Energy, economic and environmental evaluations for the separation of ethyl acetate/ethanol/water mixture via distillation and pervaporation unit

Katherine Barahona Guananga, Mario Chimbolema Anilema, Roger Lujano Conforme, Grace Sevilla Miniguano.
Escuela Superior Politécnica De Chimborazo (ESPOCH)
(Riobamba – Ecuador)

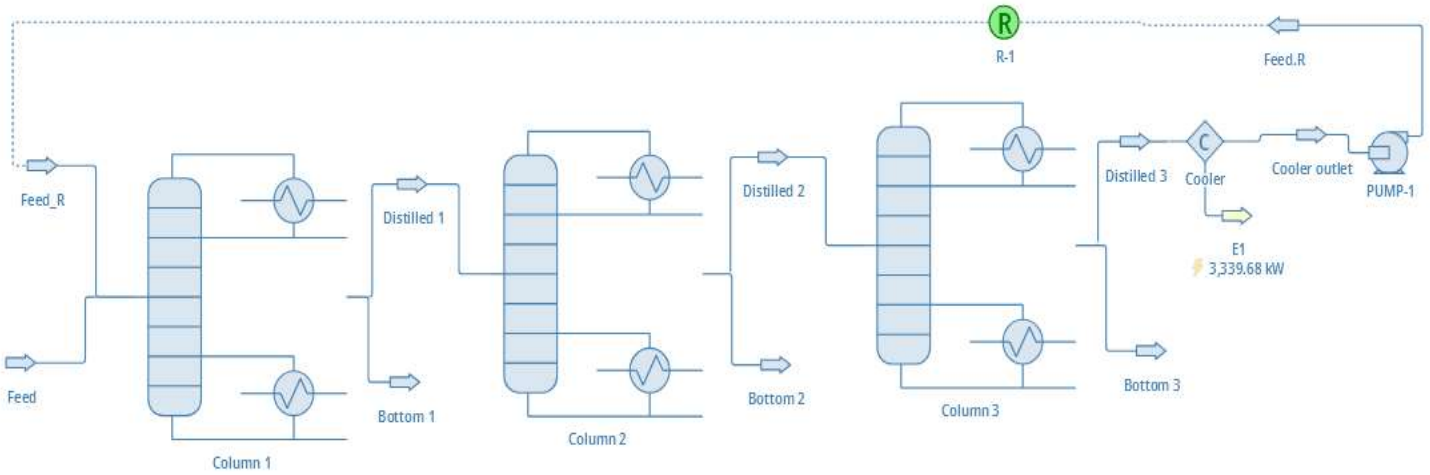
Background & Description:

Ethyl acetate (EtAC) is commonly used as an organic solvent in the biochemical and food industries; it can also be used as a cleaning agent in the textile industry and as a dragging agent in the extraction of natural flavors. Moreover, it is an important raw material in the pharmaceutical industry and in organic synthesis.

The Feed stream (1124 kmol/h, 1 atm, 45°C) with 0.1858 water, 0.276 ethanol, 0.5387 EtAC (mole fraction) feeds (stage 25) the first azeotropic distillation column (Column 1) operating at a pressure of 9 atm. At the bottom of Column 1 a flow (158.924 °C) is obtained which is composed of 0.254, 0.944 EtAC (mole fraction), while in the distillate (Distilled 1) exits at a temperature of 144.176 °C with a fraction of 0.217, 0.529, 0254 for water, ethanol, and EtAC respectively. Distilled 1 is fed (stage 21) to the second column (Column 2) at 0.37 atm. After distillation in Column 2, 0.999 water is obtained at 74.29 °C, in the residue (Bottom 2) and in the distillate (48.169 °C) 0.104 water, 0.605 ethanol, and 0.290 EtAC. Distilled 2 is fed (stage 5) to the third column (Column 3) operating at a pressure of 3.88 atm, obtaining as final product a distillate containing 0.130 water, 0.528 ethanol and 0.342 EtAc and a bottom stream (Bottom 3) with an ethanol fraction of 0.888 at 115.63 °C. Finally, Distillate 3 (Distilled 3 - 1126.71Kmol/h) is recirculated to Column 1 (Stage 9) at 45°C and 1 atm, for which a chiller with 100% efficiency was used followed by a centrifugal pump.

Thermodynamic package: Material Streams (UNIQUAC), Distillation column (Prausnitz/Ideal gas law/UNIFAC/API-SRK).

Background & Description:



Results:

The results of the simulation obtained are shown in Table 1, they are in agreement with those obtained by Meng et al. (2020)**,** who used Aspen Plus for the design and simulation of the process.

Table 1: Simulation results

Master Property Table								
Object	Feed.R	Distilled 3	Distilled 2	Distilled 1	Bottom 3	Bottom 2	Bottom 1	
Temperature	45	112.894	48.1615	144.174	115.485	74.2906	158.422	C
Molar Flow	1125.82	1125.82	1436.83	1643.93	311.01	207.1	605.002	kmol/h
Molar Fraction (Mixture) / Ethyl acetate	0.340648	0.340648	0.290179	0.253622	0.107487	1.43505E-12	0.936797	
Molar Fraction (Mixture) / Ethanol	0.5278	0.5278	0.602605	0.526689	0.873388	3.43034E-07	0.0630127	
Molar Fraction (Mixture) / Water	0.131552	0.131552	0.107217	0.219688	0.0191253	1	0.000190404	

After obtaining the results through the simulation in DWSIM, it is necessary to validate the results obtained with the scientific reference, by comparing the results to calculate the percentage error. The article used for the validation of the results was carried out by Meng et al. (2020). In the validation of the results, the most relevant results were considered. Table 2 shows the validation results.

Table 2: Simulation validation (% Error)

Variable	COLUMN 1						COLUMN 2						COLUMN 3					
	DISTILLED 1			BOTTOM 1			DISTILLED 2			BOTTOM 2			DISTILLED 3			BOTTOM 3		
	ASPEN	DWSIM	%ERROR	ASPEN	DWSIM	%ERROR	ASPEN	DWSIM	%ERROR	ASPEN	DWSIM	%ERROR	ASPEN	DWSIM	%ERROR	ASPEN	DWSIM	%ERROR
Molar Flow (Kmol/h	1643.930	1643.930	0.000	605.000	605.000	0.000	1435.940	1436.830	0.062	207.100	207.100	0.000	1124.930	1125.820	0.079	311.010	311.010	0.000
X_EtAC	0.230	0.254	10.069	0.999	0.937	6.236	0.264	0.290	9.932	-	-	-	0.337	0.340	0.980	-	-	-
X_Water	0.220	0.220	0.046	-	-	-	0.107	0.107	0.281	0.999	0.999	0.000	0.136	0.132	2.509	-	-	-
X_Ethanol	0.550	0.527	4.237	-	-	-	0.630	0.603	4.210	-	-	-	0.528	0.528	0.000	0.999	0.873	12.613

References:

Meng, D., Dai, Y., Xu, Y., Wu, Y., Cui, P., Zhu, Z., Ma, Y., & Wang, Y. (2020). Energy, economic and environmental evaluations for the separation of ethyl acetate/ethanol/water mixture via distillation and pervaporation unit. *Process Safety and Environmental Protection*, *140*, 14–25. https://doi.org/10.1016/j.psep.2020.04.039