Supporting Information

Liquid-liquid equilibrium for the ternary systems (methyl isobutyl ketone + quinoline or isoquinoline + water) at 298.15, 318.15, and 338.15 K

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The reliability of the experimental tie-line data was evaluated by using the Hand[27] and Bachman[28] equations, given by equations (S1) and (S2), respectively.

$$\ln\left(\frac{w_2}{w_1}\right)^o = a_1 + b_1 \ln\left(\frac{w_2}{w_3}\right)^w \quad \text{(S1)}$$

$$w_1^o = a_2 + b_2\left(\frac{w_1^o}{w_3^w}\right) \quad \text{(S2)}$$

where a_1, b_1 and a_2, b_2 are the parameters of the Hand and Bachman equations. The subscript 1, 2 and 3 represents methyl isobutyl ketone, quinoline or isoquinoline and water, respectively. The superscript O and W represents organic phase and aqueous phase, respectively. The fitting parameters of straight lines calculated from Hand or Bachman equations, together with corresponding linear correlation coefficients (R^2), are given in Table S3.

Figures

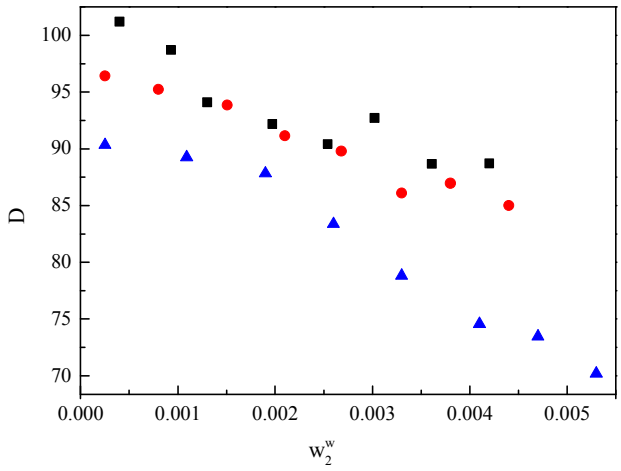

Figure S1. Distribution coefficients plotted versus mass fraction of quinoline in the aqueous phase at different temperatures. (■) T = 298.15 K, (●) T = 318.15 K, (▲) T = 338.15 K.

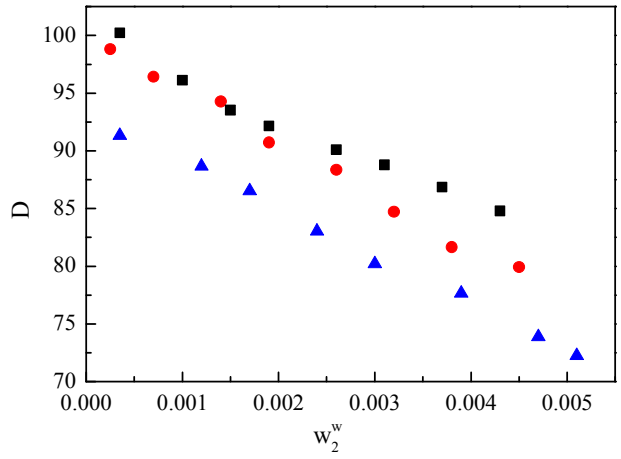

Figure S2. Distribution coefficients plotted versus mass fraction of isoquinoline in the aqueous phase at different temperatures. (■) T = 298.15 K, (●) T = 318.15 K, (▲) T = 338.15 K.

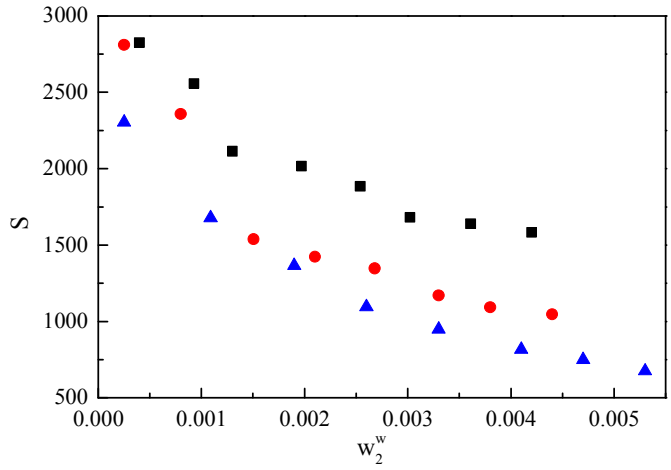

Figure S3. Separation factors plotted versus mass fraction of quinoline in the aqueous phase at different temperatures. (■) T = 298.15 K, (●) T = 318.15 K, (▲) T = 338.15 K.

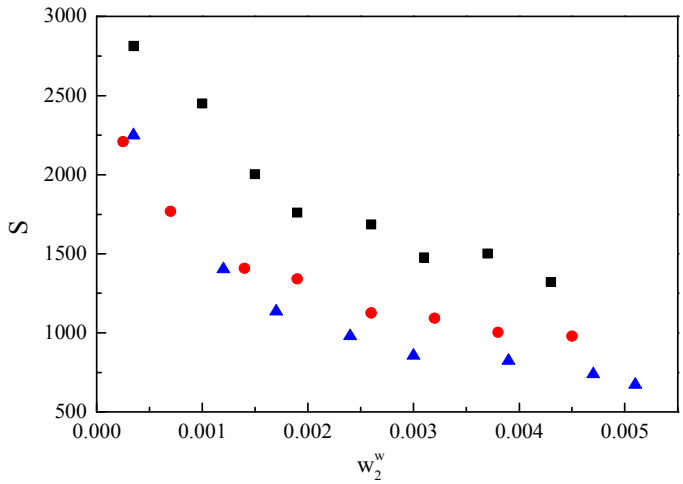

Figure S4. Separation factors plotted versus mass fraction of isoquinoline in the aqueous phase at different temperatures. (■) T = 298.15 K, (●) T = 318.15 K, (▲) T = 338.15 K.

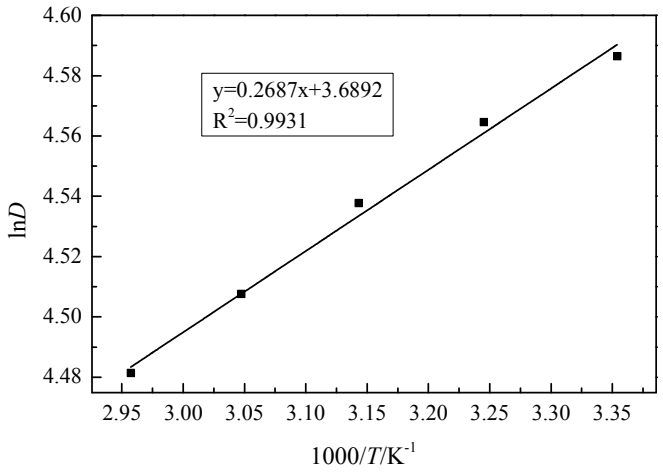

Figure S5. ln*D* plotted versus 1000/*T*/K^{-1} in quinoline extraction.

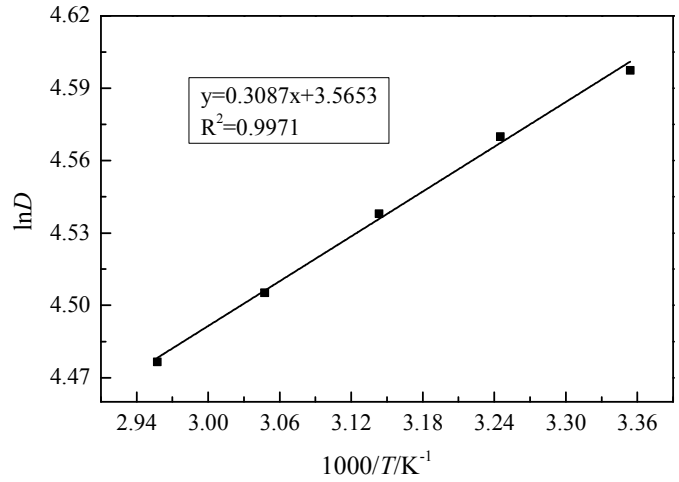

Figure S6. ln*D* plotted versus 1000/*T*/K^{-1} in isoquinoline extraction.

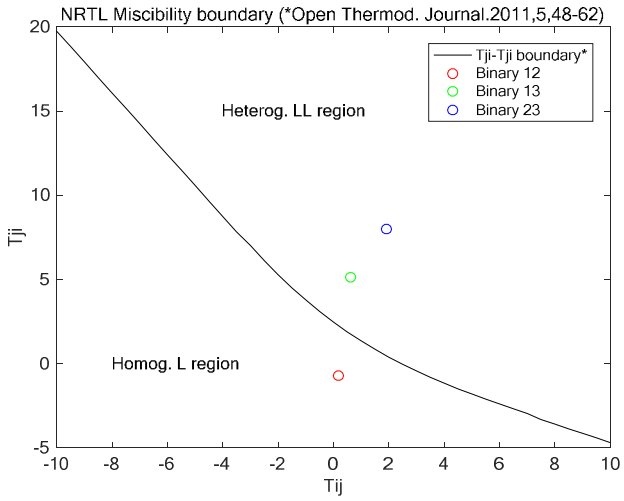

Figure S7. NRTL binary parameter boundary for total and partial miscibility for the ternary system {methyl isobutyl ketone (1) + quinoline (2) + water (3)} at 298.15 K.

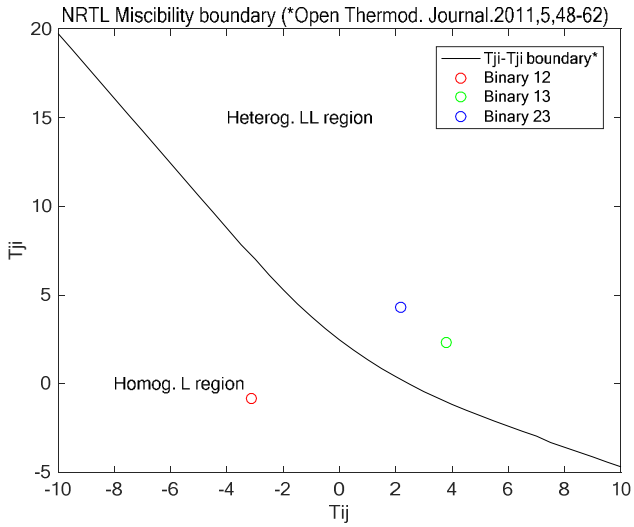

Figure S8. NRTL binary parameter boundary for total and partial miscibility for the ternary system {methyl isobutyl ketone (1) + isoquinoline (2) + water (3)} at 298.15 K.

Tables

Table S1. Chemical Oxygen Demand (COD) of Nitrogen-Containing Compounds in the Lurgi Coal Gasification Wastewater.[a]

Organic pollutant	COD(mg/L)
Quinoline	596.00
Isoquinoline	258.80
4-Methyl-2-quinolone	15.60
7,8-Benzoquinoline	30.68
Alkyl quinoline	105.60
Copper quinolate	14.56
Methylquinoline	286.40
Alkyl pyridine	13.00
5-Ethyl-5-methylhydantoin	346.80
Pyridine	60.40
Benzoylpyridine	28.60
Dimethyl pyrrole	3.12
Hydantoin	358.50
Benzimidazole	20.40
Nitrophthalic acid	48.60
Malonylurea	250.30
Phenylacetonitrile	57.60
Indole	80.00
6(5H)-Phenanthridone	23.40
Carbazole	18.20
Benzonitrile	39.60
5,5-Dimethylhydantoin	435.65

[a] from reference 3

Table S2. Experimental and Literature Values of Mutual Solubility (Mass Fraction) of Methyl Isobutyl Ketone and Water at T = (298.15, 318.15 and 338.15) K and p = 0.1 Mpa.[a]

T/K	Water in methyl isobutyl ketone (w_3^o)		Methyl isobutyl ketone in water (w_1^w)	
	This work	Reference[23]	This work	Reference[23]
298.15	0.0237	0.0230	0.0163	0.0161
318.15	0.0275	0.0268	0.0152	0.0149
338.15	0.0334	0.0340	0.0137	0.0139

[a] Standard uncertainties u are $u(T)$ = 0.1 K, $u(p)$ = 1 kPa, $u(w)$ = 0.0048.

Table S3. Hand and Bachman Equations Parameters and Regression Coefficients R^2 for the Ternary Systems (Methyl Isobutyl Ketone + Quinoline or Isoquinoline + Water).

T/K	Hand			Bachman		
	a_1	b_1	R^2	a_2	b_2	R^2
methyl isobutyl ketone (1) + quinoline (2) + water (3)						
298.15	5.4119	1.0913	0.9902	-0.0041	0.9879	1.0000
318.15	4.8469	0.9895	0.9880	-0.0034	0.9888	1.0000
338.15	4.5939	0.9657	0.9879	-0.0044	0.9906	1.0000
methyl isobutyl ketone (1) + isoquinoline (2) + water (3)						
298.15	5.0369	1.0316	0.9863	-0.0041	0.9880	1.0000
318.15	4.7502	0.9854	0.9865	-0.0040	0.9894	1.0000
333.15	4.7900	0.9977	0.9860	-0.0043	0.9905	1.0000

[c] a_1 and b_1 are the parameters of the Hand equations, and a_2 and b_2 are the parameters of the Bachman equations.

Table S4. Distribution Coefficient for Quinoline and Isoquinoline in Methyl Isobutyl Ketone at Different Temperatures

T/K	D	1000/T/K^{-1}	ln$D$
methyl isobutyl ketone + quinoline + water			
298.15	98.15	3.3540	4.5865
308.15	96.03	3.2452	4.5647
318.15	93.48	3.1432	4.5377
328.15	90.71	3.0474	4.5077
338.15	88.36	2.9573	4.4814
methyl isobutyl ketone + isoquinoline + water			
298.15	99.23	3.3540	4.5974
303.15	96.54	3.2452	4.5700
318.15	93.50	3.1432	4.5380
328.15	90.49	3.0474	4.5052
338.15	87.93	2.9573	4.4765