Simulation control of vapor recompression assisted extractive distillation for separating n-hexane and ethyl acetate using NMP

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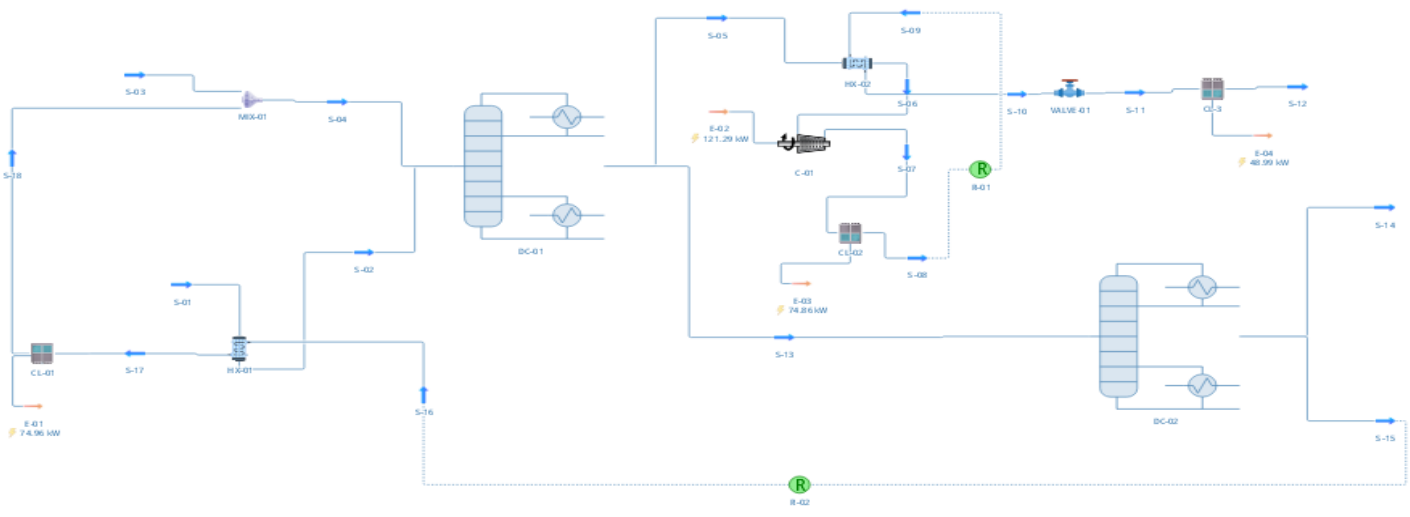
Background & Description:

Ethyl acetate is an organic compound used in different industries, its low cost and level of toxicity make it a diluent and solvent for paints, the perfume industry, food and beverages, it is synthesized chemically through Fischer esterification between acetic acid and ethanol, and n-hexane is used in the extraction of soybean oil, is sometimes used as an alcohol denaturant, and as a cleaning agent in the textile, furniture, and leather industries. Fresh feed (S-01) is fed to the middle of the EDC (Extractive Distillation Column) section after preheating by the recovered recycle skidder, while the cooled recycle skidder (S-04) is fed to the upper EDC section after mixing with the stream. replacement NMP (S-03). High purity n-hexane (99.13wt%) is obtained at the top of EDC, which goes through a compression stage, while the mixture of ethyl acetate and NMP with a small amount of n-hexane is obtained at the bottom of EDC, which is then fed into ERC (Extractive Recovery Column). High purity ethyl acetate (99.98wt%) is obtained at the top of ERC while pure NMP (99.71wt%) is obtained at the bottom of ERC. The flow rate of the fresh feed (61% by weight n-hexane and 39% by weight ethyl acetate) is set to 100 kmol/h (= 8691.94 kg/h), and the desired purity of the acetate product of ethyl and n-hexane is established at 99.9% by weight. The temperature of the fresh feed stream is set to 25 °C. Considering that the feed temperature after preheated by the recycle skidder from the bottom of ERC is set at 64 °C, which is the saturation temperature of the fresh feed at 1 atm.

Thermodynamic package: Material Streams (Wilson), Extractive Distillation Column and Recovery Column (DECHEMA/UNIFAC/Antoine/None)

Flowsheet:



Results:

The results of the simulation obtained are shown in Table 1-2, they are in agreement with those obtained by Feng et al., (2020), who used Aspen Plus for the simulation of the process.

Table 1: Simulation results

Separating n-hexane and ethyl acetate using NMP									
Object	**S-15**	**S-14**	**S-13**	**S-12**	**S-04**	**S-03**	**S-02**	**S-01**	
Temperature	160.201	42.7334	121.981	68.72	100.767	25	61.5044	25	**C**
Pressure	0.33	0.28	1.2	1.01	0.33	1.2	1.2	1.2	**bar**
Mass Flow	8507.71	3389.41	11897.1	5303.75	8508.09	0.38562	8692.8	8692.8	**kg/h**
Molar Flow	85.8499	38.47	124.32	61.5339	85.8538	0.00389	100	100	**kmol/h**
Molar Fraction (Liquid 1) / Ethyl acetate	0.00283776	0.999898	0.311371	0.00866771	0.0028482	0	0.39	0.39	
Molar Fraction (Liquid 1) / N-hexane	7.17498E-11	6.17608E-05	1.91115E-05	0.99132	4.7743E-12	0	0.61	0.61	
Molar Fraction (Liquid 1) / N-methyl-2-pyrrolidone	0.997162	4.023E-05	0.688609	1.18519E-05	0.997152	1	0	0	

Table 2: Compressor Results

Compressor (C-01)		
Property	**Value**	**Unit**
Power Required	**112.704**	**Kw**
Outlet Temperature	**150.68**	**°C**

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 **Feng et al., (2020).** In the validation of the results, the most relevant results were considered. Table 2 shows the validation results.

Table 3: Simulation validation (% Error)

Variable	**Description**	**Units**	**DWSIM**	**Feng et al., (2020).**	**Error (%)**
X_HE	N_hexane: Molar fraction at the top of the extractive distillation column	-	0.9913	0.9990	0.777
X_AE2	Ethyl Acetate: Molar fraction at the bottom of the recovery column.	-	0.9998	0.9990	0.08
X_NMP2	N-methyl-2-pyrrolidone: Molar fraction at the bottom of the recovery column	-	0.9971	0.9997	0.261

References:

FENG, Z., SHEN, W., RANGAIAH, G.P. y DONG, L., 2020. Design and control of vapor recompression assisted extractive distillation for separating n-hexane and ethyl acetate. *Separation and Purification Technology*, vol. 240. ISSN 18733794. DOI 10.1016/j.seppur.2020.116655.