

Aniline Process Creation for Conversion Improvement Using Hydrogenation Process

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Table S1. Mass and energy balances of Aspen HYSYS simulation of unmodified process of aniline production

Total Phase Porportion for Unmodified Process											
	Unit	NitroBenzene INPUT	Hydrogen INPUT	Aniline Vapor OUT	Aniline Liquid OUT	AnilinCamLiq1	Hydrogen	Aniline+Stream	Stream	Aniline	Aniline+Hot Stream
Vapour Fraction		0	1	1	0	0.98	1	0	1	0	0.99
Temperature	°C	240	240	200	200	10	10	10	170	170	170
Pressure	atm	2.3	2.3	2.3	2.3	1.96	1.96	1.96	1.62	1.62	1.62
Molar Flow	kgmole/h	100	10000	10001	0	10001	9764.57	236.43	235.23	1.21	236.43
Mass Flow	kg/h	12310.94	20160.00	32471.09	0	32471.09	20781.76	11689.33	11579.23	110.11	11689.33
Liquid Volume Flow	m3/h	10.20	288.58	292.69	0	292.69	281.23	11.46	11.35	0.11	11.46
Heat Flow	kJ/h	5344778.89	61674930.05	13201269.74	0	-54646012.5	-18519959.6	-36126052.91	-22207979.1	65844.01	-22142135.05
Composition for Unmodified Process											
Comp Mole Frac (NitroBZ)	mole	1	0	1.00E-04	0.005	1.00E-04	2.17E-06	0.004	0.004	0.006	0.004
omp Mole Frac (Hydrogen)	mole	0	1	0.97	0.04	0.97	0.99	6.15E-05	6.18E-05	2.76E-08	6.15E-05
Comp Mole Frac (Aniline)	mole	0	0	0.01	0.91	0.01	0.0001	0.41	0.41	0.97	0.41
Comp Mole Frac (H ₂ O)	mole	0	0	0.02	0.04	0.02	0.006	0.58	0.59	0.03	0.58

Table S2. Mass and energy balances of Aspen HYSYS simulation of modified process of aniline production

Total Phase Porportion for Unmodified Process											
	Unit	NitroBenzene INPUT	Hydrogen INPUT	Aniline Vapor OUT	Aniline Liquid OUT	AnilinCamLiq 1	Hydrogen	Aniline+Stream	Stream	Aniline	Aniline+Hot Stream
Vapour Fraction		0	1	1	0	0.98	1	0	1	0	0.99
Temperature	°C	240	240	200	200	10	10	10	170	170	170
Pressure	atm	2.3	2.3	2.3	2.3	1.96	1.96	1.96	1.62	1.62	1.62
Molar Flow	kgmole/h	100	10000	10001	0	10001	9764.57	236.43	235.23	1.21	236.43
Mass Flow	kg/h	12310.94	20160.00	32471.09	0	32471.09	20781.76	11689.33	11579.23	110.11	11689.33
Liquid Volume Flow	m3/h	10.20	288.58	292.69	0	292.69	281.23	11.46	11.35	0.11	11.46
Heat Flow	kJ/h	5344778.89	61674930.05	13201269.74	0	-54646012.5	-18519959.6	-36126052.91	-22207979.1	65844.01	-22142135.05
Composition for Unmodified Process											
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omp Mole Frac (Hydrogen)	mole	0	1	0.97	0.04	0.97	0.99	6.15E-05	6.18E-05	2.76E-08	6.15E-05
Comp Mole Frac (Aniline)	mole	0	0	0.01	0.91	0.01	0.0001	0.41	0.41	0.97	0.41
Comp Mole Frac (H ₂ O)	mole	0	0	0.02	0.04	0.02	0.006	0.58	0.59	0.03	0.58