Improved Design and Efficiency of the Extractive Distillation Process for Acetone-Methanol with Water

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Supporting information

Appendix S1 Sizing and economic cost calculation

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

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 100% in this work.

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

$A = \frac{Q}{u \times \triangle T}$ 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:

$$Shell\,\mathrm{cost} = 22522.8 D^{1.066} H^{0.802}$$

$$Tray\,\mathrm{cost} = 1423.7 D^{1.55} H$$

$$HeatExchanger\,\mathrm{cost} = 9367.8 A^{0.65}$$

Table S1. Binary Interaction Parameters* for UNIQUAC Model of Acetone-Methanol-Water

Component i	Acetone	Acetone	Methanol
Component j	Methanol	Water	Water
Aij	0	8.6051	-1.0662
Aji	0	-4.8338	0.6437
Bij	-225.153	-3122.58	432.8785
Bji	52.7705	1612.196	-322.131

* K unit, $\tau_{ij} = \exp(A_{ij} + B_{ij}/T + C_{ij}\ln T + D_{ij}T + E_{ij}/T^2)$

Table S2. Sizing parameters for the optimal designed columns and cost data from closed loop simulation for the extractive distillation of acetone – methanol with water

	Case 1		Case 2b		Case 3opt	
column	C_1	C_2	C_1	C_2	C_1	C_2
Diameter / m	2.88	1.92	2.66	1.77	2.88	1.72
Height / m	33.53	14.63	33.53	14.63	33.53	14.63
I_{CS} / 10^6\$	1.164	0.389	1.069	0.356	1.164	0.346
A_C / m^2	601	284	518	244	679	229
A_R / m^2	551	371	469	319	412	309
I_{HE} /10^6\$	1.166	0.807	1.055	0.731	1.118	0.709
$Cost_{cap}$ / 10^6\$	2.576	1.252	2.341	1.137	2.528	1.102
$Cost_{ope}$ / 10^6\$	1.290	0.869	1.097	0.746	0.967	0.722
$Cost_{CA}$ / 10^6\$	2.148	1.287	1.877	1.125	1.809	1.089
Q_{HA} / MW	1.24		0.91		0.58	
$Cost_{HA}$ /10^6\$	0.035		0.028		0.021	
TAC / 10^6\$	3.469		3.030		2.918	
OF / kJ/kmol	36247.5		30916.2		28318.5	