Esterification of Acetic Acid with Methanol to Ethyl Acetate

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Background

Fischer Esterification is the formation of ester (along with water) when carboxylic acid is treated with alcohol along with an acid catalyst. In the reaction, the hydroxyl group of the carboxylic acid is replaced by alkoxy group of the alcohol. The reaction is an equilibrium reaction. Carboxylic esters of low molecular weight are colourless, volatile liquid with pleasant odours, slightly soluble in water. In this flowsheet, methyl acetate is the ester being produced, is a flammable liquid being weakly polar and occasionally used as solvent. Methyl acetate is primarily used as a volatile low toxicity solvent in paints, glues and nail polish removers.

Description of the Flowsheet

Two separate streams of pure methanol and pure acetic acid of equal molar flow rate are being fed to a reactive distillation column at 1 atm pressure and 298 K temperature. Reactive column used here has been ported in from ChemSep using CAPE-OPEN Unit Operation and is a simple distillation column. UNIQUAC model of activity coefficient has been used to account for non-ideal vapor-liquid equilibrium. Extended Antoine model has been used for vapor pressure. The values of interaction parameters has been adapted from the literature. The reaction is an elementary pseudo-homogeneous reversible reaction.

In a 40 stages simple distillation column, acetic acid is fed in its 3rd stage and methanol is fed in its 27th stage. The column is operated at constant pressure. Methyl acetate is obtained as the top product with composition of 98.7 % (mole basis) at 330 K. Water is obtained as bottom product with composition of 99.5 % (mole basis) at 373 K. Reflux ratio of the column is specified at 1.966 and the bottom product flow rate is specified at 49.65 kmol/h.

McCabe-Thiele diagram Methyl acetate - Water
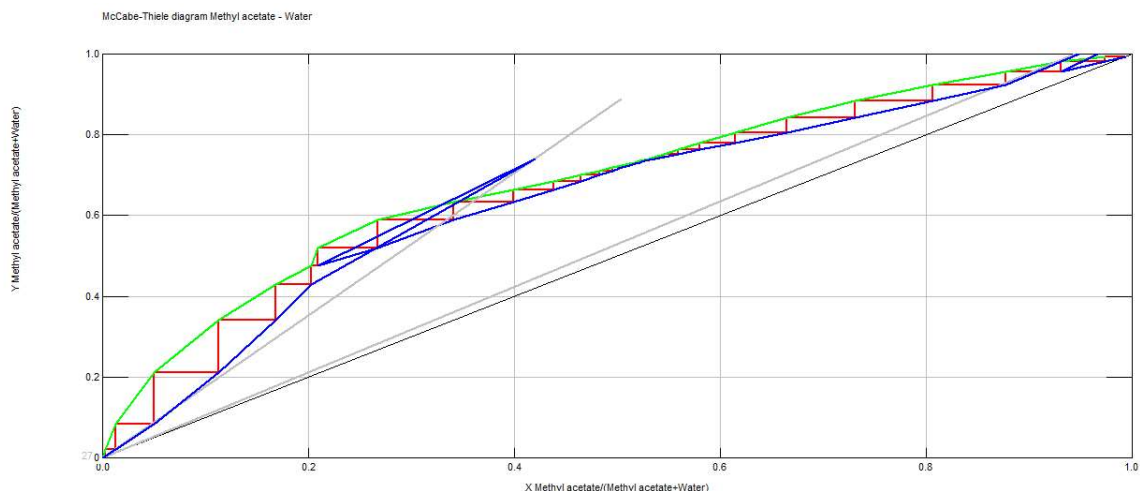
The above fig. shows the McCabe-Thiele diagram for Methyl acetate – Water which has been taken from ChemSep results.

Results

Below displayed are the results that are obtained from the ChemSep Unit Operation:

Stream	Acetic Acid	Methanol	Methyl Acetate	Water
Stage	4	27	1	40
Pressure (atm)	1	1	1	1
Vapour fraction (-)	0	0	0	0
Temperature (K)	298	298	330.658	373.215
Enthalpy (J/kmol)	-4.83E+08	-2.39E+08	-4.38E+08	-2.81E+08
Entropy (J/kmol/K)	184951	149061	248594	97785
Total molar flow (kmol/h)	50	50	50.35	49.6501
Total mass flow (kg/s)	0.83407	0.445028	1.02781	0.251276
Liquid std.vol.flow (m3/s)	7.94E-04	5.61E-04	0.0010956	2.52E-04
Mole flows (kmol/h)				
Methanol	0	50	0.271022	2.08E-05
Acetic acid	50	0	0.0296629	0.24138
Methyl acetate	0	0	49.729	2.14E-07
Water	0	0	0.320278	49.4087
Mole fractions (-)				
Methanol	0	1	0.00538277	4.19E-07
Acetic acid	1	0	5.89E-04	0.00486162
Methyl acetate	0	0	0.987667	4.31E-09
Water	0	0	0.00636104	0.995138

References

1. William L. Luyben and Cheng-Ching Yu, "Steady-State Design in Acetic Acid Esterification," in *Reactive Distillation Design and Control*. New York: Wiley Online Library, 2008, ch. 7, pp. 147-177.

Source: http://www.chemsep.com/downloads/data/MeAce_RD_Luyben2008p148.png