

SUPPORTING INFORMATION (SI)

**Benzene Purity Improvement and Feed Amount Reduction on
Benzene Production**

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Table S1. Mass balance and energy balance of the basic (unmodified) benzene production process through the hydrodealkylation process calculated using ASPEN HYSYS

Total Phase Properties							
Parameters	Unit	Toluene	H2 Feed	S1	S2	S3	S4
Vapour Fraction		0	1	1	0	0	0.7333923
Temperature	C	25	25	25	25	25.8562	24.766037
Pressure	kPa	190	2550	190	190	2580	2550
Molar Flow	kgmole/h	108	299.1	0	108	108	407.1
Mass Flow	kg/h	9951.2064	812.7579	0	9951.206	9951.206	10763.964
Liquid Volume Flow	m3/h	11.43759	9.001239	0	11.43759	11.43759	20.438828
Heat Flow	kJ/h	1309903.8	-1112574	0	1309904	1346595	234020.17
Composition							
Comp Mole Frac (Benzene)	mole	0	0	0	0	0	0
Comp Mole Frac (Toluene)	mole	1	0	1	1	1	0.265291
Comp Mole Frac (Oxygen)	mole	0	0	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0	0	0
Comp Mole Frac (Methane)	mole	0	0.05	0	0	0	0.036735
Comp Mole Frac (Hydrogen)	mole	0	0.95	0	0	0	0.697973
Comp Mole Frac (H2O)	mole	0	0	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0	0	0
Total Phase Properties							
Parameters	Unit	S5	S6	Air	Fuel Gas	Flue Gas	S7
Vapour Fraction		1	1	1	1	1	1
Temperature	C	300	625.686461	25	25	773.734322	626.794889
Pressure	kPa	2520	2520	101.325	100	100	2520
Molar Flow	kgmole/h	407.1	407.1	210	100	291.369508	407.1
Mass Flow	kg/h	10763.964	10763.964	6058.557	902.945	6961.50179	10763.9612
Liquid Volume Flow	m3/h	20.438828	20.438828	7.003696	4.122133	9.56875328	20.4447931
Heat Flow	kJ/h	11034056.15	21911526.4	-1429.26	-3745423	-14624465.5	21911526.4
Composition							
Comp Mole Frac (Benzene)	mole	0	0	0	0	0	0.00199
Comp Mole Frac (Toluene)	mole	0.265291	0.265291	0	0	0	0.263301
Comp Mole Frac (Oxygen)	mole	0	0	0.21	1.249E-16	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0.79	2.498E-16	0.569386	0
Comp Mole Frac (Methane)	mole	0.036735	0.036735	0	0.5	0.127903	0.038725
Comp Mole Frac (Hydrogen)	mole	0.697973	0.697973	0	0.5	0	0.695984
Comp Mole Frac (H2O)	mole	0	0	0	0	0.259009	0
Comp Mole Frac (CO)	mole	0	0	0	0	0.043702	0
Total Phase Properties							
Parameters	Unit	S8	S9	S10	S11	S12	S15
Vapour Fraction		1	1	1	1	1	1
Temperature	C	0	0.734435	1	0	0.007748	0.010161
Pressure	kPa	626.7949	38	38	38	39.35486	90
Molar Flow	kgmole/h	2520	2510	2510	2510	290	260
Mass Flow	kg/h	0	407.1	298.9885	108.1115	108.1115	108.1115
Liquid Volume Flow	m3/h	0	10763.96	903.5438	9860.417	9860.417	9860.417
Heat Flow	kJ/h	0	20.44479	9.081532	11.36326	11.36326	11.36326
Composition							
Comp Mole Frac (Benzene)	mole	0.001988	0.00199	7.094E-05	0.007296	0.007296	0.007296
Comp Mole Frac (Toluene)	mole	0.263069	0.263301	0.0030797	0.98296	0.98296	0.98296
Comp Mole Frac (Oxygen)	mole	0	0	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0	0	0
Comp Mole Frac (Methane)	mole	0.038735	0.038725	0.0515472	0.003265	0.003265	0.003265
Comp Mole Frac (Hydrogen)	mole	0.696208	0.695984	0.9453021	0.006479	0.006479	0.006479
Comp Mole Frac (H2O)	mole	0	0	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0	0	0

Table S1. Continued

Total Phase Properties					
Parameters	Unit	S8	S9	S10	S11
Vapour Fraction		0	0	1	0
Temperature	C	-264.676	150.2041	90	90
Pressure	kPa	250	280	260	260
Molar Flow	kgmole/h	0.658278	106.3547	1.098509	107.0129
Mass Flow	kg/h	38.59589	9795.127	26.69406	9833.723
Liquid Volume Flow	m3/h	0.050008	11.2578	0.05545	11.30781
Heat Flow	kJ/h	-511.265	3609736	-1265.73	2434597
Composition					
Comp Mole Frac (Benzene)	mole	0.707154	0.003	0.003844	0.007332
Comp Mole Frac (Toluene)	mole	0.0005	0.997	0.21236	0.99087
Comp Mole Frac (Oxygen)	mole	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0
Comp Mole Frac (Methane)	mole	0.196791	0	0.203385	0.001211
Comp Mole Frac (Hydrogen)	mole	0.095555	0	0.580411	0.000588
Comp Mole Frac (H2O)	mole	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0

Table S2. Mass balance and energy balance of the modified benzene production process through the hydrodealkylation process calculated using ASPEN HYSYS

Total Phase Properties							
Parameters	Unit	Toluene-2	H2 Feed-2	S1-2	S2-2	S3-2	S4-2
Vapour Fraction		0	1	1	0	0	0.301901
Temperature	C	25	25	25.03149	25.031488	25.888061	25.93561
Pressure	kPa	190	2550	190	190	2580	2550
Molar Flow	kgmole/h	108	299.1	0	901.04512	901.04512	1302.304
Mass Flow	kg/h	9951.206	812.7579	0	82989.638	82989.638	84126.41
Liquid Volume Flow	m3/h	11.43759	9.001239	0	95.382622	95.382622	107.5135
Heat Flow	kJ/h	1309904	-1112574	0	11021824.	11327809	9803983
Composition							
Comp Mole Frac (Benzene)	mole	0	0	0.007654	0.00264	0.00264	0.001835
Comp Mole Frac (Toluene)	mole	1	0	0.992346	0.99736	0.99736	0.690301
Comp Mole Frac (Oxygen)	mole	0	0	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0	0	0
Comp Mole Frac (Methane)	mole	0	0.05	0	0	0	0.01635
Comp Mole Frac (Hydrogen)	mole	0	0.95	0	0	0	0.291515
Comp Mole Frac (H2O)	mole	0	0	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0	0	0
Total Phase Properties							
Parameters	Unit	S5-2	S6-2	Air-2	Fuel Gas-2	Flue Gas-2	S7-2
Vapour Fraction		0.646023506	0.91238071	1	1	1	1
Temperature	C	225	240.121135	25	25	559.684898	239.948351
Pressure	kPa	2520	2520	101.325	100	100	2520
Molar Flow	kgmole/h	1302.303534	1302.30353	160	100	237.86905	1207.18125
Mass Flow	kg/h	84126.41259	84126.4126	4616.043	902.945	5518.98827	75027.734
Liquid Volume Flow	m3/h	107.5135425	107.513542	5.336149	4.122133	8.07362068	97.2094686
Heat Flow	kJ/h	57231293.98	67763137.2	-1088.96	-3745423	-14278498.7	62385530.5
Composition							
Comp Mole Frac (Benzene)	mole	0.001835	0.001835	0	0	0	0.006988
Comp Mole Frac (Toluene)	mole	0.690301	0.690301	0	0	0	0.65771
Comp Mole Frac (Oxygen)	mole	0	0	0.21	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0.79	0	0.53139	0
Comp Mole Frac (Methane)	mole	0.01635	0.01635	0	0.5	0.186099	0.023345
Comp Mole Frac (Hydrogen)	mole	0.291515	0.291515	0	0.5	0	0.311957
Comp Mole Frac (H2O)	mole	0	0	0	0	0.258408	0
Comp Mole Frac (CO)	mole	0	0	0	0	0.024103	0

Table S2. Continued.

Total Phase Properties							
Parameters	Unit	S8-2	S9-2	S10-2	S11-2	S20	S21
Vapour Fraction		0	0.329393	1	0	1	1
Temperature	C	239.9484	38	38	38	38	38
Pressure	kPa	2520	2510	2510	2510	2510	2510
Molar Flow	kgmole/h	100.4986	1207.181	397.637	809.54425	107.362	290.275
Mass Flow	kg/h	9115.706	75027.73	1265.468	73762.266	341.6764	923.7918
Liquid Volume Flow	m3/h	10.51843	97.20947	12.18928	85.020191	3.291105	8.898172
Heat Flow	kJ/h	5355864	9896214	-1644992	11541206.1	-444148	-1200844
Composition							
Comp Mole Frac (Benzene)	mole	0.006924	0.006988	0.000101	0.010371	0.000101	0.000101
Comp Mole Frac (Toluene)	mole	0.977932	0.65771	0.003086	0.979252	0.003086	0.003086
Comp Mole Frac (Oxygen)	mole	0	0	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0	0	0
Comp Mole Frac (Methane)	mole	0.001857	0.023345	0.062783	0.003974	0.062783	0.062783
Comp Mole Frac (Hydrogen)	mole	0.013287	0.311957	0.93403	0.006403	0.93403	0.93403
Comp Mole Frac (H2O)	mole	0	0	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0	0	0
Total Phase Properties							
Parameters	Unit	S25	S12-2	S13-2	S14-2	S15-2	S26
Vapour Fraction		1	0.0081270 4	1	0	0.00021879	1
Temperature	C	38.72169	39.342136	39.34214	39.342136	90	39.34151
Pressure	kPa	260	290	290	290	260	289
Molar Flow	kgmole/h	290.275	809.54425	6.579197	802.96505	802.96505	6.579197
Mass Flow	kg/h	923.7918	73762.266	53.12832	73709.137	73709.137	53.12832
Liquid Volume Flow	m3/h	8.898172	85.020191	0.24533	84.774862	84.774862	0.24533
Heat Flow	kJ/h	-1200844	11541206. 1	-113667	11654872.7	18303753.8	-113667
Composition							
Comp Mole Frac (Benzene)	mole	0.000101	0.010371	0.000877	0.010449	0.010449	0.000877
Comp Mole Frac (Toluene)	mole	0.003086	0.979252	0.026705	0.987056	0.987056	0.026705
Comp Mole Frac (Oxygen)	mole	0	0	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0	0	0
Comp Mole Frac (Methane)	mole	0.062783	0.003974	0.255628	0.001912	0.001912	0.255628
Comp Mole Frac (Hydrogen)	mole	0.93403	0.006403	0.71679	0.000582	0.000582	0.71679
Comp Mole Frac (H2O)	mole	0	0	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0	0	0
Total Phase Properties							
Parameters	Unit	S16-2	S17-2	F.G	S22	S23	S24
Vapour Fraction		1	0	1	1	1	1
Temperature	C	90	90.014516	39.14758	39.87402	39.87402	39.87402
Pressure	kPa	260	260	260	2550	2550	2550
Molar Flow	kgmole/h	2.002982	800.96207	298.8572	107.362	101.9939	5.3681
Mass Flow	kg/h	25.57293	73683.564	1002.493	341.6764	324.5926	17.08382
Liquid Volume Flow	m3/h	0.095764	84.679098	9.239266	3.291105	3.12655	0.164555
Heat Flow	kJ/h	-110434	18414188. 2	-1424945	-438191	-416281	-21909.5
Composition							
Comp Mole Frac (Benzene)	mole	0	0.010475	0.000118	0.000101	0.000101	0.000101
Comp Mole Frac (Toluene)	mole	0	0.989525	0.003585	0.003086	0.003086	0.003086
Comp Mole Frac (Oxygen)	mole	0	0	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0	0	0
Comp Mole Frac (Methane)	mole	0.766487	0	0.071744	0.062783	0.062783	0.062783
Comp Mole Frac (Hydrogen)	mole	0.233513	0	0.924553	0.93403	0.93403	0.93403
Comp Mole Frac (H2O)	mole	0	0	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0	0	0

Table S2. Continued.

Total Phase Properties							
Parameters	Unit	S18-2	S19-2	Benzene 2	R_S24	R_S23	R_S19-2
Vapour Fraction		0	0	0	1	1	0
Temperature	C	112.9	150.20412	38	39.87441	39.87442	25
Pressure	kPa	250	280	230	2550	2550	250
Molar Flow	kgmole/h	6.008391	794.95368	6.008391	5.376306	102.1584	793.0451
Mass Flow	kg/h	469.3576	73214.207	469.3576	17.05376	324.0171	73038.43
Liquid Volume Flow	m ³ /h	0.532041	84.147056	0.532041	0.164709	3.129681	83.94503
Heat Flow	kJ/h	369981.9	26981166.9	306590.6	-21651.8	-411251	9711921
Composition							
Comp Mole Frac (Benzene)	mole	0.9995	0.003	0.9995	9.78765E-05	9.78755E-05	0.003
Comp Mole Frac (Toluene)	mole	0.0005	0.997	0.0005	0.003085945	0.003085914	0.997
Comp Mole Frac (Oxygen)	mole	0	0	0	0	0	0
Comp Mole Frac (Nitrogen)	mole	0	0	0	0	0	0
Comp Mole Frac (Methane)	mole	0	0	0	0.062056075	0.062034175	0
Comp Mole Frac (Hydrogen)	mole	0	0	0	0.934760104	0.934782035	0
Comp Mole Frac (H ₂ O)	mole	0	0	0	0	0	0
Comp Mole Frac (CO)	mole	0	0	0	0	0	0
Total Phase Properties							
Parameters	Unit	S8					
Vapour Fraction		0					
Temperature	C	25					
Pressure	kPa	250					
Molar Flow	kgmole/h	794.9537					
Mass Flow	kg/h	73214.21					
Liquid Volume Flow	m ³ /h	84.14706					
Heat Flow	kJ/h	9735293					
Composition							
Comp Mole Frac (Benzene)	mole	0.003					
Comp Mole Frac (Toluene)	mole	0.997					
Comp Mole Frac (Oxygen)	mole	0					
Comp Mole Frac (Nitrogen)	mole	0					
Comp Mole Frac (Methane)	mole	0					
Comp Mole Frac (Hydrogen)	mole	0					
Comp Mole Frac (H ₂ O)	mole	0					
Comp Mole Frac (CO)	mole	0					