Desing of a triple column extractive hybrid distillation process for ternary multi-azeotrope dehydration

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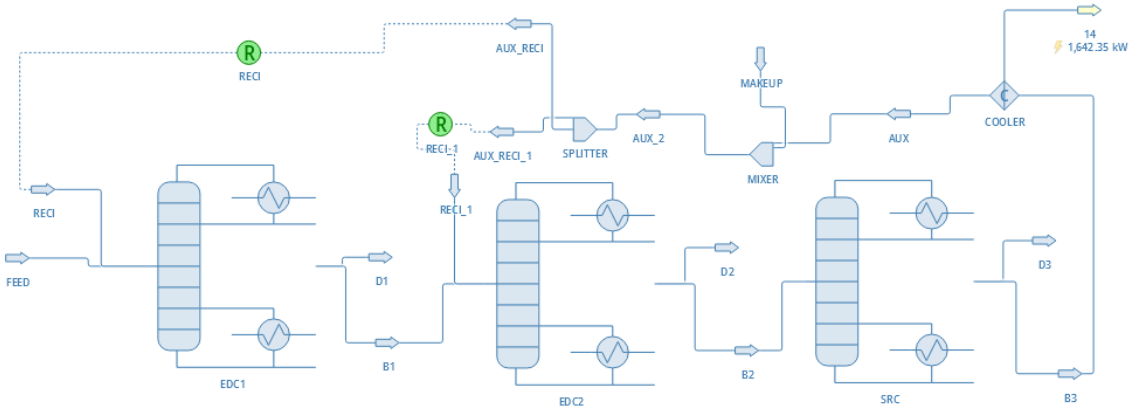
Background & description:

Multi-azeotrope and multi-limit complexes pose enormous challenges in the selection of solvents for the separation of the multi-azeotrope ternary system. In principle, integrating reactive distillation (DR) with extractive distillation (ED) is essential to achieve greater energy efficiencies and reduce process costs and environmental impacts. However, these hybrid distillation processes that can overcome the challenges have not been fully investigated.

The FEED stream (100 kmol/h) with 0.3 EA, 0.2 EtOH and 0.5 Water (molar fraction) is fed (stage 29) to a first extractive distillation column (45 stages) where in the upper stage (T=350.079 K) and in the lower stage (T= 377.81 K) it operates at a constant pressure of 1 atm. Consequently, in the distillate EA is obtained, while the liquid phase enters (stage 10) a second extractive distillation column (19 stages) in the distillate EtOH is obtained, the liquid part feeds (stage 5) to a third column recovery (10 stages) obtaining in the lower part of the latter a molar flow of 238.80 kmol/h, which enters a cooler and leaves with a temperature of 323 K, thus entering a mixer with the MAKEUP stream (0.192 kmol /h EG), the resulting stream enters a separator where the RECI (143 kmol/h) and RECI_1 (96 kmol/h) streams enter the first column (stage 6) and second column (stage 5) respectively. The final concentration of EA (X_EA) in the distillate from the first extractive distillation column (EDC1) is 0.996, the final concentration of EtOH (X_EtOH) in the second extractive distillation column (EDC2) is 0.994 and in the lower part of Solvent Recovery Column (SRC) final concentration of EG (X_EG) is 0.996.

Thermodynamic package: Material Streams (UNIFAC), Extractive Distillation Columns: EDC1 (DECHEMA/ Modified UNIFAC (D)/Antoine/Ideal); EDC2 (DECHEMA/ Wilson/Antoine/Ideal); Solvent Recovery Column: SRC (DECHEMA/ UNIQUAC/Antoine/Ideal).

Flowsheet:



Results:

The results of the simulation obtained are shown in Table 1, they are in agreement with those obtained by Wang et al., (2021), who used Aspen Plus for the design and simulation of the process.

Table 1: Simulation results

Triple column extractive distillation process for ternary multi-azeotrope							
Object	D3	D2	D1	B3	B2	B1	
Temperature	358.198	351.671	350.313	468.583	430.961	386.38	K
Molar Flow	52.0423	19.4038	28.7459	238.808	290.85	214.254	kmol/h
Molar Fraction (Mixture) / Water	0.951806	0.0011848	0.000311657	0.00200157	0.171951	0.233449	
Molar Fraction (Mixture) / Ethylene glycol	0.0119575	2.61273E-05	0.000265152	0.997904	0.821487	0.667223	
Molar Fraction (Mixture) / Ethanol	0.0129595	0.995968	6.83919E-08	2.87567E-08	0.00231888	0.093347	
Molar Fraction (Mixture) / Ethyl acetate	0.0232774	0.00282064	0.999423	9.39873E-05	0.00424223	0.00598074	

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 Wang et al., (2021). In the validation of the results, the most relevant results were considered. Table 2 shows the validation results.

Table 2: Simulation validation (% Error)

Variable	Description	Units	DWSIM	Wang et al., (2021)	Error (%)
X_D3	Molar fraction at the top of the column.		0.9518	0.9967	4.505
X_D2	Molar fraction at the top of the column.		0.9959	0.9954	0.05023
X_D1	Molar fraction at the top of the column.		0.9994	0.9947	0.4725
X_B3	Molar fraction at the bottom of the column.		0.9979	0.999	0.2000
X_B2	Molar fraction at the bottom of the column.		0.9994	0.9947	0.4725
X_B1	Molar fraction at the bottom of the column.		0.6672	0.6711	0.5811

References:

Wang, C., Zhuang, Y., Liu, L., Zhang, L., & Du, J. (2021). Design and comparison of energy-saving double column and triple column reactive-extractive hybrid distillation processes for ternary multi-azeotrope dehydration. *Separation and Purification Technology*, *259*(December), 118211. https://doi.org/10.1016/j.seppur.2020.118211