Simulated annealing-based optimal design of energy efficient ternary extractive dividing wall distillation process for separating benzene-isopropanol-water mixtures.

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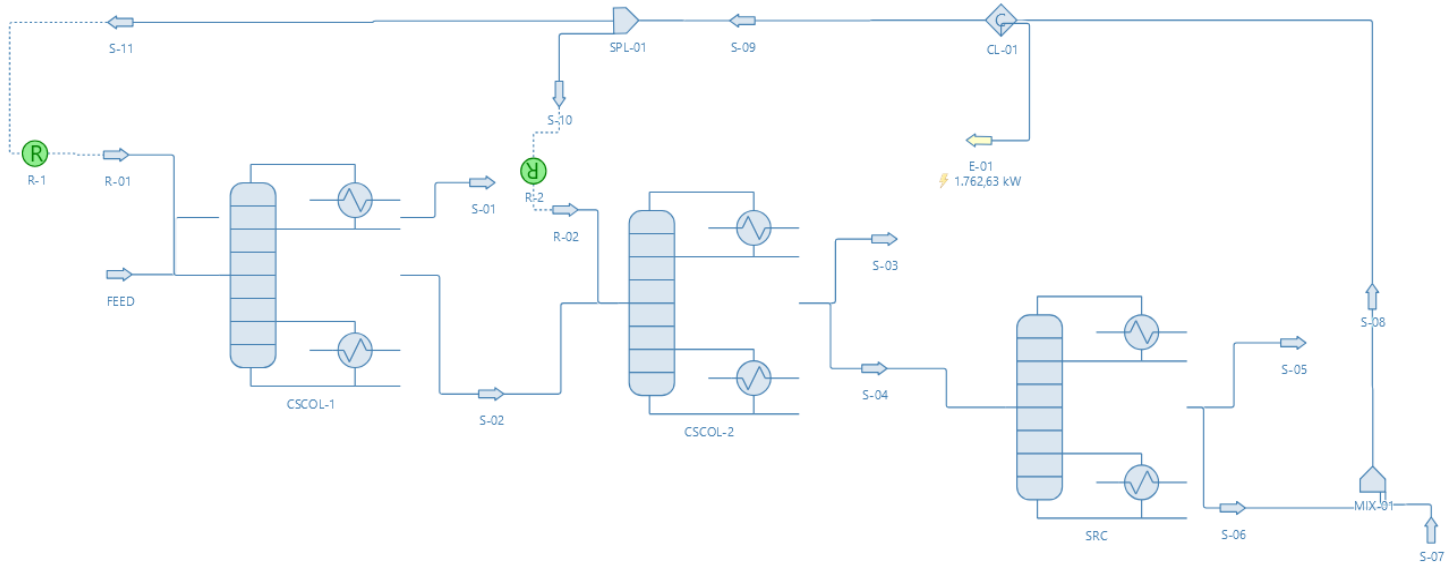
Background & Description:

Benzene (BZ) and isopropanol (IPA) are both good organic solvents and important fundamental chemicals. IPA is also used as alkylation reagent of benzene to produce isopropyl benzene or n-propyl benzene. A ternary mixture containing most of benzene and isopropanol and a small amount of water is often generated in chemical and pharmaceutical industries. This mixture must be separated in order to improve the efficient use of resources and protect the environment.
The FEED stream (100 kmol/h, 1.2 atm, 298.15 K) with 0.3 benzene, 0.1 water, 0.6 IPA (mole fraction) feed (stage 11) to the first column of extractive distillation (27 stages) where in the upper stage (352.83 K) and in the lower stage (378.40 K) operates at a constant pressure of 1 atm. Therefore in the distillate BZ is obtained, while the liquid phase enters (stage 23) to a second column of extractive distillation (29 stages) in the distillate IPA is obtained, the liquid part feeds (stage 10) to a third column recovery (31 stages), obtaining in the final part of the latter a molar flow of 253.14 kmol/h in which it enters a mixer with the current S-07 (0.035 kmol/h EG), the resulting current enters a cooler and exits with a temperature of 323 K, thus entering a current separator where R-01 (116.48 kmol/h) enters the first column (stage 3) and R-02 (136.7 kmol/h) enters the second column (stage 7). The final concentration of BZ (X_BZ) in the distillate of the first extractive distillation column (CSCOL-1) is 0.999, the final concentration of IPA (X_I PA) in the second column of extractive distillation (CSCOL-2) is 0.992 and in the lower part of Solvent Recovery Column (SRC) the final concentration of EG (X_EG) is 1.

Thermodynamic package: Material streams (UNIFAC), extractive distillation columns CSCOL-1, CSCOL-2, and SRC (DECHEMA/UNIFAC/Riedel/Peng-Robinson 78)

Flowsheet:



Results:

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

Table 1: Simulation results

Tabla maestra de propiedades							
Objeto	S-06	S-05	S-04	S-03	S-02	S-01	
Temperatura	470,084	376,845	450,354	355,37	375,916	353,318	K
Presión	1	1	1	1	1	1	atm
Flujo másico	4,36456	0,0512992	4,41586	1,00966	3,06892	0,642724	kg/s
Flujo molar	253,149	10,011	263,16	60,4301	186,905	29,6243	kmol/h
Molar Fraction (Mixture) / Benzene	2,57866E-21	3,26836E-11	1,24334E-12	0,00641488	0,00207406	0,999597	
Molar Fraction (Mixture) / Water	4,26188E-20	0,99	0,0376613	0,00147251	0,0535027	2,63957E-06	
Molar Fraction (Mixture) / Ethylene glycol	1	0,00570581	0,962175	2,02993E-13	0,623423	0,000282615	
Molar Fraction (Mixture) / Isopropanol	6,94849E-20	0,00429419	0,000163358	0,992113	0,321	0,000118064	

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 (Li 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	Li et al., (2020)	Error (%)
X_S-06	Molar fraction at the bottom of the column.	-	1	0.999	0.100
X_S-05	Molar fraction at the top of the column.	-	0.990	0.999	0.900
X_S-04	Molar fraction at the bottom of the column.	-	0.962	0.963	0.103
X_S-03	Molar fraction at the top of the column.	-	0.992	0.995	0.301
X_S-02	Molar fraction at the bottom of the column.	-	0.663	0.625	6.080
X_S-01	Molar fraction at the top of the column.	-	0.999	0.995	0.400

References:

Li, M., Cui, Y., Shi, X., Zhang, Z., Zhao, X., Zhu, X., & Gao, J. (2021). Simulated annealing-based optimal design of energy efficient ternary extractive dividing wall distillation process for separating benzene-isopropanol-water mixtures. In *Chinese Journal of Chemical Engineering* (Vol. 33, pp. 203–210). Materials China. https://doi.org/10.1016/j.cjche.2020.08.041