

SUPPORTING INFORMATION (SI)

**Minimizing Energy Usage in the Production of Benzene through
Hydrodealkylation Toluene Process by Optimizing Heat Transfer
Unit in Reactor System**

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Table S1. Material and energy balances of the modified process

	Unit	Hydrogen Feed	Toluene Feed	H2 K-01	H2 HE-01	Tol. P-01	Fuel	H2 FH-01	Tol. FH-01	Flue Gas	Vapour Product	Product TEE-01	Product RCY-1 in	Product HE-01
Total Phase Properties														
Vapour Fraction		1	0	1	1	0	1	1	1	1	1	1	1	1
Temperature	C	35	30	96.2	192.0	62.6	28.8	643.4	312.9	407.1	635.9	635.9	635.9	600.6
Pressure	atm	20	1	34.1	34	34	34	34	34	1	34	34	34	33.7
Molar Flow	kgmole/h	2860	572	2860	2860	572	266	2860	572	1159.434889	6864	3432	3432	3432
Mass Flow	kg/h	5816.6169	52562.9107	5816.6169	5816.6169	52562.9107	1186.4585	5816.6169	52562.9107	30193.1834	116755.3561	58377.6780	58377.6780	58377.6780
Liquid Volume Flow	m3/h	82.6238	60.4016	82.6238	82.6238	60.4016	8.7268	82.6238	60.4016	35.9468	293.1592	146.5796	146.5796	146.5796
Heat Flow	kJ/h	541620.3738	8241604.2428	5565836.4305	13472310.9410	11209686.5426	-2824561.7307	51656857.4003	49394233.0020	-78819274.8085	244416262.9143	122208131.4571	122208131.4571	114301656.9467
Std Gas Flow	STD_m3/h	67623.0882	13524.6176	67623.0882	67623.0882	13524.6176	6289.4201	67623.0882	13524.6176	27414.1845	162295.4117	81147.7058	81147.7058	81147.7058
Molecular Weight		2.0338	91.8932	2.0338	2.0338	91.8932	4.4604	2.0338	91.8932	26.0413	17.0098	17.0098	17.0098	17.0098
Vapor Phase Properties														
Phase Mass Flow (Vapour Phase)	kg/h	5816.6169		5816.6169	5816.6169		1186.4585	5816.6169	52562.9107	30193.1834	116755.3561	58377.6780	58377.6780	58377.6780
Phase Molecular Weight (Vapour Phase)		2.0338		2.0338	2.0338		4.4604	2.0338	91.8932	26.0413	17.0098	17.0098	17.0098	17.0098
Phase Mass Density (Vapour Phase)	kg/m3	1.5971		2.2618	1.7929		6.0686	0.9138	116.5697	0.4665	7.6925	7.6925	7.6925	7.9334
Phase Actual Gas Flow (Vapour Phase)	ACT_m3/h	3641.8741		2571.6643	3244.1773		195.5077	6365.0182	450.9139	64727.1132	15177.7353	7588.8677	7588.8677	7358.4303
Phase Z Factor (Vapour Phase)		1.0072		1.0118	1.0104		1.0087	1.0061	0.5574	1.0001	1.0079	1.0079	1.0079	1.0078
Phase Cp/Cv (Vapour Phase)		1.4176		1.4148	1.4075		1.4018	1.3791	1.4752	1.3305	1.1477	1.1477	1.1477	1.1505
Phase Viscosity (Vapour Phase)	cP	0.0090		0.0105	0.0125		0.0090	0.0209	0.0172	0.0289	0.0288	0.0288	0.0288	0.0278
Phase Mass Heat Capacity (Vapour Phase)	kJ/kg-C	14.0601		14.1409	14.2340		6.7890	14.8894	2.9835	1.2873	3.8689	3.8689	3.8689	3.8139
Phase Thermal Conductivity (Vapour Phase)	W/m-K	0.1801		0.2076	0.2459		0.1399	0.3922	0.0419	0.0503	0.2314	0.2314	0.2314	0.2238
Liquid Phase Properties														
Phase Mass Flow (Liquid Phase)	kg/h		52562.9107			52562.9107	0.0000				0.0000	0.0000	0.0000	
Phase Molecular Weight (Liquid Phase)			91.8932			91.8932	80.3134				17.0015	17.0015	17.0015	
Phase Mass Density (Liquid Phase)	kg/m3		859.8474			832.3299	863.2614				7.6888	7.6888	7.6888	
Phase Actual Liquid Flow (Liquid Phase)	m3/s		0.0170			0.0175	0.0000				0.0000	0.0000	0.0000	
Phase Z Factor (Liquid Phase)			0.0043			0.1363	0.1277				1.0079	1.0079	1.0079	
Phase Cp/Cv (Liquid Phase)			1.3744			1.3507	1.7455				1.1477	1.1477	1.1477	
Phase Viscosity (Liquid Phase)	cP		0.5166			0.3694	0.5433				0.0047	0.0047	0.0047	
Phase Mass Heat Capacity (Liquid Phase)	kJ/kg-C		1.5818			1.7138	1.5584				3.8697	3.8697	3.8697	
Phase Thermal Conductivity (Liquid Phase)	W/m-K		0.1347			0.1266	0.1301				0.0580	0.0580	0.0580	
Composition														
Comp Mole Frac (Toluene)		0.0000	0.9824	0.0000	0.0000	0.9824	0.0005	0.0000	0.9824	0.0000	0.0234	0.0234	0.0234	0.0234
Comp Mole Frac (Hydrogen)		0.9987	0.0000	0.9987	0.9987	0.0000	0.8474	0.9987	0.0000	0.0000	0.6933	0.6933	0.6933	0.6933
Comp Mole Frac (Benzene)		0.0000	0.0176	0.0000	0.0000	0.0176	0.0043	0.0000	0.0176	0.0000	0.1405	0.1405	0.1405	0.1405
Comp Mole Frac (Methane)		0.0013	0.0000	0.0013	0.0013	0.0000	0.1479	0.0013	0.0000	0.0000	0.1414	0.1414	0.1414	0.1414
Comp Mole Frac (BiPhenyl)		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014	0.0014	0.0014	0.0014

Table S1 (continued)

	Unit	Product RCY-1 out	Tol. Mixed	Product WHB-01	Air	Tol. H-01	Product PC-01	Tol. Mixed Heated	Crude Product	Liquid Product
Total Phase Properties										
Vapour Fraction		1	1	1	1	0	1	1	1	0
Temperature	C	635.9	510.4	503.5	30.0	61.0	490.8	570.4	191.3	635.9
Pressure	atm	34	34	33.3	1	1	33.2	34	33.2	34
Molar Flow	kgmole/h	3432	4004	3432	1005.42298	572	3432	4004	3432	0
Mass Flow	kg/h	58377.6780	110940.5888	58377.6780	29006.7248	52562.9107	58377.6780	110940.5888	58377.6780	0
Liquid Volume Flow	m3/h	146.5796	206.9812	146.5796	33.5318	60.4016	146.5796	206.9812	146.5796	0
Heat Flow	kJ/h	122207665.1336	171601898.1356	93145595.9978	138634.8676	10927528.6404	90459671.6002	192757959.0845	32954974.3484	0
Std Gas Flow	STD_m3/h	81147.7058	94672.3235	81147.7058	23772.6597	13524.6176	81147.7058	94672.3235	81147.7058	0
Molecular Weight		17.0098	27.7074	17.0098	28.8503	91.8932	17.0098	27.7074	17.0098	17.0015
Vapor Phase Properties										
Phase Mass Flow (Vapour Phase)	kg/h	58377.6780	110940.5888	58377.6780	29006.7248		58377.6780	110940.5888	58377.6780	0
Phase Molecular Weight (Vapour Phase)		17.0098	27.7074	17.0098	28.8503		17.0098	27.7074	17.0098	17.0098
Phase Mass Density (Vapour Phase)	kg/m3	7.6926	14.6050	8.8248	1.1604		8.9453	13.5413	14.8946	7.6925
Phase Actual Gas Flow (Vapour Phase)	ACT_m3/h	7588.8504	7596.0769	6615.2035	24997.6255		6526.0501	8192.7401	3919.3929	0
Phase Z Factor (Vapour Phase)		1.0079	1.0032	1.0072	0.9995		1.0071	1.0050	0.9948	1.0079
Phase Cp/Cv (Vapour Phase)		1.1477	1.1140	1.1598	1.4005		1.1612	1.1087	1.2257	1.1477
Phase Viscosity (Vapour Phase)	cP	0.0288	0.0278	0.0252	0.0191		0.0249	0.0293	0.0172	0.0288
Phase Mass Heat Capacity (Vapour Phase)	kJ/kg-C	3.8689	3.1266	3.6449	1.0131		3.6208	3.2284	2.9143	3.8689
Phase Thermal Conductivity (Vapour Phase)	W/m-K	0.2314	0.1645	0.2027	0.0263		0.2000	0.1758	0.1317	0.2314
Liquid Phase Properties										
Phase Mass Flow (Liquid Phase)	kg/h					52562.9107				0
Phase Molecular Weight (Liquid Phase)						91.8932				17.0015
Phase Mass Density (Liquid Phase)	kg/m3					830.5322				7.6888
Phase Actual Liquid Flow (Liquid Phase)	m3/s					0.0176				1.1477
Phase Z Factor (Liquid Phase)						0.0040				0.0047
Phase Cp/Cv (Liquid Phase)						1.3600				3.8697
Phase Viscosity (Liquid Phase)	cP					0.3740				
Phase Mass Heat Capacity (Liquid Phase)	kJ/kg-C					1.7151				
Phase Thermal Conductivity (Liquid Phase)	W/m-K					0.1269				0.058041002
Composition										
Comp Mole Frac (Toluene)		0.0234	0.1604	0.0234	0.0000	0.9824	0.0234	0.1604	0.0234	0.0234
Comp Mole Frac (Hydrogen)		0.6933	0.5943	0.6933	0.0000	0.0000	0.6933	0.5943	0.6933	0.6934
Comp Mole Frac (Benzene)		0.1405	0.1229	0.1405	0.0000	0.0176	0.1405	0.1229	0.1405	0.1404
Comp Mole Frac (Methane)		0.1414	0.1212	0.1414	0.0000	0.0000	0.1414	0.1212	0.1414	0.1414
Comp Mole Frac (BiPhenyl)		0.0014	0.0012	0.0014	0.0000	0.0000	0.0014	0.0012	0.0014	0.0014