

Improving Purity Propylene Glycol by Modifying Glycerol Hydrogenolysis Process

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Table S1. Heat and material balance before modification

Stream No	1	2	3	4	5	6	7	8
Total Phase Properties								
Vapour Fraction	1	0	0.8343	0	1	1	0.004	0
Temperature (°C)	226.96	219.85	219.85	219.85	219.85	-123.35	-123.3	348.71
Pressure (kPa)	4000	4000	4000	4000	4000	3000	3000	3600
Molecular Weight	2.016	92.095	17.063	65.213	6.8776	2.016	18.2	79.448
Molar Flow (kgmole/h)	52.232	10.475	62.707	10.949	51.758	1.91E-07	2.545	8.4044
Mass Flow (kg/h)	105.3	964.7	1070	714.03	355.97	3.84E-07	46.32	667.71
Heat Flow (kJ/h)	302427	-7E+06	-6E+06	-5E+06	-2E+06	-0.0008	-8E+05	-4E+06
Std Gas Flow (STD_m ³ /h)	1235	247.68	1482.7	258.89	1223.8	4.51E-06	60.17	198.72
Vapor Phase Properties								
Mass Flow (kg/h)	105.3		119.36	0	355.97	3.84E-07	0.023	
Molecular Weight	2.016		2.2816	6.8776	6.8776	2.016	2.016	
Mass Density (kg/m ³)	1.9394		2.2265	6.7116	6.7116	4.85582	4.856	
Actual Volume Flow (m ³ /h)	54.296		53.61	0	53.039	7.92E-08	0.005	
Z Factor	1		1	1	1	1.00001	1	
Cp/Cv	1.4033		1.3961	1.3149	1.3149	1.41975	1.42	
Viscosity (cP)	0.0131		0.013	0.0128	0.0128	0.00501	0.005	
Mass Heat Capacity (kJ/kg°C)	14.351		12.844	5.0479	5.0479	13.9495	13.95	
Thermal Conductivity (W/mK)	0.2596		0.2545	0.188	0.188	0.10322	0.103	
Liquid Phase Properties								
Mass Flow (kg/h)		964.7	950.64	714.03	0			667.71
Molecular Weight		92.095	91.483	65.213	65.213			79.448
Mass Density (kg/m ³)		944.01	935.23	745.54	745.54			534.14

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Actual Volume Flow (m ³ /h)		1.0219	1.0165	0.9577	0			1.2501
Z Factor		0.0952	0.0955	0.0854	0.0854			0.1036
Cp/Cv		1.0305	1.0307	3.3936	3.3936			0.2072
Viscosity (cP)		2.2625	2.2135	0.5142	0.5142			0.1183
Mass Heat Capacity (kJ/kg°C)		3.0471	3.0488	3.5803	3.5803			10.982
Thermal Conductivity (W/mK)		0.1622	0.1616	0.2045	0.2045			0.0418
Composition								
Glycerol	0	1	0.901589	0.246746	0.006421	0	0	0.2639
H ₂ O	0	0	0	0.064555	0.302563	0	0.9890	0.0011
Hydrogen	1	0	0.098411	4.41E-05	0.247372	1	0.0061	0
12-C3diol	0	0	0	0.688655	0.443644	0	0.0049	0.7350
Total Mass Fractions	1	1	1	1	1	1	1	1

Table S2. Heat and material balance after modification

Stream No	1	2	3	4	5	6	7	8	9
Total Phase Properties									
Vapour Fraction	0	1	0.8353	1	0	0.985	1	0	1
Temperature (°K)	500	509	500	547.2	547.2	547.2	547.2	547.2	547.2
Pressure (kPa)	4000	4000	4000	4000	4000	4000	4000	4000	4000
Molecular Weight	92.095	2.016	17.03	16.18	72.83	17.03	16.16	72.79	16.16
Molar Flow (kgmole/s)	0.009049	0.04524	0.05429	0.05347	0.0008170	0.05429	0.05346	0.0008316	0.03437
Mass Flow (kg/s)	0.833	0.0912	0.9245	0.8650	0.0594	0.9245	0.86401	0.06053	0.5556
Heat Flow (kJ/s)	-5661.636	273.56	-5388.07	-5012.45	-375.66	-5388.11	-5007.082	-382.13	-3219.523
Std Gas Flow (STD_m ³ /s)	0.213	1.069	1.283	1.264	0.0193	1.283	1.264	0.019	0.812
Vapor Phase Properties									
Mass Flow (kg/s)		0.0912	0.106	0.865	0	0.865	0.864	0	0.555
Molecular Weight		2.016	2.3551	16.176	16.177	16.177	16.162	16.162	16.161
Mass Density (kg/m ³)		1.906	2.2661	14.222	14.222	14.222	14.213	14.213	14.213
Actual Volume Flow (m ³ /s)		0.0478	0.0471	0.0608	0	0.0608	0.0607	0	0.0390
Z Factor		1	1	1	1	1	1	1	1
Cp/Cv		1.403	1.3936	1.198	1.198	1.198	1.1981	1.1981	1.1981
Viscosity (cP)		0.000013	0.000013	0.0000172	0.0000172	0.0000172	0.0000172	0.0000172	0.0000172
Mass Heat Capacity (kJ/kg°C)		14.36	12.499	3.1103	3.1104	3.1104	3.1114	3.1114	3.1114

Thermal Conductivity (W/mK)		0.263	0.2563	0.1419	0.1419	0.1419	0.1419	0.1419	0.1419
Liquid Phase Properties									
Mass Flow (kg/h)	0.833		0.817	0	0.0594	0.0594	0	0.0605	0
Molecular Weight	92.095		91.449	72.826	72.826	72.826	72.787	72.787	72.787
Mass Density (kg/m³)	931.839		922.64	685.63	685.63	685.63	685.63	685.63	685.63
Actual Volume Flow (m³/h)	8.94289 181674 135e-004		0.0000886	0	0.0000886	0.0000886	0	0.0000828	0
Z Factor	0.0951		0.0954	0.0934	0.0934	0.0934	0.0934	0.0934	0.0934
Cp/Cv	1.0303		1.0305	1.0297	1.0297	1.0297	1.0297	1.0297	1.0297
Viscosity (cP)	2.02639		1.9811	0.3263	0.3263	0.3263	0.3258	0.3258	0.3258
Mass Heat Capacity (kJ/kg°K)	3.071		3.072	3.964	3.964	3.964	3.964	3.964	3.964
Thermal Conductivity (W/mK)	0.1599		0.159	0.144	0.144	0.144	0.1443	0.1443	0.1443
Composition									
Glycerol	1	0	0.9013	0.0242	0.3478	0.0451	0.024	0.3458	0.024
H ₂ O	0	0	0	0.1768	0.0319	0.1675	0.17699	0.03201	0.17699
Hydrogen	0	1	0.0987	0.0854	6.42E-05	0.0799	0.0855	6.40E-05	0.0855
12-C3diol	0	0	0	0.7135	0.62018	0.7075	0.71351	0.62209	0.71351
Total Mass Fractions	1	1	1	0.1768243 98845616	0.0319	0.167	0.176	0.032	1

Table S2. Heat and material balance after modification (continuous)

Stream No	10	11	12	13	14	15	16	17
Total Phase Properties								
Vapour Fraction	1	0	1	1	1	0	0	1
Temperature (°K)	1088.1	557.7	1088.1	263.4	561.2	619.3	-102.09	349.307
Pressure (Pa)	4000	4000	4000	4000	4000	4000	4999	4999
Molecular Weight	2.01	46.98	2.016	2.016	23.81	71.59	27.056	77.5915
Molar Flow (kgmole/s)	0.01308	0.00603	0.01308	0.0321	0.00307	0.00376	0	11.2338
Mass Flow (kg/s)	0.0263	0.2820	0.0263	0.0648	0.0731	0.269	361.77	871.645
Heat Flow (kJ/s)	305.2	-2092.7	305.2	-31.6	-765.6	-1515.5	-4E+06	-5E+06
Std Gas Flow (STD_m³/s)	0.309	0.141	0.309	0.760	0.0726	0.0889	316.15	265.616
Vapor Phase Properties								
Mass Flow (kg/s)	0.0263	0	0.0263	0.0648	0.0731	233.41	0.0115	
Molecular Weight	2.016	26.86	2.01	2.01	23.81	58.66	2.016	
Mass Density (kg/m³)	0.8913	23.172	0.8913	3.68	25.50	56.94	7.086	
Actual Volume Flow (m³/s)	0.0295	0	0.0295	0.017	0.002	0	0.0016	
Z Factor	1	1	1	1	1	1	1	
Cp/Cv	1.36	1.139	1.36	1.415	1.13	1.06	1.4189	
Viscosity (cP)	0.00002	0.00001	0.00003	0.000008	0.00002	0.00002	0.0056	
Mass Heat Capacity (kJ/kg°K)	15.27	2.523	15.27	14.06	2.96	2.20	13.969	
Thermal Conductivity (W/mK)	0.44	0.042	0.4455	0.161	0.0453	0.04.2	0.1167	
Liquid Phase Properties								
Mass Flow (kg/h)	0			1232.9				871.645
Molecular Weight	72.787			50.15				77.5915
Mass Density (kg/m³)	685.63			598.33				483.37

Actual Volume Flow (m³/h)	0			2.0605				1.80326
Z Factor	0.0934			0.0725				0.15505
Cp/Cv	1.0297			1.7711				1.00803
Viscosity (cP)	0.3258			0.1402				0.06181
Mass Heat Capacity (kJ/kg°C)	3.9649			4.4978				13.4566
Thermal Conductivity (W/mK)	0.1444			0.2436				0.03113
Composition								
Glycerol	0.024	0.024	0	0.0262	0	0	0	0.105
H ₂ O	0.17699	0.17699	0	0.193	0	0	0.6803	0.0251
Hydrogen	0.0855	0.0855	1	0	1	1	0.0001	0
12-C3diol	0.71351	0.71351	0	0.7802	0	0	0.319	0.869
Total Mass Fractions	1	1	1	1	1	1	1	1