Investigation on ternary system tetrahydrofuran/ethanol/water with three azeotropes separation via the combination of reactive and extractive distillation

Angie Serrano, Karla Panchi, Margorie Ruiz, Paulina Lopez
Escuela Superior Politécnica De Chimborazo (ESPOCH)
(Riobamba – Ecuador)

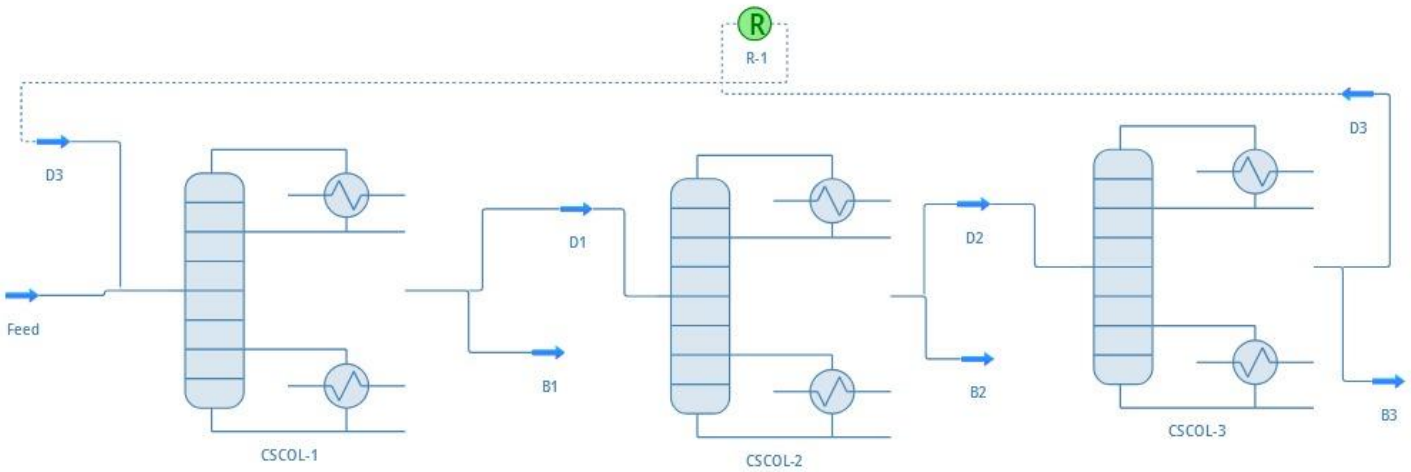
Background & Description:

The principal end uses of Tetrahydrofuran include pharmaceutical solvent, adhesives, PVC cement and magnetic tape, ethanol is one of many kinds of alcohol and is the only type of alcohol that can be consumed and water is the universal solvent.

In this process the theoretical stages of the three columns C1, C2, and C3 are 29, 72, and 70. The recirculation exits through stream D3 and re-enters column C1 for which a recycling logic block was used. Stream D3 (recycled stream) and the Feed Stream are fed to the 7th and 24th trays of the column C1, at the botton 99.9 mol% water is obtained and the reflux is 0.408, at the top 99.5 mol% ethanol is obtained while the stream D1 feeds at the 6th stage of column C2 and the reflux ratio is 1.350, on the other hand, in the column C3 while the feed is at the 37th stage 99.5 mol% THF is obtained and the reflux ratio is 1.762. The process operating pressures are 0.10 MPa for column C1, 0.52 MPa for column C2 and 1.00 MPa for column C3.

Thermodynamic package: Material Streams (NRTL), Distillation Column 1 (DECHEMA/ Ideal Gas Law/ Wilson/ T correlation/ Ideal), Distillation Column 2 (DECHEMA/ Ideal Gas Law/ Wilson/ T correlation/ None), Distillation Column 3 (DECHEMA/ Ideal Gas Law/ Wilson/ T correlation/ None).

Flowsheet:



Results:

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

Table 1: Simulation results

Tabla maestra de propiedades							
Object	D3	D2	D1	B3	B2	B1	
Temperature	420,424	393,577	340,444	432,198	400,162	372,738	K
Pressure	1	0,52	0,1	1	0,52	0,1	MPa
Molar Flow	157,5	190,681	225,936	33,1819	35,2541	31,8343	kmol/h
Molar Fraction (Mixture) / Tetrahydrofuran	0,447773	0,543	0,45874	0,995	0,003	4,556E-07	
Molar Fraction (Mixture) / Ethanol	0,326418	0,270486	0,373847	0,00499971	0,932903	0,000999544	
Molar Fraction (Mixture) / Water	0,225809	0,186514	0,167413	2,93402E-07	0,0640974	0,999	

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 Yang Su 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)

	COLUMN 1						COLUMN 2						COLUMN 3					
	D1			*B1*			*D2*			*B2*			*D3*			*B3*		
	Aspen	Dwsim	%Error	Aspen	Dwsim	%Error	Aspen	Dwsim	%Error	Aspen	Dwsim	%Error	Aspen	Dwsim	%Error	Aspen	Dwsim	%Error
TEMPERATURE (K)	340.100	340.410	0.091	377.600	372.738	1.288	393.700	393.576	0.031	403.000	400.160	0.705	421.500	420.423	0.256	434.800	432.198	0.598
X TETRAHIDOFURANO	0.455	0.460	1.187	0.000	0.002	0.000	0.543	0.543	0.000	0.003	0.003	0.000	0.435	0.448	2.943	0.995	0.995	0.000
X ETHANOL	0.374	0.371	0.695	0.001	0.008	670.000	0.254	0.270	6.417	0.995	0.932	6.312	0.314	0.326	3.854	0.005	0.005	2.000
X WATER	0.171	0.168	0.455	0.999	0.999	0.000	0.203	0.187	8.079	0.002	0.000	100.000	0.251	0.226	10.000	0.000	0.000	0.000
MOLAR FLOW (kmol/h)	203.857	225.949	0.374	34.000	32.146	5.452	170.858	191.418	12.033	33.000	34.532	4.642	137.857	158.130	14.706	33.000	33.280	0.848
ERROR RATE			**0.171**			**2.246**			**5.312**			**3.886**			**6.351**			**0.482**

References:

Yang Su, Ao Yang, Saimeng Jin, Weifeng Shen, Peizhe Cui, Jingzheng Ren, Investigation on ternary system tetrahydrofuran/ethanol/water with three azeotropes separation via the combination of reactive and extractive distillation, Journal of Cleaner Production, Volume 273, 2020, 123145, ISSN 0959-6526, https://doi.org/10.1016/j.jclepro.2020.123145. (https://www.sciencedirect.com/science/article/pii/S0959652620331905)