Nature of Invention: Process design

Applicant: Catalysta Industries Pvt. Ltd

Inventors:

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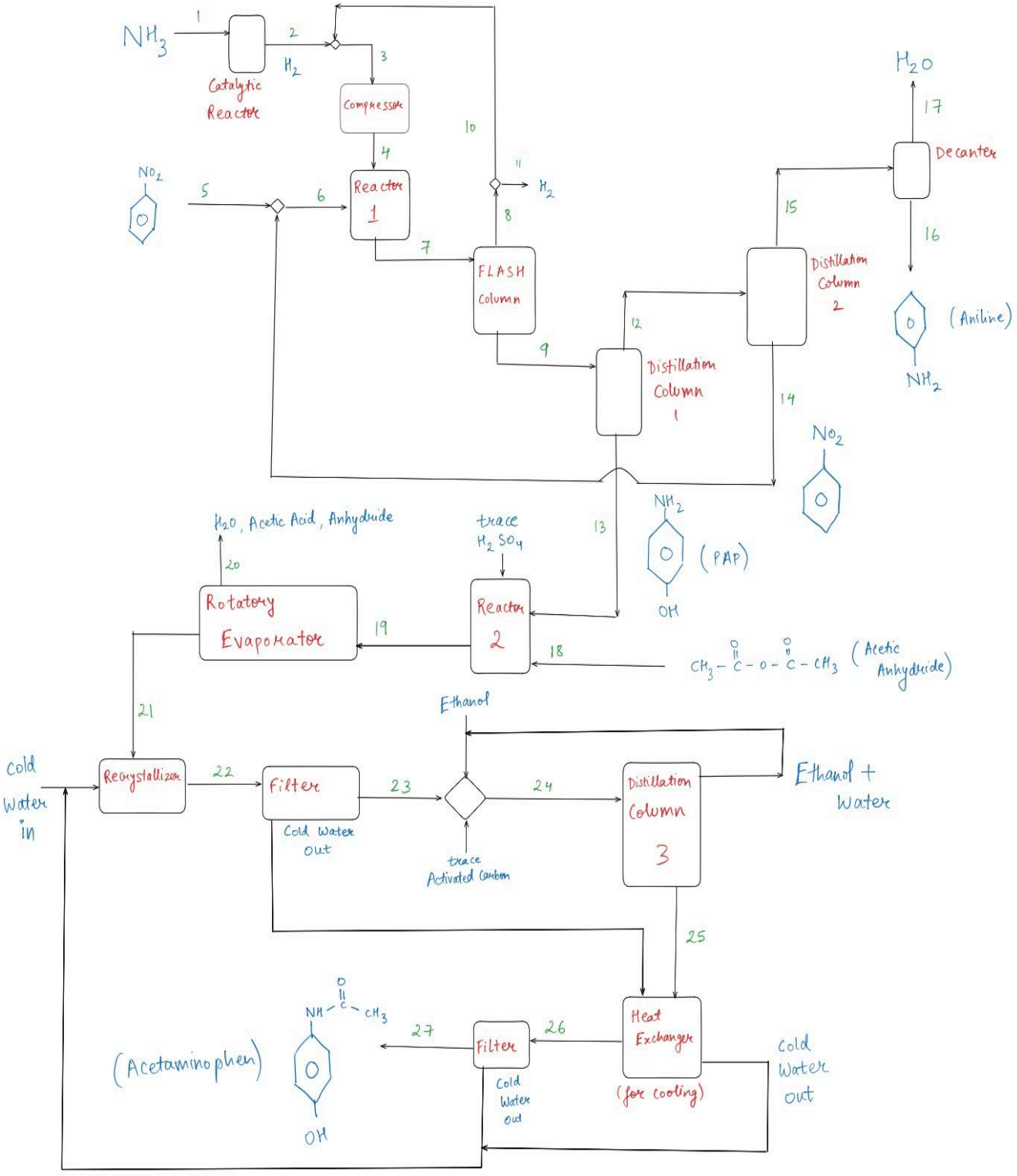
Chemical Formula: $C_8H_9NO_2$ ($HOC_6H_4NHCOCH_3$)

Chemical Name: Acetaminophen

Process Title: Integrated Process for the Production and Purification of Paracetamol from Nitrobenzene.

Process Description:

Block Diagram:



Unit operations and process conditions:

unit operation	design gauge pressure (barg)	design temperature(C)
Reactor 1	4.71	121.11
Reactor 2	0	121.11
Flash drum	4.71	121.11

unit operation	design gauge pressure bottom(barg)	design temperature bottom(C)	operating bottom temperature(C)	bottom tray type
Distillation column 1	1.034	311.264	283.487	sieve
Distillation column 2	1.034	236.729	208.952	sieve
Distillation column 3	1.034	150	130	sieve

unit operation	design gauge pressure (barg)	vacuum design gauge pressure(barg)	operating temperature (C)	design temperature (C)
Decanter	1.03425	-1.00667	30	121.11

Material balance scaled-up process:

Specie data:

Species	Molar Weight	Average Density (kg/m3)
Ammonia	17	701
Hydrogen	2	0.08988
Nitrobenzene	123.11	1109
Aniline	93.13	998
Water	18	947.99
Para aminophenol	109.13	1250
Acetic Anhydride	102.09	1080
Acetic Acid	60.05	1050
Ethanol	46.07	789
Acetaminophen	151.163	1263

Material balance:

Assumptions:

- 100% conversion of NH3 to H2 and N2 is separated out.
- In flash drum 100% hydrogen move to stripper.
- In Distillation column 1 100% para aminophenol gets separated in stream 13 and all other species move to stream 12.
- In Distillation column 2 100% nitrobenzene is separated in stream 14 and all other species move to stream 15.

			kmol /day	kg/day		kmol /day	kg/day	kg/m3	m3 / day

Stream	Remarks	Relevant Species	Molar Flow Rate	Mass Flow Rate	Mass Fraction	Total Molar Flow	Total Mass Flow	Average Density	Volume Flow Rate
1	90% conversion to pure H2	Ammonia	24.49	416.28	1	24.49	416.28	701	0.5938440377
2		Hydrogen	33.06	66.12	1	33.06	66.12	0.08988	735.6008077
3		Hydrogen	94.88	189.77	1	94.88	189.77	0.08988	2111.368564
4	PAP formed = 0.7 * 0.6 * every 2 Hydrogen required; Aniline formed = 0.3 * 0.6 * every 3 Hydrogen Required	Hydrogen	94.88	189.77	1	94.88	189.77	0.08988	2111.368564
5		Nitrobenzene	11.39	1401.75	1	11.39	1401.75	1109	1.263979849
6	Conversion of NB = 60%	Nitrobenzene	18.98	2336.26	1	18.98	2336.26	1109	2.106633082
7	NB used = PAP and Aniline formed	Paraaminophenol	7.97	869.80	0.3443052238	102.48	2526.25	1066.278673	2.369224558
	Selectivity of PAP = 70%	Aniline	3.42	318.12	0.1259250913				
	Used H2 = 2*PAP + 3*Aniline	Hydrogen	68.70	137.39	0.05438620213				

	Unreacted = 40% of Fed	Nitrobenzene	7.59	934.50	0.3699163174				
	Water = 2*Aniline + PAP	Water	14.80	266.44	0.1054671655				
8		Hydrogen	68.70	137.39	1	68.70	137.39	0.08988	1528.63084
9		Paraaminophenol	7.97	869.80	0.3641076564	33.78	2388.86	1127.599647	2.118535851
		Aniline	3.42	318.12	0.1331675696				
		Nitrobenzene	7.59	934.50	0.391191751				
		Water	14.80	266.44	0.111533023				
10		Hydrogen	61.83	123.65	1	61.83	123.65	0.08988	1375.767756
11		Hydrogen	6.87	13.74	1	6.87	13.74	0.08988	152.863084
12		Aniline	3.42	318.12	0.2094184196	25.81	1519.06	1057.514033	1.436442367
		Nitrobenzene	7.59	934.50	0.6151855026				
		Water	14.80	266.44	0.1753960778				
13	PAP needed = Acetaminophen formed	Paraaminophenol	7.97	869.80	1	7.97	869.80	1250	0.695841854
14		Nitrobenzene	7.59	934.50	1	7.59	934.50	1109	0.8426532329
15		Aniline	3.42	318.12	0.5442061591	18.22	584.56	975.20575	0.5994176366

		Water	14.80	266.44	0.4557938409				
16		Aniline	3.42	318.12	1	3.42	318.12	998	0.3187562299
17		Water	14.80	266.44	1	14.80	266.44	947.99	0.2810544503
18	PAP : Anhydride = 1 : 3	Acetic Anhydride	23.91	2441.07	1	23.91	2441.07	1080	2.260253281
19	Post Filter Yield : 83%	Acetaminophen	7.97	1204.82	0.3639035805	31.88	3310.82	1142.257498	2.898488365
		Acetic Anhydride	15.94	1627.38	0.4915345227				
		Acetic Acid	7.97	478.62	0.1445618968				
20		Acetic Anhydride	15.94	1627.38	0.772735874	23.91	2106.00	1073.182076	1.962389084
		Acetic Acid	7.97	478.62	0.227264126				
21		Acetaminophen	7.97	1204.82	1	7.97	1204.82	1263	0.9539345029
22		Acetaminophen	7.97	1204.82	1	7.97	1204.82	1263	0.9539345029
23	Recrystallisation Filter causes drop by 10%	Acetaminophen	7.17	1084.34	1	7.17	1084.34	1263	0.8585410526
24		Acetaminophen	7.17	1084.34	1	7.17	1084.34	1263	0.8585410526

25		Acetaminophen	7.17	1084.34	1	7.17	1084.34	1263	0.8585410526
26	Last Filter causes remaining drop	Acetaminophen	7.17	1084.34	1	7.17	1084.34	1263	0.8585410526
27	Basis Given	Acetaminophen	6.62	1000.00	1	6.62	1000.00	1263	0.7917656374

Capital cost (only for the reactor):

Equipment	Design Capacity (L)	No. of units	Cost/unit ($ for year 2014)	Total Cost ($ for year 2014)
Reactor 1 (Jacketed reactor, agitated, Carbon steel, 25 - 150psi pressure)	118.46	1	10,000	10,000
Reactor 2 (Jacketed reactor, agitated, Carbon steel, atm-25 psi pressure)	207.034	1	8,100	8,100

References: Provide reference for a research paper or an actual patent.

1. Matches' Reactor cost - autoclave, fermenter, kettle, mixer settler.
2. e-journal: Multistep Synthesis of Paracetamol in Continuous Flow

3. Patent: FR3109581A1 - Continuous paracetamol synthesis process - Google Patents
4. link: Synthesis of paracetamol from p-aminophenol - Labmonk
5. https://arxiv.org/ftp/arxiv/papers/2110/2110.15750.pdf

List the contributions of each author:

- Authors 1 and 2 contributed to the block diagram and calculations.
- Author 3 contributed to block diagram and deciding process conditions.
- Author 4 calculated the capital cost of the reactors.
- Author 5 helped find good resources and references.
- Author 6 proofread the document and helped in correcting some information.

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