

# Supporting Information

## **Separation of Azeotropic Mixture Methanol and Toluene Using Extractive Distillation: Entrainers Determination, Vapor-liquid Equilibrium Measurement and Modelling**

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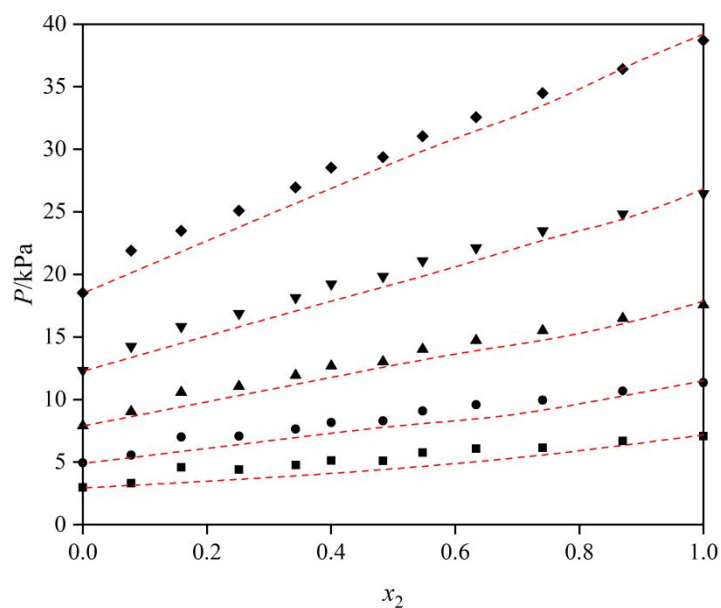


Figure S1. Comparison of the predicted experimental vapor pressures with the reference data for the mixture toluene + triethylamine: (■), 293.15 K from ref. 34; (●), 303.15 K from ref. 34; (▲), 313.15 K from ref. 34; (▼), 323.15 K from ref. 34; (◆), 333.15 K from ref. 34; (---); predicted data of Wilson model parameters.

Table S1. Experimental isobaric VLE data of the mixture methanol (1) + toluene (2) + butyl butanoate (3) under 101.3 kPa.<sup>a</sup>

T/K	x			y			$\alpha_{12}$
	$x_1$	$x_2$	$x_3$	$y_1$	$y_2$	$y_3$	
348.26	0.2408	0.2574	0.5018	0.8807	0.0960	0.0233	9.57
350.34	0.2044	0.2615	0.5341	0.8690	0.1026	0.0284	10.54
353.51	0.1703	0.2691	0.5606	0.8495	0.1175	0.0330	11.29
357.19	0.1363	0.2724	0.5913	0.8284	0.1317	0.0399	12.01
366.37	0.0896	0.2742	0.6362	0.7652	0.1699	0.0649	13.10
375.82	0.0566	0.2648	0.6786	0.6880	0.2152	0.0968	14.61
384.08	0.0422	0.2469	0.7109	0.6035	0.2559	0.1406	15.83
393.46	0.0285	0.2162	0.7553	0.5067	0.2886	0.2047	17.22
402.67	0.0152	0.1808	0.8040	0.4086	0.2965	0.2949	18.98

<sup>a</sup> The standard uncertainties of  $u$  are  $u(P)=0.35$  kPa,  $u(T)=0.35$  K,  $u(x)=0.0069$  and  $u(y)=0.0062$ . The feed ratio (mole fraction) of methanol: toluene: butyl butanoate is 0.25: 0.25: 0.5.

Table S2. Isobaric VLE data of the mixture methanol (1) + toluene (2) + butyl butanoate (3) predicted by the NRTL and UNIFAC models under 101.3 kPa.<sup>a</sup>

<i>T</i> /K	<i>x</i>			<i>y</i>		
	<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>y</i> <sub>1</sub>	<i>y</i> <sub>2</sub>	<i>y</i> <sub>3</sub>
NRTL model						
348.26	0.2331	0.2572	0.5097	0.8825	0.0956	0.0219
350.34	0.2019	0.2652	0.5329	0.8700	0.1030	0.0270
353.51	0.1668	0.2731	0.5601	0.8542	0.1155	0.0303
357.19	0.1312	0.2782	0.5906	0.8308	0.1319	0.0373
366.37	0.0899	0.2786	0.6315	0.7687	0.1710	0.0603
375.82	0.0512	0.2631	0.6857	0.6833	0.2215	0.0952
384.08	0.0387	0.2443	0.7170	0.6065	0.2544	0.1391
393.46	0.0221	0.2135	0.7644	0.5042	0.2855	0.2103
402.67	0.0141	0.1750	0.8109	0.4055	0.2966	0.2979
UNIFAC model						
348.26	0.2399	0.2525	0.5076	0.8793	0.0967	0.0240
350.34	0.2066	0.2602	0.5332	0.8688	0.1038	0.0274
353.51	0.1690	0.2681	0.5629	0.8516	0.1155	0.0329
357.19	0.1374	0.2733	0.5893	0.8298	0.1300	0.0402
366.37	0.0877	0.2750	0.6373	0.7663	0.1703	0.0634
375.82	0.0578	0.2651	0.6771	0.6869	0.2156	0.0975
384.08	0.0407	0.2478	0.7115	0.6072	0.2538	0.1390
393.46	0.0272	0.2179	0.7549	0.5085	0.2873	0.2042
402.67	0.0180	0.1787	0.8033	0.4079	0.2985	0.2936

<sup>a</sup> The feed ratio (mole fraction) of methanol: toluene: butyl butanoate is 0.25: 0.25: 0.5.