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Journal of Chemical Engineering Research Progress, 1 (1), 2024, 8

SUPPORTING INFORMATION (SI)

Maximizing Chlorobenzene Product Yield by Modifying the Benzene Chlorination Process

Michael Natan Syalom*[a], Fauzan Akmal Danuwijaya[b], Lalu Muhammad Imam Rusully[c], Muhammad Arif Tirtana Aradhea[d]

Department of Chemical Engineering, Faculty of Engineering, Universitas Diponegoro, Indonesia.

[a] *michaelnatan21@gmail.com* ; [b] *fauzandanuwijaya@students.undip.ac.id;* [c] *rusully.imam25@gmail.com;* [d] *arifaradhea1992@gmail.com*

Table S1. Heat and material balance for basic chlorination process

	Unit	Cl_2 in	Cl_2 out	Benzene in	Liquid Product	Benzene to Reactor	Dichlorobenzene (Side Product)	Chlorobenzene (Main Product)	HCl (Side Product)	Upper Product	Bottom Product
Total Phase Properties											
Vapour Fraction		0	1	0	0	1	0	0	1	1	2.05E-06
Temperature	*C*	-50	-30	30	40	64.83	173.8	117.78	40	64.81	133
Pressure	*psia*	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50
Molecular Weight		70.91	70.91	78.11	120.6	61.65	146.9	107.7	39.25	61.64	123.7
Molar Flow	*MMSCFD*	0.9025	0.9025	0.7128	0.7016	0.0351	0.2717	0.3947	0.9489	0.0351	0.6664
Mass Flow	*lb/hr*	7027	7027	6113	9288	237.9	4383	4668	4090	237.8	9051
Heat Flow	*kJ/h*	-1.055E+06	-8.762E+04	1.778E+06	3.153E+04	2.747E+04	2.716E+04	6.101E+05	-3.971E+06	2.737E+04	5.739E+05
Std Gas Flow	*STD_m3/h*	1063	1063	839.4	826.2	41.38	320	464.8	1117	41.38	784.8
Vapor Phase Properties											
Phase Mass Flow	*lb/hr*		7027		0	237.9		6.063E-03	4090	237.8	0.0158
Phase Molecular Weight			70.91		39.25	61.65		98.12	39.25	61.64	105.1
Phase Mass Density	*kg/m3*		3.581		1.517	2.234		3.107	1.517	2.234	3.202
Phase Actual Gas Flow	*ACT_m3/h*		890.2		0	48.30		8.851E-04	1223	48.29	2.233E-03
Phase Z Factor			0.9795		0.9938	0.9821		0.9716	0.9938	0.9822	0.9722
Phase Cp/Cv			1.356		1.349	1.146		1.083	1.349	1.146	1.077
Phase Viscosity	*cP*		0.0111		0.0140	0.0104		9.213E-03	0.0140	0.0104	9.529E-03
Phase Mass Heat Capacity	*kJ/kg-C*		0.4751		0.8377	1.123		1.222	0.8377	1.123	1.210
Phase Thermal Conductivity	*W/m-K*		7.298E-03		0.0172	0.0149		0.0149	0.0172	0.0149	0.0154
Liquid Phase Properties											
Phase Mass Flow	*lb/hr*	7027		6113	9288		4383	4668	0		9051
Phase Molecular Weight		70.91		78.11	120.6		146.9	107.7	120.6		123.7
Phase Mass Density	*kg/m3*	1599		866.8	1139		1099	966.4	1139		1038
Phase Actual Liquid Flow	*m3/s*	5.538E-04		8.887E-04	1.028E-03		5.026E-04	6.086E-04	0		1.099E-03
Phase Z Factor		2.391E-03		3.575E-03	4.068E-03		3.598E-03	3.429E-03	4.068E-03		3.530E-03
Phase Cp/Cv		1.845		1.962	1.058		1.041	1.366	1.058		1.047
Phase Viscosity	*cP*	0.6037		0.5650	0.8214		0.3173	0.3449	0.8214		0.3538
Phase Mass Heat Capacity	*kJ/kg-C*	0.8660		1.603	1.260		1.446	1.561	1.260		1.490
Phase Thermal Conductivity	*W/m-K*	0.1374		0.1297	0.1198		0.0912	0.1072	0.1198		0.1017
Composition											
Comp Mole Frac (Benzene)	*mole%*	0	0	1	0.1175	0.6001	8.00E-08	0.1556	0.0291	0.5998	0.0921
Comp Mole Frac (Cl2)	*mole%*	1	1	0	0	0	0	0	0	0	0
Comp Mole Frac (Cl-BZ)	*mole%*	0	0	0	0.4683	0.0026	0.003	0.8300	0.0175	0.0026	0.4928
Comp Mole Frac (14-Cl-BZ)	*mole%*	0	0	0	0.3943	4.85E-06	0.9970	0.0144	0.0022	4.84E-06	0.4151
Comp Mole Frac (HCl)	*mole%*	0	0	0	0.0199	0.3973	1.62E-2	1.30E-08	0.9511	0.3976	7.70E-09

Table S2. Heat and material balance for chlorination process after process modification

	Unit	Cl_2 in	Cl_2 out	Benzene in	Vapour Product	Liquid Product	HCl (Side Product)	Bottom Product	Upper Product	Bottom Product-1	Dichlorobenzene (Side Product)	Chlorobenzene (Main Product)	Benzen to Recycle	Benzene to Reactor
Total Phase Properties														
Vapour Fraction		0	1	0	1	0	1	2.05E-06	3.96E-06	0	0	0	4.36E-4	5.344E-4
Temperature	*C*	-50	-30	30	40	40	-85.01	133	-35.37	138.25	168.27	130.06	-37.32	-37.35
Pressure	*psia*	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50	14.50
Molecular Weight		70.91	70.91	78.11	39.59	115.07	36.46	123.7	81.27	121.7326	143.9950	112.32	82.8287	82.8356
Molar Flow	*MMSCFD*	0.9025	0.9025	0.7128	0.9628	0.85328	0.9026	0.6664	0.1405	0.7127	0.2118	0.5010	0.2008	0.2008
Mass Flow	*lb/hr*	7027	7027	6113	4185.4543	1.078E+04	3613.4930	9051	1254.2250	9526.9780	3348.2830	6178.69	1826.19	1826.38
Heat Flow	*kJ/h*	-1.055E+06	-8.762E+04	1.778E+06	-3.999E+06	2.941E+05	-4.302E+06	5.739E+05	1.057E+05	7.148E+05	3.918E+04	7.046E+5	1.150E+5	1.144E+5
Std Gas Flow	*STD_m3/h*	1063	1063	839.4	1133.86	1004.8764	1062.9190	70.9452	165.5179	839.3585	249.3871	589.9714	236.4631	236.4686
Vapor Phase Properties														
Phase Mass Flow	*lb/hr*		7027		4185.4543	0	3613.4930		0.0022				0.3513	0.4306
Phase Molecular Weight			70.91		39.5896	39.59	36.4608		36.5657				36.5440	36.5437
Phase Mass Density	*kg/m3*		3.581		1.5302	1.53	2.3781		1.8701				1.8848	1.8851
Phase Actual Gas Flow	*ACT_m3/h*		890.2		1240.7331	0	689.2374		5.416E-04				0.0845	0.1036
Phase Z Factor			0.9795		0.9937	0.9937	0.9801		0.9891				0.9888	0.9888
Phase Cp/Cv			1.356		1.3444	1.3444	1.4110		1.4023				1.4028	1.4028
Phase Viscosity	*cP*		0.0113		0.0140	0.0140	0.0085		0.01078				0.0107	0.0107
Phase Mass Heat Capacity	*kJ/kg-C*		0.4751		0.8389	0.8388	0.8308		0.8212				0.8215	0.8215
Phase Thermal Conductivity	*W/m-K*		7.298E-03		0.0172	0.0172	0.0107		0,0135				0.0134	0.0134
Liquid Phase Properties														
Phase Mass Flow	*lb/hr*	7027		6113	0	10781.2030		571.9613	1254.2227	9526.9780	3348.28297	6178.696	1825.835	1825.9504
Phase Molecular Weight		70.91		78.11	115.0678	115.0678		86.4655	81.2701	121.7326	143.9950	112.3220	82.8489	82.8603
Phase Mass Density	*kg/m3*	1599		866.8	1107.1827	1107.1827		1078.3560	1016.4668	1020.3066	1092.7687	978.1960	1035.177	1035.3742
Phase Actual Liquid Flow	*m3/s*	5.538E-04		8.887E-04	0	1.227E-03		6.68E-05	1.555E-04	1.176E-03	3.861E-04	7.959E-04	2.224E-04	2.222E-04
Phase Z Factor		2.391E-03		3.575E-03	3.992E-03	3.992E-03		4.165E-03	4.044E-03	3.489E-03	3.590E-03	3.425E-03	4.082E-03	4.082E-03
Phase Cp/Cv		1.845		1.962	1.0599	1.060E-03		1.090	1.0904	1.3107	1.0415	1.3266	1.0905	1.0905
Phase Viscosity	*cP*	0.6037		0.5650	0.7821	0.7821		1.9123	1.6260	0.3400	0.3232	0.3349	1.7106	1.7118
Phase Mass Heat Capacity	*kJ/kg-C*	0.8660		1.603	1.2795	1.2795		1.1591	1.2336	1.5085	1.4501	1.5499	1.2098	1.2094
Phase Thermal Conductivity	*W/m-K*	0.1374		0.1297	0.1213	0.1213		0.1457	0.1451	0.1013	0.0926	0.1045	0.1453	0.1453
Composition														
Comp Mole Frac (Benzene)	*mole%*	0	0	1	0.0282	0.1141	1.15E-20	0.4514	0.6452	9.404E-3	1.66E-07	0.01338	0.5871	0.5864
Comp Mole Frac (Cl2)	*mole%*	1	1	0	0	0	0	0	0	0	0	0	0	0
Comp Mole Frac (Cl-BZ)	*mole%*	0	0	0	0.0237	0.6351	5.39E-27	0.3795	0.2311	0.7148	0.0873	0.9800	0.2756	0.2759
Comp Mole Frac (14-Cl-BZ)	*mole%*	0	0	0	1.318E-03	0.2309	1.32E-35	0.0211	3.197E-03	0.2758	0.9127	6.614E-03	8.558E-03	8.626E-03
Comp Mole Frac (HCl)	*mole%*	0	0	0	0.9467	0.0199	1	0.1481	0.1205	3.16E-10	3.26E-25	4.50E-10	0.1288	0.1290