Recovery of Diisopropyl Ether and Isopropanol

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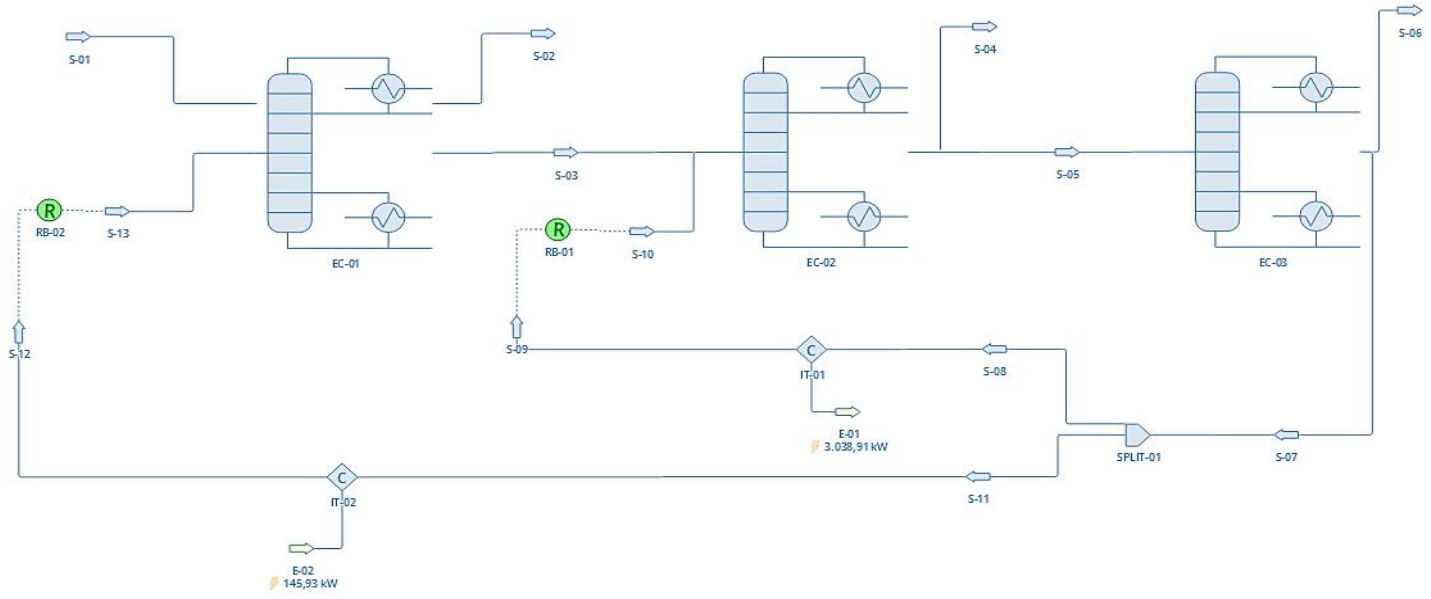
Background & Description:

The Isopropyl Alcohol (IPA) is an industrial conventional solvent can be used as a feedstock for the synthesis of glycerin, isopropyl acetate and methylisobutylocetone. The Diisopropyl Ether (DIPE) is an industrial effluent by-product of IPA, it has also gradually demonstrated its potential as a petroleum additive due to its high octane and resistance to explosions.

Stream S-01 (500 kmol/h, 1.2 atm, 298.15 K) with 0.30 DIPE, 0.40 IPA, 0.3 water (molar fraction) feeds (stage 12) the first extractive distillation column (EC-01), where in the top stage (T=340.24 K) and in the bottom stage (T=364.21 K) work with a pressure of 1 atm. In addition, in the distillate, DIPE is obtained, while the lower part is the feed (stage 52) of the second column (EC-02) and, in the distillate, IPA is obtained, while, the bottom feeds (stage 7) the recovery column (EC-03), obtaining at the bottom of the latter, a molar flow of 694.881 kmol/h that enters the separator (SPLIT-01), where streams S-08 and S-11 are preheated before entering columns ED-02 and ED-01 through stage 2, respectively. The final concentration of DIPE (X_DIPE) in the distillate from the first extractive distillation column (EC-01) is 0.996, the final concentration of IPA (X_IPA) in the distillate from the second extractive distillation column (EC-02) is 0.962 and at the bottom of the recovery column (EC-03), the final concentration of the ionic liquid ethylene glycol EG (X_EG3) is 0.999.

Thermodynamic package: Material Streams (UNIFAC), Extractive Distillation Columns: ED-01 & ED-03: (DECHEMA/UNIFAC/Riedel/Peng-Robinson 78); ED-02: (DECHEMA/UNIFAC/Antoine/Soave-RK).

Flowsheet:



Results:

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

Table 1: Simulation results

Recovery of Diisopropyl Ether and Isopropanol										
Object	S-13	S-10	S-07	S-06	S-05	S-04	S-03	S-02	S-01	
Temperature	323,15	343,15	469,449	370,303	415,758	355,697	364,217	340,254	298,15	K
Pressure	1	1	1	1	1	1	1	1	1,2	atm
Mass Flow	3,42399	8,548	11,972	0,744951	12,7169	3,43082	7,53334	4,25896	8,34653	kg/s
Molar Flow	198,736	496,145	694,881	147,578	842,459	207,261	549,72	150,28	500	kmol/h
Molar Fraction (Mixture) / Diisopropyl ether	0	0	0	1,78353E-20	3,12437E-21	0,0010305	0,000388527	0,996716	0,3	
Molar Fraction (Mixture) / Water	0,001	0,001	0,001	0,99627	0,175347	0,01406	0,273115	0,000421445	0,3	
Molar Fraction (Mixture) / Ethylene glycol	0,999	0,999	0,999	1,07373E-06	0,824	0,022596	0,362675	0,00286292	0	
Molar Fraction (Mixture) / Isopropanol	2,19738E-11	2,19738E-11	2,19738E-11	0,00372862	0,000653162	0,962314	0,363822	4,82622E-08	0,4	

After obtaining the results 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 Qi 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	Description	Units	DWSIM	Qi et al., (2020)	Error (%)
X_DIPE	Molar fraction at the top of the column ED-01.		0.996	0.999	0.30
X_IPA	Molar fraction at the top of the column ED-02.		0.962	0.999	3.703
X_EG1	Molar fraction at the bottom of the column ED-01.		0.362	0.364	0.549
X_EG2	Molar fraction at the bottom of the column ED-02.		0.824	0.824	0
X_EG3	Molar fraction at the bottom of the column ED-03.		0.999	0.999	0
X_WATER	Molar fraction at the top of the column ED-03.		0.996	0.999	0.30
F_S-02	Molar flow out of the top at the ED-01 column.	kmol/h	150.28	150.10	0.12
F_S-13	Molar flow at the inlet of the ED-01 column.	kmol/h	198.736	199.98	0.622
F_S-03	Molar flow at the bottom of the ED-01 column.	kmol/h	549.72	549.9	0.03
F_S-10	Molar flow at the inlet of the ED-02 column.	kmol/h	496.145	500.00	0.771
F_S-05	Molar flow at the bottom of the ED-02 column.	kmol/h	842.459	849.88	0.873
F_S-07	Molar flow at the bottom of the ED-03 column.	kmol/h	694.881	699.98	0.728

References:

Qi, J., Zhu, R., Han, X., Zhao, H., Li, Q., & Lei, Z. (2020). Ionic liquid extractive distillation for the recovery of diisopropyl ether and isopropanol from industrial effluent: Experiment and simulation. *Journal of Cleaner Production*, *254*, 120132. https://doi.org/10.1016/J.JCLEPRO.2020.120132