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Research Article

Enhancing Mass and Yield Product of Propylene Glycol Production through Glycerol Hydrogenolysis

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Table S1. Material balance and composition of process before modification

Stream	Unit	Glycerol In	Hydrogen In	High Press. Glycerol	Feed + Recycle	Reactor Inlet
Vapour Fraction		0	1	0	1	0.960464332
Temperature	K	298.15	493	299.3571936	439.2655095	448.8214608
Pressure	kPa	1000	4000	4000	4000	4000
Molar Flow	kgmole/h	15.49422466	77.47112332	15.49422466	539.496345	554.9905697
Mass Flow	tonne/year	12500	1368.152455	12500	14045.63041	26545.63041
Liquid Volume Flow	m^3/h	1.131791911	2.235668458	1.131791911	15.4189956	16.55078752
Heat Flow	kJ/h	-10499984.9	432626.2603	-10495564.19	-4092830.357	-14111132.83
Comp Mole Frac (Glycerol)		1	0	1	0.0000158	0.0279333
Comp Mole Frac (Hydrogen)		0	1	0	0.9544173	0.9277719
Comp Mole Frac (12-C3diol)		0	0	0	0.0038834	0.0037750
Comp Mole Frac (H2O)		0	0	0	0.0416836	0.0405198

Stream	*Unit*	Vapor Phase	Liquid Phase	HE-01 Inlet	High Temp. Glycerol		Sep-01 Inlet
Vapour Fraction		1	0	0.991897893	0		0.985464888
Temperature	*K*	490.75	490.75	490.7500204	423.15		475.0669713
Pressure	*kPa*	4000	4000	4000	3990		3990
Molar Flow	*kgmole/h*	550.4939842	4.496585404	554.9905697	15.49422466		554.9905697
Mass Flow	*tonne/year*	23626.39348	2919.247984	26545.64146	12500		26545.64146
Liquid Volume Flow	*m3/h*	16.12798307	0.287662017	16.41564509	1.131791911		16.41564509
Heat Flow	*kJ/h*	-10939621.93	-2272637.83	-13212259.8	-10018320.33		-13689503.62
Comp Mole Frac (Glycerol)		0.0012722	0.4820666	0.0051677	1.0000000		0.0051677
Comp Mole Frac (Hydrogen)		0.9123764	0.0027188	0.9050063	0.0000000		0.9050063
Comp Mole Frac (12-C3diol)		0.0238845	0.3517195	0.0265406	0.0000000		0.0265406
Comp Mole Frac (H2O)		0.0624669	0.1634951	0.0632855	0.0000000		0.0632855

Stream	*Unit*	Feed Glycerol for Reactor	Top Result	Bottom Result	Purge	Tee-Out
Vapour Fraction		0	1	0	1	1
Temperature	*K*	423.1543969	430.15	430.15	430.15	430.15
Pressure	*kPa*	4000	3990	3990	3990	3990
Molar Flow	*kgmole/h*	15.49422466	530.4841449	24.50642474	53.04841449	477.4357304
Mass Flow	*tonne/year*	12500	14555.22844	11990.41302	1455.522844	13099.7056
Liquid Volume Flow	*m3/h*	1.131791911	15.1367389	1.278906189	1.51367389	13.62306501
Heat Flow	*kJ/h*	-10018302.48	-5201398.58	-10147916.7	-520139.8576	-4681258.719
Comp Mole Frac (Glycerol)		1	0.0000184	0.11663	0.00002	0.00002
Comp Mole Frac (Hydrogen)		0	0.9467810	0.00072	0.94678	0.94678
Comp Mole Frac (12-C3diol)		0	0.0045338	0.50292	0.00453	0.00453
Comp Mole Frac (H2O)		0	0.0486668	0.37973	0.04867	0.04867

Stream	*Unit*	Compre-01 Out	H2O Out	Bottom COL-01	Propylene Glycol Out	Glycerol out	Recycle
Vapour Fraction		1	0.001480202	0	0	0	1
Temperature	*K*	430.553713	161.2801861	621.0056944	612.2877613	684.0213799	430.5537117
Pressure	*kPa*	4000	3800	3999	3700	3800	4000
Molar Flow	*kgmole/h*	477.4357304	10.14396326	14.36245809	10.94998706	3.412471016	462.0252217
Mass Flow	*tonne/year*	13099.7056	2021.255594	9969.157368	7303.97612	2665.181238	12677.47795
Liquid Volume Flow	*m3/h*	13.62306501	0.229104822	1.049801268	0.800464475	0.249336793	13.18332715
Heat Flow	*kJ/h*	-4675558.712	-3179373.58	-6286101.25	-4465924.929	-1814222.262	-4525456.618
Comp Mole Frac (Glycerol)		0.0000184	0.0000001	0.1990074	0.0066208	0.8163407	0.0000184
Comp Mole Frac (Hydrogen)		0.9467810	0.0017376	0.0000000	0.0000000	0.0000000	0.9467741
Comp Mole Frac (12-C3diol)		0.0045338	0.0819361	0.8002459	0.9923999	0.1836593	0.0045345
Comp Mole Frac (H2O)		0.0486668	0.9163262	0.0007467	0.0009794	0.0000000	0.0486729

Table S2. Material balance and composition of process after modification

Stream	*Unit*	Glycerol in	Hydrogen in	High Press. Glycerol	Feed+Recycle 01	Reactor Inlet	Vapour Phase
Vapour Fraction		0	1	0	1	0.956071752	1
Temperature	*C*	25	219.85	26.20719238	165.361601	175.7177114	217.6
Pressure	*kPa*	1000	4000	4000	4000	4000	4000
Molar Flow	*kgmole/h*	15.49422466	77.47112332	18.97473554	590.157614	609.1323495	602.9087001
Mass Flow	*tonne/year*	12500	1368.152455	15307.90355	15467.94457	30775.84812	26780.09157
Liquid Volume Flow	*m3/h*	1.131791911	2.235668458	1.386029333	16.86067621	18.24670554	17.6848546
Heat Flow	*kJ/h*	-10499984.9	432626.2603	-12853205.15	-4654730.523	-16923465.46	-12849177.33
Comp Mole Frac (Glycerol)		1.00000000	0.00000000	0.99999817	0.00001579	0.03116567	0.00118333
Comp Mole Frac (Hydrogen)		0.00000000	1.00000000	0.00000000	0.95328071	0.92358560	0.90743096
Comp Mole Frac (12-C3diol)		0.00000000	0.00000000	0.00000169	0.00391447	0.00379259	0.02558299
Comp Mole Frac (H2O)		0.00000000	0.00000000	0.00000015	0.04278903	0.04145614	0.06580272
Comp Mole Frac (Glycerol)		1.00000000	0.00000000	0.99999817	0.00001579	0.03116567	0.00118333

	Unit	Liquid Phase	HE-01 Inlet	High Temp. Glycerol	Inlet Sep-01	Feed Glycerol for Reactor	Top result
Vapour Fraction		0	0.989782734	0	0.98177267	0	1
Temperature	*C*	217.6	217.6000429	150	201.4878517	150.0043969	157
Pressure	*kPa*	4000	4000	3990	3990	4000	3990
Molar Flow	*kgmole/h*	6.223649415	609.1323495	18.97473554	609.1323495	18.97473554	578.5694849
Mass Flow	*tonne/year*	3995.77009	30775.86165	15307.90355	30775.86165	15307.90355	15953.64267
Liquid Volume Flow	*m3/h*	0.396360892	18.0812155	1.386029333	18.0812155	1.386029333	16.49952487
Heat Flow	*kJ/h*	-3104055.347	-15953232.68	-12268756.8	-16537681.03	-12268734.94	-5832252.629
Comp Mole Frac (Glycerol)		0.44967196	0.00576565	0.99999817	0.00576565	0.99999817	0.00001789
Comp Mole Frac (Hydrogen)		0.00255009	0.89818558	0.00000000	0.89818558	0.00000000	0.94559438
Comp Mole Frac (12-C3diol)		0.37887065	0.02919261	0.00000169	0.02919261	0.00000169	0.00447623
Comp Mole Frac (H2O)		0.16890730	0.06685616	0.00000015	0.06685616	0.00000015	0.04991150
Comp Mole Frac (Glycerol)		0.44967196	0.00576565	0.99999817	0.00576565	0.99999817	0.00001789

	Unit	Bottom Result	Purge	Tee-Out	Compre-01 Out	H2O Out	Propylene Glycol Out
Vapour Fraction		0	1	1	1	2.83E-06	0
Temperature	*C*	157	157	157	157.4036527	-108.1969272	340.4618668
Pressure	*kPa*	3990	3990	3990	4000	3700	3800
Molar Flow	*kgmole/h*	30.56286459	57.85694849	520.7125364	520.7125364	11.8736421	15.18737758
Mass Flow	*tonne/year*	14822.21899	1595.364267	14358.2784	14358.2784	1873.355379	10123.84689
Liquid Volume Flow	*m3/h*	1.581690628	1.649952487	14.84957238	14.84957238	0.214852007	1.111048325
Heat Flow	*kJ/h*	-12598471.71	-583225.2629	-5249027.366	-5242810.427	-3495495.047	-6165277.793
Comp Mole Frac (Glycerol)		0.11457339	0.00001789	0.00001789	0.00001789	0.00000000	0.00000036
Comp Mole Frac (Hydrogen)		0.00071464	0.94559438	0.94559438	0.94559438	0.00182903	0.00000000
Comp Mole Frac (12-C3diol)		0.49708539	0.00447623	0.00447623	0.00447623	0.00042915	0.99999000
Comp Mole Frac (H2O)		0.38762657	0.04991150	0.04991150	0.04991150	0.99774182	0.00000963
Comp Mole Frac (Glycerol)		0.11457339	0.00001789	0.00001789	0.00001789	0.00000000	0.00000036

	Unit	Top COL-01	Glycerol Out	Recycle	Feed+Rycycle 02	Valve-01 Out	Cooler-01 Out	Cycle 2
Vapour Fraction		0.000800431	0	1	0	0.734287449	0	0
Temperature	*C*	-85.2827725	454.5469661	157.4036855	25	383.8048421	25	25
Pressure	*kPa*	3800	3999	4000	1000	1000	1000	1000
Molar Flow	*kgmole/h*	27.0610199	3.501720629	512.6864906	18.97473554	3.501720629	3.501720629	3.48051088
Mass Flow	*tonne/year*	11997.20228	2825.01452	14099.79211	15307.90355	2825.01452	2825.01452	2807.90355
Liquid Volume Flow	*m3/h*	1.325900339	0.255786709	14.62500775	1.386029333	0.255786709	0.255786709	0.25423742
Heat Flow	*kJ/h*	-11369592.5	-1895182.204	-5087356.783	-12858618.89	-1895182.204	-2373007.187	-2358634
Comp Mole Frac (Glycerol)		0.00000020	0.99999000	0.00001818	0.99999817	0.99999000	0.99999000	0.99999000
Comp Mole Frac (Hydrogen)		0.00080254	0.00000000	0.94622104	0.00000000	0.00000000	0.00000000	0.00000000
Comp Mole Frac (12-C3diol)		0.56140978	0.00000920	0.00450598	0.00000169	0.00000920	0.00000920	0.00000920
Comp Mole Frac (H2O)		0.43778748	0.00000080	0.04925480	0.00000015	0.00000080	0.00000080	0.00000080
Comp Mole Frac (Glycerol)		0.00000020	0.99999000	0.00001818	0.99999817	0.99999000	0.99999000	0.99999000