Energy-saving thermally coupled ternary extractive distillation process that saves energy by combining with the mixed entrainer to separate the ternary mixture containing bioethanol

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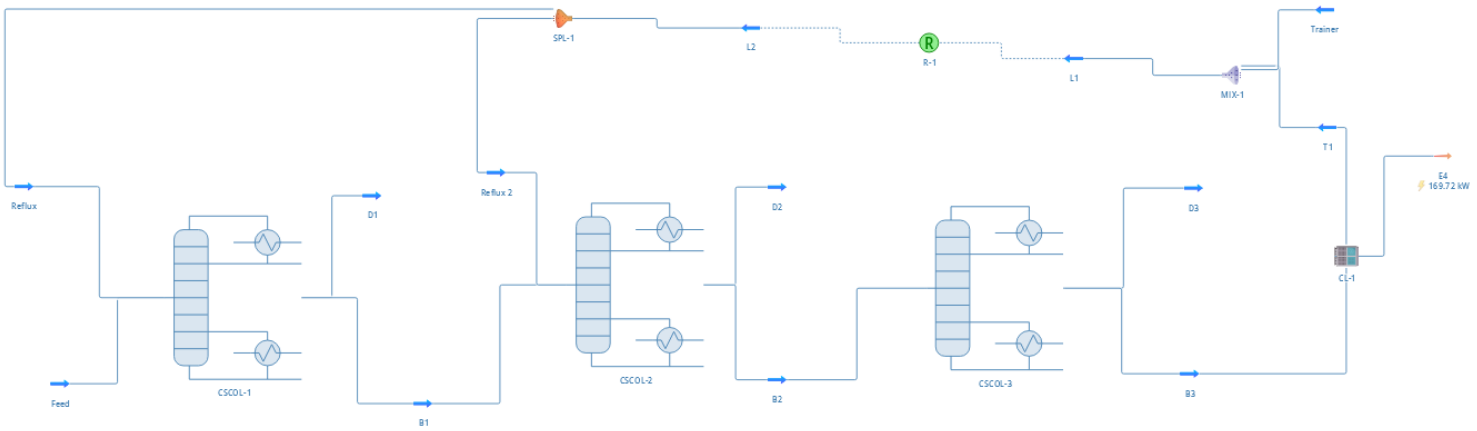
Background & Description:

At present the problem of extractive distillation is high energy consumption, to reduce energy consumption, thermally coupled ternary extractive distillation processes have been studied to separate azeotropic mixtures (tetrahydrofuran (THF)/ethanol/water) with a solvent (dimethyl sulfoxide (DMSO)). Azeotropic distillation can separate the mixtures with the help of a carrier, extractive distillation is widely used to separate multiple azeotropes in the chemical industry.
This simulation shows an extractive distillation process to reduce energy consumption, three extractive distillation towers are shown, fed with 100 kmol/h and compositions of 0.3 THF, O.3 ethanol and 0.4 water, the first tower has 39 stages and two feed sources with a recirculation in stage 4, at the distillate outlet there is a composition of 0.91 of THF, in the second tower there are 52 stages and 2 feedings being one of these a recirculation, in the exit of the distillate there is an increase of the components, while in the exit of the waste it increases the values of its components with a molar flux of 99.99kmol/h, the third tower there is only one feeding, in which in the exit of the distillate we have a molar flux of 40.01kmol/h being this the highest value of molar flux in the three towers, from the third tower comes out the recirculation for tower 2 and for tower 1 where a Cooler (cooler) was added at 50ºC and a power of 261kW to this reflux enters 0.02kmol/h and 1 of DMSO, a mixing system is added for the first recirculation that goes to tower 2, a current divider was added so that the recirculated enters to tower 2 as to tower 1, in tower 2 it enters 35kmol/h and 0.99999 of DMSO, in tower 1 it enters 25kmol/h.

Thermodynamic package: Column1(Wilson-Peng-ROBINSON 78), Column 2 y 3(DECHEMA-Wilson, T correlation, ideal)

Flowsheet:



Results:

The results obtained from the simulation are shown in Stem 1 and 2, these are compared with the results obtained by Zhao et al., (2018), who used the commercial software Aspen Plus (V 8.4) for the simulation of the process.

Tabla 1.: Simulation results

Master Property Table												
Object	Reflux 2	Reflux	L2	L1	Feed	D3	D2	D1	B3	B2	B1	
Temperature	50	50	50	50	50	53.6617	53.5595	65.8152	124.751	114.055	90.4541	C
Pressure	0.15	0.15	0.15	0.15	0.15	0.15	0.4	1	0.15	0.4	1	atm
Mass Flow	0.751616	0.536942	1.28625	1.28625	1.18495	0.203625	0.402221	0.581846	1.28582	1.48944	1.14005	kg/s
Molar Flow	34.998	25.002	60	60	100	40.01	29.9879	30.0221	59.98	99.99	94.9799	kmol/h
Molar Fraction (Mixture) / Tetrahydrofuran	6.57687E-21	6.57687E-21	7.99501E-21	7.99501E-21	0.3	3.81491E-07	0.0889231	0.910442	7.99767E-21	1.5265E-07	0.0280757	
Molar Fraction (Mixture) / Ethanol	2.40116E-15	2.40116E-15	3.69923E-15	3.69923E-15	0.3	0.00289539	0.907018	0.0894213	3.70046E-15	0.00115856	0.287591	
Molar Fraction (Mixture) / Water	0.0136389	0.0136389	0.0159376	0.0159376	0.4	0.99336	0.00378964	0.000135304	0.0159429	0.407047	0.424689	
Molar Fraction (Mixture) / Dimethyl sulfoxide	0.986361	0.986361	0.984062	0.984062	0	0.00374416	0.000268772	1.83058E-06	0.984057	0.591794	0.259644	

After obtaining the simulation results in DWSIM, it is necessary to validate these obtained results with a scientific reference, comparing the calculated results with a percentage error. The article used for the validation of the results was made by Zhao et al., (2018). For the validation of the results the most relevant parameters were considered. Table 2 shows the validation of the results.

Table 2: Simulation Validation (% Error)

	COLUMN 1						COLUMN 2		
	D1			B1			D2		
Object	*ASPEN*	*DWSIM*	*%ERROR*	*ASPEN*	*DWSIM*	*%ERROR*	*ASPEN*	*DWSIM*	*%ERROR*
Molar Flow (kmol/h)	30.02	30.02	0.00	94.98	94.98	0.00011	29.99	29.98	0.03334
Molar Fraction THF	0.99	0.91	8.08	-	-	-	-	-	-
Molar Fraction Ethanol	-	-	-	0.316	0.2876	8.98734	0.99	0.9064	8.44455
Molar Fraction Water	-	-	-	0.421	0.4252	0.99762	-	-	-
Molar Fraction DMSO	-	-	-	0.263	0.259	1.52091	-	-	-
Temperature (°C)	65.97	65.81	0.24	98.87	90.494	8.47173	56.7	53.554	5.54815

	COLUMN 2			COLUMN 3					
	B 2			D3			B3		
Object	*ASPEN*	*DWSIM*	*%ERROR*	*ASPEN*	*DWSIM*	*%ERROR*	*ASPEN*	*DWSIM*	*%ERROR*
Molar Flow (kmol/h)	99.99	99.99	0	40.01	40.01	0	59.98	59.98	0
Molar Fraction THF	-	-	-	-	-	-	-	-	-
Molar Fraction Ethanol	-	-	-	-	-	-	-	-	-
Molar Fraction Water	0.4	0.4	0	0.99	0.99	0	-	-	-
Molar Fraction DMSO	0.6	0.5904	1.6	-	-	-	0.99	0.9823	0.77778
Temperature (°C)	128.3	113.89	11.2307	54.19	53.507	1.2613	146.8	124.52	15.1713

References:

Zhao, Y., Ma, K., Bai, W., Du, D., Zhu, Z., Wang, Y., & Gao, J. (2018). Energy-saving thermally coupled ternary extractive distillation process by combining with mixed entrainer for separating ternary mixture containing bioethanol. *Energy* , *148* , 296–308. https://doi.org/10.1016/j.energy.2018.01.161