# ESTERIFICATION OF ACETIC ACID WITH 1-BUTANOL TO N-BUTYLACETATE

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Background

Esterification is a chemical process for making ester. The most common method of making esters are heating carboxylic acid with an alcohol and removing water from it. Esters are normally produced by a batch process in industries using mineral acid catalyst like H_2So_4. The Esterification of acetic acid with 1-butanol is expressed as:-

1-butanol + Acetic acid <--> N-butyl acetate +Water
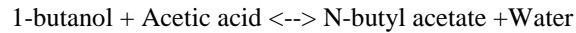
The reaction is a reversible reaction. N-Butyl acetate is used as a flavoring ingredient, solvent in the production of lacquers and other products. It is also used in synthetic fruit flavoring.

Description of flow sheet

Two pure streams of 1-butanol and acetic acid at were fed into reactive distillation column at 50 kmol/hr, 1 atm and 298.15 K. Reactive distillation column was introduced from CAPE-OPEN and chemsep was used to input the data. In a 34 stages simple distillation column acetic acid was fed at 13 stage and 1-butanol at 16 stage. Water and small fraction of N-butyl acetate is obtained from top and from bottom N-Butyl acetate is obtained. To separate the water and N-butyl acetate a decanter is used. Decanter was introduced from CAPE-OPEN using chemsep data. Reflux ratio to operate the column is 2. Molar flow rate of product (N-butyl acetate) is 50.036 Kmol/hr and for by-product (water) is 49.96 Kmol/hr.

Results

Stream	Feed1	Feed2	Top	Bottom
Stage	13	16	1	34
Pressure (N/m2)	101325	101325	101325	101325
Vapour fraction (-)	0	0	0	0
Temperature (K)	298.15	298.15	373.174	399.462
Enthalpy (J/kmol)	-4.8E+08	-3.3E+08	-2.8E+08	-5E+08
Entropy (J/kmol/K)	185017	269885	97592	420247
Total molar flow (kmol/s)	0.0138889	0.0138889	0.0138889	0.0138889
Total mass flow (kg/s)	0.834069	1.02949	0.252502	1.61104
Vapour std.vol.flow (m3/s)				
Liquid std.vol.flow (m3/s)	0.00079401	0.00126619	0.00025333	0.00182191
Mole flows (kmol/s)				
1-butanol	0	0.0138889	9.4514E-09	3.3993E-05
Water	0	0	0.0138486	6.3127E-06
N-butyl acetate	0	0	1.0665E-05	0.0138442
Acetic acid	0.013888	0	0.00002964	4.362E-06

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Mole fractions (-)				
1-butanol	0	1	6.805E-07	0.00244753
Water	0	0	0.997097	0.00045452
N-butyl acetate	0	0	0.00076791	0.996784
Acetic acid	1	0	0.00213414	0.00031407
Mass flows (kg/s)				
1-butanol	0	1.02949	7.0057E-07	0.0025197
Water	0	0	0.249482	0.00011372
N-butyl acetate	0	0	0.00123889	1.60814
Acetic acid	0.834069	0	0.00178002	0.00026195
Mass fractions (-)				
1-butanol	0	1	2.7745E-06	0.00156402
Water	0	0	0.988041	7.0591E-05
N-butyl acetate	0	0	0.00490648	0.998203
Acetic acid	1	0	0.00704956	0.0001626
Combined feed fractions (-)				
1-butanol	0	1	6.805E-07	0.00244753
Water	0	0	0	0
N-butyl acetate	0	0	0	0
Acetic acid	1	0	0.00213414	0.00031407
Liquid:				
Mole weight (kg/kmol)	60.053	74.123	18.1801	115.995
Density (kg/m3)	1061.25	822.503	1180.7	779.238
Std.density (kg/m3)	1050.45	813.055	996.722	884.257
Viscosity (N/m2.s)	0.00111877	0.00252161	0.00027903	0.00025209
Heat capacity (J/kmol/K)	123864	177760	76267.1	265566
Thermal cond. (J/s/m/K)	0.161234	0.153213	0.665839	0.108722
Surface tension (N/m)	0.0270536	0.024356	0.0589498	0.0144902

References

[1] William L. Luyben; 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.