

Enhancing Propylene Glycol Product Yield by Modifying the Glycerol Hydrogenation Process

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Table S1. Heat and material balance for modified glycerol hydrogenation process

	Unit	1	2	3	4	5	6	7	8	9	10	11	12
Total Phase Properties													
Vapour Fraction		0.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.9818	1.0000	0.0000	0.9992	1.0000
Temperature	C	219.0000	-9.6840	220.8042	200.0000	21.2066	28.8076	300.0000	258.7780	215.0000	215.0000	215.0000	273.9000
Pressure	kPa	101.3250	3000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000
Molecular Weight		92.0950	2.0160	92.0950	92.0950	2.0160	2.0160	2.0160	4.5926	4.5315	78.7921	4.5926	4.5926
Molar Flow	kgmole/h	32.5800	1000.0000	32.5800	32.5800	1000.0000	1106.4235	1106.4235	1139.0035	1138.0668	0.9367	1139.0035	1139.0035
Mass Flow	kg/h	3000.4551	2016.0000	3000.4551	3000.4551	2016.0000	2230.5499	2230.5499	5231.0050	5157.2006	73.8075	5231.0081	5231.0081
Heat Flow	kJ/h	-20457002.6602	-984488.4126	-20440506.2471	-20628798.8190	-107803.1029	119759.2796	8752507.6336	-11876291.1854	-14274250.5663	-484472.1840	-14758722.7503	-12511642.9918
Std Gas Flow	STD_m3/h	770.3357	23644.4364	770.3357	770.3357	23644.4364	26160.7606	26160.7606	26931.0963	26908.9477	22.1486	26931.0963	26931.0963
Vapor Phase Properties													
Mass Flow	kg/h		2016.0000			2016.0000	2230.5499	2230.5499	3340.1270	5157.2006	0.0000	5157.2006	5231.0081
Molecular Weight			2.0160			2.0160	2.0160	2.0160	2.9868	4.5315	4.5315	4.5315	4.5926
Mass Density	kg/m3		2.7610			3.2950	3.2120	1.6922	2.7014	4.4661	4.4661	4.4661	4.0389
Actual Volume Flow	m3/h		730.1802			611.8438	694.4390	1318.1245	1236.4419	1154.7495	0.0000	1154.7495	1295.1463
Z Factor			1.0000			1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Cp/Cv			1.4151			1.4136	1.4133	1.3993	1.3742	1.3459	1.3459	1.3459	1.3379
Viscosity	cP		0.0079			0.0087	0.0089	0.0143	0.0138	0.0130	0.0130	0.0130	0.0142
Mass Heat Capacity	kJ/kg-C		14.0608			14.0945	14.1030	14.4534	10.2232	7.1384	7.1384	7.1384	7.1677
Thermal Conductivity	W/m-K		0.1604			0.1755	0.1789	0.2856	0.2616	0.2241	0.2241	0.2241	0.2425
Liquid Phase Properties													
Phase Mass Flow	kg/h	3000.4551		3000.4551	3000.4551				1890.8780	0.0000	73.8075	73.8075	0.0000
Phase Molecular Weight		92.0950		92.0950	92.0950				91.2845	78.7921	78.7921	78.7921	74.9863
Phase Mass Density	kg/m3	945.4823		942.3472	978.5003				864.9093	813.6310	813.6310	813.6310	4165.9036
Phase Actual Volume Flow	m3/h	3.1735		3.1840	3.0664				2.1862	0.0000	0.0907	0.0907	0.0000
Phase Z Factor		0.0024		0.0952	0.0957				0.0955	0.0954	0.0954	0.0954	0.0158
Phase Cp/Cv		1.0306		1.0305	1.0312				1.0293	1.0327	1.0327	1.0327	1.0299
Phase Viscosity	cP	2.2936		2.2282	3.1694				1.2493	0.9366	0.9366	0.9366	1.3234
Phase Mass Heat Capacity	kJ/kg-C	3.0443		3.0504	2.9837				3.1960	3.3319	3.3319	3.3319	3.8141

Phase Thermal Conductivity	<i>W/m-K</i>	0.1624		0.1619	0.1685				0.1487	0.1637	0.1637	0.1637	0.1441
Phase Surface Tension	<i>dyne/cm</i>	36.9960		36.7149	39.9540				30.5105	26.8176	26.8176	26.8176	17.7073
Composition													
Comp Mole Frac (Propylene Glycol)	<i>mole%</i>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0268	0.4668	0.0272	0.0272
Comp Mole Frac (Glycerol)	<i>mole%</i>	1.0000	0.0000	1.0000	1.0000	0.0000	0.0000	0.0000	0.0286	0.0011	0.4550	0.0014	0.0014
Comp Mole Frac (H2O)	<i>mole%</i>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0271	0.0756	0.0272	0.0272
Comp Mole Frac (Hydrogen)	<i>mole%</i>	0.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.9714	0.9450	0.0026	0.9442	0.9442
Total Mole Fractions		1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	<i>Unit</i>	13	14	15	16	17	18	19	20	21	22	23	24
Total Phase Properties													
Vapour Fraction		0.0000	1.0000	1.0000	1.0000	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
Temperature	<i>C</i>	273.9000	273.9000	273.9000	100.0000	100.0000	100.0000	252.6872	113.9805	100.0000	343.4889	-10.7188	30.0000
Pressure	<i>kPa</i>	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	4000.0000	3000.0000	101.3250
Molecular Weight		74.9863	4.5926	4.5926	2.1971	52.2200	2.0160	20.6345	47.1016	2.0160	76.1365	18.7817	76.1365
Molar Flow	<i>kgmole/h</i>	0.0000	1025.1032	113.9004	108.4458	5.4545	107.3910	1.0548	6.5093	106.4235	3.2141	3.2952	3.2141
Mass Flow	<i>kg/h</i>	0.0000	4707.9073	523.1008	238.2662	284.8346	216.5003	21.7659	306.6005	214.5498	244.7103	61.8903	244.7103
Heat Flow	<i>kJ/h</i>	0.0000	11260478.6926	-1251164.2992	-30262.4497	2169050.7301	229631.1416	-289852.8835	-2458903.6136	227562.3825	-1299753.3293	-956600.9742	-1595548.4422
Std Gas Flow	<i>STD_m3/h</i>	0.0000	24237.9867	2693.1096	2564.1409	128.9687	2539.1999	24.9409	153.9097	2516.3242	75.9955	77.9142	75.9955
Vapor Phase Properties													
Mass Flow	<i>kg/h</i>	0.0000	4707.9073	523.1008	238.2662	0.0000	216.5003	0.0000		214.5498			
Molecular Weight		4.5926	4.5926	4.5926	2.1971	2.1971	2.0160	18.3810		2.0160			
Mass Density	<i>kg/m3</i>	4.0389	4.0389	4.0389	2.8327	2.8327	2.5992	16.8171		2.5992			
Actual Volume Flow	<i>m3/h</i>	0.0000	1165.6317	129.5146	84.1130	0.0000	83.2948	0.0000		82.5444			
Z Factor		1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000		1.0000			
Cp/Cv		1.3379	1.3379	1.3379	1.4079	1.4079	1.4099	1.1224		1.4099			
Viscosity	<i>cP</i>	0.0142	0.0142	0.0142	0.0105	0.0105	0.0106	0.0141		0.0106			
Mass Heat Capacity	<i>kJ/kg-C</i>	7.1677	7.1677	7.1677	13.0617	13.0617	14.1865	4.1487		14.1865			
Thermal Conductivity	<i>W/m-K</i>	0.2425	0.2425	0.2425	0.2062	0.2062	0.2099	0.0428		0.2099			
Liquid Phase Properties													
Phase Mass Flow	<i>kg/h</i>	0.0000	0.0000	0.0000	0.0000	284.8346			306.6005		244.7103		244.7103
Phase Molecular Weight		74.9863	74.9863	74.9863	52.2200	52.2200			47.1016		76.1365		76.1365

Phase Mass Density	<i>kg/m3</i>	4165.9036	4165.9036	4165.9036	870.8062	870.8062			851.4841		462.9629		1022.1686
Phase Actual Volume Flow	<i>m3/h</i>	0.0000	0.0000	0.0000	0.0000	0.3271			0.3601		0.5286		0.2394
Phase Z Factor		0.0158	0.0158	0.0158	0.0773	0.0773			0.0687		0.1283		0.0030
Phase Cp/Cv		1.0299	1.0299	1.0299	1.4564	1.4564			1.3510		1.0118		1.0397
Phase Viscosity	<i>cP</i>	1.3234	1.3234	1.3234	1.7517	1.7517			1.2003		0.0599		20.4281
Phase Mass Heat Capacity	<i>kJ/kg-C</i>	3.8141	3.8141	3.8141	3.2321	3.2321			3.3299		9.3323		2.8630
Phase Thermal Conductivity	<i>W/m-K</i>	0.1441	0.1441	0.1441	0.3175	0.3175			0.3587		0.0406		0.1826
Phase Surface Tension	<i>dyne/cm</i>	17.7073	17.7073	17.7073	40.4262	40.4262			41.0506		1.0233		35.2790
Composition													
Comp Mole Frac (Propylene Glycol)	<i>mole%</i>	0.4761	0.0272	0.0272	0.0004	0.5871	0.0000	0.0451	0.4993	0.0000	0.9975	0.0133	0.9975
Comp Mole Frac (Glycerol)	<i>mole%</i>	0.3996	0.0014	0.0014	0.0000	0.0015	0.0000	0.0000	0.0013	0.0000	0.0025	0.0000	0.0025
Comp Mole Frac (H2O)	<i>mole%</i>	0.1067	0.0272	0.0272	0.0093	0.4111	0.0000	0.9549	0.4993	0.0000	0.0000	0.9862	0.0000
Comp Mole Frac (Hydrogen)	<i>mole%</i>	0.0176	0.9442	0.9442	0.9903	0.0003	1.0000	0.0000	0.0002	1.0000	0.0000	0.0005	0.0000
Total Mole Fractions		1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000