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Process Design and Optimization for Separation of Ethylene Oxide & Water Using Simulator

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Abstract

Ethylene Oxide was first reported in 1859 as being prepared from the reaction of potassium hydroxide on ethylene chlorohydrins. But nowadays it is mainly prepared by direct oxidation of ethylene with oxygen on silver based catalyst. In its final product stream along with ethylene oxide many other impurities like formaldehyde, acetaldehyde, unconverted ethylene, water and other inert gases are also present. So its purification consist of many stages which includes stripping zone, scrubbing zone, phase separator, an ethylene oxide purification zone and their interconnections. In its scrubbing step ethylene oxide is scrubbed from other impurities with help of excess of water which needs to be removed so it can be reused for scrubbing purpose as well as to get pure ethylene oxide. For commercial purpose like its use in epoxy paints, as surfactants demands highly pure ethylene oxide having purity of more than 99.5%. Present study aims to separate Ethylene oxide from water at minimum cost and high purity using distillation process as a means of purifying technique and then designing its heat exchangers as well as storage tanks to store crude Ethylene oxide as well purified ethylene oxide and finally preparing its process flow diagram to show how exactly the whole purifying stages are connected. Distillation operation is a widely used separation technology because of its ability to provide highly pure components although at high energy cost. In present study Distillation is evaluated has separation technology for separation of Ethylene oxide from water. Simulation of Distillation column were carried out using chemical simulators and then results obtained from simulation were verified for column efficiency by manual calculation as well as program was prepared using Excel to check efficiency. Distillation operation was able to provide purity of around 99% and efficiency of column was achieved around 60%.

Introduction

Ethylene Oxide is widely used petrochemical compound derived from ethylene. Ethylene Oxide was first prepared in 1859 by Wurtz from 2-chloroethanol (ethylene Chlorohydrins) and aqueous potassium hydroxide. Ethylene Oxide can be manufactured mainly by two processes which include: **1)** Direct oxidation of Ethylene with Oxygen and **2)** Production from ethylene Chlorohydrins. But now it is produced mainly by direct oxidation process. Molecular Weight of Ethylene Oxide is 44.05 kg/kmole. The boiling point of ethylene oxide at atmospheric conditions is 10^{o}C. Even though in final purification stage of Ethylene Oxide production recovery of Ethylene Oxide from aqueous solution is easy due to high volatility difference between water and Ethylene Oxide, separation process is highly energy intensive process because of high solubility of Ethylene Oxide in water. So this paper describes the optimal design of recovery process of Ethylene Oxide from water [5,6, 7].

Selection of Fluid Package

Fluid package selection can do mainly in two ways. One is in which it can be selected by using the selection chart or decision tree available from literature and second is it can done by cross verifying VLE data obtained from simulator with that of the data available in literature which is very accurate method and gives surety of the results of process simulation with that particular property package. So from literature we sorted out three fluid packages i.e. NRTL (non-random two liquids), WILSON & UNIQUAC, which gives binary coefficients of our desired compound which in turn gives physical and chemical properties of our compound (Ethylene Oxide & water). Next we collected VLE data of Ethylene Oxide and water from literature with different temperature & Pressure condition. After that we generated VLE data using UNISIM at the same temperature pressure condition as that collected from literature and calculated deviation of UNISIM from that of literature. The table 1, 2 & 3 shows the comparison of VLE data of UNISIM with that of literature and also shows the deviation of both the data [11].

Table shows individual deviation and overall deviation of NRTL, WILSON & UNIQUAC is 12%, 6.8% and 4.8%. Similarly VLE data were compared at other temperature and pressure condition and was found that average deviation of all three fluid packages were nearly same. So conclusion was we can select any fluid package for predicting binary coefficients of our compounds (Ethylene Oxide & water). So we had chosen UNIQUAC as a fluid package to simulate our distillation column.

Tray Type Selection

Many different types of trays are available in market for satisfying our process requirement and for the process of separating EO from water main things which we considered were the Vapor flow rates and that was sufficiently high so this helped to ignore selection of bubble cap tray from Sieve type. Another thing to be kept in mind was achievement of desired turn down ratio which we assumed to be in sieve tray 70 % and weeping didn't occurred at that ratio and so it satisfied our requirement and thus helped in avoiding Valve tray for our process which helped indirectly in fixed cost reduction for the process [12].

After deciding pressure of 2 atmosphere we made a run for converging distillation column by shortcut method and found that minimum number of stages were 7 with feed at

Next step for our project to converge distillation column taking some design basis. We have taken feed composition as 50% ethylene oxide and 50% water and chilled water at 12^{o}C. We have taken column pressure as 2 atmosphere absolute because at 2 atmosphere 30^{o}C is bubble point of pure ethylene oxide and so it provides sufficient temperature difference between outlet temperature of chilled water and inlet temperature of feed to condenser i.e. temperature of vapor at top most tray of distillation column.

the 5th stage and minimum reflux ratio of 2 to get 99% pure Ethylene Oxide in distillate. Following this we designed a sieve tray for the column whose detail tray design is mentioned in the table 4 & 5 and then finally calculated tray efficiency using rigorous AIChE method which gave average column efficiency of 70% and so actual number of tray calculated were 10.

Using results of tray efficiency and that obtained from shortcut distillation column we simulated our column using rigorous distillation method. On converging column by rigorous distillation method we used the results obtained from them to calculate tray efficiency and then finally designing tray for the same. So tray efficiency result came out to be 60% which gave actual number of

trays to be 16 for separating EO from water with a purity of 99% in distillate.

The next step after getting actual number of trays of distillation column was to feed individual tray efficiency into the column and then simulating the column to get distillate composition of EO which came out as 99% as desired.

Analyzing the results obtained above we can interpret the optimization of reflux ratio led to reduction in requirement of utility to around half of that required initially without compromising product quality and quantity.

Conclusion

Finally we designed a distillation column to separate EO from water Using UNISIM with 16 trays and average efficiency of 60 % and optimal reflux ratio as 0.5 which satisfies our process requirements of 99% pure Ethylene Oxide in distillate stream.

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Table 1: VLE Data Comparison for EO-Water at 10^0C Temperature for NRTL

A (mole fraction)	B (mm Hg)	D (mm Hg)	% Deviation
0.0253	132.8	169.58	27.70
0.0408	202.9	248.27	22.36
0.0562	260	290.19	11.61
0.0727	336	375.18	11.66
0.1231	473.3	507.04	6.45
0.154	552	560.07	1.46
0.2299	617	637.02	3.24

Table 2: VLE Data Comparison for EO-Water at 10^0C Temperature for WILSON

A (mole fraction)	B (mm Hg)	D (mm Hg)	% Deviation
0.0253	132.8	150.16	13.07
0.0408	202.9	218.71	7.79
0.0562	260	255.09	1.88
0.0727	336	328.97	2.09
0.1231	473.3	446.21	6.32
0.154	552	495.71	10.19
0.2299	617	575.29	6.75

Table 3: VLE Data Comparison for EO-Water at 10^0C Temperature for UNIQUAC

A (mole fraction)	B (mm Hg)	D (mm Hg)	% Deviation
0.0253	132.8	142.13	7.03
0.0408	202.9	210.09	3.54
0.0562	260	254.49	2.12
0.0727	336	324.1	3.54
0.1231	473.3	451.16	5.27
0.154	552	506.14	8.31
0.2299	617	593.59	3.79

Table 4. Summary of Tray Design for Column Simulated Using Short cut Method

	Tray 1	Tray 2	Tray 3	Tray 4	Tray 5	Tray 6	Tray 7
Liq Flow (kmol/hr)	231.59	230.5	230.45	230.4	529	510	519.73
Vapour Flow (kmol/hr)	345.78	345.7	344	34308	215	210	242.53
ρL (kg/m3)	859.5	859	858	858	951	951	952.5
ρv (kg/m3)	3.48	3.47	3.45	3.44	3	1.17	1.252
Flooding Velocity (m/s)	1.62	1.65	1.68	1.7	2.11	3.23	3.43
An (m2)	0.865	0.86	0.864	0.8	0.75	0.35	0.37
Dowmcomer area (m2)	0.117	0.117	0.117	0.117	0.058	0.054	0.054
Column Diameter (m)	1.19	1.19	1.19	1.19	1	0.73	0.73
Active area (m2)	1.019	1.019	1.019	1.019	1.019	1.019	1.019
vh min (m2)	6.28	6.26	6.25	6.2	8	9.95	10.65
ht (mm LC)	107.26	106.5	106.4	100	95	94	91.63
hdc (mm)	2.226	2.22	2.225	2.6	2.3	2.2	2.19
hb (m)	178.47	178.47	178.46	170	200	167.8	167.7
lt+hw/2	329.9	329.9	329.9	329.9	329.9	329.9	329.9
Liq Residence time (s)	6.74	6.74	6.75	5	3	2.7	2.778
Entrainment (%)	10	10	10	10	12	12	12

Table 5. Summary of Tray Design for Column Simulated Using Short cut Method

	Tray 1	Tray 2	Tray 3	Tray 4	Tray 5	Tray 6	Tray 7	Tray 8	Tray 9	Tray 10
Liq Flow (kmol/hr)	116.86	116.8	116.66	116.3	115.36	116.6	489.7	438.6	469	473.52
Vapour Flow (kmol/hr)	230.37	230.36	230	229.78	228.86	225	212.11	161.1	166.9	195.95
ρL (kg/m3)	858.1	858.1	858	858.3	858.3	860	921	960.1	943.3	930.4
ρv (kg/m3)	3.549	3.548	3.546	3.53	3.524	3.54	3	1.445	1.134	1.116
Flooding Velocity (m/s)	1.59	1.595	1.597	1.6	1.6	1.64	2.11	3.23	3.51	3.52
An (m2)	0.58	0.585	0.58	0.58	0.578	0.563	0.45	0.259	0.25	0.292
Dowmcomer area (m2)	0.079	0.079	0.079	0.079	0.078	0.076	0.06	0.035	0.034	0.039
Column Diameter (m)	0.92	0.92	0.91	0.918	0.91	0.9	0.808	0.61	0.6	0.65
Active area (m2)	0.5	0.5	0.504	0.503	0.49	0.48	0.389	0.223	0.21	0.252
vh min (m2)	6.22	6.22	6.22	6.23	6.25	6.15	6.98	9.92	11.19	11.289
ht (mm LC)	152.18	152.13	151099	152.2	152.7	100	200	193.04	183.5	181.8
hdc (mm)	3.29	3.3	3.3	3.31	3.34	3.4	3.71	3.811	3	2.57
hb (m)	219.5	219.48	219.34	219.5	220	167.5	289	272	259.69	256.2
lt+hw/2	329.9	329.9	329.9	329.9	329.9	329.9	329.9	329.9	329.9	329.9
Liq Residence time (s)	10.52	10.52	10.52	10.54	10.59	8	2.9	3.29	3.46	4
Entrainment (%)	12	12	12	12	5	12	5	5	5	7

Optimization of Distillation Column

Table 6. Distillation Column Optimization Using Reflux as Optimizing Parameter

EO Purity in Distillate = 99% and Number of stages =16

Reflux ratio	Condenser Duty	Reboiler Duty	Steam flow rate (kg/hr)	Chilled water flow rate (kg/hr)
2	9.00E+06	8.80E+06	13552.32	623700
1.8	8.20E+06	8.20E+06	12628.3	568260
1.6	7.60E+06	7.60E+06	11704.28	526681
1.4	7.00E+06	7.00E+06	10780.3	485100
1.2	6.50E+06	6.50E+06	10010	450450
1	5.80E+06	5.80E+06	8932	401940
0.8	5.30E+06	5.30E+06	8162	367290
0.5	4.61E+06	4.60E+06	7084	319743