Separation of ternary azeotropic mixture Acetonitrile/ethanol/water using DMSO as entrainer

Ms.Para Preethi
NIT Rourkela

Unit system: C5

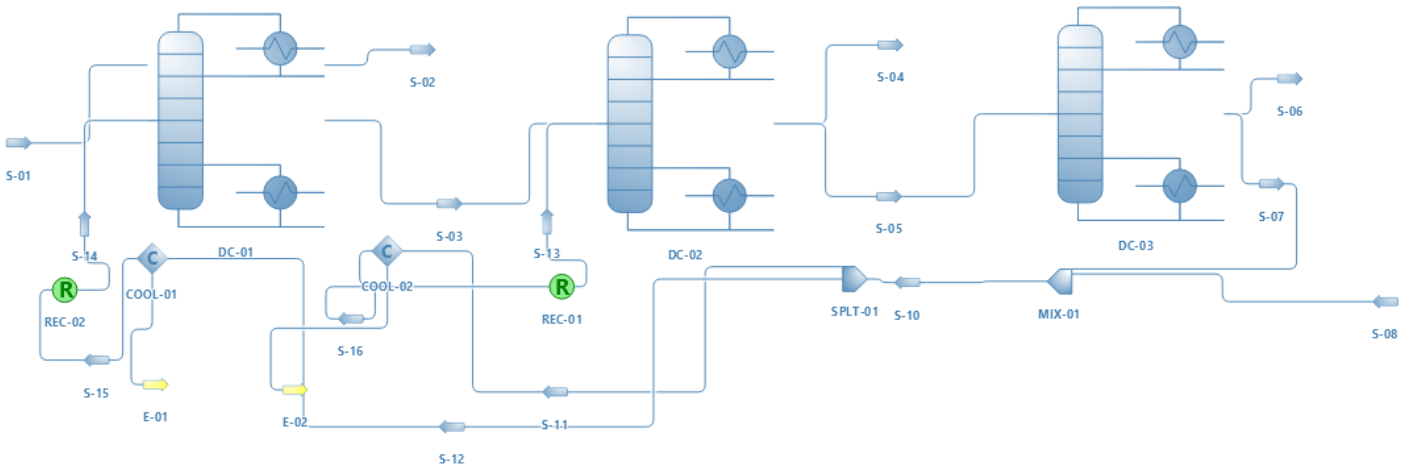
Thermodynamic Package: NRTL is chosen to describe vapor-liquid equilibrium

Background:

Acetonitrile and ethanol are used as mobile phase organic solvents in HPLC (High-Performance Liquid Chromatography), which results in the production of waste ternary mixture ACN/EtOH/water. Such ternary mixtures are also generated from the production process of Acetonitrile by dehydrogenation of ethanol and ammonia. Lower the absorbance of organic solvent, lower the noise in UV detection, and hence is an excellent solvent for HPLC. Separating mixtures is necessary to obtain pure substances for economic benefits, industrial purposes, and research work. Acetonitrile is used as a solvent to make pesticides, pharmaceuticals, batteries, and rubber products. At the same time, ethanol is used to manufacture drugs, plastics, lacquers, polishes, plasticizers, beverages, and cosmetics. It is also used as a disinfectant in a lab/hospital and an antidote for ethylene glycol or methanol overdose.

Description:

ACN/EtOH/water ternary mixture cannot be separated by simple distillation since it forms an azeotropic mixture. An azeotropic assortment, also called the constant boiling mixture, has the same liquid and vapor composition. The separation of such mixtures can be achieved using the "Triple column extractive distillation" method. Here Acetonitrile/ethanol/water forms a ternary azeotropic mixture with three binary azeotropes (ACN/EtOH, ACN/Water, EtOH/Water) and a ternary azeotrope (ACN/EtOH/water). DMSO (Dimethyl sulfoxide) is chosen as an entrainer because of its high separation efficiency and low energy consumption. This ternary mixture can be separated using three distillation columns with recycling for the 1st and 2nd distillation columns. The initial feed is given to the DC-01, i.e., in S-01, is 100 Kmol/hr with compositions 0.453 ACN, 0.131 EtOH, 0.416 water. The feed is given at stages 26, 23, 7 to DC-01, DC-02, DC-03. Recycle stream enters DC-01 at 7th stage, recycle stream to DC-02 enters at 4th stage. We obtain 99.9% purity of Acetonitrile in the top distillate from the first distillation column, 99.9% purity of ethanol, and 99.9% of the water from the top distillates 2nd and 3rd distillation columns.



ACN/EtOH/Water separation using DMSO as entrainer

Results:

Stream wise compositions																
Object	S-16	S-15	S-14	S-13	S-12	S-11	S-10	S-08	S-07	S-06	S-05	S-04	S-03	S-02	S-01	
Temperature	50	50	50	50	97.0553	97.0553	97.0553	150	97.0508	88.4438	95.2768	77.1156	91.7443	79.1716	10	C
Pressure	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	bar
Mass Flow	1751.93	3180.31	3180.31	1751.93	3180.31	1751.93	4932.24	3.12534	4929.11	1303.22	6232.33	467.512	4948.3	1443.89	3212.58	kg/h
Molar Flow	61.9938	112.538	112.538	61.9938	112.538	61.9938	174.532	0.04	174.492	41.5972	216.089	13.1078	167.206	45.3269	100	kmol/h
Molar Fraction (Mixture) / Acetonitrile	0.240004	0.240004	0.240004	0.240004	0.240004	0.240004	0.240004	0	0.240059	0.575498	0.304631	0.492814	0.343204	0.330153	0.453	
Molar Flow (Mixture) / Acetonitrile	14.8788	27.0097	27.0097	14.8788	27.0097	14.8788	41.8885	0	41.8885	23.9391	65.8276	6.4597	57.3859	14.9648	45.3	kmol/h
Molar Fraction (Mixture) / Ethanol	1.68342E-08	1.68342E-08	1.68342E-08	1.68342E-08	1.68342E-08	1.68342E-08	1.68342E-08	0	1.6838E-08	0.00202175	0.000389201	0.224521	0.0181038	0.222228	0.131	
Molar Flow (Mixture) / Ethanol	1.04361E-06	1.89449E-06	1.89449E-06	1.04361E-06	1.89449E-06	1.04361E-06	2.9381E-06	0	2.9381E-06	0.0840993	0.0841023	2.94297	3.02708	10.0729	13.1	kmol/h
Molar Fraction (Mixture) / Water	0.681557	0.681557	0.681557	0.681557	0.681557	0.681557	0.681557	0	0.681713	0.42248	0.631811	0.282661	0.586053	0.447619	0.416	
Molar Flow (Mixture) / Water	42.2523	76.7013	76.7013	42.2523	76.7013	42.2523	118.954	0	118.954	17.574	136.528	3.70507	97.9916	20.2892	41.6	kmol/h
Molar Fraction (Mixture) / Dimethyl sulfoxide	0.0784388	0.0784388	0.0784388	0.0784388	0.0784388	0.0784388	0.0784388	1	0.0782275	9.49135E-09	0.0631687	3.17735E-06	0.0526392	4.14859E-07	0	
Molar Flow (Mixture) / Dimethyl sulfoxide	4.86272	8.82737	8.82737	4.86272	8.82737	4.86272	13.6901	0.04	13.6501	3.94814E-07	13.6501	4.1648E-05	8.8016	1.88043E-05	0	kmol/h

Conclusion:

Here we obtain, 99.9% purity of Acetonitrile in the top distillate from the first distillation column, 99.9% purity of ethanol, and 99.9% of the water from the top distillates of 2nd and 3rd distillation columns.