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Vapor–Liquid Equilibrium in Mixtures of Water + Quinoline + Hydrogen

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Vapor-liquid equilibrium was experimentally investigated in ternary mixtures of water + quinoline + hydrogen at three temperatures, 462, 544, and 622 K, pressures from 5 to 20 MPa, and water concentrations in the liquid from 3 to 47 mol %.

Introduction

Phase equilibrium data of water in mixtures with hydrocarbon and/or light gases are of fundamental interest in chemical, petroleum, natural gas, and fossil-fuel technologies. Previous studies have been confined largely to near-ambient conditions. As the industrial processes have become increasingly complex, operating at more diverse conditions, demand has arisen for new information on phase equilibrium over wider ranges of temperatures and pressures. In this work, we investigate vapor-liquid equilibrium (VLE) in ternary mixtures of water + quinoline + hydrogen at the temperatures 462, 544, and 622 K, pressures from 5 to 20 MPa, and water concentrations from 3 to 47 mol % in the liquid.

Vapor-liquid equilibrium in binary mixtures of quinoline + hydrogen has been reported by Sebastian et al. (*1*) at temperatures up to 702 K. The solubility of compressed hydrogen in water has been studied at elevated temperatures (*2–4*). Zegalska (*5*) reported liquid-liquid equilibrium data for water + quinoline up to the upper consolute temperature of 497 K.

Experimental Section

The measurements were made in a flow apparatus to minimize thermal decomposition of the samples at the high temperatures of this investigation. Details of the apparatus and experimental procedure have been described by Lin and coworkers (*6*).

Compositions of both cell effluents, overhead and bottom, were determined by first measuring the volume of gas collected upon flashing the effluent and cooling down to ambient conditions. The collected condensates were analyzed for water content by Karl Fischer titration using a Labindustries aquameter with a platinum electrode. The reagent titer was standardized with reagent-grade water.

Table I. VLE Data of Water + Quinoline + Hydrogen Mixtures Obtained from a Liquid Feed of 5 wt % Water (x_W = 0.274)

p, MPa	y_H	y_W	y_Q	x_H	x_W	x_Q	K_H	K_W	K_Q
				462.6 K					
5.09	0.9293	0.0640	0.0067	0.0167	0.1008	0.8825	55.7	0.635	0.0076
10.31	0.9560	0.0403	0.0037	0.0333	0.1217	0.8450	28.7	0.331	0.0044
15.06	0.9620	0.0352	0.0028	0.0468	0.1432	0.8100	20.6	0.246	0.0035
20.27	0.9650	0.0327	0.0023	0.0631	0.1721	0.7648	15.3	0.190	0.0030
				544.4 K					
5.01	0.8249	0.1257	0.0494	0.0233	0.0547	0.9220	35.4	2.30	0.0536
9.82	0.8991	0.0738	0.0271	0.0475	0.0624	0.8901	18.9	1.18	0.0304
15.31	0.9261	0.0557	0.0182	0.0724	0.0691	0.8585	12.8	0.766	0.0212
20.06	0.9393	0.0452	0.0155	0.0913	0.0727	0.8360	10.3	0.622	0.0185
				623.5 K					
5.05	0.6882	0.1251	0.1867	0.0253	0.0342	0.9405	27.2	3.66	0.199
10.10	0.7799	0.1160	0.1041	0.0549	0.0652	0.8799	14.2	1.78	0.118
15.34	0.8096	0.1106	0.0798	0.0824	0.0825	0.8351	9.83	1.34	0.0956
20.20	0.8303	0.1070	0.0627	0.1105	0.1059	0.7836	7.51	1.01	0.0800

Table II. VLE Data of Water + Quinoline + Hydrogen Mixtures Obtained from a Liquid Feed of 10 wt % Water (x_W = 0.443)

p, MPa	y_H	y_W	y_Q	x_H	x_W	x_Q	K_H	K_W	K_Q
				463.6 K					
5.20	0.8947	0.0990	0.0063	0.0151	0.1707	0.8142	59.3	0.580	0.0077
10.44	0.9326	0.0637	0.0037	0.0308	0.2055	0.7637	30.3	0.310	0.0048
14.94	0.9482	0.0490	0.0028	0.0436	0.2122	0.7442	21.8	0.231	0.0038
20.27	0.9562	0.0416	0.0022	0.0581	0.2435	0.6984	16.5	0.171	0.0032
				543.6 K					
4.99	0.7210	0.2282	0.0508	0.0178	0.1061	0.8761	40.5	2.15	0.0580
10.16	0.7943	0.1788	0.0269	0.0398	0.1627	0.7975	20.0	1.10	0.0337
15.17	0.8452	0.1361	0.0187	0.0622	0.1744	0.7634	13.6	0.780	0.0245
20.15	0.8812	0.1041	0.0147	0.0831	0.1793	0.7376	10.6	0.581	0.0199
				622.2 K					
10.07	0.5358	0.3702	0.0940	0.0388	0.2091	0.7521	13.8	1.77	0.125
15.51	0.6690	0.2582	0.0719	0.0684	0.2017	0.7299	9.79	1.28	0.0985
20.15	0.7760	0.1725	0.0615	0.1021	0.1742	0.7237	7.60	0.990	0.0850

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Table III. VLE Data of Water + Quinoline + Hydrogen Mixtures Obtained from a Liquid Feed of 15 wt % Water (x_W = 0.559)

p, MPa	y_H	y_W	y_Q	x_H	x_W	x_Q	K_H	K_W	K_Q
463.1 K									
5.03	0.7412	0.2536	0.0043	0.0114	0.4721	0.5205	65.0	0.537	0.0083
10.07	0.8753	0.1218	0.0029	0.0253	0.4403	0.5424	34.6	0.277	0.0053
15.30	0.9097	0.0880	0.0023	0.0379	0.4048	0.5653	24.0	0.217	0.0041
20.30	0.9342	0.0638	0.0020	0.0511	0.3953	0.5883	18.3	0.161	0.0034
543.1 K									
10.21	0.6739	0.3014	0.0247	0.0315	0.2955	0.6730	21.4	1.02	0.0367
15.22	0.7879	0.1945	0.0176	0.0531	0.2726	0.6743	14.8	0.714	0.0261
20.26	0.8453	0.1398	0.0149	0.0726	0.2509	0.6755	11.6	0.557	0.0221
620.9 K									
10.24	0.4748	0.4337	0.0915	0.0325	0.2507	0.7198	14.6	1.73	0.128
15.22	0.6742	0.2531	0.0727	0.0648	0.2026	0.7326	10.4	1.25	0.0992
17.29	0.7271	0.2057	0.0672	0.0777	0.1834	0.7387	9.36	1.12	0.0909
20.09	0.7795	0.1568	0.0637	0.0971	0.1610	0.7419	8.03	0.974	0.0859

The concentration of quinoline in most condensate samples from the cell overhead effluent exceeded the solubility of quinoline in water at ambient temperature; a heterogeneous mixture was obtained upon cooling. Those samples were homogenized by addition of a weighed amount of dry pyridine before titration. Pyridine was purchased from Aldrich Chemical Co. with a minimum purity of 99% and was further dried over 3-Å molecular sieves.

Hydrogen was obtained from Airco with a claimed purity of 99.95+%. Quinoline of 99+% purity purchased from Aldrich Chemical Co. was decolorized by vacuum distillation prior to use.

Results

Tables I–III present the experimental results obtained with liquid feeds containing 5, 10, and 15 wt % water in quinoline, respectively. The tabulated compositions represent average values from at least two replicate samples taken at a condition of temperature, pressure, and flows. The equilibrium compositions from multiple samples are generally reproducible to within 2% in mole fraction of hydrogen and 3% in mole fraction of water.

Glossary

K	equilibrium vaporization ratio, $K \equiv y/x$
p	pressure
T	temperature
x	mole fraction in liquid phase
y	mole fraction in vapor phase

Subscripts

H	hydrogen
Q	quinoline
W	water

Registry No. Quinoline, 91-22-5; hydrogen, 1333-74-0.

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