Improved design and optimization for separating azeotropes with heavy component as distillate through energy-saving extractive distillation by varying pressure

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1 Process utility

Table S1. Process utility

Name	Pressure /MPa	Temperature /K	Price / $/GJ
LP steam	0.5	433	7.72
MP steam	1.0	457	8.22
HP steam	1.5	527	9.88
Cooling water	0.1	298	0.278

Table S2. Pressure correlation factor (F_p) for column shell*

Pressure / psi	Up to 50	100	200	300
Pressure / atm	Up to 3.45	6.9	13.8	20.7
F_p	1.00	1.05	1.15	1.20

* Douglas, J. M. Conceptual Design of Chemical Processes; McGraw-Hill: New York, 1988.

Table S3. Recovery, entrainer makeup and OF for design 1, design 16, and design A.

	Mole fraction		Recovery	makeup entrainer kmol/h	OF kJ/kmol
	D1 stream	D2 stream			
	Design 1 with D1=271.2 and D2=271.2 kmol/h				
Acetone	0.0010	0.9950	0.9994	2.4	50165.9
Methanol	0.9950	0.0002	0.9994		
water	0.0040	0.0048			
	Design 16 with D1=271 and D2=270.8 kmol/h				
Acetone	0.001306	0.995739	0.9987	1.8	33165.3
Methanol	0.995001	0.001310	0.9987		
water	0.003694	0.002951			
	Design A with D1=271 and D2=270.8 kmol/h				
Acetone	0.000415	0.996449	0.9994	1.8	36093.2
Methanol	0.995718	0.000593	0.9994		
water	0.003867	0.002958			

2 Capital cost formulas

The diameter of a distillation column is calculated using the *tray sizing* tool in Aspen Plus.

The height of a distillation column is calculated from the equation:

$H = \frac{N}{e_T} \times 0.6096$ N tray stage except condenser and reboiler, e_T tray efficiency is taken as 85% for calculating TAC.

The heat transfer areas of the condenser and reboiler are calculated using following equations:

$A = \frac{Q}{u \times \Delta T}$ u: overall heat transfer coefficient($kW \cdot K^{-1} \cdot m^{-2}$), u=0.852 for condenser, 0.568 for reboiler.

The capital costs of a distillation column are estimated by the following equations:

$$Shell\ cost = \left(\frac{CEPCI}{100}\right) \times 902.8 \times D^{1.066} H^{0.802} \times (2.18 + F_C) = 226886 D^{1.066} H^{0.802}$$ Unit of D and H: m

$$Tray\ cost = \left(\frac{CEPCI}{100}\right) \times 93.1 \times D^{1.55} H F_C = 1426.0 D^{1.55} H$$ Unit of D and H: m

$$HeatExchanger\ cost = \left(\frac{CEPCI}{100}\right) \times 457.4 \times A^{0.65} \times (2.29 + F_C) = 9367.8 A^{0.65}$$ Unit of A: m^2

3 Binary parameter of uniquac model

Table S2. Binary parameters of unqiuac model for acetone-methanol with chlorobenzene system

Component i Component j	Acetone methanol	Acetone chlorobenzene	Methanol chlorobenzene
Aij	0	-3.2083	-0.2317
Aji	0	3.9310	1.7617
Bij	-225.1533	1102.0709	149.5426
Bji	52.7705	-1388.0554	-1255.4807