

Vapor-liquid equilibria and conceptual design of extractive distillation for separating ethanol and ethyl propionate

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Table S1. Parameters of Antoine equation

	C _{1i}	C _{12i}	C _{3i}	C _{4i}	C _{5i}	C _{6i}	C _{7i}	C _{8i}	C _{9i}
ethanol	66.3962	-7122.3	0	0	-7.1424	2.89E-6	2	159.05	514
Ethyl propionate	65.4022	-6944.3	0	0	-7.298	3.79E-6	2	174.3	561
Isobutyl acetate	98.7322	-8007	0	0	-12.477	9.00E-6	2	199.25	546

Table S2. van der Waals areas (q) and volumes (r) of pure components for the UNIQUAC model

	Ethanol	Ethyl propionate	Isobutyl acetate
q	1.972	3.656	4.192
r	2.10547	4.15293	4.82663

Table S3. Liquid molar volume of pure components for the Wilson equation.

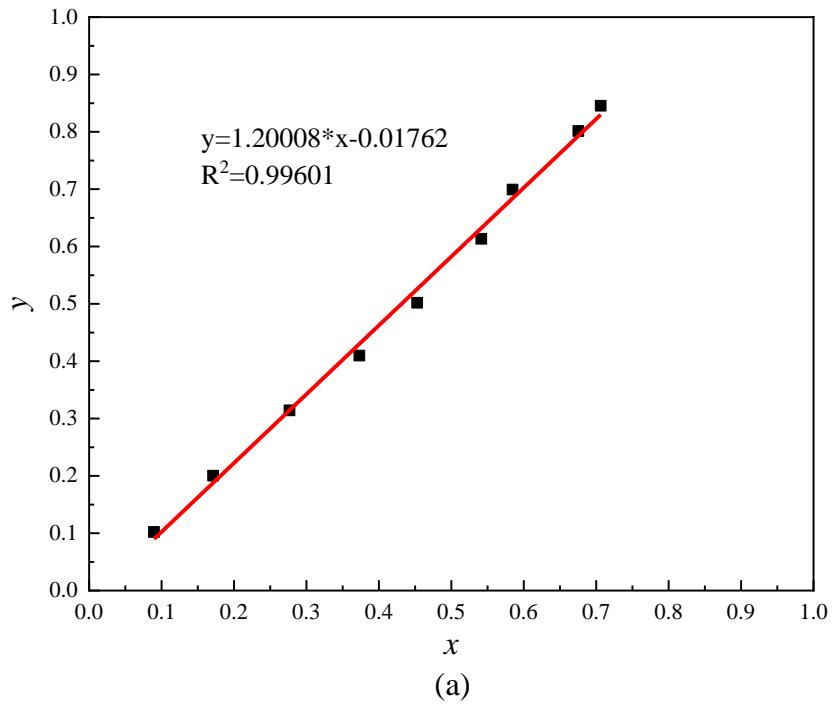
	Ethanol	Ethyl propionate	Isobutyl acetate
V_L (ml/mol)	58.6197	133.811	115.622

Table S4. The binary parameters for ethanol + ethyl propionate

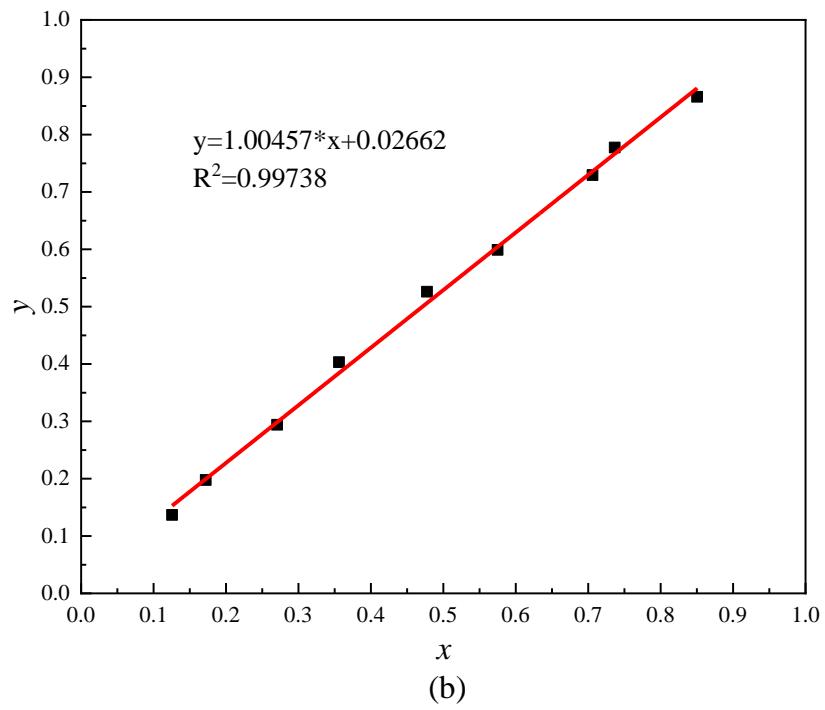
Model	Binary parameters			
	a_{ij}	a_{ji}	b_{ij}	b_{ji}
NRTL	0	0	398.01	-16.592
UNIQUAC	0	0	12.475	-180.58
Wilson	0	0	-53.459	-342.106

Table S5. Cost estimating formulas for TAC.

Project	Formula
Column diameter (D)	Aspen tray sizing
Column length (H)	$(NT -2) \times 0.61 \times 1.2$
column shell cost (\$)	$(CEPCI /119)(957.9D^{1.066} H^{0.802})(2.18 + F_m F_p)$, where the coefficient $F_m=1$, $F_p=0.983$.
column tray cost (\$)	$(CEPCI /119)(97.2D^{1.55} H)(F_t + F_m)$, where the coefficient $F_t=0$.
heat exchange area (m^2)	$A = Q / (U * \Delta T)$, where Q is the duty of the heat exchanger; U is the heat transfer coefficient; ΔT is the temperature difference.
Heat-transfer coefficient (Condensers)	$U=0.852 \text{ kW/K-m}^2$
Heat-transfer coefficient (Reboilers)	$U= 0.568 \text{ kW/K-m}^2$
heat exchanger cost (\$)	$(CEPCI /119)(474.7A^{0.65})[2.29+ F_m(F_p + F_t)]$, where the coefficient $F_p = 0$; $F_d = 1.35$ for kettle reboiler and 0.8 for fixed-tube sheet
LP steam (5 barg, 160 °C)	\$7.78/GJ
Cooling water (320K)	\$0.354/GJ



(a)



(b)

Figure S1. Calibration curves for (a) ethanol + isobutyl acetate; (b) ethyl propionate + isobutyl acetate binary systems.

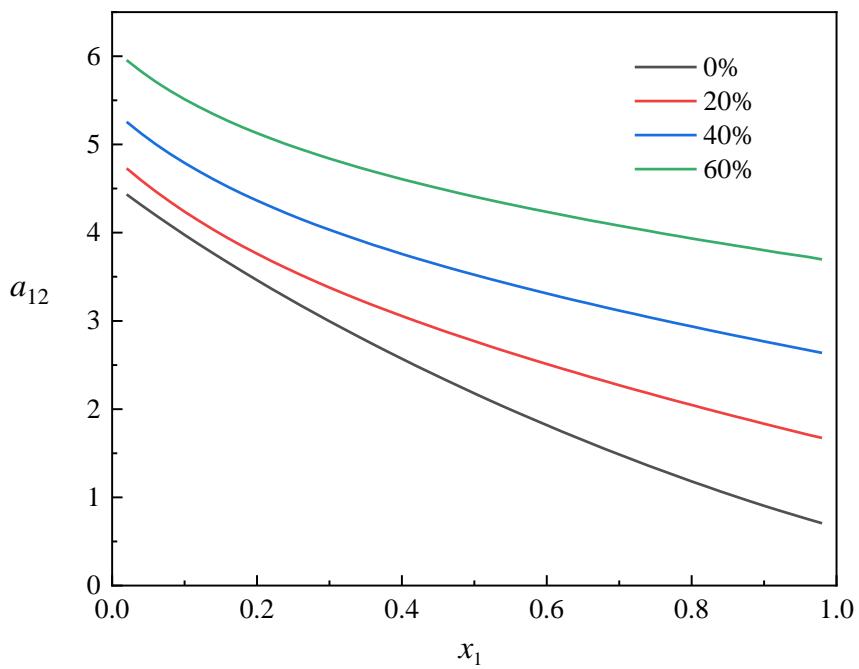


Figure S2. Relative volatility for ethanol (1) + ethyl propionate (2) binary system at 101.3 kPa