Entrainer effect of *n*-hexanol reactant on coproducing *n*-butyl and *n*-hexyl acetate in energy-efficient reactive distillation

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Unit System: Temperature - C , Pressure-bar , Molar flowrate - kmol/hr, Mass flowrate kg/hr Volumetric flowrate m3/h (other units SI)

Background

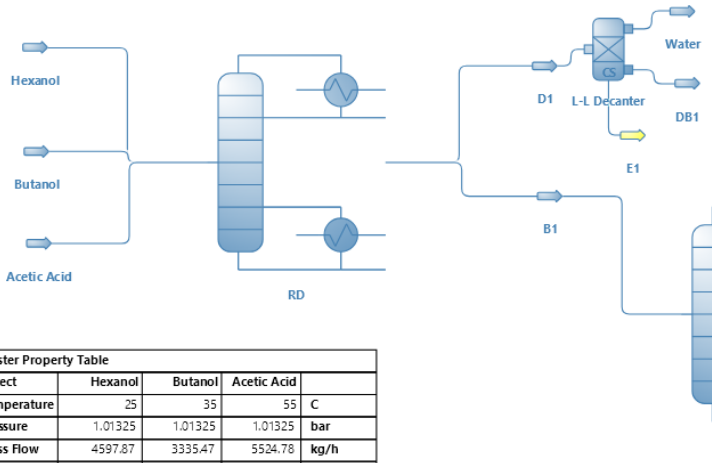
We demonstrate the formation and separation of the two esters n-butyl acetate and n-hexyl acetate . N-Hexanol which is one of the reactant of this double esterification reaction , was to found to have an entrainer effect on the mixture in the direct sequence method of reactive distillation. It facilitated production of water with high purity and also increased the extent of the reaction.

Description of Flowsheet

The flowsheet comprises two distillation columns of which the first one is a reactive distillation column,named RD with 60 stages, followed by a non-reactive distillation column, named NRD with 40 stages. The three feed streams of hexanol, butanol and acetic acid enter the 2^{nd},6^{th} and 6^{th} stage of the first

column respectively. Water obtained as the distillate,D1, is further purified by decantation to 99.9059% purity in the stream named ‘water’. The esters n-hexyl acetate and n-butyl acetate are produced after the reactive distillation in the first column and were separated in the NRD column following it. N-Hexyl Acetate was obtained as the bottom product ,in B2,with 99.57% purity and n-butyl acetate as the top product,in D2, with 98.74% purity.

THE FLOWSHEET



Master Property Table			
Object	Water		
Temperature	96.7935	C	
Pressure	1.01325	bar	
Mass Flow	1300.41	kg/h	
Molar Flow	71.9661	kmol/h	
Molar Fraction (Overall Liquid) / Water	0.999059		

Master Property Table				
Object	Hexanol	Butanol	Acetic Acid	
Temperature	25	35	55	C
Pressure	1.01325	1.01325	1.01325	bar
Mass Flow	4597.87	3335.47	5524.78	kg/h
Molar Flow	45	45	92	kmol/h

Master Property Table			
Object	D2	B2	
Temperature	103.84	231.749	C
Pressure	0.506625	4.053	bar
Molar Flow	28.7726	32.3227	kmol/h
Molar Fraction (Mixture) / N-hexyl acetate	2.95217E-05	0.9957	
Molar Fraction (Mixture) / N-butyl acetate	0.987484	5.50855E-06	

RESULTS

Master Property Table										
Object	Water	Hexanol	DB1	D2	D1	Butanol	B2	B1	Acetic Acid	
Temperature	96.7935	25	96.7935	103.84	96.7935	35	231.749	142.796	55	C
Pressure	1.01325	1.01325	1.01325	0.506625	1.01325	1.01325	4.053	1.01325	1.01325	bar
Molar Flow	71.9661	45	48.9385	28.7726	120.905	45	32.3227	61.0953	92	kmol/h
Molar Fraction (Mixture) / Water	0.999059	0	0.011848	1.46147E-14	0.599466	0	3.18206E-24	6.88271E-15	0	
Molar Fraction (Mixture) / 1-hexanol	6.16134E-05	1	0.25159	0.00462515	0.101873	0	0.00429444	0.00445019	0	
Molar Fraction (Mixture) / 1-butanol	0.00016451	0	0.100557	1.03653E-06	0.0408005	1	7.31974E-16	4.88151E-07	0	
Molar Fraction (Mixture) / N-hexyl acetate	1.30539E-06	0	0.00462883	2.95217E-05	0.00187439	0	0.9957	0.526793	0	
Molar Fraction (Mixture) / N-butyl acetate	0.000174897	0	0.237885	0.987484	0.0963927	0	5.50855E-06	0.465055	0	
Molar Fraction (Mixture) / Acetic acid	0.000538923	0	0.39349	0.00785996	0.159594	0	4.98945E-08	0.00370164	1	

REFERENCE

https://www.sciencedirect.com/science/article/pii/S0255270120305092