A Heuristic Predictive Model for Screening Green Entrainer Comparing Life Cycle Assessment Indexes and Economics

Electronic Supplementary Information

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Table S1: The thermodynamic data of Methanol-Toluene azeotrope.

Azeotrope	Methanol-toluene	
	$x_{methanol}$ /mol	Temperature /K
Experimental data	0.8820-0.8860	336.41-336.95
NRTL model	0.887	337.02
UNIQUAC model	0.8843	336.91

Table S2: The method of accounting the necessary parameters to evaluate TAC.

Project	Content	Unit
ID	Aspen tray sizing	m
H	0.61×(NT/0.75-3) +6	m
Column shell cost	$C_1 = \left(\frac{M\&S}{280}\right) \times 937.636 \times D^{1.066} \times H^{0.802} \times (2.18 + F_C)$	$
	F_C=Fm·Fp, Fm=3.67, Fp = 1.05, P≤ 6.8atm; Fp = 1.00, P≤ 3.4atm	
A_C	$A_C = \frac{Q_C}{K_C \Delta T_C}$	m^2
Kc	0.852	$kW\cdot m^{-2}\cdot K^{-1}$
EH cost	$C_2 = \left(\frac{M\&S}{280}\right) \times 474.668 \times A^{0.65} \times (2.29 + F_C)$	$
$F_C=(F_d+F_p)\cdot F_m$, F_m=3.75, F_d=1.35(kettle reboiler), F_d= (fixed tube sheet heat exchangers), F_p=0		
A_R	$A_R = \frac{Q_R}{K_R \Delta T_C}$	m^2
K_R	0.568	$kW\cdot m^{-2}\cdot K^{-1}$
Energy costs		
LP steam /433 K)	7.78	$\$\cdot GJ^{-1}$
MP steam /457 K	8.22	$\$\cdot GJ^{-1}$
HP steam /537 K	9.88	$\$\cdot GJ^{-1}$
M&S	1431.7	
Membrane Material Cost	327.62 × A_M	$
Vacuum Pump Cost	$C_3 = 4200 \times \left(\frac{60 \times F_P \times 8.314 \times 273.15}{3600 \times 101.325}\right)^{0.55}$	$
Fp	Aspen simulation results	$kmol\cdot h^{-1}$
TAC	$TAC = \frac{capital\ cost}{paybackperiod} + energy\ cost$	$\$\cdot y^{-1}$
Payback period	3	years

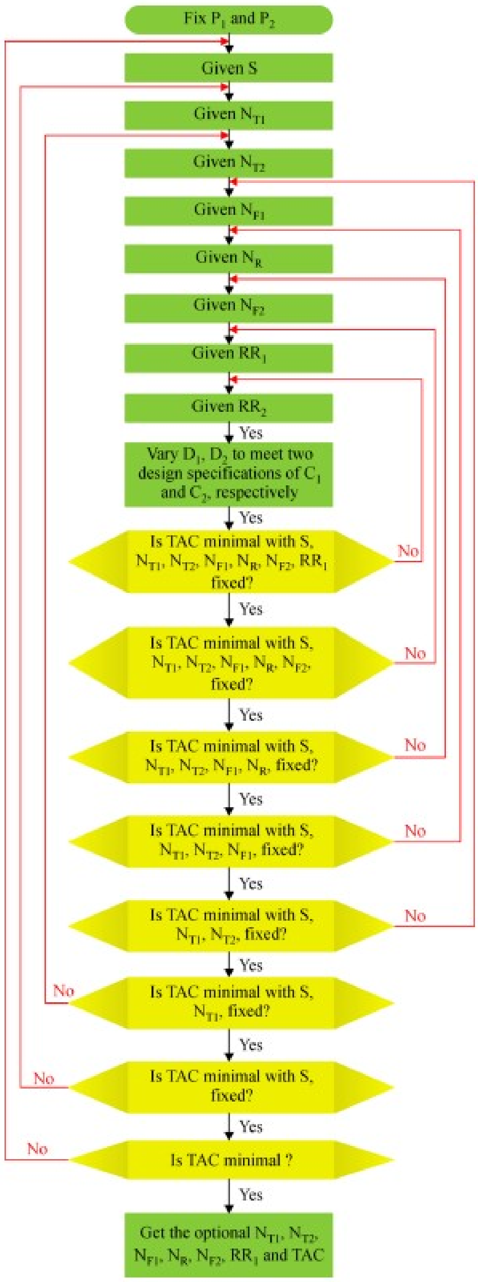

Fig. S1 The simulated and optimized procedure of the extractive distillation process.

Table S3: The detailed life cycle inventory of each entrainer for separating TOL+META azeotropes with the extractive distillation process.

Project	Unit	NMP	Aniline	DMF	Styrene	o-xylene	p-xylene	m-xylene
GWP	kg·y^{-1}CO_2 Eq.	289.703	281	285.973	335.708	345.655	407.781	494.128
AP	kg·y^{-1}SO_2 Eq.	0.5176	0.5021	0.511	0.5998	0.6176	0.7287	0.8775
HTP	kg DCB Eq.	8.9837	8.7138	8.8681	10.4103	10.7188	12.6447	15.2299
FETP	kg DCB Eq.	0.1545	0.1499	0.1525	0.1791	0.1844	0.2175	0.262
TETP	kg DCB Eq.	0.1611	0.1563	0.159	0.1867	0.1922	0.2268	0.2731
TEDI		0.56	0.58	0.79	1.62	1.74	2.75	2.81
LTEDI	□	0.3815	0.4156	0.5319	0.7431	0.7772	0.9981	1.0178

Table S4: The detailed life cycle inventory of each entrainer for separating ACT+META azeotropes with the extractive distillation process.

Project	Unit	MEA	DMSO	Water	DMF	Ethanol
GWP	kg·y^{-1}CO_2 Eq.	273.415	353.737	516.617	487.398	1883.69
AP	kg·y^{-1}SO_2 Eq.	0.488513	0.632023	0.923043	0.870837	3.36561
HTP	kg DCB Eq.	8.4786	10.9694	16.0203	15.1142	58.4134
FETP	kg DCB Eq.	0.1458	0.1887	0.2756	0.26	1.0048
TETP	kg DCB Eq.	0.152	0.1967	0.2873	0.271	1.0495
TEDI		1.06	2.21	4.5	7.32	12.77
LTEDI	□	0.5209	0.7985	1.4536	1.6221	2.8898

Table S5: The theoretical derivation formula for process assumption of the TAC model of Zhu et al..

V_i= D +L= $D_i \times$ (R_i+1)
F(TAC)$_i$ = $C_1 \times N_i \times V_i$
$R_{i,min} = \frac{1}{\lvert\alpha_i - 1\rvert} \times (\frac{x_{D,LK}}{x_{F,LK}} - \alpha_i \times \frac{x_{D,HK}}{x_{F,HK}}) = \frac{1}{\lvert\alpha_i - 1\rvert} \times \frac{x_{D,LK}}{x_{F,LK}}$
$R_{i,min} = C_2 \times \frac{1}{\lvert\alpha_i - 1\rvert}$
$V_i \approx \frac{C_3}{\lvert\alpha_i - 1\rvert}$
$N_{i,min} = \frac{\log_{10}(\frac{x_{D,LK}}{x_{D,HK}} \times \frac{x_{W,HK}}{x_{W,LK}})}{\log_{10}\alpha_i} = C_4 \times \frac{1}{\log_{10}\alpha_i}$
$N_i = C_5 \times \frac{C_4}{\log_{10}\alpha_i}$
F(TAC)$_i$ $= C_1 \times N_i \times V_i = C_1 \times C_2 \times C_3 \times C_4 \times C_5 \times \frac{1}{\lvert\alpha_i - 1\rvert} \times \frac{1}{\log_{10}\alpha_i} = \frac{C}{\lvert\alpha_i - 1\rvert \log_{10}\alpha_i}$
F(TAC) = $\sum_{i=1}^{n} \frac{C}{\lvert\alpha_i - 1\rvert \log_{10}\alpha_i}$ (i=1,2,,,,n)