500.6
Comp. Mass fraction														
Water	0.0000	1.0000	0.0000	0.9843	0.9843	0.9843	0.6876	0.9866	0.9866	0.9982	0.9387	0.9387	0.9975	0.4043
Glycerol	1.0000	0.0000	0.0000	0.0134	0.0134	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<i>E. coli</i>	0.0000	0.0000	1.0000	0.0023	0.0023	0.0023	0.3030	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Succinic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0002	0.0003	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000
Lactic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0002	0.0003	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000
Acetic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0002	0.0003	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000
Butyric acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0006	0.0009	0.0009	0.0006	0.0023	0.0023	0.0023	0.0021
Ethanol	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0006	0.0009	0.0009	0.0000	0.0045	0.0045	0.0001	0.0448
Butanol	0.0000	0.0000	0.0000	0.0000	0.0000	0.0107	0.0075	0.0107	0.0107	0.0000	0.0545	0.0545	0.0001	0.5488

Table S.3. Process streams for butanol production (continuation).

Stream	15	16	17	18	19	20
Temperature (°C)	112.2	112.2	112.2	78.5	115.6	35.1
Pressure (atm)	1.3	1.3	1.3	1.0	1.0	1.0
Vapor mass fraction	1.0000	1.0000	0.0000	0.0000	0.0000	0.0000
Liquid mass fraction	0.0000	0.0000	1.0000	1.0000	1.0000	1.0000
Solid mass fraction	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Mass enthalpy (kJ/kg)	-7,556.0	-12,018.5	-4,396.5	-7,009.2	-4,185.8	-4,440.3
Molar flow (kmol/h)	46.3	34.5	11.8	1.6	10.2	10.2
Volume flow (m ³ /h)	1,084.2	810.8	1.1	0.1	1.1	0.9
Mass flow (kg/h)	1,500.6	688.0	812.6	60.6	752.1	752.1
Comp. Mass fraction						
Water	0.4043	0.8701	0.0100	0.1177	0.0013	0.0013
Glycerol	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<i>E. coli</i>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Succinic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Lactic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Acetic acid	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Butyric acid	0.0021	0.0005	0.0034	0.0000	0.0037	0.0037
Ethanol	0.0448	0.0098	0.0745	0.8758	0.0100	0.0100
Butanol	0.5488	0.1197	0.9121	0.0065	0.9850	0.9850

Table S.4. Equipment details for ethanol production.

Heat Exchangers			
HE-1		HE-2	
Duty (GJ.h ⁻¹)	5.16	Duty (GJ.h ⁻¹)	0.47
Area (m ²)	6.75	Area (m ²)	5.04
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Utility flowrate - LP Steam (kg.h ⁻¹)	2,353.21	Utility flowrate - Cooling Water (kg.h ⁻¹)	22,441.70
Cost (US\$)	8,037.09	Cost (US\$)	3,835.58
Compressor			
CP-1			
Volume flowrate (m ³ .h ⁻¹)	366.90		
Pressure increase (kPa)	278.68		
Power (kW)	18.22		
Cost (US\$)	99,709.03		
Adsorption Vessels			
PSA-1			
Number of Vessels	4		
Height / diameter (m)	0.9 / 0.3		
Cycle time (min)	11.50		
Total Cost (US\$)	53,145.63		
Reactors			
R-1			
Number of Vessels	10		
Height / diameter (m)	13.84 / 6.92		
Cycle time (min)	70.00		
Total Cost (US\$)	6,358,772.64		
Distillation Column			
C-1		Condenser (Partial)	
Temperature - top / bottom (°C)	78.16 / 99.99	Duty (GJ.h ⁻¹)	2.55
Pressure - top / bottom (kPa)	101.33 / 101.33	Area (m ²)	17.18
Height / diameter (m)	21.93 / 1.03	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Number of stages	62	Utility flowrate – Cooling Water (kg.h ⁻¹)	122,055.00
Reflux ratio (molar)	5	Cost (US\$)	4,666.79
Cost (US\$)	238,934.56		
Reboiler			
Duty (GJ.h ⁻¹)	30.91		
Area (m ²)	81.51		
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01		
Utility flowrate - LP Steam (kg.h ⁻¹)	14,101.30		
Cost (US\$)	50,467.03		
Other			
CFG-1			
Solid mass flowrate (ton.h ⁻¹)	0.04		
Cost (US\$)	92,232.66		

Table S.5. Equipment details for propanol production.

Heat Exchangers			
HE-1		HE-2	
Duty (GJ.h ⁻¹)	0.67	Duty (GJ.h ⁻¹)	0.60
Area (m ²)	0.85	Area (m ²)	8.70
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Utility flowrate - LP Steam (kg.h ⁻¹)	4,129.02	Utility flowrate - Cooling Water (kg.h ⁻¹)	28,972.90
Cost (US\$)	5,768.13	Cost (US\$)	4,185.59
Compressor			
CP-1			
Volume flowrate (m ³ .h ⁻¹)	1,087.53		
Pressure increase (kPa)	33.57		
Power (kW)	11.95		
Cost (US\$)	76,449.58		
Adsorption Vessels			
PSA-1			
Number of Vessels	4		
Height / diameter (m)	6.92 / 2.31		
Cycle time (min)	480		
Total Cost (US\$)	434,943.00		
Reactors			
R-1			
Number of Vessels	10		
Height / diameter (m)	11.7 / 5.85		
Cycle time (min)	140		
Total Cost (US\$)	5,038,920.35		
Distillation Column			
C-1		Condenser (Partial)	
Temperature - top / bottom (°C)	89.85 / 100.08	Duty (GJ.h ⁻¹)	0.06
Pressure - top / bottom (kPa)	101.33 / 101.33	Area (m ²)	0.48
Height / diameter (m)	19.72 / 0.91	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Number of stages	56	Utility flowrate – Cooling Water (kg.h ⁻¹)	2,957.36
Reflux ratio (molar)	0.04	Cost (US\$)	2,636.36
Cost (US\$)	201,330.25		
Reboiler			
Duty (GJ.h ⁻¹)	9.05		
Area (m ²)	45.30		
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01		
Utility flowrate - LP Steam (kg.h ⁻¹)	4,129.02		
Cost (US\$)	42,393.12		
Other			
CFG-1			
Solid mass flowrate (ton.h ⁻¹)	0.19		
Cost (US\$)	145,276.72		

Table S.6. Equipment details for butanol production.

Heat Exchangers			
HE-1		HE-2	
Duty (GJ.h ⁻¹)	3.86	Duty (GJ.h ⁻¹)	195.08
Area (m ²)	5.04	Area (m ²)	612.41
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01
Utility flowrate - LP Steam (kg.h ⁻¹)	1,759.55	Utility flowrate - Cooling Water (kg.h ⁻¹)	89,001.50
Cost (US\$)	7,671.61	Cost (US\$)	147,322.19
HE-3		HE-4	
Duty (GJ.h ⁻¹)	22.78	Duty (GJ.h ⁻¹)	0.19
Area (m ²)	100.73	Area (m ²)	2.65
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Utility flowrate - LP Steam (kg.h ⁻¹)	10,394.20	Utility flowrate - Cooling Water (kg.h ⁻¹)	9,173.47
Cost (US\$)	54,564.43	Cost (US\$)	3,460.05
Compressor			
CP-1			
Volume flowrate (m ³ .h ⁻¹)	1,371.12		
Pressure increase (kPa)	33.57		
Power (kW)	15.06		
Cost (US\$)	88,423.42		
Adsorption Vessels			
PSA-1			
Number of Vessels	4		
Height / diameter (m)	7.70 / 2.57		
Cycle time (min)	480		
Total Cost (US\$)	530,690.07		
Reactors			
R-1			
Number of Vessels	10		
Height / diameter (m)	11.14 / 5.57		
Cycle time (min)	47		
Total Cost (US\$)	4,714,986.88		
Distillation Columns			
C-1		C-1 Condenser (Total)	
Temperature - top / bottom (°C)	89.85 / 100.08	Duty (GJ.h ⁻¹)	0.06
Pressure - top / bottom (kPa)	101.33 / 101.33	Area (m ²)	0.48
Height / diameter (m)	19.72 / 0.91	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Number of stages	56	Utility flowrate – Cooling Water (kg.h ⁻¹)	2,957.36
Reflux ratio (molar)	0.04	Cost (US\$)	2,636.36
Cost (US\$)	201,330.25		
C-1 Reboiler		C-2	
Duty (GJ.h ⁻¹)	9.05	Temperature - top / bottom (°C)	91.94 / 99.99
Area (m ²)	45.30	Pressure - top / bottom (kPa)	101.33 / 101.33
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01	Height / diameter (m)	5.29 / 1.16
Utility flowrate - LP Steam (kg.h ⁻¹)	4,129.02	Number of stages	6.0
Cost (US\$)	42,393.12	Reflux ratio (molar)	12.00
		Cost (US\$)	134,799.47
C-2 Reboiler		C-2 Condenser (Partial)	
Duty (GJ.h ⁻¹)	2.70	Duty (GJ.h ⁻¹)	23.12
Area (m ²)	13.46	Area (m ²)	175.44
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Utility flowrate - LP Steam (kg.h ⁻¹)	1,231.82	Utility flowrate – Cooling Water (kg.h ⁻¹)	1,107,790.00
Cost (US\$)	8,976.44	Cost (US\$)	55,650.30

Table S.6. Equipment details for butanol production (continuation).

Distillation Columns			
C-3		C-3 Condenser (Total)	
Temperature - top / bottom (°C)	78.5 / 115.63	Duty (GJ.h ⁻¹)	0.76
Pressure - top / bottom (kPa)	101.33 / 101.33	Area (m ²)	7.28
Height / diameter (m)	3.95 / 0.56	U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	2,045.75
Number of stages	8.0	Utility flowrate – Cooling Water (kg.h ⁻¹)	36,390.60
Reflux ratio (molar)	11.30	Cost (US\$)	4,068.10
Cost (US\$)	56,525.45		
C-3 Reboiler			
Duty (GJ.h ⁻¹)	0.76		
Area (m ²)	10.48		
U (kJ.°C ⁻¹ .m ⁻² .h ⁻¹)	8,183.01		
Utility flowrate - LP Steam (kg.h ⁻¹)	346.53		
Cost (US\$)	4,312.02		
Other			
CFG-1			
Solid mass flowrate (ton.h ⁻¹)	0.18		
Cost (US\$)	142,364.40		