

Improving Yield Conversion with Triple Conversion Reactor for Styrene Production from Ethylbenzene

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

Data	Unit	Fresh HCl	Fresh Acetylene	Pressed Act	Acetylene	Pressed HCl	HCl	Mixed Feed	Liquid Product	Vapour Product	Dowtherm A
Vapour Fraction		1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.000	1.000	0.000
Temperature	C	25.000	25.000	114.540	180.000	177.285	180.000	179.999	180.000	180.000	60.029
Pressure	atm	1.000	1.000	3.165	2.961	3.165	2.961	2.961	2.961	2.961	1.817
Molar Flow	kgmole/h	424.461	382.600	382.600	382.600	424.461	1913.000	2295.600	0.000	1913.552	1050.310
Mass Flow	kg/h	15476.176	9962.138	9962.138	9962.138	15476.176	70512.435	80474.572	0.000	80471.974	174351.393
Liquid Volume Flow	m3/h	17.782	23.887	23.887	23.887	17.782	81.512	105.399	0.000	91.513	163.864
Heat Flow	kJ/h	-39220289.986	86792475.600	88397576.102	89683294.865	-37322076.904	-156819277.549	-67135982.683	0.000	-106059388.122	-9550987.373
Std Gas Flow	STD_m3/h	10036.133	9046.360	9046.360	9046.360	10036.133	45231.802	54278.162	0.000	45244.852	24833.979
Master Comp Mass Flow (Acetylene)	kg/h	0.000	9962.138	9962.138	9962.138	0.000	509.196	10471.334	0.000	523.567	0.000
Master Comp Mass Flow (DTRM-A)	kg/h	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	174351.393
Master Comp Mass Flow (H2O)	kg/h	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Master Comp Mass Flow (HCl)	kg/h	15476.176	0.000	0.000	0.000	15476.176	67682.383	67682.383	0.000	53752.606	0.000
Master Comp Mass Flow (VinylCl)	kg/h	0.000	0.000	0.000	0.000	0.000	2320.856	2320.856	0.000	26195.802	0.000
Phase Mass Flow (Liquid Phase)	kg/h	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	174351.393
Phase Mass Flow (Vapour Phase)	kg/h	15476.176	9962.138	9962.138	9962.138	15476.176	70512.435	80474.572	0.000	80471.974	0.000
Phase Molecular Weight (Liquid Phase)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	42.036	42.036	166.000
Phase Molecular Weight (Vapour Phase)		36.461	26.038	26.038	26.038	36.461	36.860	35.056	42.054	42.054	0.000
Phase Mass Density (Liquid Phase)	kg/m3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	3.371	3.371	1028.422
Phase Mass Density (Vapour Phase)	kg/m3	1.499	1.072	2.615	2.084	3.138	2.950	2.805	3.372	3.372	0.000
Phase Actual Volume Flow (Liquid Phase)	m3/h	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	169.533
Phase Actual Volume Flow (Vapour Phase)	m3/h	10322.873	9295.310	3808.922	4780.661	4931.108	23905.717	28686.331	0.000	23864.315	0.000
Phase Z Factor (Liquid Phase)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.993	0.993	0.011
Phase Z Factor (Vapour Phase)		0.994	0.993	0.990	0.995	0.995	0.995	0.995	0.993	0.993	0.000
Phase Cp/Cy (Liquid Phase)		0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.282	1.282	1.285
Phase Cp/Cy (Vapour Phase)		1.400	1.231	1.211	1.195	1.400	1.381	1.329	1.281	1.281	0.000
Phase Viscosity (Liquid Phase)	cP	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.002	1.621
Phase Viscosity (Vapour Phase)	cP	0.014	0.010	0.013	0.016	0.021	0.021	0.020	0.019	0.019	0.000
Phase Mass Heat Capacity (Liquid Phase)	kJ/kg-C	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.930	0.930	1.182
Phase Mass Heat Capacity (Vapour Phase)	kJ/kg-C	0.816	1.751	1.919	2.016	0.819	0.838	0.984	0.930	0.930	0.000
Phase Thermal Conductivity (Liquid Phase)	W/m-K	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.036	0.036	0.117
Phase Thermal Conductivity (Vapour Phase)	W/m-K	0.017	0.023	0.032	0.039	0.025	0.025	0.027	0.024	0.024	0.000

Dowtherm A to HE-01	Exp. Vap. Product	Act & HCl	VCM	HCl to Heater	Recycled HCl	Pressed Act & HCl	Fresh Dowtherm A	Dowtherm A to HE-02	Dowtherm A to RE-01	BFW	BFW In	CW Out	Waste	VCM 99.9%
0.000	1.000	1.000	0.000	1.000	1.000	1.000	0.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000
210.000	107.285	-73.247	-35.812	58.894	26.333	26.271	60.000	205.868	182.133	30.000	30.048	160.039	-77.286	-15.921
1.612	1.000	1.000	1.000	3.165	3.165	3.165	1.000	1.408	1.204	1.000	6.202	6.100	1.000	1.000
1050.310	1913.552	1500.412	413.139	1913.000	1488.539	1500.412	1050.310	1050.310	1050.310	632.348	632.348	632.348	46.547	366.593
174351.393	80471.974	55468.897	25003.078	70512.435	55036.259	55468.897	174351.393	174351.393	174351.393	11391.806	11391.806	11391.806	2103.687	22899.391
163.864	91.513	64.231	27.282	81.512	63.730	64.231	163.864	163.864	163.864	11.415	11.415	11.415	2.370	24.912
29372418.065	-111248825.689	-132115556.863	705778.215	-163965323.528	-126643246.623	-127693795.773	-9569690.325	28086699.303	20940653.324	-180745266.891	-180737289.533	-150226945.885	-3183869.187	4325403.335
24833.979	45244.852	35476.406	9768.446	45231.802	35195.669	35476.406	24833.979	24833.979	24833.979	14951.503	14951.503	14951.503	1100.572	8667.874
0.000	523.567	512.809	10.757	509.196	509.196	512.809	0.000	0.000	0.000	0.000	0.000	0.000	10.638	0.119
174351.393	0.000	0.000	0.000	0.000	0.000	0.000	174351.393	174351.393	174351.393	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	11391.806	11391.806	11391.806	0.000	0.000
0.000	53752.606	52632.411	1120.194	67682.383	52206.207	52632.411	0.000	0.000	0.000	0.000	0.000	0.000	1106.829	13.366
0.000	26195.802	2323.676	23872.126	2320.856	2320.856	2323.676	0.000	0.000	0.000	0.000	0.000	0.000	986.220	22885.906
174351.393	0.000	0.000	25003.078	0.000	0.000	0.000	174351.393	174351.393	174351.393	0.000	0.000	0.000	2103.687	22899.391
0.000	80471.974	55468.897	0.000	70512.435	55036.259	55468.897	0.000	0.000	0.000	0.000	0.000	11391.806	0.000	0.000
166.000	0.000	0.000	60.520	0.000	0.000	0.000	166.000	166.000	166.000	0.000	0.000	0.000	45.195	62.466
0.000	42.054	36.969	0.000	36.860	36.973	36.969	0.000	0.000	0.000	0.000	0.000	18.015	0.000	0.000
900.484	0.000	0.000	1003.111	0.000	0.000	0.000	1028.382	904.243	925.617	0.000	0.000	0.000	1126.756	965.905
0.000	1.353	2.295	0.000	4.344	4.856	4.857	0.000	0.000	0.000	0.000	0.000	3.207	0.000	0.000
193.620	0.000	0.000	24.926	0.000	0.000	0.000	169.540	192.815	188.362	0.000	0.000	0.000	1.867	23.708
0.000	59490.834	24168.704	0.000	16233.337	11332.942	11420.873	0.000	0.000	0.000	0.000	0.000	3552.129	0.000	0.000
0.007	0.000	0.000	0.003	0.000	0.000	0.000	0.006	0.007	0.006	0.000	0.000	0.000	0.002	0.003
0.000	0.996	0.982	0.000	0.986	0.981	0.981	0.000	0.000	0.000	0.000	0.000	0.964	0.000	0.000
1.236	0.000	0.000	1.125	0.000	0.000	0.000	1.285	1.237	1.247	0.000	0.000	0.000	1.992	1.714
0.000	1.293	1.402	0.000	1.399	1.403	1.404	0.000	0.000	0.000	0.000	0.000	1.356	0.000	0.000
0.369	0.000	0.000	0.322	0.000	0.000	0.000	1.622	0.380	0.455	0.000	0.000	0.000	0.439	0.264
0.000	0.016	0.009	0.000	0.015	0.014	0.014	0.000	0.000	0.000	0.000	0.000	0.014	0.000	0.000
1.789	0.000	0.000	1.234	0.000	0.000	0.000	1.182	1.773	1.679	0.000	0.000	0.000	1.392	1.277
0.000	0.886	0.829	0.000	0.835	0.840	0.840	0.000	0.000	0.000	0.000	0.000	1.993	0.000	0.000
0.099	0.000	0.000	0.149	0.000	0.000	0.000	0.117	0.099	0.102	0.000	0.000	0.000	0.173	0.141
0.000	0.020	0.011	0.000	0.019	0.017	0.017	0.000	0.000	0.000	0.000	0.000	0.029	0.000	0.000