CONVENTIONAL/ UNUSUAL PRESSURE SWING DISTILLATION OF ISOBUTANOL AND N-HEPTANE

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About Flowsheet

Here simulation is carried out for separation of Isobutanol and N-heptane which generated during production of triisobutyl vanadate. This mixture is separated for the reuse of the reactants to reduce cost of raw material. For the separation of this mixture special distillation techniques may used like Azeotropic distillation, Extractive distillation, Pressure Swing distillation etc. But among this pressure swing distillation (PSD) received research attention because of its advantages like simple configuration, possibility of heat integration and main not to require third component as used in Azeotropic distillation.

Pressure Swing Distillation is commonly used for azeotrope separation in which based on changing pressure the separation makes easier as pressure is changed the composition of mixture also changes which then form minimum or maximum azeoptrope. Herein case for isobutanol if pressure is increased then minimum azeotrope will move to maximum azeotrope [1].

PROCESS: Here two flowsheet are simulated for the separation of isobutanol and N-heptane. For simulation data are obtained from Yinglong Wang's works .Two flowsheet simulated one of conventional pressure swing distillation and second one unusual pressure swing distillation. Both are same except unusual pressure swing distillation in which one of the product is carried out from top of the column and in conventional all products withdrawn from bottom of columns. In both flowsheet feed is contains 0.2 mol N-heptane and 0.8 mol isobutanol. However recycle stream having different proportion of mole fraction of both component and also molar flow. For getting nearer results to literature here NRTL method used and also coefficient data are fitted. Below data are used for column set-up.

Variables	CPSD	UPSD
P1/P2 (atm)	1/4	1/12
NT1/NT2	18/36	23/18
NF1/NFR/NF2	12/8/3	11/18/15
RR1/RR2	0.42/0.13	0.55/2.16

1) Conventional Pressure Swing Distillation:



Figure 1: Process of CPSD

For simulation I assumed here that feed stream will have temeperature of 40°C and also Isobutanol is taken as 2-methyl-1-propanol due to unavailability in DWSIM database for isobutanol component. LPC (low pressure column) operates at 1 atm pressure in which isobutanol is separated at bottom of the column at a rate of 80.06 Kmol/h and top product of the column is sent to HPC (high pressure column) which operates at 4 atm pressure from this column N-heptane is obtained as bottom product and top product is recycle back to LPC at a rate of 49.07 Kmol/h.

From simulation following results are obtained;

Simulation data										
Object	feed	Recyle back to first column	N-heptane	MSTR-003	Isobutanol					
Temperature	40	131.14185	153.67059	101.61649	107.64705	С				
Molar Flow	100	49.07762	19.939889	69.017509	80.060131	kmol/h				
Molar Fraction (Mixture) / 2-methyl-1-propanol	0.8	0.46483501	0.001	0.33082816	0.999					
Molar Fraction (Mixture) / N-heptane	0.2	0.53516499	0.999	0.66917184	0.001					

2) Unusual Pressure Swing Distillation:

Here same condition assumed that feed will have temperature of 40°C and enters in LPC which operates at 1 atm pressure from the column as bottom product isobutanol is obtained at a rate of

80.08 Kmol/h and top product is sent to HPC which operates at 12 atm pressure from which as a top product N-heptane is obtained and bottom product is recycle back to LPC at a rate of 51.55 Kmol/h.



(Note: Feed location of columns are already shown in Table 1.1)

From the simulation below results are obtained;

simulation data									
Object	Recycle from HPC	N-HEPTANE	MSTR-022	MSTR-019	ISOBUTANOL	Feed2			
Temperature	166.79426	152.13762	166.79426	101.61631	107.64705	40	С		
Molar Flow	51.552206	19.948773	51.552206	71.500979	80.080959	100	kmol/h		
Molar Fraction (Mixture) / 2-methyl-1-propanol	0.4585724	0.0006393891	0.4585724	0.33080915	0.999	0.8			
Molar Fraction (Mixture) / N-heptane	0.5414276	0.99936061	0.5414276	0.66919085	0.001	0.2			

During simulation it's observed that process has sensitivity toward selection of proper coefficient calculation method because the selections of method directly influence the purity data of both columns.

References:

[1] Wang, Y., Zhang, Z., Xu, D., Liu, W., & Zhu, Z. (2016). Design and control of pressure-swing distillation for azeotropes with different types of boiling behavior at different pressures. *Journal of Process Control*, *42*, 59-76.