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SUPPORTING INFORMATION (SI)

Enhancing Energy Efficiency of Cumene Production Through Reactor Output Recycling Modification in a Heat Exchanger

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Table S1. Heat and material balance of modified process using Aspen HYSYS

Stream No.	Unit	Benzene	Propylene	1	2	3	4	5	6	7	8
Total Phase Properties											
Vapour Fraction		0	1	0	0	0	1	0	1	1	0
Temperature	°C	30	30	45.4018484	56.49	57.6770691	84.99006681	104.326593	350	370	370
Pressure	atm	1	10	1	0.90002467	25	25	25	25	25	25
Molecular Weight		78.22912451	42.17703104	86.1380078	86.1380078	86.1380078	42.17703104	66.5041999	66.50419991	115.7143539	115.7143495
Molar Flow	kgmole/h	141.0589735	147.246021	182.444427	182.444427	182.444427	147.246021	329.690448	329.6904477	189.4861756	0
Mass Flow	kg/h	11034.92	6210.4	15715.3994	15715.3994	15715.3994	6210.4	21925.7994	21925.79944	21926.27038	0
Liquid Volume Flow	m3/h	12.51029876	11.93797838	17.9591797	17.9591797	17.9591797	11.93797838	29.8971581	29.8971581	25.64444304	0
Heat Flow	kJ/h	7116124.493	2015846.934	6234558.86	6526553.79	6587471.2	2398720.178	8986191.38	26461772.8	13536583.74	0
Std Gas Flow	STD_m3/h	3335.259932	3481.549185	4313.79565	4313.79565	4313.79565	3481.549185	7795.34483	7795.344835	4480.293833	0
Vapor Phase Properties											
Mass Flow	kg/h		6210.4				6210.4		21925.79944	21926.27038	0
Molecular Weight			42.17703104				42.17703104		66.50419991	115.7143539	115.7143539
Mass Density	kg/m3		20.14687225				48.31206052		35.90687212	78.77873149	78.77873149
Actual Gas Flow	ACT_m3/h		308.2562853				128.5476118		610.6296134	278.3272841	0
Cp/Cv			1.261678201				1.370192118		1.092382862	1.138232764	1.138232764
Viscosity	cP		0.009162052				0.011696981		0.017640745	0.015798812	0.015798812
Heat Capacity	kJ/kg.°C		1.722384767				2.18995696		2.381349172	2.70867014	2.70867014
Thermal Conductivity	W/m.K		0.018625537				0.026205357		0.049103588	0.045970639	0.045970639
Liquid Phase Properties											
Mass Flow	kg/h	11034.92		15715.3994	15715.3994	15715.3994		21925.7994		0	0
Molecular Weight		78.22912451		86.1380078	86.1380078	86.1380078		66.5041999		115.7143495	115.7143495
Mass Density	kg/m3	866.7933217		851.655097	839.95476	840.58325		643.620958		78.77872463	78.77872463
Actual Liquid Flow	m3/s	0.003536317		0.00512577	0.00519717	0.00519329		0.00946287		0	0
Viscosity	cP	0.564521723		0.48690286	0.42700868	0.42184647		0.12728482		0.014013069	0.014013069
Heat Capacity	kJ/kg.°C	1.542366042		1.6516258	1.70118739	1.7001464		2.25425128		2.708670093	2.708670093
Thermal Conductivity	W/m.K	0.129749754		0.12690651	0.12403041	0.12372193		0.08983853		0.002617556	0.002617556
Surface Tension	dyne/cm	26.96081611		24.9986707	23.6712106	23.5299061		10.0246697		0.014840774	0.014840774
Composition											
Benzene	weight %	0.991509828	0	0.77792359	0.77792359	0.77792359	0	0.43048813	0.430488127	0.016495102	0.01649511
Propylene	weight %	0	0.952176984	1.03E-11	1.03E-11	1.03E-11	0.952176984	0.42526034	0.425260341	7.40E-11	7.40E-11
Cumene	weight %	0	0	0.18624211	0.18624211	0.18624211	0	0.10306284	0.103062841	0.904440762	0.904440702
14-iP-BZ	weight %	0	0	3.48E-08	3.48E-08	3.48E-08	0	1.93E-08	1.93E-08	0.007399216	0.007399211
Propane	weight %	0	0.047823016	0.0065064	0.0065064	0.0065064	0.047823016	0.02495918	0.024959184	0.043426938	0.043426986
Toluene	weight %	0.008490172	0	0.02932788	0.02932788	0.02932788	0	0.01622949	0.016229489	0.028237983	0.02823799
Total		**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**

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Table S1. Continued

9	10	11	12	13	14	15	16	17	Cumene	PDIB	18
1	1	1	0.117376318	1	0	0	0	0	0	0	0
370	315.7787714	309.8517781	144.76	144.76	144.76	80.26282714	153.866136	153.8828648	153.5430093	166.0692694	80.26068784
25	1.6	1.50002467	1.3	1.3	1.3	1	1	1.3	1	1	1
115.7178799	115.7178799	115.7178799	115.7178799	92.89151695	118.7534594	113.0947891	120.622757	120.6227571	120.1783869	134.9291865	113.0947973
188.8304922	188.8304922	188.8304922	188.8304922	22.16422784	166.6662643	41.38549643	125.280766	125.2807655	121.5066629	3.774102501	41.38545322
21851.06421	21851.06421	21851.06421	21851.06421	2058.868746	19792.19546	4680.483989	15111.7113	15111.71135	14602.47475	509.2365803	4680.479445
25.5561748	25.5561748	25.5561748	25.5561748	2.630793987	22.92538081	5.448886199	17.4764944	17.47649439	16.8861794	0.590314977	5.448880959
13490758.48	11745722.45	11453727.52	-2074039.16	-160308.117	-1913731.05	-881546.7	-1345396.4	-1344570.59	-1216108.3	-126183.191	-881565.636
4464.790569	4464.790569	4464.790569	4464.790569	524.0606762	3940.729893	978.5367395	2962.1931	2962.193097	2872.956568	89.23652667	978.535718
21851.06421	21851.06421	21851.06421	2058.868746	2058.868746	0						
115.7178799	115.7178799	115.7178799	92.89151695	92.89151695	92.89151695						
78.78442008	3.919291729	3.70899155	3.642296593	3.642296593	3.642296593						
277.3526059	5575.258419	5891.376111	565.266637	565.266637	0						
1.138251287	1.035708734	1.03583416	1.059042425	1.059042425	1.059042425						
0.015798785	0.011779899	0.011636734	0.009166064	0.009166064	0.009166064						
2.708702704	2.295206765	2.278741015	1.811952067	1.811952067	1.811952067						
0.045969926	0.037551065	0.036894579	0.022616102	0.022616102	0.022616102						
			19792.19546	0	19792.19546	4680.483989	15111.7113	15111.71135	14602.47475	509.2365803	4680.479445
			118.7534594	118.7534594	118.7534594	113.0947891	120.622757	120.6227571	120.1783869	134.9291865	113.0947973
			749.228376	749.228376	749.228376	806.6551235	741.669954	741.7085865	741.7777278	735.6019953	806.6571057
			0.007337992	0	0.007337992	0.00161176	0.00565979	0.005659497	0.005468273	0.000192298	0.001611754
			0.217868984	0.217868984	0.217868984	0.369542265	0.20493179	0.204914572	0.205080155	0.196586181	0.369550197
			2.175442701	2.175442701	2.175442701	1.897234316	2.21459737	2.214495667	2.213350929	2.262562186	1.897225082
			0.109509584	0.109509584	0.109509584	0.122278453	0.10813715	0.108133079	0.108038286	0.110933051	0.12227899
			15.85303395	15.85303395	15.85303395	21.40769697	15.2080549	15.20653535	15.21959058	14.73194043	21.40790952
0.016458356	0.016458356	0.016458356	0.016458356	0.046984212	0.012398854	0.049932099	4.65E-08	4.65E-08	4.79E-08	1.35E-13	0.049932151
7.42E-11	7.42E-11	7.42E-11	7.42E-11	5.48E-10	1.13E-11	4.54E-11	1.00E-30	1.00E-30	1.00E-30	1.00E-30	4.54E-11
0.904409873	0.904409873	0.904409873	0.904409873	0.588396455	0.946435135	0.821032904	0.98786077	0.987860773	0.99836035	0.649828464	0.821033275
0.007423619	0.007423619	0.007423619	0.007423619	0.001244152	0.008245399	1.53E-07	0.01096915	0.01096915	0.000433244	0.350171072	1.53E-07
0.043381866	0.043381866	0.043381866	0.043381866	0.316039051	0.007122362	0.028682888	1.13E-23	1.13E-23	1.17E-23	1.00E-30	0.028682918
0.028326287	0.028326287	0.028326287	0.028326287	0.047336129	0.02579825	0.100351956	0.00117003	0.00117003	0.001206358	4.65E-07	0.100351502
1	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**

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