

Liquid-Liquid Equilibria of Water + Solutes (Acetic Acid/Acetol/Furfural/Guaiacol/Methanol/Phenol/Propanal) + Solvents (Isopropyl acetate/Toluene) Ternary Systems for Pyrolysis Oil Fractionation

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Supplementary work

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Ternary systems LLE experimental data and consistency tests

Tables 1 to 8 present the measured data with the uncertainties for the ternary systems LLE. and Figures 1 to 8 present the Othmer-Tobias consistency test for the experimental LLE ternary data.

Table 1 : Ternary LLE experimental data for water (1) - acetol (2) - toluene (3) system at atmospheric pressure ($P = 101.3 \text{ kPa}$)^a

Organic phase						Aqueous phase					
x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$	x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$
$T = 298.15\text{K}^b$											
0.0038	0.0110	0.9852	0.0003	0.0005	0.0005	0.9381	0.0616	0.0003	0.0029	0.0029	0.0000
0.0038	0.0220	0.9742	0.0003	0.0009	0.0010	0.8552	0.1441	0.0007	0.0061	0.0061	0.0000
0.0038	0.0321	0.9641	0.0003	0.0014	0.0014	0.7860	0.2127	0.0014	0.0083	0.0083	0.0001

0.0040	0.0425	0.9535	0.0003	0.0018	0.0018	0.7353	0.2624	0.0022	0.0096	0.0096	0.0001
0.0043	0.0771	0.9185	0.0004	0.0031	0.0031	0.5651	0.4229	0.0120	0.0120	0.0120	0.0006
0.0038	0.1068	0.8894	0.0003	0.0042	0.0042	0.4378	0.5333	0.0289	0.0118	0.0121	0.0013
0.0045	0.1414	0.8541	0.0004	0.0053	0.0053	0.3129	0.6258	0.0614	0.0101	0.0111	0.0029
$T = 323.15\text{K}^b$											
0.0043	0.0112	0.9845	0.0004	0.0005	0.0005	0.9490	0.0504	0.0006	0.0024	0.0024	0.0000
0.0041	0.0325	0.9634	0.0004	0.0014	0.0014	0.8515	0.1475	0.0010	0.0063	0.0062	0.0000
0.0042	0.0616	0.9343	0.0004	0.0025	0.0026	0.7370	0.2609	0.0021	0.0096	0.0096	0.0001
0.0042	0.0952	0.9005	0.0004	0.0038	0.0038	0.6248	0.3666	0.0086	0.0115	0.0115	0.0004
0.0040	0.1223	0.8737	0.0004	0.0047	0.0047	0.5074	0.4722	0.0204	0.0121	0.0122	0.0009
0.0040	0.1657	0.8303	0.0003	0.0061	0.0061	0.4289	0.5358	0.0353	0.0117	0.0121	0.0016

^au(P) = 1.0 kPa. ^bu(T) = 0.10 K

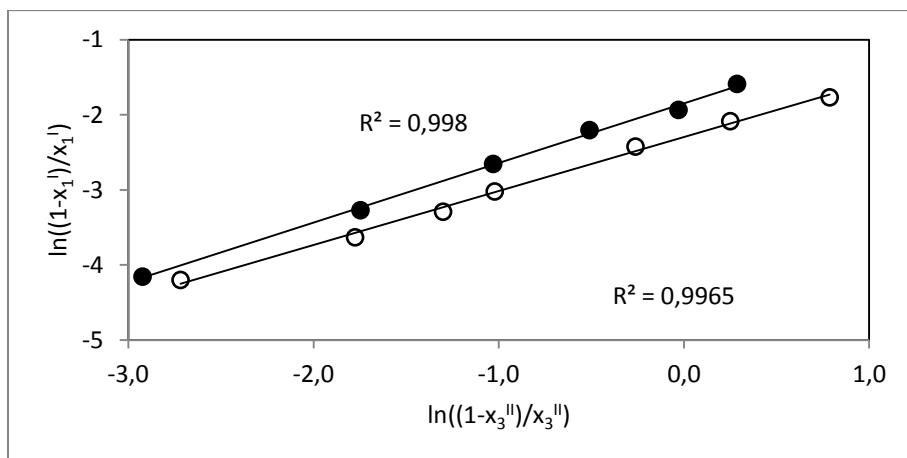


Figure 1: Data treatment of the ternary system water (1) - acetol (2) - toluene (3) using the Othmer-Tobias correlation
 (o): 298.15 K. and (●): 323.15 K

Table 2 : Ternary LLE experimental data for water (1) - propanal (2) - toluene (3) system at atmospheric pressure (P = 101.3 kPa)^a

Organic phase						Aqueous phase					
x1	x2	x3	u(x1)	u(x2)	u(x3)	x1	x2	x3	u(x1)	u(x2)	u(x3)
$T = 298.15\text{K}^b$											
0.0010	0.0987	0.9004	0.0000	0.0040	0.0040	0.9899	0.0099	0.0002	0.0005	0.0005	0.00001
0.0013	0.2288	0.7699	0.0001	0.0079	0.0080	0.9789	0.0208	0.0003	0.0010	0.0010	0.00001
0.0024	0.4221	0.5754	0.0001	0.0110	0.0110	0.9621	0.0373	0.0005	0.0018	0.0018	0.00002
0.0919	0.5860	0.3221	0.0035	0.0102	0.0091	0.9398	0.0596	0.0006	0.0028	0.0027	0.00002
0.1468	0.6895	0.1637	0.0056	0.0088	0.0056	0.9225	0.0773	0.0002	0.0035	0.0035	0.00001
$T = 313.15\text{K}^b$											
0.0002	0.0849	0.9149	0.00001	0.0035	0.0035	0.9943	0.0056	0.0001	0.0003	0.0003	0.00000
0.0002	0.2397	0.7601	0.00001	0.0082	0.0082	0.9856	0.0142	0.0002	0.0007	0.0007	0.00001
0.0003	0.4421	0.5577	0.00001	0.0111	0.0111	0.9708	0.0290	0.0002	0.0014	0.0014	0.00001
0.0634	0.6228	0.3139	0.00253	0.0100	0.0092	0.9541	0.0456	0.0003	0.0021	0.0021	0.00001

0.1258	0.7180	0.1561	0.00496	0.0083	0.0055		0.9410	0.0587	0.0003	0.0027	0.0027	0.00001
^a u(P) = 1.0 kPa. ^b u(T) = 0.10 K												

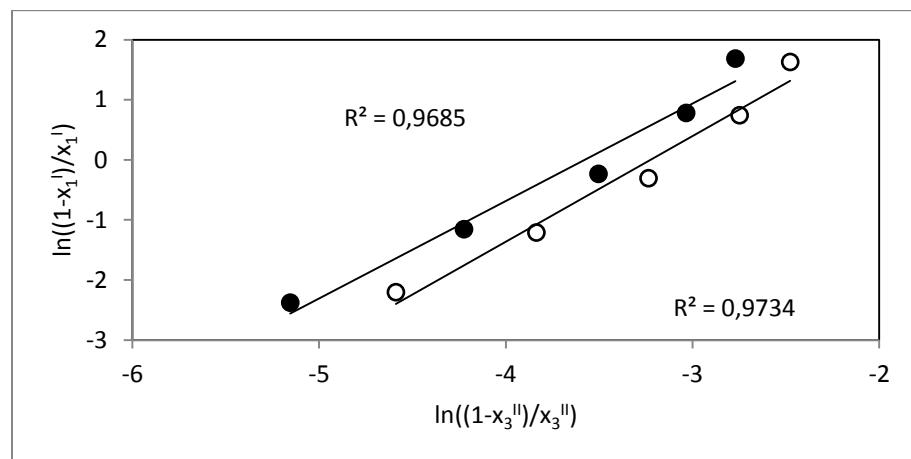


Figure 2: Data treatment of the ternary system water (1) - propanal (2) - toluene (3) using the Othmer-Tobias correlation (o): 298.15 K, and (●): 313.15 K

Table 3 : Ternary LLE experimental data for water (1) - acetol (2) – isopropyl acetate (3) system at atmospheric pressure (P = 101.3 kPa)^a

Organic phase						Aqueous phase					
x1	x2	x3	u(x1)	u(x2)	u(x3)	x1	x2	x3	u(x1)	u(x2)	u(x3)
T = 298.15K ^b											
0.0555	0.0236	0.9209	0.0019	0.0008	0.0023	0.9546	0.0405	0.0049	0.0017	0.0016	0.0002
0.0855	0.0614	0.8530	0.0028	0.0021	0.0039	0.8884	0.1035	0.0081	0.0039	0.0038	0.0003
0.0916	0.0618	0.8466	0.0030	0.0021	0.0040	0.8853	0.1072	0.0075	0.0040	0.0039	0.0003
0.0890	0.1470	0.7640	0.0028	0.0045	0.0056	0.7864	0.1994	0.0142	0.0066	0.0065	0.0005
0.1315	0.2036	0.6649	0.0039	0.0057	0.0069	0.7410	0.2391	0.0199	0.0076	0.0073	0.0007
T = 323.15K ^b											
0.1032	0.0293	0.8675	0.0034	0.0010	0.0038	0.9581	0.0374	0.0045	0.0016	0.0015	0.0002
0.1201	0.0664	0.8135	0.0038	0.0022	0.0048	0.9045	0.0882	0.0073	0.0034	0.0033	0.0003
0.1223	0.1045	0.7732	0.0038	0.0033	0.0054	0.8490	0.1410	0.0100	0.0051	0.0049	0.0004
0.1395	0.1625	0.6980	0.0042	0.0048	0.0065	0.7877	0.1979	0.0144	0.0066	0.0064	0.0005
0.2380	0.2408	0.5211	0.0062	0.0062	0.0077	0.7155	0.2604	0.0241	0.0080	0.0077	0.0009

^au(P) = 1.0 kPa. ^bu(T) = 0.10 K

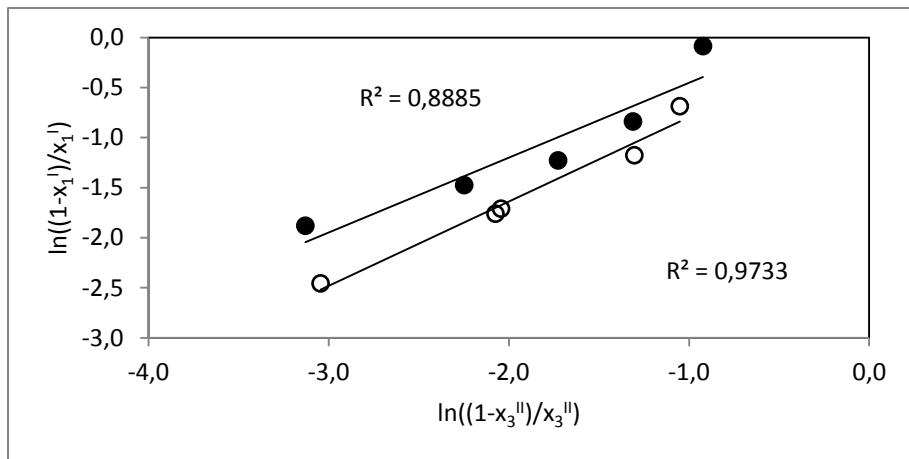


Figure 3: Data treatment of the ternary system water (1) - acetol (2) – isopropyl acetate (3) using the Othmer-Tobias correlation (o): 298.15 K, and (●): 323.15 K

Table 4 : Ternary LLE experimental data for water (1) - furfural (2) – isopropyl acetate (3) system at atmospheric pressure ($P = 101.3 \text{ kPa}$)^a

Organic phase						Aqueous phase					
x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$	x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$
$T = 298.15 \text{ K}^b$											
0.0747	0.1192	0.8061	0.0026	0.0023	0.0037	0.9941	0.0022	0.0037	0.0003	0.0001	0.0002
0.0724	0.2480	0.6796	0.0025	0.0040	0.0048	0.9905	0.0045	0.0050	0.0004	0.0002	0.0003
0.0909	0.3671	0.5419	0.0030	0.0049	0.0054	0.9897	0.0064	0.0040	0.0004	0.0003	0.0002
0.1270	0.5086	0.3644	0.0040	0.0053	0.0051	0.9866	0.0097	0.0037	0.0005	0.0004	0.0002
0.1520	0.6107	0.2373	0.0047	0.0053	0.0040	0.9857	0.0116	0.0027	0.0006	0.0005	0.0001
0.1591	0.7275	0.1134	0.0049	0.0051	0.0022	0.9848	0.0137	0.0015	0.0006	0.0005	0.0001
$T = 323.15 \text{ K}^b$											
0.0868	0.1233	0.7899	0.0030	0.0023	0.0040	0.9943	0.0024	0.0033	0.0002	0.0001	0.0002
0.0890	0.2251	0.6859	0.0030	0.0037	0.0048	0.9925	0.0043	0.0033	0.0003	0.0002	0.0002
0.1431	0.3509	0.5060	0.0045	0.0048	0.0056	0.9904	0.0068	0.0029	0.0004	0.0003	0.0002
0.1747	0.5123	0.3130	0.0052	0.0055	0.0048	0.9878	0.0097	0.0025	0.0005	0.0004	0.0001
0.1985	0.5822	0.2193	0.0058	0.0058	0.0038	0.9856	0.0124	0.0020	0.0006	0.0005	0.0001
0.2217	0.6728	0.1055	0.0064	0.0062	0.0021	0.9838	0.0150	0.0012	0.0006	0.0006	0.0001

^a $u(P) = 1.0 \text{ kPa}$. ^b $u(T) = 0.10 \text{ K}$

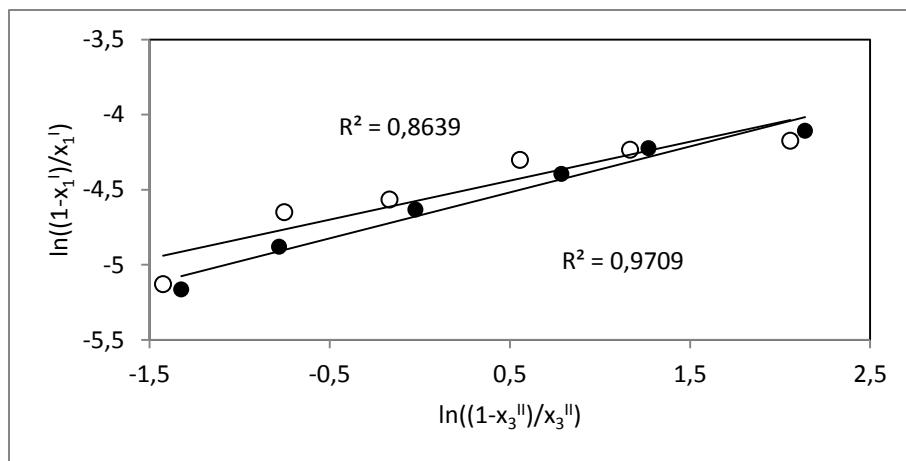


Figure 4: Data treatment of the ternary system water (1) - furfural (2) – isopropyl acetate (3) using the Othmer-Tobias correlation (o): 298.15 K, and (●): 323.15 K

Table 5: Ternary LLE experimental data for water (1) - guaiacol (2) – isopropyl acetate (3) system at atmospheric pressure ($P = 101.3 \text{ kPa}$)^a

Organic phase						Aqueous phase					
x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$	x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$
$T = 298.15\text{K}^b$											
0.0980	0.1031	0.7989	0.0034	0.0035	0.0048	0.9951	0.0004	0.0045	0.0002	0.00002	0.00024
0.0961	0.2291	0.6748	0.0033	0.0067	0.0069	0.9952	0.0009	0.0039	0.0002	0.00004	0.00021
0.1084	0.3683	0.5233	0.0038	0.0088	0.0082	0.9956	0.0015	0.0029	0.0002	0.00006	0.00016
0.1199	0.5063	0.3739	0.0043	0.0095	0.0079	0.9962	0.0019	0.0019	0.0002	0.00008	0.00010
0.1408	0.6249	0.2343	0.0052	0.0090	0.0061	0.9963	0.0025	0.0013	0.0002	0.00010	0.00007
0.1533	0.7068	0.1399	0.0059	0.0083	0.0041	0.9958	0.0034	0.0008	0.0002	0.00014	0.00004
$T = 323.15\text{K}^b$											
0.0816	0.1242	0.7942	0.0029	0.0042	0.0050	0.9960	0.0006	0.0035	0.0002	0.00002	0.00018
0.1013	0.2029	0.6959	0.0035	0.0062	0.0066	0.9962	0.0009	0.0029	0.0002	0.00004	0.00015
0.1245	0.3308	0.5447	0.0042	0.0084	0.0079	0.9960	0.0015	0.0024	0.0002	0.00006	0.00013
0.1727	0.4833	0.3440	0.0058	0.0096	0.0073	0.9959	0.0023	0.0018	0.0002	0.00010	0.00010
0.1593	0.5898	0.2508	0.0057	0.0093	0.0062	0.9960	0.0026	0.0014	0.0002	0.00011	0.00007
0.1817	0.6528	0.1655	0.0066	0.0091	0.0046	0.9960	0.0033	0.0007	0.0002	0.00014	0.00004

^a $u(P) = 1.0 \text{ kPa}$. ^b $u(T) = 0.10 \text{ K}$

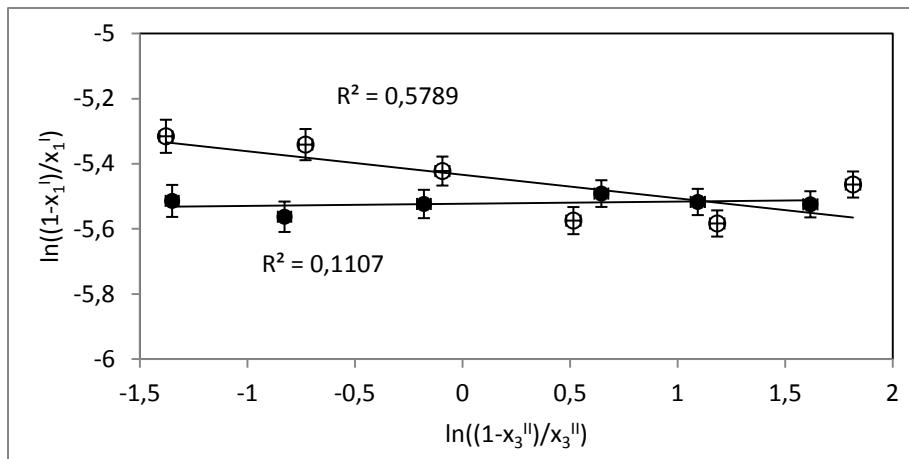


Figure 5: Data treatment of the ternary system water (1) - guaiacol (2) – isopropyl acetate (3) using the Othmer-Tobias correlation (○): 298.15 K, and (●): 323.15 K

Table 6: Ternary LLE experimental data for water (1) - methanol (2) – isopropyl acetate (3) system at atmospheric pressure ($P = 101.3 \text{ kPa}$)^a

Organic phase						Aqueous phase					
x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$	x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$
$T = 298.15 \text{ K}^b$											
0.0897	0.0126	0.8977	0.0025	0.0003	0.0026	0.9753	0.0201	0.0046	0.0008	0.0007	0.0002
0.1002	0.0346	0.8652	0.0028	0.0007	0.0029	0.9475	0.0469	0.0056	0.0016	0.0015	0.0002
0.1179	0.0747	0.8074	0.0032	0.0014	0.0034	0.9043	0.0894	0.0063	0.0029	0.0027	0.0002
0.1604	0.1249	0.7147	0.0041	0.0022	0.0043	0.8534	0.1368	0.0099	0.0041	0.0039	0.0003
0.2435	0.2102	0.5463	0.0056	0.0035	0.0052	0.7755	0.2055	0.0190	0.0057	0.0054	0.0005
0.3612	0.2813	0.3575	0.0070	0.0047	0.0049	0.6982	0.2587	0.0431	0.0069	0.0062	0.0011
$T = 323.15 \text{ K}^b$											
0.1334	0.0181	0.8485	0.0036	0.0004	0.0036	0.9773	0.0191	0.0036	0.0007	0.0006	0.0001
0.1579	0.0469	0.7952	0.0041	0.0009	0.0041	0.9530	0.0443	0.0027	0.0015	0.0014	0.0001
0.1817	0.0956	0.7228	0.0046	0.0018	0.0046	0.9103	0.0852	0.0045	0.0027	0.0026	0.0001
0.2140	0.1498	0.6362	0.0051	0.0026	0.0050	0.8642	0.1285	0.0072	0.0039	0.0037	0.0002
0.3354	0.2332	0.4313	0.0068	0.0040	0.0053	0.7819	0.1959	0.0222	0.0056	0.0052	0.0006
0.4264	0.2730	0.3006	0.0075	0.0049	0.0046	0.7146	0.2371	0.0483	0.0066	0.0058	0.0013

^a $u(P) = 1.0 \text{ kPa}$. ^b $u(T) = 0.10 \text{ K}$

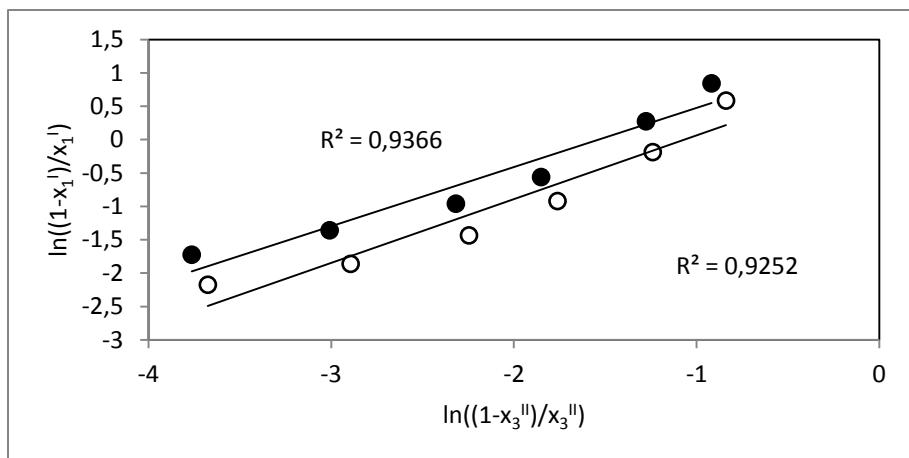


Figure 6: Data treatment of the ternary system water (1) - methanol (2) – isopropyl acetate (3) using the Othmer-Tobias correlation (o): 298.15 K, and (●): 323.15 K

Table 7: Ternary LLE experimental data for water (1) - phenol (2) – isopropyl acetate (3) system at atmospheric pressure ($P = 101.3 \text{ kPa}$)^a

Organic phase						Aqueous phase					
x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$	x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$
$T = 323.15 \text{ K}^b$											
0.1308	0.1012	0.7680	0.0043	0.0028	0.0051	0.9966	0.0007	0.0027	0.0002	0.0000	0.00014
0.1554	0.2172	0.6275	0.0049	0.0051	0.0064	0.9961	0.0016	0.0023	0.0002	0.0001	0.00012
0.2513	0.3360	0.4127	0.0071	0.0069	0.0066	0.9946	0.0039	0.0015	0.0002	0.0002	0.00008
0.3311	0.4303	0.2386	0.0086	0.0083	0.0049	0.9915	0.0075	0.0010	0.0004	0.0003	0.00005
0.4782	0.4117	0.1101	0.0101	0.0093	0.0028	0.9874	0.0119	0.0007	0.0005	0.0005	0.00004
0.6132	0.3490	0.0378	0.0099	0.0095	0.0011	0.9843	0.0154	0.0003	0.0007	0.0007	0.00002

^a $u(P) = 1.0 \text{ kPa}$. ^b $u(T) = 0.10 \text{ K}$

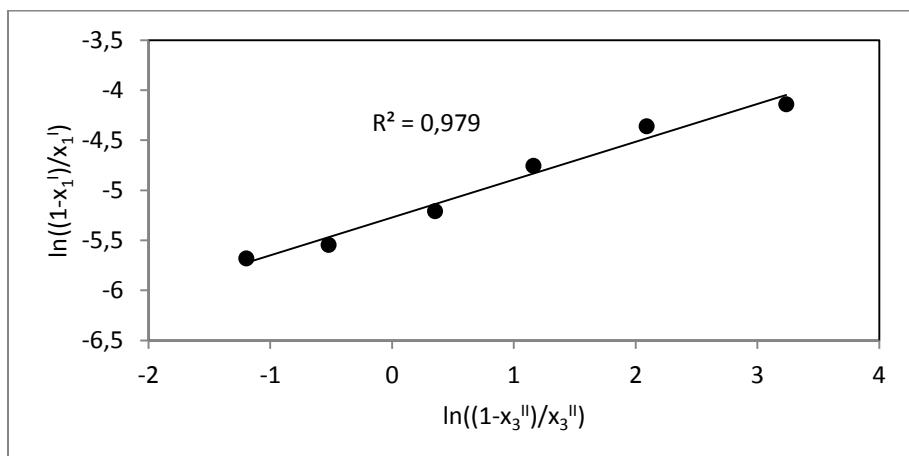


Figure 7: Data treatment of the ternary system water (1) - phenol (2) – isopropyl acetate (3) using the Othmer-Tobias correlation (●): 323.15 K

Table 8: Ternary LLE experimental data for water (1) - propanal (2) – isopropyl acetate (3) system at atmospheric pressure ($P = 101.3 \text{ kPa}$)^a

Organic phase						Aqueous phase					
x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$	x1	x2	x3	$u(x1)$	$u(x2)$	$u(x3)$
$T = 298.15\text{K}^b$											
0.1001	0.0780	0.8220	0.0023	0.0013	0.0027	0.9896	0.0064	0.0040	0.0003	0.0002	0.00011
0.1099	0.1826	0.7075	0.0024	0.0027	0.0035	0.9786	0.0173	0.0041	0.0005	0.0005	0.00012
0.1574	0.3227	0.5199	0.0033	0.0039	0.0042	0.9663	0.0298	0.0039	0.0009	0.0008	0.00011
0.1626	0.4856	0.3518	0.0034	0.0045	0.0038	0.9518	0.0451	0.0031	0.0012	0.0012	0.00009
0.1906	0.5875	0.2220	0.0039	0.0046	0.0029	0.9382	0.0594	0.0023	0.0016	0.0015	0.00006
0.2398	0.6716	0.0886	0.0048	0.0049	0.0014	0.9162	0.0821	0.0017	0.0021	0.0021	0.00005
$T = 313.15\text{K}^b$											
0.1213	0.0776	0.8010	0.0027	0.0013	0.0030	0.9917	0.0049	0.0034	0.0002	0.0001	0.00010
0.1505	0.1926	0.6569	0.0032	0.0028	0.0039	0.9864	0.0119	0.0017	0.0004	0.0003	0.00005
0.1655	0.3420	0.4926	0.0034	0.0040	0.0042	0.9724	0.0243	0.0033	0.0007	0.0006	0.00009
0.1692	0.4992	0.3316	0.0035	0.0045	0.0037	0.9621	0.0354	0.0025	0.0010	0.0009	0.00007
0.1967	0.5895	0.2138	0.0040	0.0046	0.0028	0.9566	0.0418	0.0016	0.0011	0.0011	0.00005
0.2269	0.6842	0.0890	0.0046	0.0048	0.0014	0.9396	0.0596	0.0009	0.0015	0.0015	0.00002

^a $u(P) = 1.0 \text{ kPa}$. ^b $u(T) = 0.10 \text{ K}$

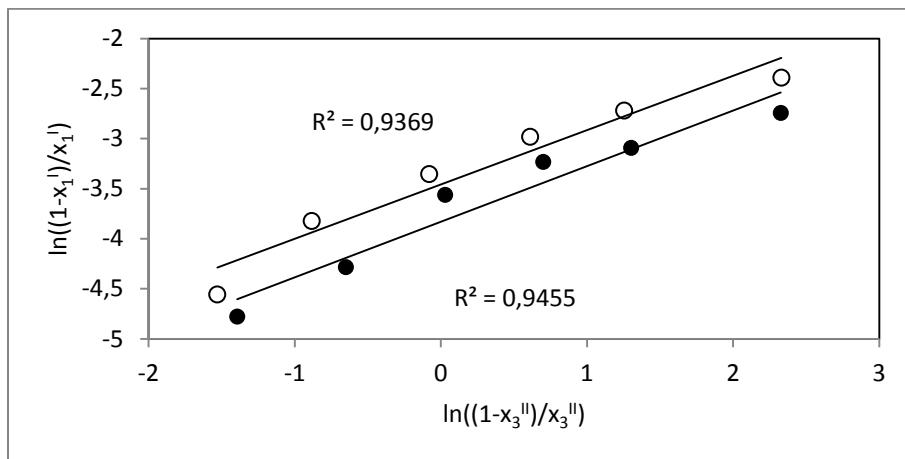


Figure 8: Data treatment of the ternary system water (1) - propanal (2) – isopropyl acetate (3) using the Othmer-Tobias correlation (o): 298.15 K, and (●): 323.15 K

Binary system LLE calculated data and charts

Tables 9 to 14 present the calculated data for the binary systems LLE with UNIQUAC and NRTL models. The average absolute deviation is calculated from the literature data [9]-[14]. The Figures 9 to 14 represent the experimental LLE data for binary systems and the calculated data with both models.

Table 9: Calculation of Binary LLE data for furfural (1) – water (2) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviation calculated based on the literature data [9].

Temperature (K)	UNIQUAC				NRTL			
	organic phase		aqueous phase		organic phase		aqueous phase	
	x1	x2	x1	x2	x1	x2	x1	x2
273.15	0.8433	0.1567	0.0172	0.9828	0.8549	0.1451	0.0139	0.9861
283.15	0.8212	0.1788	0.0168	0.9832	0.8259	0.1741	0.0149	0.9851
293.03	0.7969	0.2031	0.0169	0.9831	0.7954	0.2046	0.0161	0.9839
293.15	0.7965	0.2035	0.0169	0.9831	0.7950	0.2050	0.0161	0.9839
303.15	0.7692	0.2308	0.0173	0.9827	0.7628	0.2372	0.0175	0.9825
303.39	0.7685	0.2315	0.0174	0.9826	0.7620	0.2380	0.0175	0.9825
313.15	0.7391	0.2609	0.0182	0.9818	0.7296	0.2704	0.0190	0.9810
313.67	0.7375	0.2625	0.0183	0.9817	0.7279	0.2721	0.0191	0.9809
323.15	0.7062	0.2938	0.0196	0.9804	0.6961	0.3039	0.0207	0.9793
323.73	0.7042	0.2958	0.0197	0.9803	0.6941	0.3059	0.0208	0.9792
333.15	0.6701	0.3299	0.0215	0.9785	0.6624	0.3376	0.0226	0.9774
333.41	0.6691	0.3309	0.0215	0.9785	0.6616	0.3384	0.0226	0.9774
343.15	0.6307	0.3693	0.0241	0.9759	0.6289	0.3711	0.0246	0.9754
343.64	0.6287	0.3713	0.0242	0.9758	0.6273	0.3727	0.0247	0.9753
353.15	0.5877	0.4123	0.0276	0.9724	0.5957	0.4043	0.0270	0.9730
353.51	0.5860	0.4140	0.0277	0.9723	0.5945	0.4055	0.0271	0.9729
363.15	0.5405	0.4595	0.0324	0.9676	0.5629	0.4371	0.0296	0.9704
363.27	0.5399	0.4601	0.0325	0.9675	0.5625	0.4375	0.0296	0.9704
AAD	0.0055	0.0055	0.0009	0.0009	0.0091	0.0090	0.0013	0.0013

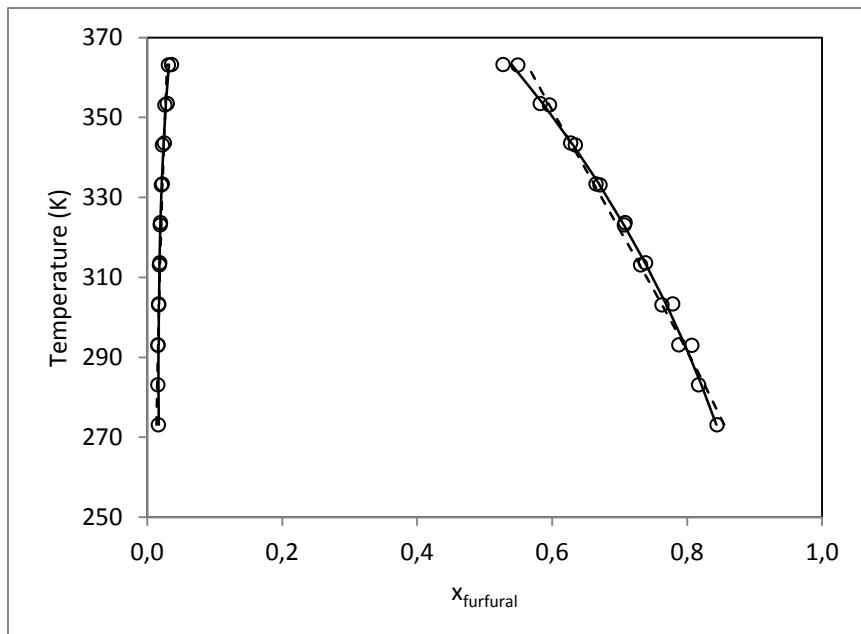


Figure 9: Binary diagram for furfural-water system LLE at atmospheric pressure, (o): experimental data [9], (—): UNIQUAC model, (- - -): NRTL model

Table 10: Calculation of Binary LLE data for guaiacol (1) – water (2) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviation calculated based on the literature data [10].

Temperature (K)	UNIQUAC				NRTL			
	organic phase		aqueous phase		organic phase		aqueous phase	
	x1	x2	x1	x2	x1	x2	x1	x2
298.15	0.7544	0.2456	0.0039	0.9961	0.7577	0.2423	0.0036	0.9964
303.15	0.7368	0.2632	0.0038	0.9962	0.7359	0.2641	0.0037	0.9963
308.15	0.7172	0.2828	0.0037	0.9963	0.7142	0.2858	0.0038	0.9962
313.15	0.6957	0.3043	0.0038	0.9962	0.6927	0.3073	0.0039	0.9961
318.15	0.6721	0.3279	0.0039	0.9961	0.6716	0.3284	0.0040	0.9960
323.15	0.6465	0.3535	0.0041	0.9959	0.6508	0.3492	0.0041	0.9959
AAD	0.0024	0.0024	0.0001	0.0001	0.0038	0.0038	0.0000	0.0000

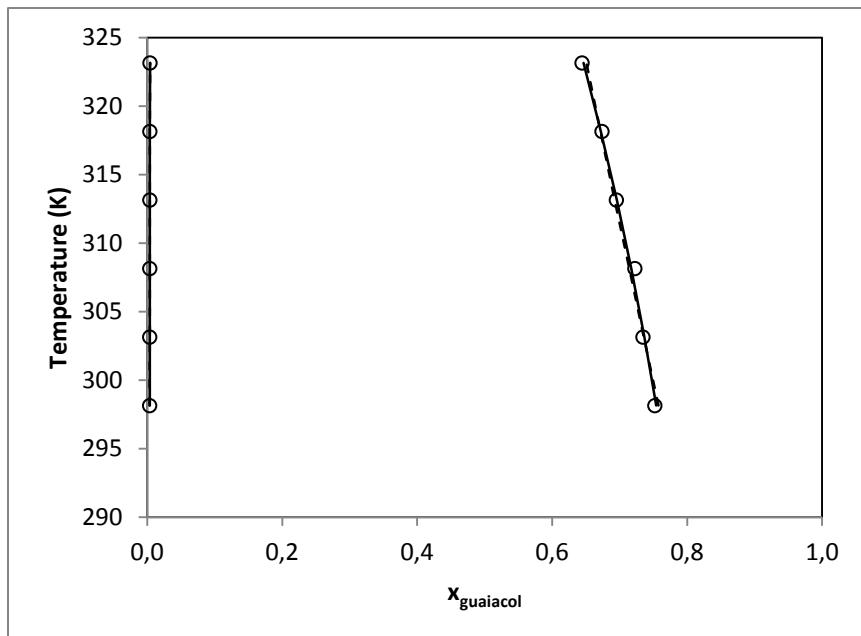


Figure 10: Binary diagram for guaiacol-water system LLE at atmospheric pressure, (o): experimental data [10], (—): UNIQUAC model, (---): NRTL model

Table 11: Calculation of Binary LLE data for isopropyl acetate (1) – water (2) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviation calculated based on the literature data [13].

Temperature (K)	UNIQUAC				NRTL			
	organic phase		aqueous phase		organic phase		aqueous phase	
	x1	x2	x1	x2	x1	x2	x1	x2
282.15	0.9272	0.0728	0.0060	0.9940	0.9274	0.0726	0.0058	0.9942
293.05	0.9185	0.0815	0.0051	0.9949	0.9181	0.0819	0.0051	0.9949
302.84	0.9100	0.0900	0.0045	0.9955	0.9094	0.0906	0.0046	0.9954
312.94	0.9007	0.0993	0.0041	0.9959	0.9000	0.1000	0.0041	0.9959
323.14	0.8908	0.1092	0.0037	0.9963	0.8903	0.1097	0.0038	0.9962
335.33	0.8782	0.1218	0.0034	0.9966	0.8784	0.1216	0.0034	0.9966
347.73	0.8647	0.1353	0.0031	0.9969	0.8660	0.1340	0.0031	0.9969
AAD	0.0026	0.0034	0.0001	0.0001	0.0028	0.0024	0.0001	0.0001

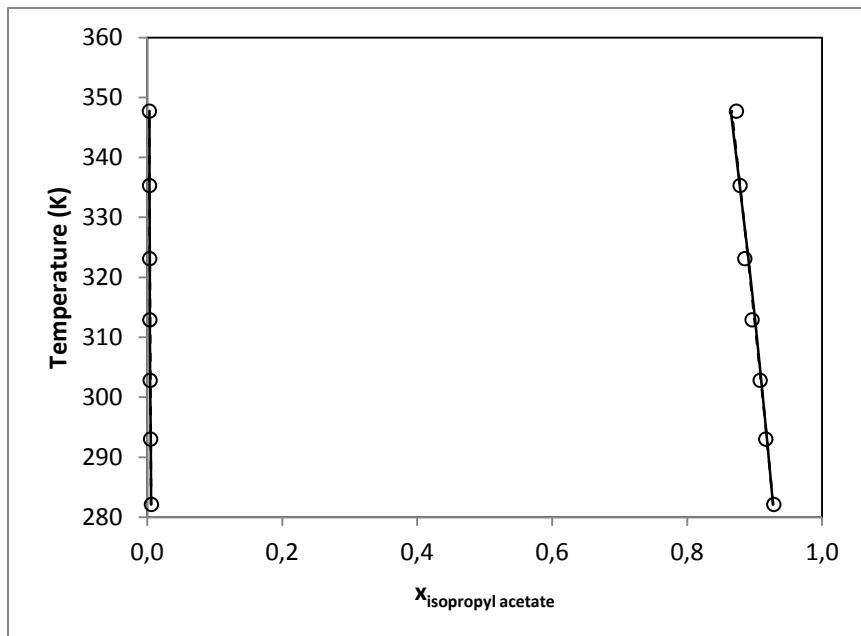


Figure 11: Binary diagram for isopropyl acetate-water system LLE at atmospheric pressure, (o): experimental data [13], (—): UNIQUAC model, (---): NRTL model

Table 12: Calculation of Binary LLE data for phenol (1) – water (2) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviation calculated based on the literature data [11].

Température (K)	UNIQUAC				NRTL			
	organic phase		aqueous phase		organic phase		aqueous phase	
	x1	x2	x1	x2	x1	x2	x1	x2
273.15	0.3750	0.6250	0.0067	0.9933	0.3644	0.6356	0.0094	0.9906
283.14	0.3515	0.6485	0.0090	0.9910	0.3500	0.6500	0.0112	0.9888
293.14	0.3268	0.6732	0.0120	0.9880	0.3295	0.6705	0.0135	0.9865
298.09	0.3141	0.6859	0.0138	0.9862	0.3174	0.6826	0.0149	0.9851
303.13	0.3007	0.6993	0.0159	0.9841	0.3039	0.6961	0.0166	0.9834
308.09	0.2871	0.7129	0.0184	0.9816	0.2896	0.7104	0.0184	0.9816
313.13	0.2727	0.7273	0.0213	0.9787	0.2740	0.7260	0.0207	0.9793
318.09	0.2579	0.7421	0.0247	0.9753	0.2576	0.7424	0.0233	0.9767
323.13	0.2420	0.7580	0.0288	0.9712	0.2398	0.7602	0.0266	0.9734
328.09	0.2254	0.7746	0.0338	0.9662	0.2210	0.7790	0.0305	0.9695
333.12	0.2070	0.7930	0.0401	0.9599	0.2004	0.7996	0.0357	0.9643
335.12	0.1992	0.8008	0.0431	0.9569	0.1916	0.8084	0.0383	0.9617
337.12	0.1910	0.8090	0.0465	0.9535	0.1825	0.8175	0.0411	0.9589
339.12	0.1822	0.8178	0.0504	0.9496	0.1728	0.8272	0.0445	0.9555
340.12	0.1776	0.8224	0.0526	0.9474	0.1677	0.8323	0.0464	0.9536
341.12	0.1728	0.8272	0.0550	0.9450	0.1624	0.8376	0.0484	0.9516
AAD	0.0145	0.0112	0.0050	0.0059	0.0097	0.0078	0.0038	0.0052

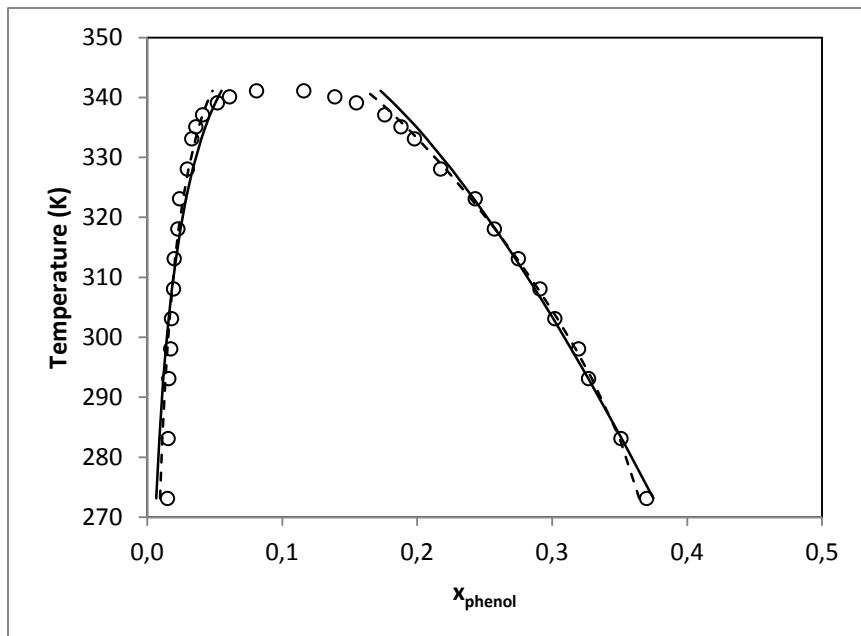


Figure 12: Binary diagram for phenol-water system LLE at atmospheric pressure, (o): experimental data [11], (—): UNIQUAC model, (---): NRTL model

Table 13: Calculation of Binary LLE data for propanal (1) – water (2) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviation calculated based on the literature data [12]

Temperature (K)	UNIQUAC				NRTL			
	organic phase		aqueous phase		organic phase		aqueous phase	
	x1	x2	x1	x2	x1	x2	x1	x2
288.00	0.6061	0.3939	0.2129	0.7871	0.6031	0.3969	0.2265	0.7735
293.14	0.6494	0.3506	0.1703	0.8297	0.6495	0.3505	0.1797	0.8203
298.14	0.6762	0.3238	0.1435	0.8565	0.6812	0.3188	0.1483	0.8517
303.14	0.6948	0.3052	0.1241	0.8759	0.7053	0.2947	0.1249	0.8751
313.15	0.7183	0.2817	0.0977	0.9023	0.7399	0.2601	0.0923	0.9077
AAD	0.0129	0.0139	0.0089	0.0096	0.0071	0.0071	0.0078	0.0078

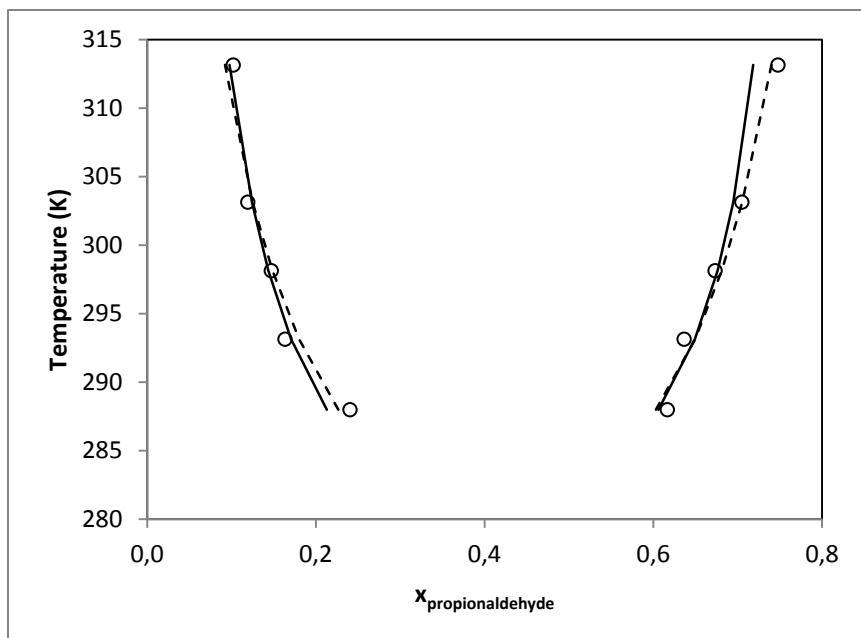


Figure 13: Binary diagram for propanal-water system LLE at atmospheric pressure, (o): experimental data [12], (—): UNIQUAC model, (---): NRTL model

Table 14: Calculation of Binary LLE data for toluene (1) – water (2) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviation calculated based on the literature data [14].

Temperature (K)	UNIQUAC				NRTL			
	organic phase		aqueous phase		organic phase		aqueous phase	
	x1	x2	x1	x2	x1	x2	x1	x2
273.15	0.9977	0.0023	0.0002	0.9998	0.9976	0.0024	0.0002	0.9998
282.65	0.9970	0.0030	0.0002	0.9998	0.9970	0.0030	0.0002	0.9998
292.95	0.9962	0.0038	0.0002	0.9998	0.9962	0.0038	0.0002	0.9998
302.85	0.9953	0.0047	0.0002	0.9998	0.9953	0.0047	0.0002	0.9998
312.75	0.9942	0.0058	0.0002	0.9998	0.9942	0.0058	0.0002	0.9998
323.15	0.9929	0.0071	0.0002	0.9998	0.9929	0.0071	0.0002	0.9998
333.25	0.9915	0.0085	0.0002	0.9998	0.9915	0.0085	0.0002	0.9998
343.55	0.9898	0.0102	0.0002	0.9998	0.9898	0.0102	0.0002	0.9998
354.15	0.9879	0.0121	0.0002	0.9998	0.9879	0.0121	0.0002	0.9998
363.35	0.9860	0.0140	0.0002	0.9998	0.9860	0.0140	0.0002	0.9998
AAD	0.0003	0.0003	0.0000	0.0000	0.0003	0.0003	0.0000	0.0000

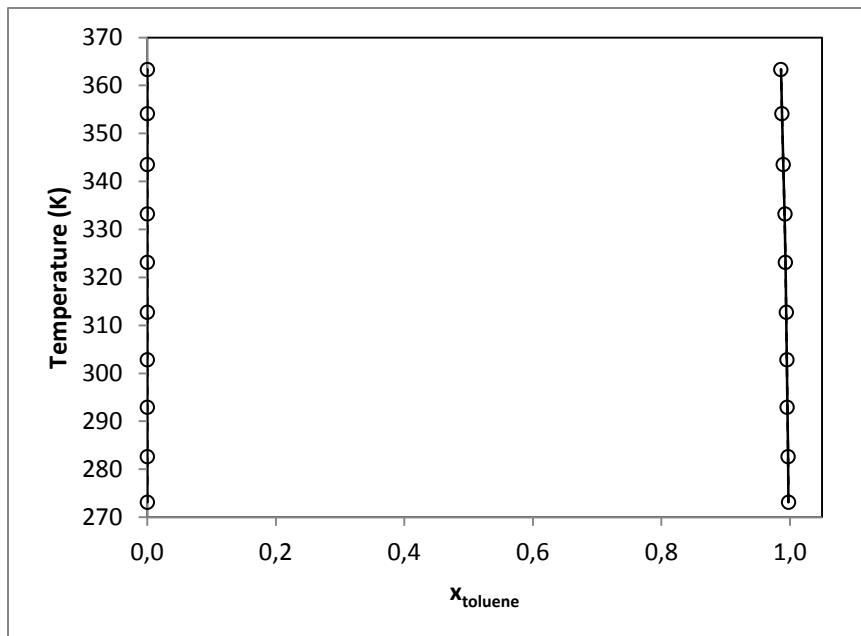


Figure 14: Binary diagram for toluene-water system LLE at atmospheric pressure, (o): experimental data [14], (—): UNIQUAC model, (---): NRTL model

Both UNIQUAC and NRTL models represent accurately the binary systems LLE. According to the AAD, either UNIQUAC or NRTL represent slightly better the data than the other model depending on the system considered but no significant difference is observed.

Ternary systems LLE calculated data and ternary diagrams

Tables 15 to 27 present the calculated LLE data for the binary systems with UNIQUAC and NRTL activity coefficient models. The average absolute deviation is calculated from experimental data realized in this work or taken from literature [15]-[20]. The Figures 15 to 39 represent the experimental LLE data for ternary systems and the calculated data with both models.

Table 15: Calculation of Ternary LLE data for water (1) – acetic acid (2) - isopropyl acetate (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data [15].

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
$T = 297.75 \text{ K}$											
0.1904	0.1141	0.6954	0.9535	0.0369	0.0096	0.2387	0.1087	0.6526	0.9534	0.0375	0.0091
0.3150	0.1942	0.4908	0.9103	0.0725	0.0172	0.3872	0.1781	0.4347	0.9101	0.0741	0.0157
0.4214	0.2291	0.3495	0.8686	0.1040	0.0274	0.4826	0.2090	0.3083	0.8668	0.1081	0.0251
0.5117	0.2379	0.2504	0.8252	0.1337	0.0412	0.5522	0.2204	0.2274	0.8247	0.1377	0.0376
No calculation						0.5820	0.2216	0.1964	0.8037	0.1512	0.0452
Average absolute difference											
0.0258	0.0091	0.0167	0.0009	0.0031	0.0034	0.0216	0.0042	0.0173	0.0045	0.0020	0.0038

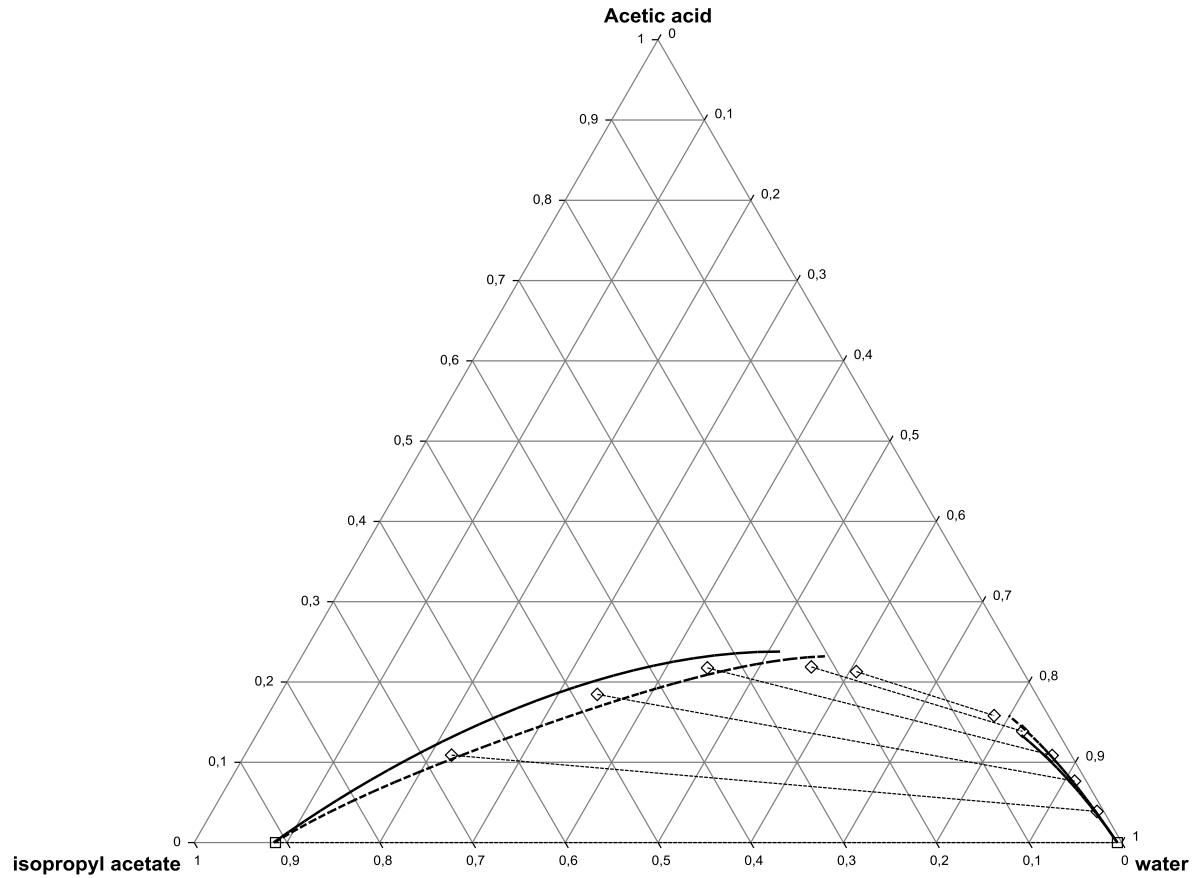


Figure 15: Ternary diagram for water - acetic acid - isopropyl acetate system LLE at 304.15K and atmospheric pressure, (□): experimental data [13], (◊): experimental data [15], (—): UNIQUAC model, (---): NRTL model (—)

Accurate representation of the data for both NRTL and UNIQUAC models

Table 16: Calculation of Ternary LLE data for water (1) - acetol (2) - isopropyl acetate (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data (this work).

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
$T = 298.15\text{K}$											
0.0878	0.0267	0.8855	0.9552	0.0379	0.0069	0.0921	0.0257	0.8823	0.9545	0.0390	0.0064
0.0896	0.0639	0.8465	0.8876	0.1012	0.0113	0.1014	0.0670	0.8316	0.8916	0.0987	0.0097
0.0897	0.0653	0.8451	0.8850	0.1036	0.0114	0.1018	0.0686	0.8296	0.8892	0.1009	0.0099
0.0909	0.1316	0.7775	0.7664	0.2126	0.0210	0.1200	0.1455	0.7344	0.7783	0.2028	0.0189
0.0913	0.1685	0.7403	0.7102	0.2634	0.0264	0.1305	0.1870	0.6825	0.7210	0.2533	0.0256
$T = 323.15\text{K}$											
0.1129	0.0329	0.8542	0.9608	0.0339	0.0053	0.1159	0.0273	0.8568	0.9550	0.0396	0.0054
0.1169	0.0718	0.8113	0.9089	0.0828	0.0083	0.1245	0.0639	0.8115	0.9011	0.0907	0.0082
0.1202	0.1102	0.7696	0.8523	0.1354	0.0123	0.1340	0.1033	0.7627	0.8451	0.1427	0.0122
0.1239	0.1590	0.7170	0.7815	0.2000	0.0186	0.1468	0.1539	0.6993	0.7748	0.2060	0.0192

0.1285	0.2192	0.6524	0.7016	0.2709	0.0275		0.1633	0.2141	0.6226	0.6934	0.2758	0.0308
Average absolute difference												
0.0190	0.0083	0.0257	0.0069	0.0061	0.0028	0.0176	0.0061	0.0213	0.0067	0.0050	0.0026	

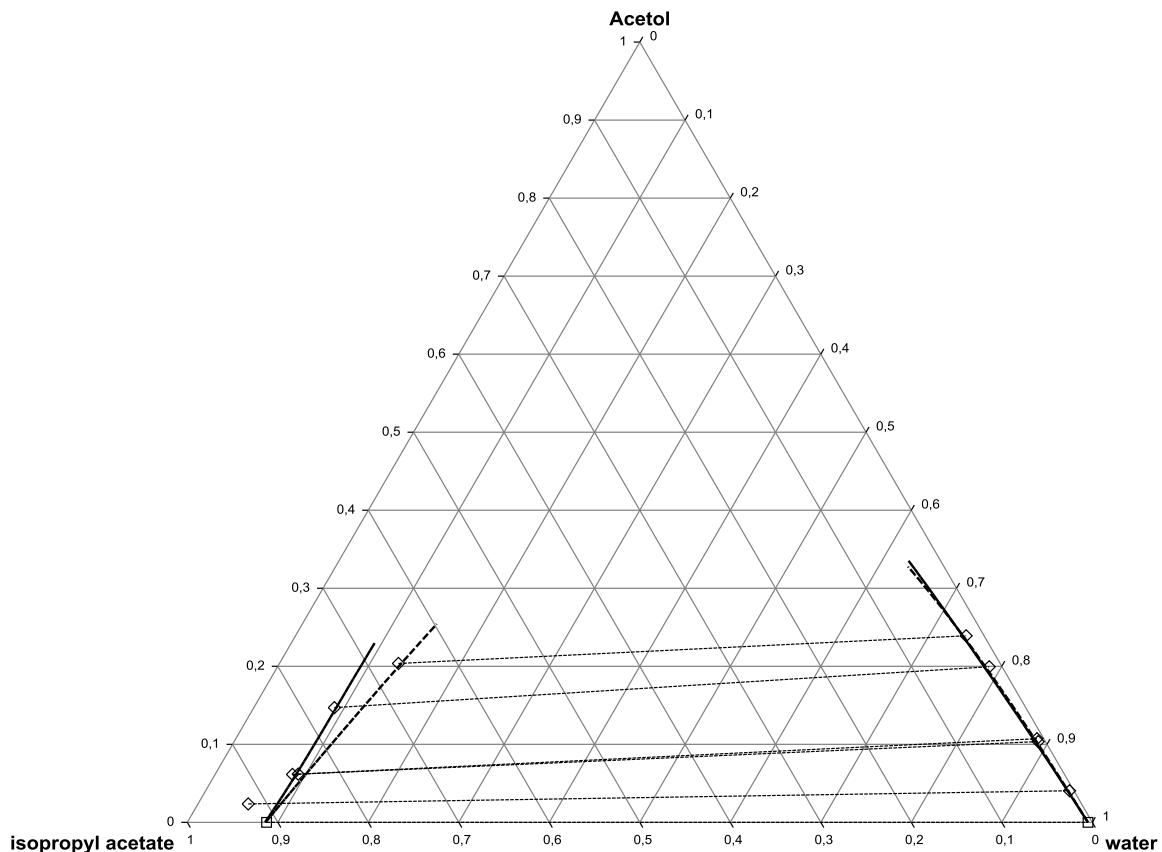


Figure 16: Ternary diagram for water - acetol - isopropyl acetate system LLE at 298.15K and atmospheric pressure, (□): experimental data [13], (◊): experimental data [this work], (—): UNIQUAC model, (---): NRTL model

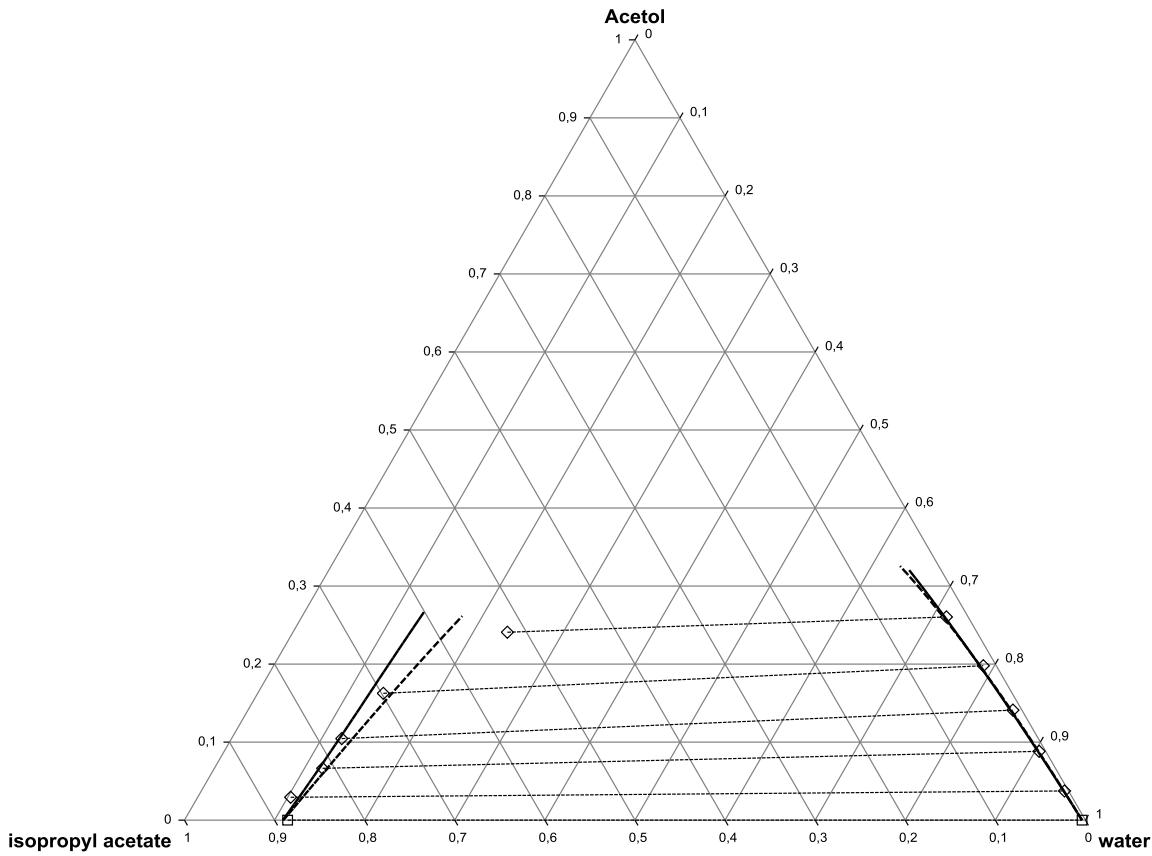


Figure 17: Ternary diagram for water - acetol - isopropyl acetate system LLE at 323.15K and atmospheric pressure, (□): experimental data [13], (◊): experimental data [this work], (—): UNIQUAC model, (---): NRTL model

The compositions calculated by the models show a significant deviation from the experimental data when approaching the liquid-liquid critical point. For acetol lower concentration, the models are accurate. NRTL model is slightly more accurate than UNIQUAC model for this system.

Table 17: Calculation of Ternary LLE data for water (1) - furfural (2) - isopropyl acetate (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data (this work).

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3									
T = 298.15K											
0.1011	0.1161	0.7827	0.9938	0.0019	0.0043	0.0961	0.1169	0.7870	0.9940	0.0017	0.0043
0.1184	0.2359	0.6457	0.9923	0.0039	0.0037	0.1078	0.2386	0.6536	0.9923	0.0040	0.0036
0.1361	0.3489	0.5150	0.9908	0.0060	0.0032	0.1213	0.3544	0.5243	0.9903	0.0067	0.0030
0.1599	0.4891	0.3510	0.9888	0.0089	0.0023	0.1447	0.4972	0.3581	0.9874	0.0104	0.0022
0.1786	0.5910	0.2304	0.9871	0.0112	0.0017	0.1692	0.5973	0.2335	0.9855	0.0129	0.0017
0.1983	0.6931	0.1086	0.9853	0.0139	0.0008	0.2002	0.6914	0.1083	0.9840	0.0149	0.0011
T = 323.15K											
0.1307	0.1176	0.7517	0.9945	0.0022	0.0034	0.1261	0.1182	0.7558	0.9944	0.0023	0.0034
0.1495	0.2104	0.6401	0.9929	0.0040	0.0030	0.1406	0.2123	0.6472	0.9924	0.0045	0.0030

0.1780	0.3366	0.4854	0.9906	0.0068	0.0025		0.1644	0.3413	0.4943	0.9892	0.0083	0.0025
0.2173	0.4852	0.2975	0.9874	0.0108	0.0018		0.2313	0.5572	0.2114	0.9829	0.0156	0.0015
0.2379	0.5531	0.2090	0.9857	0.0130	0.0014		0.2711	0.6297	0.0992	0.9810	0.0180	0.0010
0.2658	0.6343	0.0999	0.9832	0.0160	0.0007		0.3034	0.6966	0.0000	0.9793	0.0207	0.0000
Average absolute deviation												
0.0307	0.0149	0.0158	0.0006	0.0004	0.0005	0.0244	0.0130	0.0114	0.0009	0.0009	0.0005	

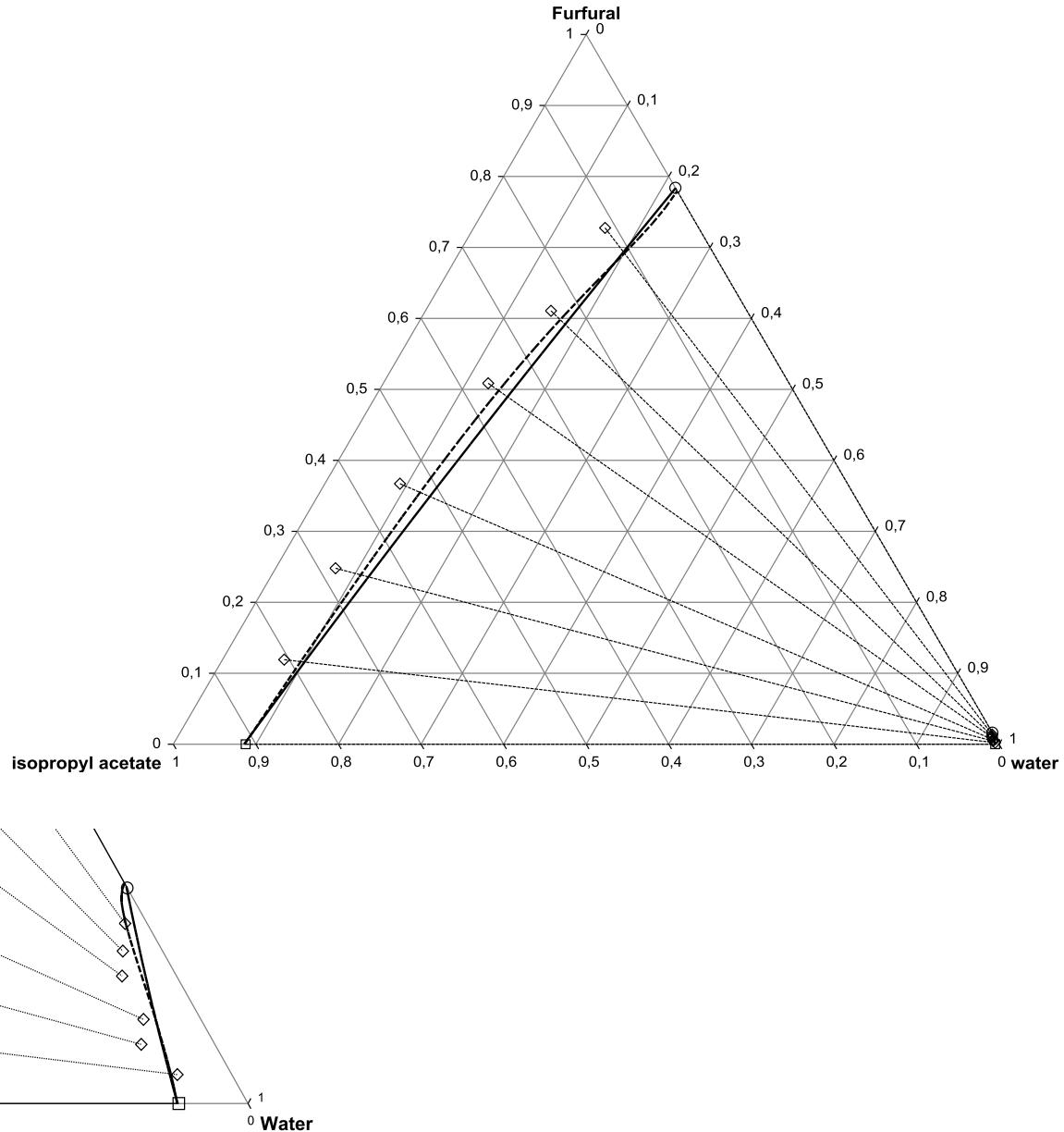


Figure 18: Ternary diagram for water - furfural - isopropyl acetate system LLE at 298.15K and atmospheric pressure, (□): experimental data [13], (o): experimental data [9], (◊): experimental data [this work], (—): UNIQUAC model, (---): NRTL model (◊); zoom on the aqueous phase data

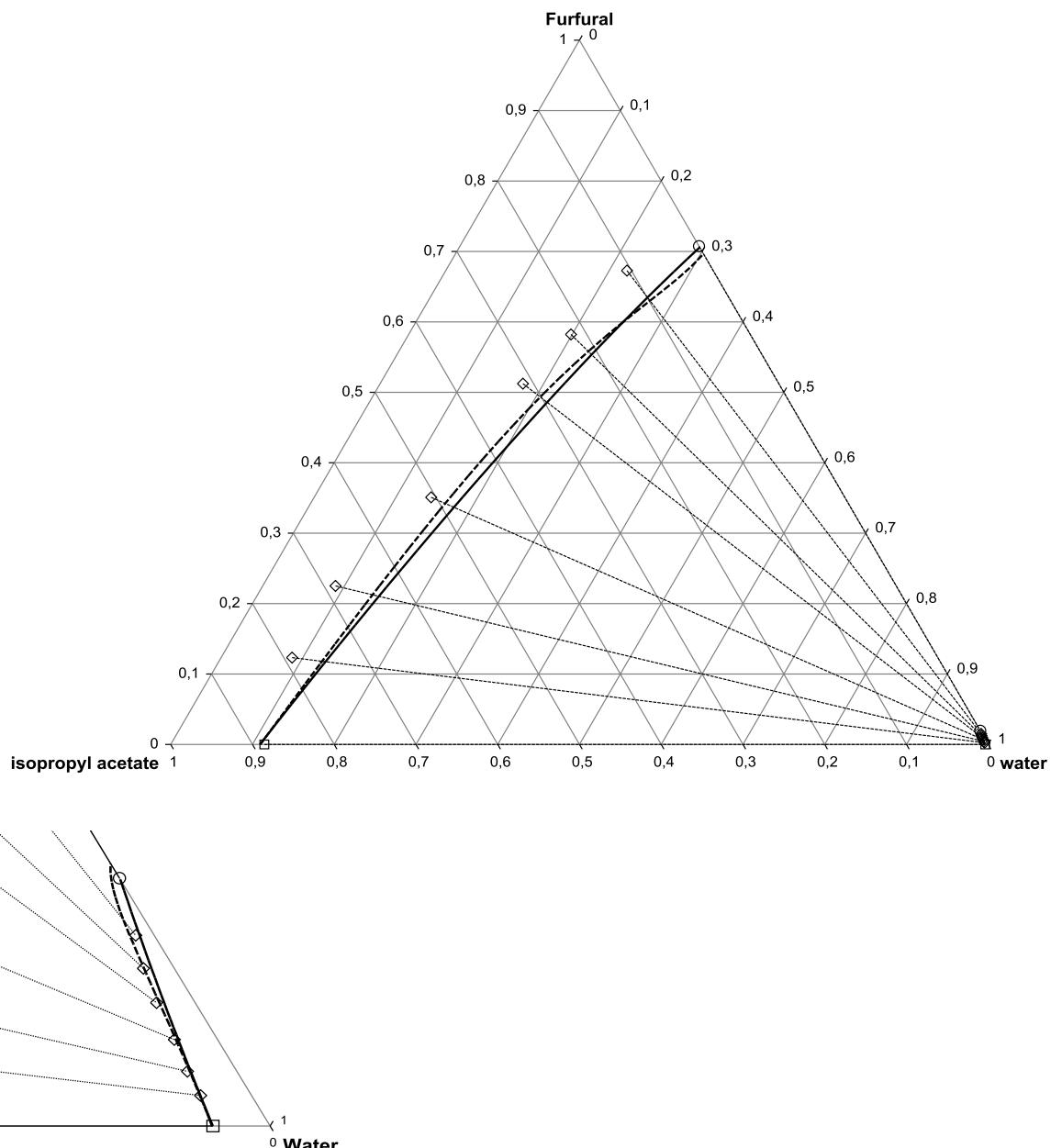


Figure 19: Ternary diagram for water - furfural - isopropyl acetate system LLE at 323.15K and atmospheric pressure, (\square): experimental data [13], (\circ): experimental data [9], (\diamond): experimental data [this work], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

Accurate representation of the data for both NRTL and UNIQUAC models

Table 18: Calculation of Ternary LLE data for water (1) - guaiacol (2) - isopropyl acetate (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data (this work).

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3									

T = 298.15K											
0.1043	0.1024	0.7933	0.9955	0.0003	0.0042	0.0996	0.1030	0.7975	0.9945	0.0004	0.0051
0.1266	0.2213	0.6521	0.9958	0.0008	0.0034	0.0934	0.2302	0.6764	0.9948	0.0006	0.0047
0.1518	0.3502	0.4979	0.9960	0.0014	0.0026	0.1028	0.3710	0.5262	0.9956	0.0011	0.0033
0.1772	0.4731	0.3496	0.9962	0.0021	0.0018	0.1255	0.5032	0.3714	0.9963	0.0017	0.0020
0.2012	0.5808	0.2180	0.9962	0.0027	0.0011	0.1574	0.6127	0.2299	0.9966	0.0024	0.0010
0.2182	0.6524	0.1293	0.9962	0.0032	0.0006	0.1864	0.6790	0.1346	0.9966	0.0029	0.0005
T = 323.15K											
0.1482	0.1153	0.7365	0.9964	0.0004	0.0032	0.1370	0.1167	0.7463	0.9954	0.0007	0.0040
0.1733	0.1867	0.6400	0.9965	0.0007	0.0028	0.1388	0.1947	0.6665	0.9954	0.0008	0.0038
0.2132	0.2973	0.4895	0.9965	0.0013	0.0022	0.1545	0.3199	0.5256	0.9957	0.0012	0.0031
0.2630	0.4304	0.3066	0.9964	0.0022	0.0014	0.1993	0.4678	0.3329	0.9961	0.0021	0.0018
0.2895	0.4982	0.2122	0.9963	0.0027	0.0010	0.2346	0.5369	0.2285	0.9962	0.0027	0.0011
0.3105	0.5500	0.1395	0.9962	0.0032	0.0006	0.2681	0.5839	0.1480	0.9961	0.0032	0.0007
Average absolute difference											
0.0533	0.0294	0.0239	0.0003	0.0001	0.0002	0.0247	0.0140	0.0107	0.0003	0.0002	0.0003

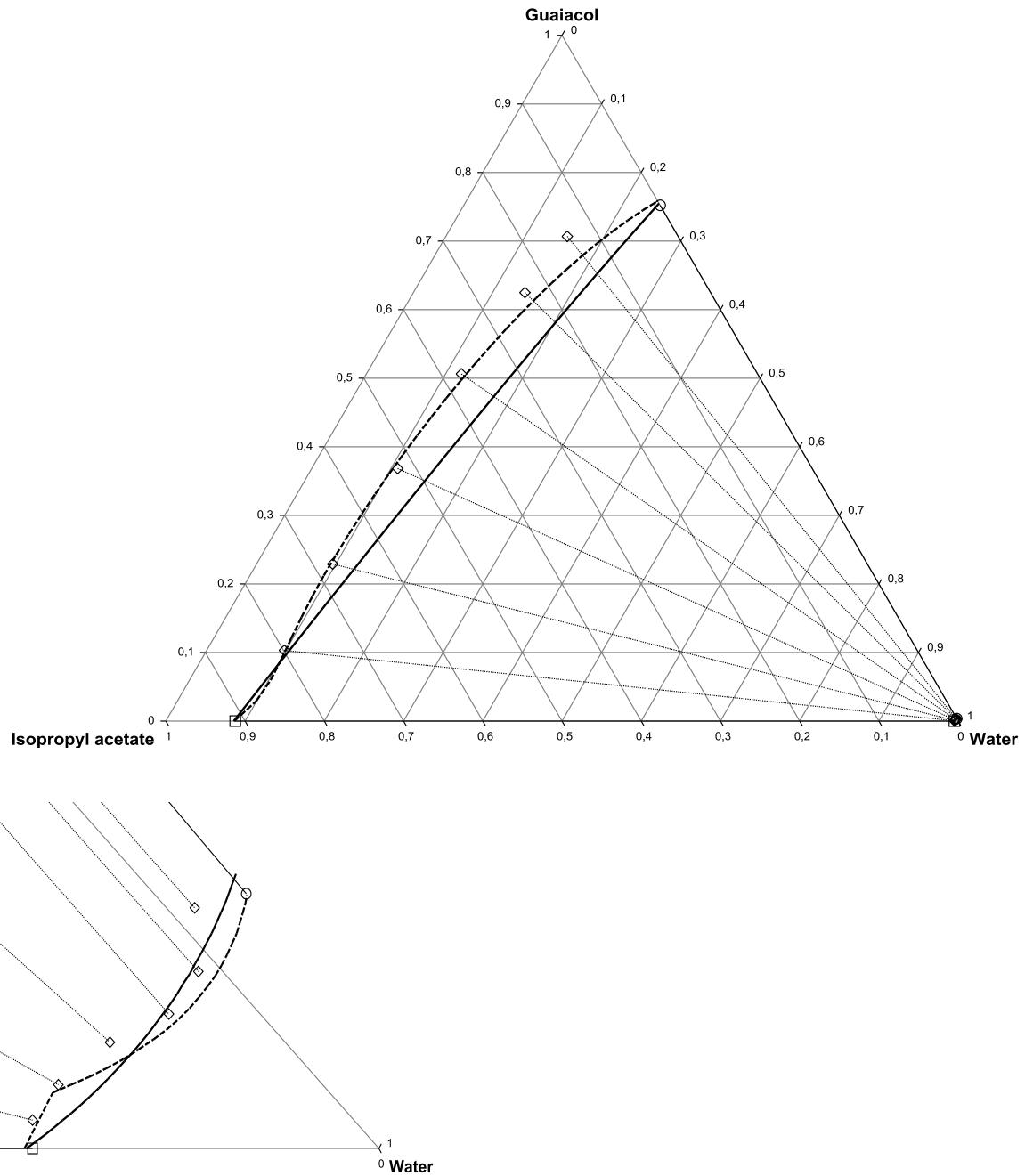


Figure 20: Ternary diagram for water - guaiacol - isopropyl acetate system LLE at 298.15K and atmospheric pressure, (□): experimental data [13], (○): experimental data [10], (◊): experimental data [this work], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

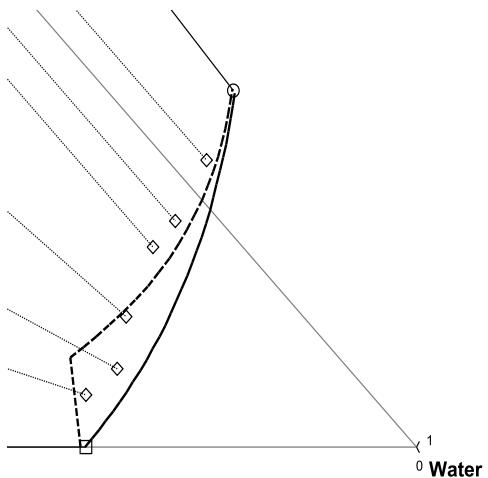
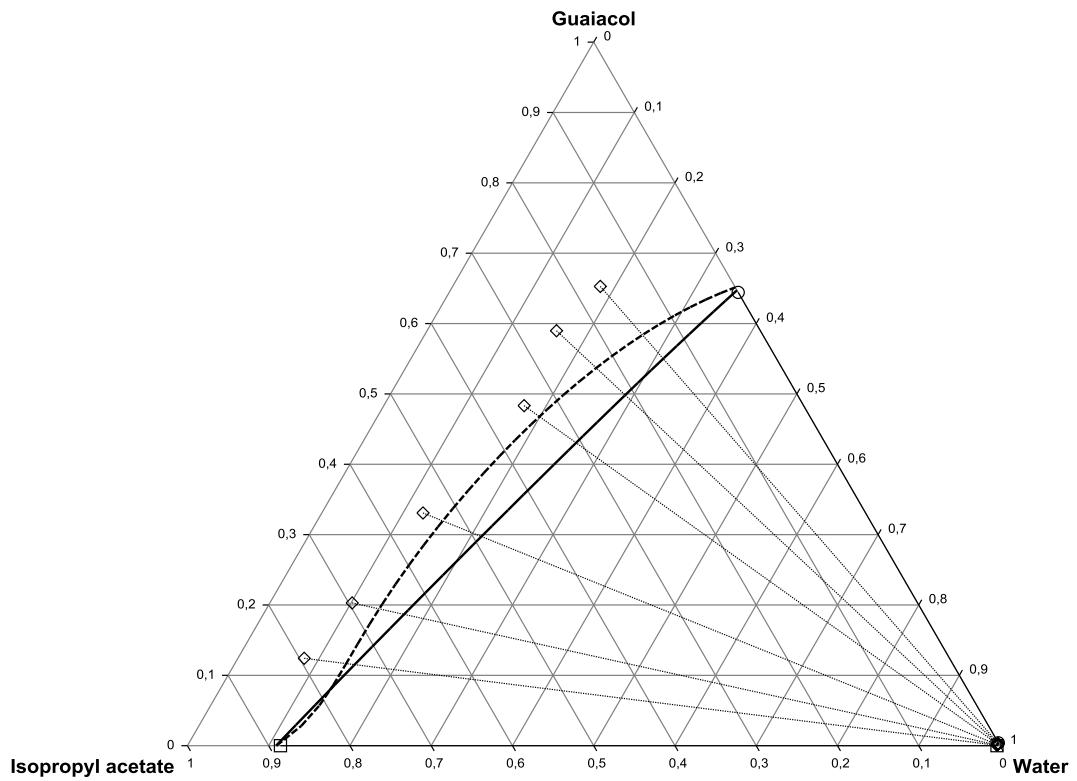


Figure 21: Ternary diagram for water - guaiacol - isopropyl acetate system LLE at 323.15K and atmospheric pressure, (\square): experimental data [13], (\circ): experimental data [10], (\diamond): experimental data [this work], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

Accurate representation of the data for NRTL model. UNIQUAC model is unable to represent accurately the experimental data.

Table 19: Calculation of Ternary LLE data for water (1) - methanol (2) - isopropyl acetate (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data (this work).

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
T = 298.15K											
0.0946	0.0135	0.8918	0.9749	0.0192	0.0059	0.0945	0.0143	0.8913	0.9754	0.0185	0.0061
0.1094	0.0351	0.8555	0.9457	0.0465	0.0079	0.1088	0.0372	0.8540	0.9473	0.0444	0.0083
0.1391	0.0755	0.7854	0.8989	0.0889	0.0122	0.1393	0.0794	0.7813	0.9019	0.0849	0.0132
0.1821	0.1284	0.6895	0.8474	0.1334	0.0191	0.1846	0.1322	0.6832	0.8494	0.1294	0.0213
0.2705	0.2173	0.5122	0.7655	0.1977	0.0367	0.2760	0.2162	0.5078	0.7575	0.1990	0.0435
0.3763	0.2853	0.3384	0.6757	0.2554	0.0689	0.3819	0.2800	0.3381	0.6513	0.2618	0.0869
T = 323.15K											
0.1200	0.0175	0.8625	0.9757	0.0197	0.0046	0.1200	0.0171	0.8629	0.9749	0.0201	0.0050
0.1375	0.0443	0.8182	0.9469	0.0469	0.0062	0.1375	0.0435	0.8190	0.9451	0.0476	0.0073
0.1707	0.0922	0.7371	0.9016	0.0887	0.0097	0.1724	0.0902	0.7374	0.8971	0.0905	0.0124
0.2130	0.1478	0.6392	0.8543	0.1308	0.0149	0.2183	0.1432	0.6385	0.8440	0.1353	0.0207
0.2942	0.2372	0.4686	0.7754	0.1960	0.0285	0.3080	0.2254	0.4666	0.7488	0.2064	0.0448
0.3513	0.2830	0.3657	0.7215	0.2358	0.0427	0.3738	0.2674	0.3588	0.6797	0.2482	0.0721
Average absolute deviation											
0.0192	0.0028	0.0200	0.0061	0.0019	0.0065	0.0176	0.0038	0.0206	0.0131	0.0046	0.0118

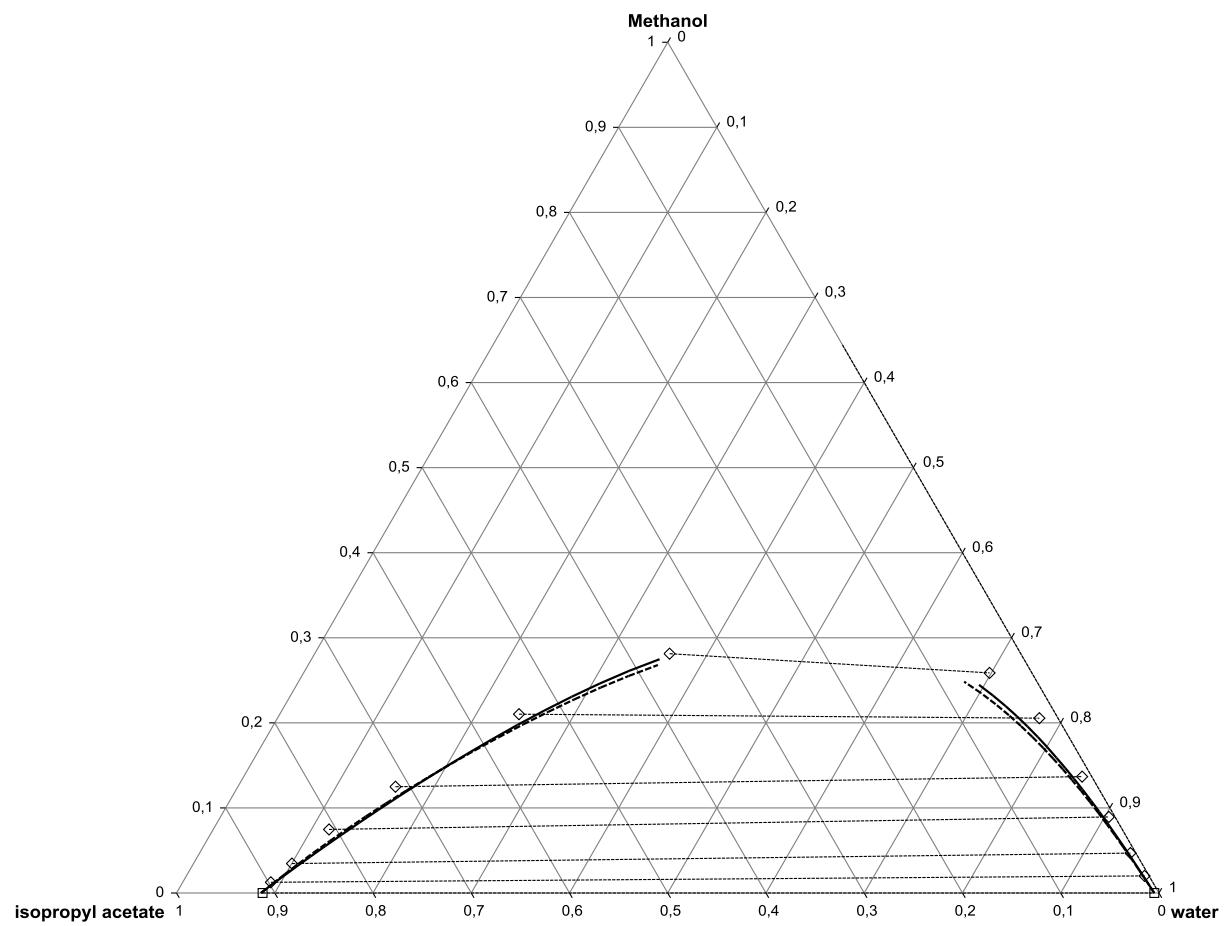


Figure 22: Ternary diagram for water - methanol - isopropyl acetate system LLE at 298.15K and atmospheric pressure, (\square): experimental data [13], (\diamond): experimental data [this work], (—): UNIQUAC model, (---): NRTL model

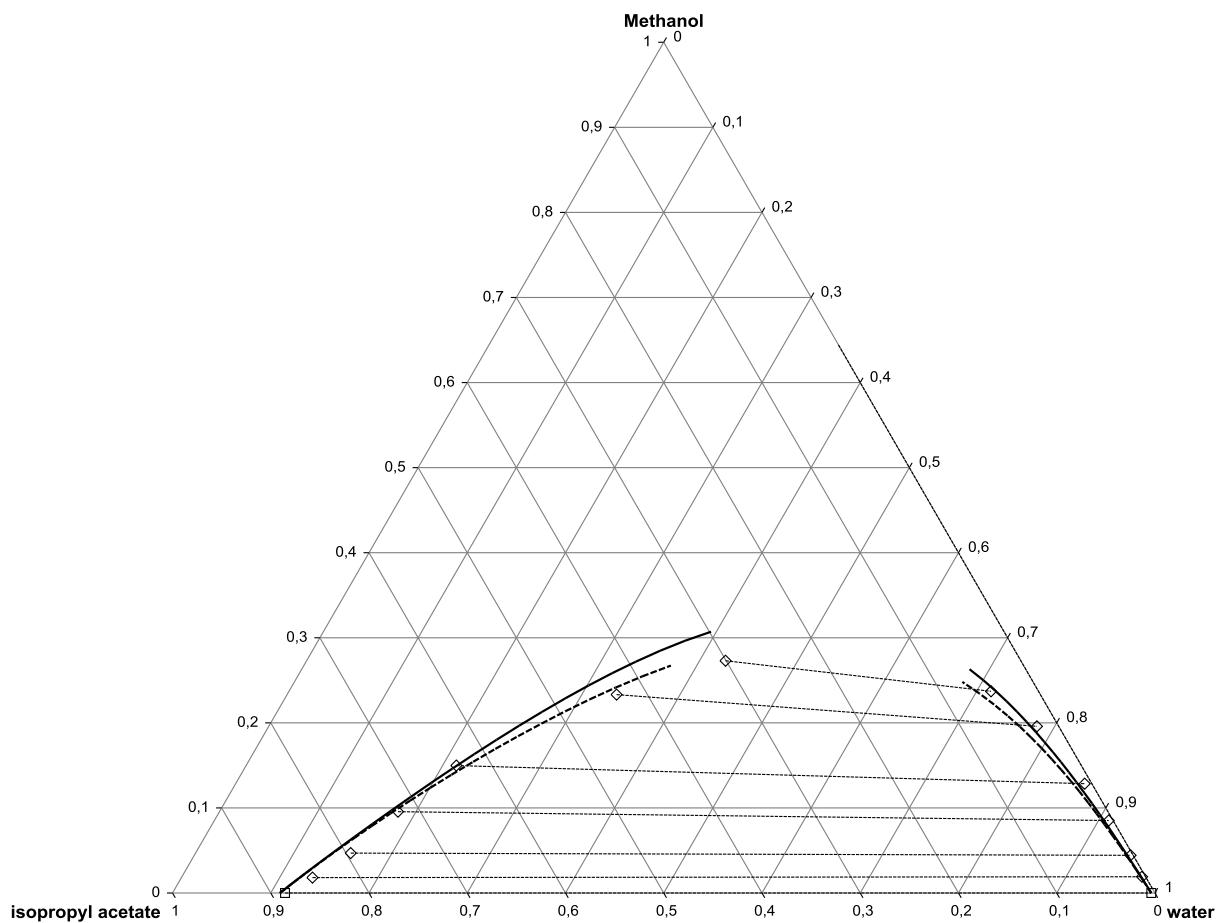


Figure 23: Ternary diagram for water - methanol - isopropyl acetate system LLE at 323.15K and atmospheric pressure, (□): experimental data [13], (◊): experimental data [this work], (—): UNIQUAC model, (---): NRTL model

Accurate representation of the data for both NRTL and UNIQUAC models

Table 20: Calculation of Ternary LLE data for water (1) - phenol (2) - isopropyl acetate (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data [16] and this work.

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3									
$T = 298.15K$											
0.1680	0.0888	0.7432	0.9957	0.0002	0.0041	0.1075	0.0952	0.7972	0.9956	0.0003	0.0042
0.2168	0.1403	0.6429	0.9959	0.0005	0.0036	0.1244	0.1568	0.7188	0.9958	0.0006	0.0037
0.2744	0.1988	0.5268	0.9961	0.0010	0.0029	0.1502	0.2328	0.6171	0.9959	0.0011	0.0030
0.3094	0.2321	0.4585	0.9960	0.0015	0.0024	0.1699	0.2788	0.5512	0.9958	0.0016	0.0026
0.3675	0.2814	0.3512	0.9955	0.0027	0.0018	0.2117	0.3504	0.4379	0.9952	0.0029	0.0019
0.4338	0.3248	0.2414	0.9942	0.0046	0.0012	0.2771	0.4142	0.3087	0.9938	0.0050	0.0012

0.4839	0.3461	0.1699	0.9929	0.0063	0.0008		0.3420	0.4406	0.2174	0.9922	0.0070	0.0008
0.5464	0.3567	0.0969	0.9909	0.0086	0.0005		0.4422	0.4381	0.1197	0.9898	0.0097	0.0005
0.5718	0.3557	0.0726	0.9900	0.0096	0.0004		0.4874	0.4253	0.0873	0.9888	0.0108	0.0004
T = 323.15K												
0.1963	0.0938	0.7099	0.9962	0.0005	0.0032		0.1507	0.0991	0.7502	0.9962	0.0005	0.0033
0.2879	0.1832	0.5289	0.9957	0.0017	0.0026		0.2075	0.2038	0.5887	0.9958	0.0017	0.0026
0.3979	0.2702	0.3319	0.9934	0.0048	0.0018		0.3001	0.3139	0.3861	0.9936	0.0047	0.0017
0.5048	0.3187	0.1765	0.9889	0.0100	0.0011		0.4221	0.3714	0.2065	0.9888	0.0102	0.0010
0.5902	0.3234	0.0864	0.9838	0.0155	0.0007		0.5405	0.3621	0.0974	0.9836	0.0158	0.0006
0.6677	0.2996	0.0327	0.9784	0.0212	0.0004		0.6513	0.3143	0.0344	0.9789	0.0207	0.0004
Average absolute difference												
0.0754	0.0398	0.0357	0.0018	0.0016	0.0002		0.0350	0.0165	0.0185	0.0014	0.0012	0.0002

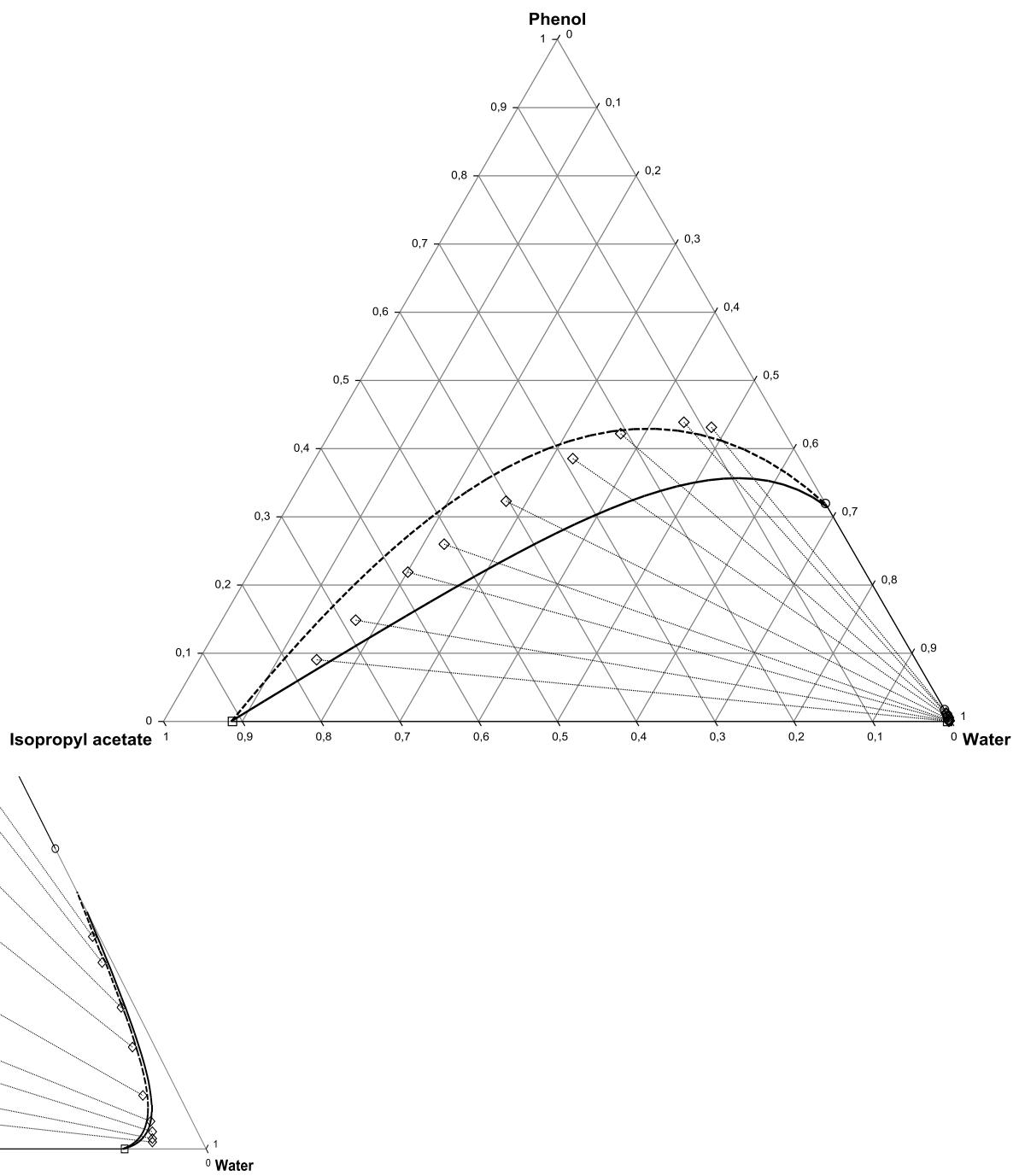


Figure 24: Ternary diagram for water - phenol - isopropyl acetate system LLE at 298.15 K and atmospheric pressure, (□): experimental data [13], (○): experimental data [11], (◊): experimental data [16], (—): UNIQUAC model, (- - -): NRTL model; zoom on the aqueous phase data

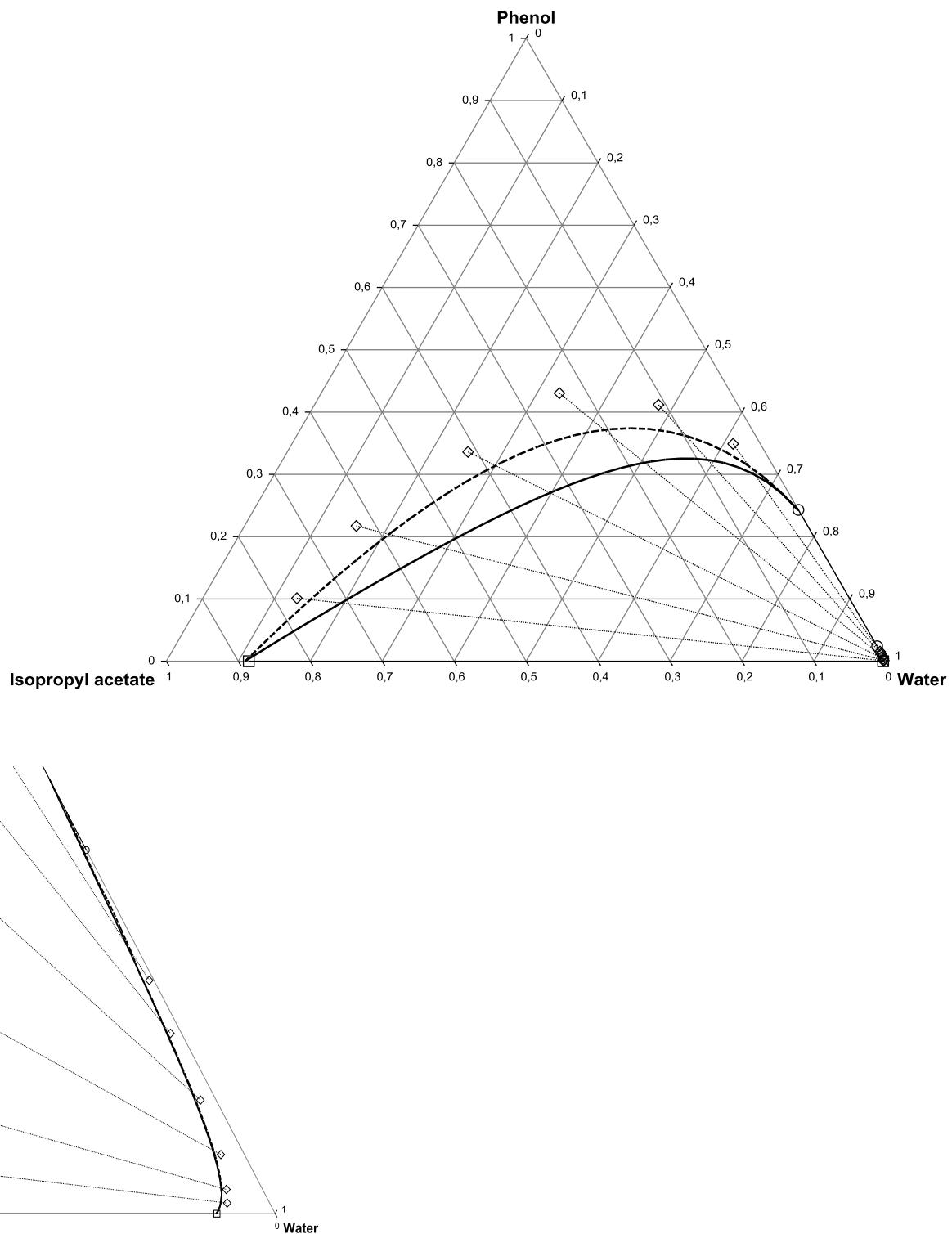


Figure 25: Ternary diagram for water - phenol - isopropyl acetate system LLE at 323.15K and atmospheric pressure, (□): experimental data [13], (○): experimental data [11], (◇): experimental data [this work], (—): UNIQUAC model, (- -): NRTL model; zoom on the aqueous phase data

Both models have significant deviations from experimental data. NRTL model is more accurate than UNIQUAC model.

Table 21: Calculation of Ternary LLE data for water (1) - propanal (2) - isopropyl acetate (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data (this work).

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
T = 298.15K											
0.0910	0.0801	0.8289	0.9903	0.0050	0.0047	0.0935	0.0797	0.8268	0.9901	0.0051	0.0047
0.0995	0.1885	0.7120	0.9827	0.0127	0.0046	0.1044	0.1871	0.7086	0.9821	0.0133	0.0046
0.1156	0.3405	0.5439	0.9694	0.0262	0.0044	0.1230	0.3367	0.5403	0.9677	0.0279	0.0044
0.1421	0.4971	0.3608	0.9500	0.0461	0.0039	0.1509	0.4907	0.3584	0.9466	0.0494	0.0040
0.1729	0.5986	0.2285	0.9304	0.0663	0.0034	0.1816	0.5911	0.2273	0.9256	0.0709	0.0035
0.2308	0.6776	0.0916	0.8990	0.0987	0.0022	0.2367	0.6717	0.0915	0.8933	0.1044	0.0023
T = 313.15K											
0.1042	0.0799	0.8159	0.9919	0.0041	0.0040	0.1058	0.0799	0.8143	0.9920	0.0040	0.0040
0.1132	0.2016	0.6852	0.9849	0.0113	0.0038	0.1157	0.2013	0.6830	0.9851	0.0110	0.0038
0.1289	0.3574	0.5137	0.9738	0.0228	0.0035	0.1315	0.3565	0.5120	0.9740	0.0225	0.0035
0.1526	0.5080	0.3394	0.9590	0.0381	0.0029	0.1536	0.5075	0.3389	0.9593	0.0377	0.0029
0.1768	0.6015	0.2217	0.9458	0.0517	0.0024	0.1753	0.6028	0.2219	0.9466	0.0510	0.0024
0.2212	0.6879	0.0909	0.9254	0.0732	0.0014	0.2130	0.6953	0.0917	0.9277	0.0709	0.0014
Average absolute deviation											
0.0181	0.0086	0.0096	0.0046	0.0044	0.0006	0.0148	0.0064	0.0084	0.0054	0.0052	0.0006

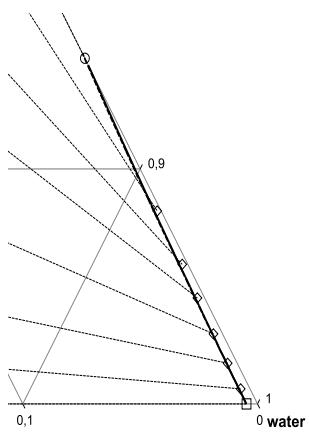
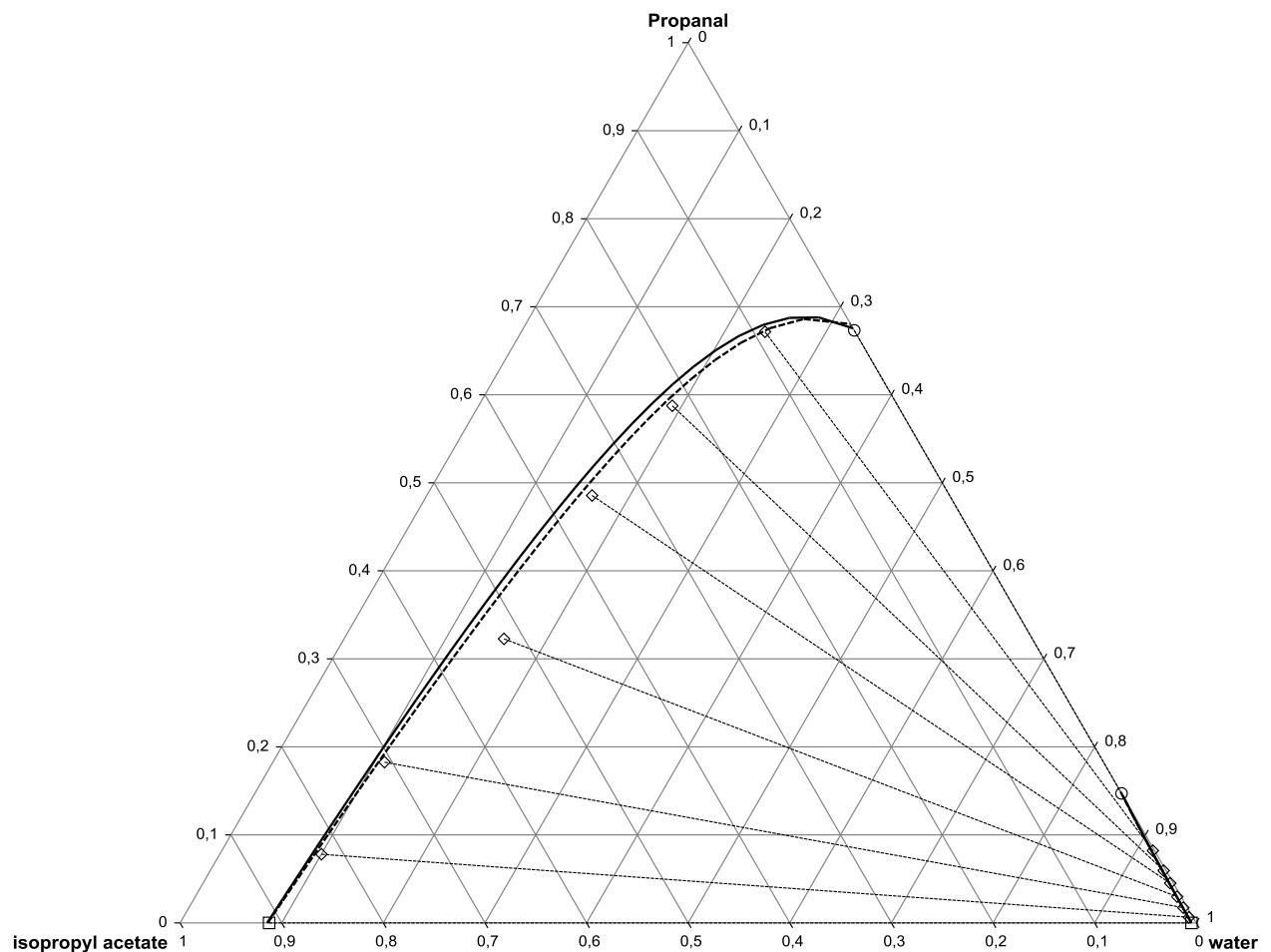


Figure 26: Ternary diagram for water - propanal - isopropyl acetate system LLE at 298.15K and atmospheric pressure, (□): experimental data [13], (○): experimental data [12], (◊): experimental data [this work], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

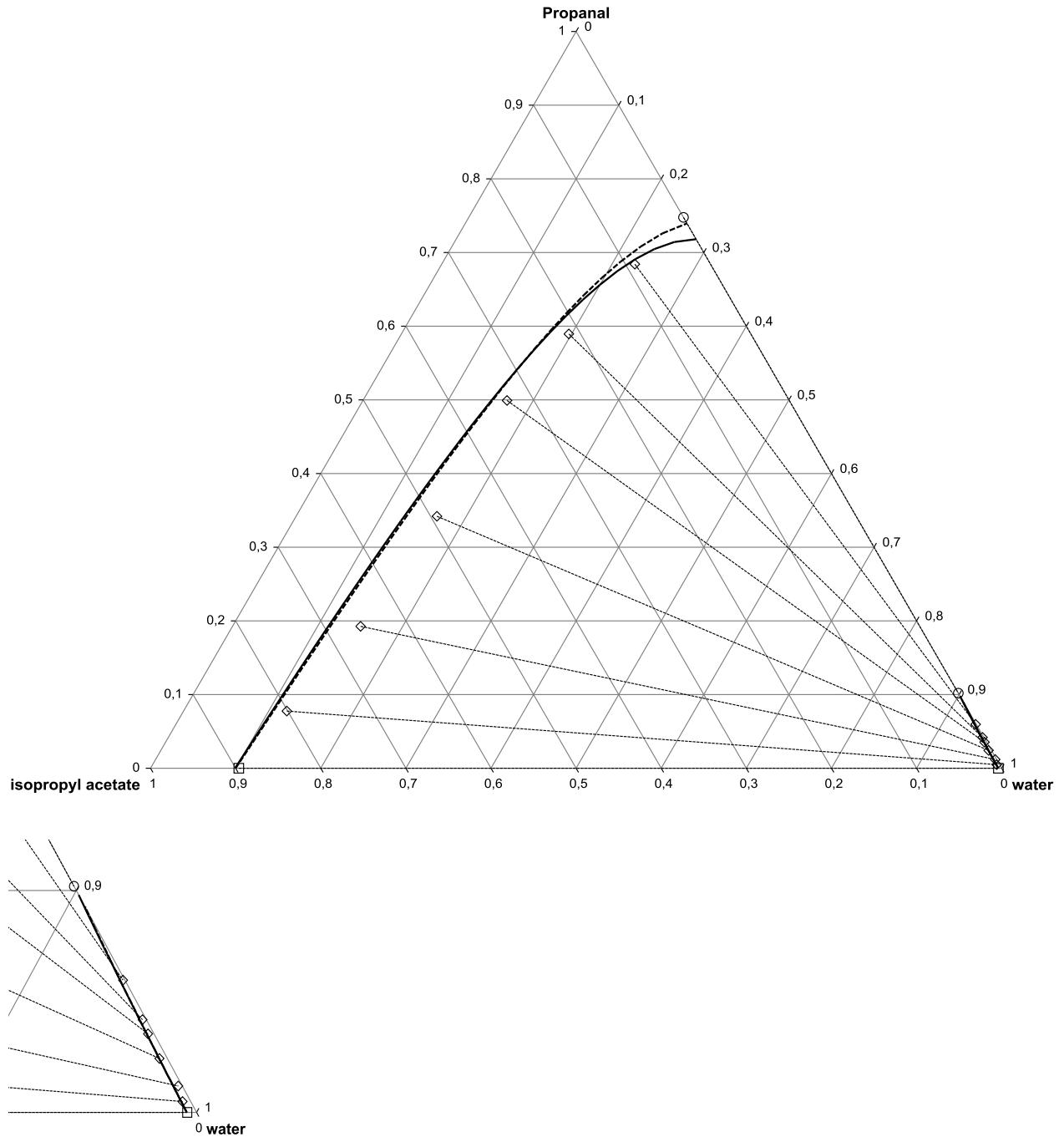


Figure 27: Ternary diagram for water - propanal - isopropyl acetate system LLE at 313.15K and atmospheric pressure, (\square): experimental data [13], (\circ): experimental data [11], (\diamond): experimental data [this work], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

Accurate representation of the data for both NRTL and UNIQUAC models

Table 22: Calculation of Ternary LLE data for water (1) – acetic acid (2) - toluene (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data [17].

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
T = 298.15K											
0.0069	0.0192	0.9738	0.9272	0.0722	0.0006	0.0060	0.0237	0.9703	0.9316	0.0679	0.0005
0.0086	0.0304	0.9610	0.8982	0.1010	0.0009	0.0069	0.0345	0.9587	0.9021	0.0971	0.0008
0.0099	0.0393	0.9508	0.8782	0.1207	0.0011	0.0076	0.0424	0.9500	0.8813	0.1176	0.0010
0.0126	0.0560	0.9314	0.8448	0.1536	0.0017	0.0090	0.0566	0.9343	0.8458	0.1527	0.0016
0.0134	0.0611	0.9255	0.8354	0.1627	0.0019	0.0095	0.0609	0.9297	0.8357	0.1625	0.0018
0.0178	0.0867	0.8955	0.7926	0.2044	0.0029	0.0119	0.0817	0.9064	0.7891	0.2080	0.0029
0.0199	0.0985	0.8816	0.7746	0.2219	0.0035	0.0131	0.0912	0.8957	0.7693	0.2271	0.0036
0.0249	0.1256	0.8495	0.7359	0.2589	0.0051	0.0162	0.1132	0.8706	0.7268	0.2679	0.0053
T = 313.15K											
0.0092	0.0232	0.9676	0.9233	0.0761	0.0006	0.0082	0.0276	0.9643	0.9275	0.0719	0.0006
0.0106	0.0326	0.9569	0.9009	0.0982	0.0009	0.0091	0.0366	0.9543	0.9049	0.0943	0.0008
0.0122	0.0429	0.9449	0.8787	0.1201	0.0011	0.0100	0.0461	0.9438	0.8819	0.1170	0.0011
0.0147	0.0583	0.9270	0.8494	0.1490	0.0016	0.0115	0.0595	0.9289	0.8508	0.1476	0.0016
0.0165	0.0691	0.9144	0.8305	0.1675	0.0020	0.0126	0.0687	0.9187	0.8306	0.1674	0.0020
0.0208	0.0941	0.8851	0.7906	0.2063	0.0031	0.0154	0.0896	0.8951	0.7874	0.2095	0.0031
0.0231	0.1064	0.8705	0.7723	0.2239	0.0037	0.0168	0.0998	0.8833	0.7675	0.2287	0.0038
0.0281	0.1334	0.8385	0.7349	0.2597	0.0053	0.0203	0.1223	0.8574	0.7267	0.2677	0.0056
Average absolute difference											
0.0034	0.0023	0.0028	0.0020	0.0021	0.0004	0.0018	0.0033	0.0047	0.0026	0.0027	0.0004

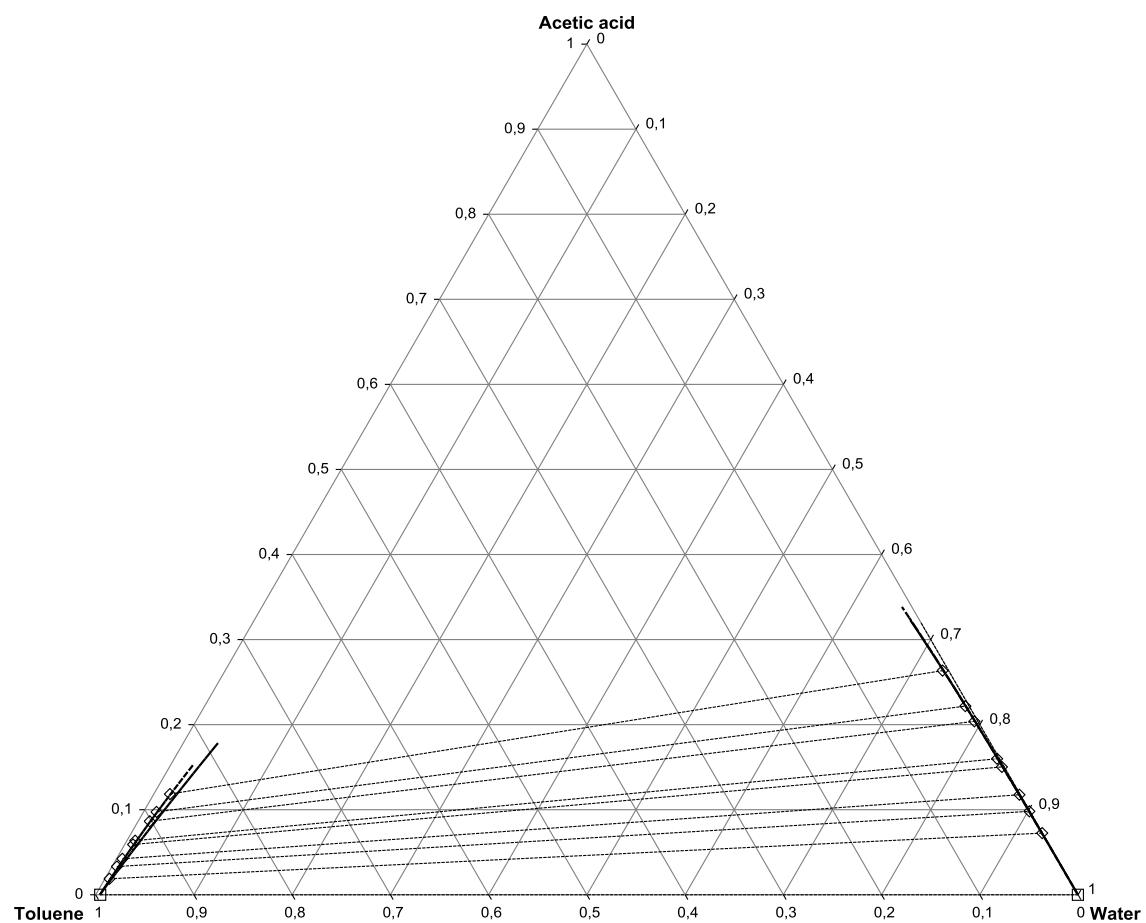


Figure 28: Ternary diagram for water – acetic acid - toluene system LLE at 298.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [17], (—): UNIQUAC model, (---): NRTL model

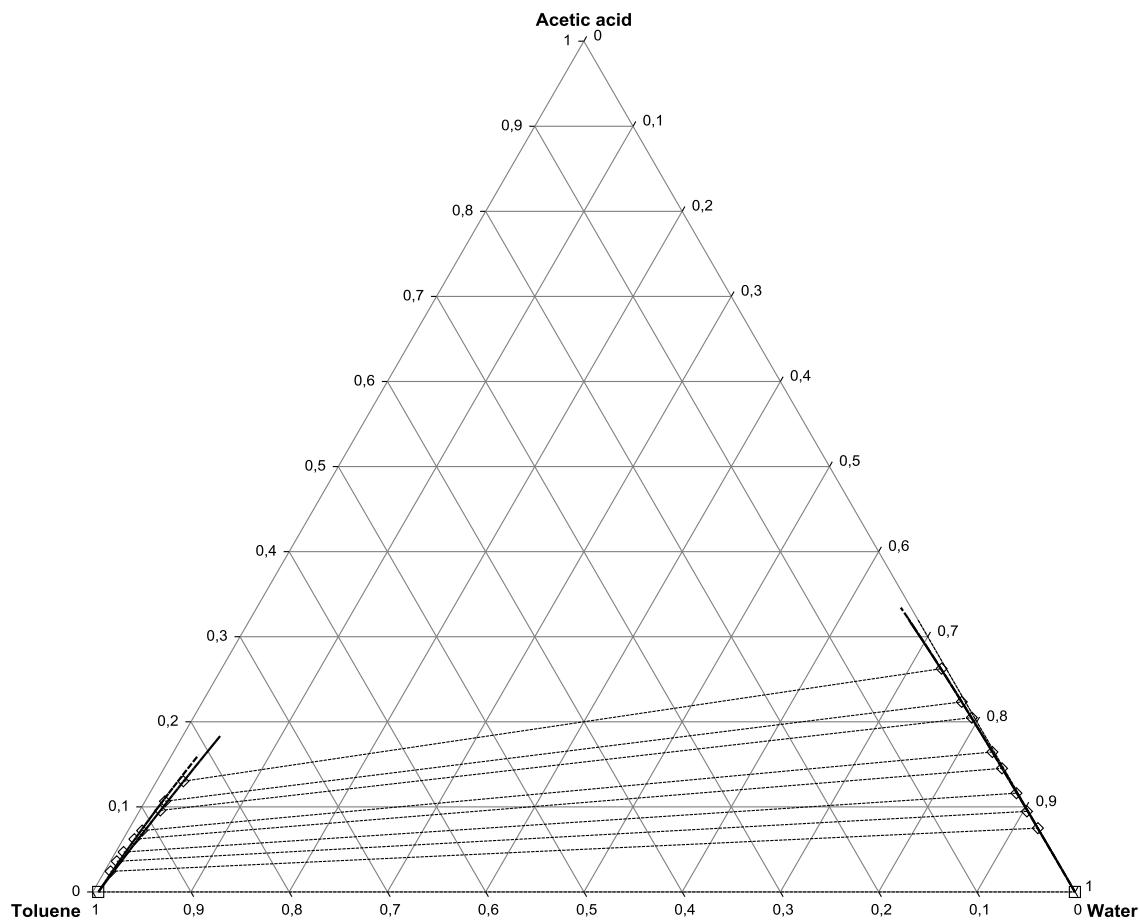


Figure 29: Ternary diagram for water – acetic acid - toluene system LLE at 313.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [17], (—): UNIQUAC model, (---): NRTL model

Accurate representation of the data for both NRTL and UNIQUAC models

Table 23: Calculation of Ternary LLE data for water (1) – acetol (2) - toluene (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data (this work).

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
$T = 298.15\text{K}$											
0.0042	0.0083	0.9874	0.9353	0.0642	0.0005	0.0044	0.0081	0.9875	0.9352	0.0644	0.0004
0.0042	0.0181	0.9777	0.851	0.1475	0.0015	0.0046	0.0199	0.9755	0.8531	0.1460	0.0008
0.0041	0.0274	0.9685	0.7809	0.2162	0.0029	0.0048	0.0314	0.9638	0.7851	0.2134	0.0015
0.004	0.0357	0.9604	0.7285	0.2671	0.0044	0.0049	0.0412	0.9539	0.7341	0.2637	0.0022
0.0036	0.0742	0.9222	0.5633	0.4244	0.0123	0.0057	0.0813	0.9130	0.5702	0.4227	0.0071

0.0034	0.1193	0.8773	0.4479	0.5299	0.0222	0.0067	0.1225	0.8708	0.4517	0.5331	0.0152
0.0035	0.1842	0.8123	0.3429	0.6204	0.0367	0.0082	0.1778	0.8140	0.3390	0.6303	0.0307
$T = 323.15K$											
0.0072	0.0104	0.9824	0.9482	0.0513	0.0005	0.0072	0.0077	0.9850	0.9458	0.0538	0.0004
0.0072	0.0279	0.9649	0.8465	0.1518	0.0017	0.0076	0.0247	0.9677	0.8443	0.1547	0.0010
0.0071	0.0525	0.9404	0.7271	0.2679	0.005	0.0081	0.0495	0.9424	0.7263	0.2709	0.0028
0.007	0.085	0.908	0.6156	0.3738	0.0107	0.0089	0.0796	0.9115	0.6143	0.3794	0.0063
0.007	0.1292	0.8638	0.511	0.4697	0.0192	0.0100	0.1173	0.8727	0.5063	0.4806	0.0131
0.0072	0.1738	0.819	0.4355	0.5361	0.0284	0.0112	0.1532	0.8356	0.4259	0.5523	0.0218
Average absolute deviation											
0.0015	0.0077	0.0076	0.0064	0.0031	0.0034	0.0016	0.0090	0.0098	0.0074	0.0017	0.0071

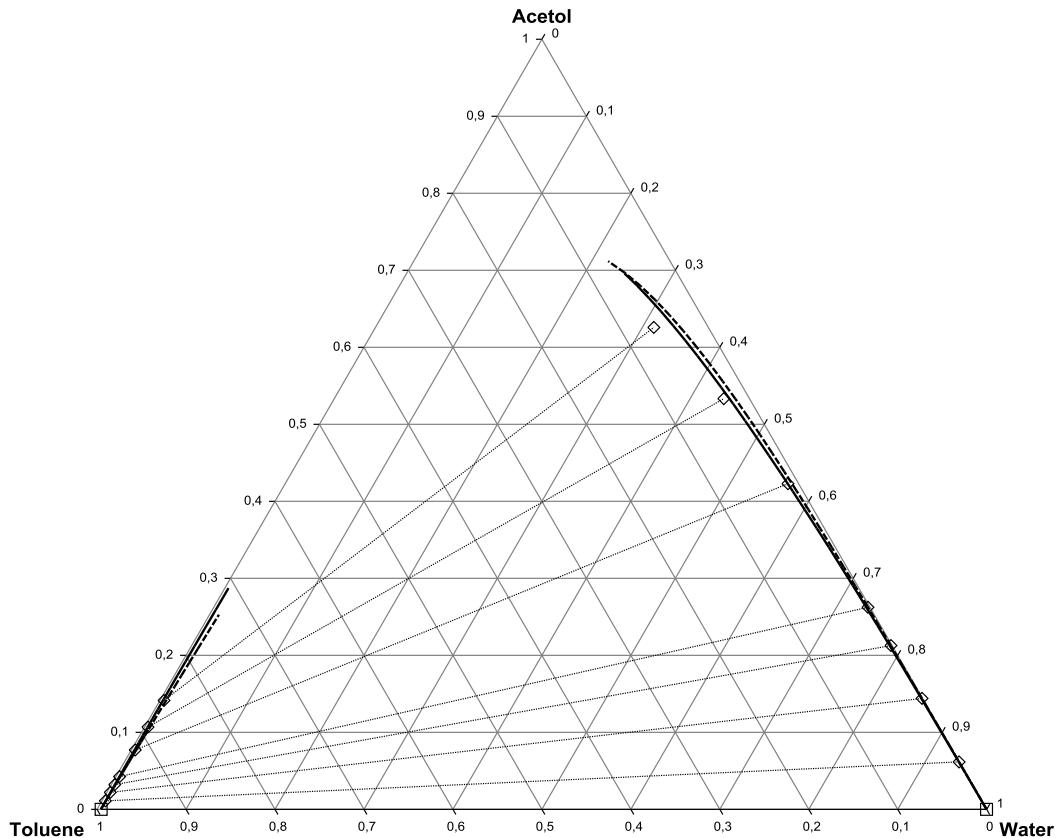


Figure 30: Ternary diagram for water – acetol - toluene system LLE at 298.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [this work], (—): UNIQUAC model, (- -): NRTL model

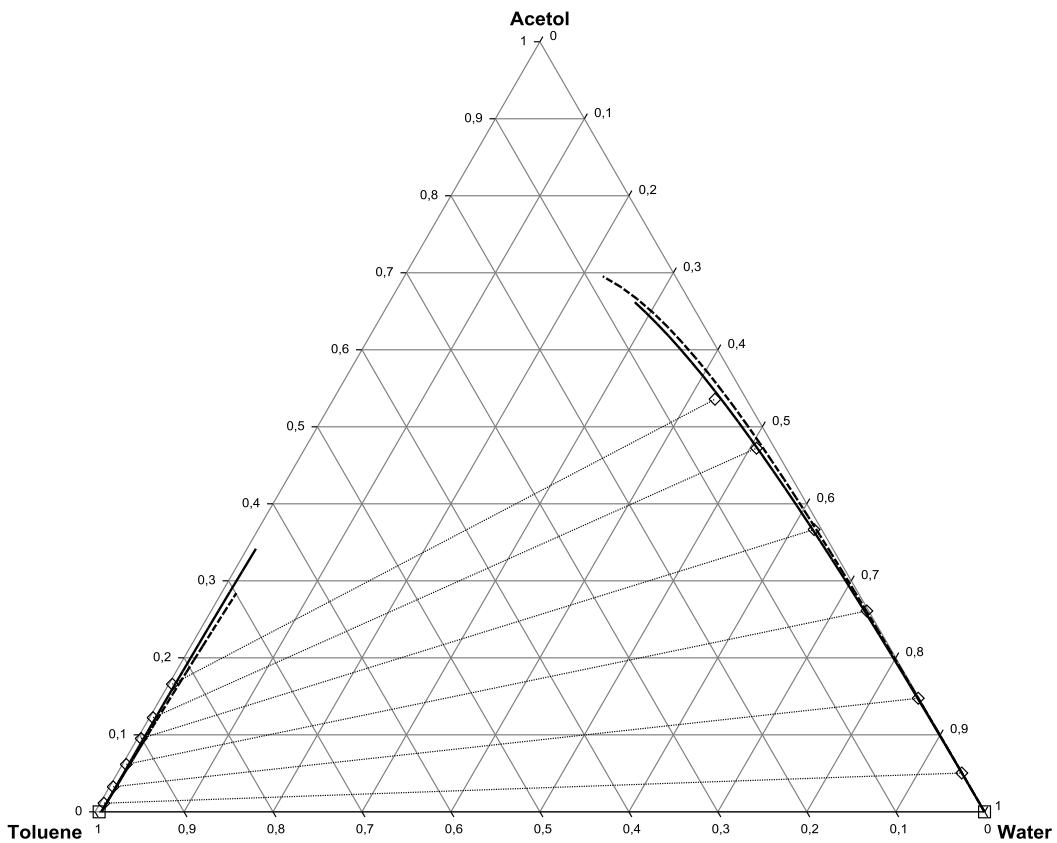


Figure 31: Ternary diagram for water – acetol - toluene system LLE at 323.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [this work], (—): UNIQUAC model, (---): NRTL model

Accurate representation of the data for both NRTL and UNIQUAC models

Table 24: Calculation of Ternary LLE data for water (1) – furfural (2) - toluene (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data [18].

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
T = 303.15K											
0.0260	0.1163	0.8577	0.9957	0.0040	0.0002	0.0084	0.1188	0.8729	0.9961	0.0037	0.0002
0.0634	0.3203	0.6163	0.9949	0.0049	0.0002	0.0227	0.3334	0.6439	0.9939	0.0059	0.0002
0.1052	0.4947	0.4000	0.9921	0.0077	0.0002	0.0507	0.5243	0.4250	0.9913	0.0085	0.0002
0.1418	0.6083	0.2498	0.9893	0.0105	0.0001	0.0873	0.6467	0.2660	0.9889	0.0109	0.0001
0.1673	0.6695	0.1632	0.9874	0.0125	0.0001	0.1198	0.7075	0.1727	0.9873	0.0126	0.0001
Average absolute difference											
0.0160	0.0060	0.0100	0.0013	0.0013	0.0001	0.0500	0.0274	0.0226	0.0009	0.0008	0.0001

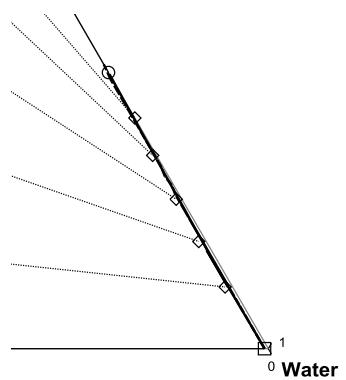
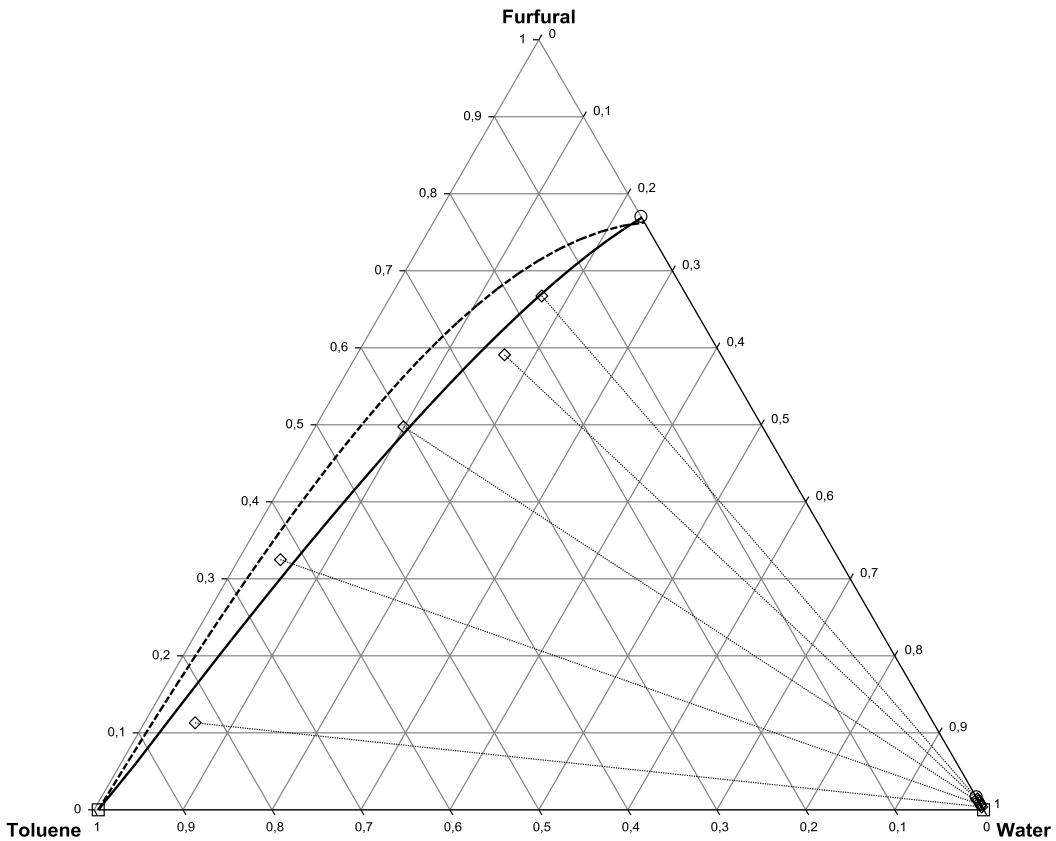


Figure 32: Ternary diagram for water – furfural - toluene system LLE at 303.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [9], (◊): experimental data [18], (—): UNIQUAC model, (- - -): NRTL model; zoom on the aqueous phase data

Accurate representation of the data for UNIQUAC model. NRTL model shows significant deviation for high furfural concentrations.

Table 25: Calculation of Ternary LLE data for water (1) – methanol (2) - toluene (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data [19].

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
$T = 298.15K$											
0.0046	0.0115	0.9839	0.8762	0.1230	0.0008	0.0040	0.0060	0.9900	0.8714	0.1277	0.0008
0.0048	0.0185	0.9767	0.8042	0.1942	0.0016	0.0039	0.0117	0.9844	0.7988	0.1995	0.0016
0.0051	0.0287	0.9663	0.7107	0.2858	0.0035	0.0038	0.0223	0.9739	0.7064	0.2901	0.0035
0.0056	0.0541	0.9403	0.5354	0.4516	0.0130	0.0041	0.0545	0.9415	0.5367	0.4511	0.0122
0.0058	0.0654	0.9288	0.4786	0.5024	0.0190	0.0043	0.0695	0.9262	0.4823	0.5002	0.0175
0.0061	0.0796	0.9143	0.4191	0.5528	0.0280	0.0047	0.0886	0.9067	0.4254	0.5494	0.0252
0.0065	0.0970	0.8966	0.3611	0.5983	0.0406	0.0052	0.1115	0.8833	0.3698	0.5945	0.0357
0.0070	0.1200	0.8730	0.3012	0.6396	0.0592	0.0060	0.1408	0.8532	0.3126	0.6364	0.0510
0.0070	0.1196	0.8735	0.3022	0.6390	0.0588	0.0060	0.1404	0.8536	0.3133	0.6359	0.0508
Average absolute difference											
0.0039	0.0057	0.0074	0.0020	0.0038	0.0027	0.0046	0.0078	0.0044	0.0066	0.0059	0.0027

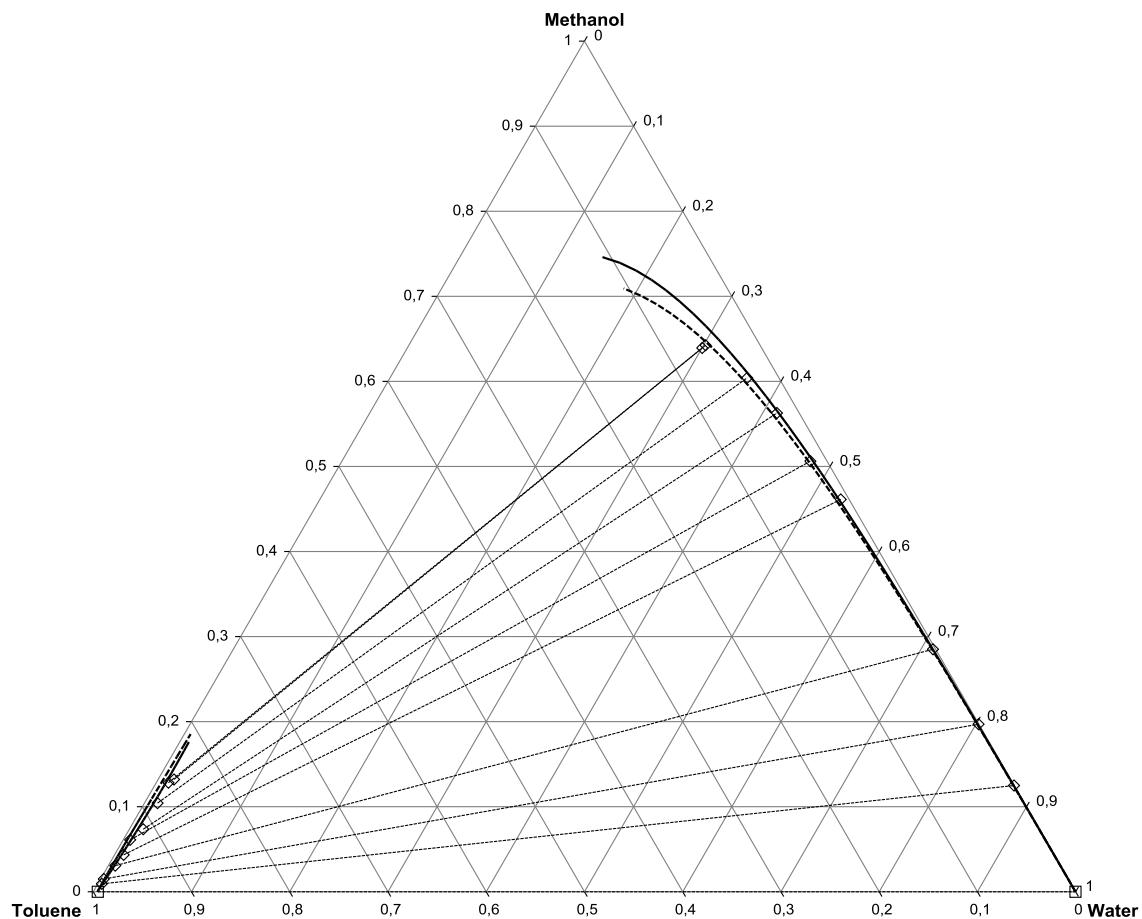


Figure 33: Ternary diagram for water – methanol - toluene system LLE at 298.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [19], (—): UNIQUAC model, (---): NRTL model

Accurate representation of the data for both NRTL and UNIQUAC models

Table 26: Calculation of Ternary LLE data for water (1) – phenol (2) - toluene (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data [20].

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
T = 293.15K											
0.0606	0.1413	0.7981	0.9950	0.0048	0.0002	0.0127	0.1491	0.8382	0.9959	0.0039	0.0002
0.0952	0.1961	0.7087	0.9943	0.0054	0.0002	0.0202	0.2125	0.7673	0.9949	0.0049	0.0002
0.1486	0.2625	0.5889	0.9938	0.0059	0.0002	0.0365	0.2964	0.6671	0.9937	0.0061	0.0002
0.2264	0.3325	0.4411	0.9933	0.0064	0.0002	0.0758	0.3956	0.5286	0.9921	0.0077	0.0002
0.2898	0.3714	0.3388	0.9929	0.0069	0.0002	0.1280	0.4541	0.4179	0.9911	0.0087	0.0002
0.3526	0.3957	0.2517	0.9924	0.0074	0.0002	0.2018	0.4862	0.3120	0.9904	0.0094	0.0002
0.4448	0.4077	0.1474	0.9915	0.0083	0.0002	0.3421	0.4822	0.1757	0.9897	0.0101	0.0002
0.5211	0.3976	0.0813	0.9906	0.0092	0.0001	0.4642	0.4443	0.0915	0.9890	0.0108	0.0002
T = 303.15K											
0.0810	0.1702	0.7488	0.9933	0.0065	0.0002	0.0205	0.1818	0.7977	0.9941	0.0057	0.0002
0.1320	0.2383	0.6297	0.9924	0.0073	0.0002	0.0372	0.2639	0.6989	0.9926	0.0072	0.0002
0.1878	0.2951	0.5171	0.9919	0.0079	0.0002	0.0643	0.3386	0.5971	0.9911	0.0086	0.0002
0.1979	0.3038	0.4983	0.9918	0.0080	0.0002	0.0704	0.3506	0.5790	0.9909	0.0089	0.0002
0.2424	0.3371	0.4205	0.9914	0.0083	0.0002	0.1028	0.3973	0.4999	0.9900	0.0098	0.0002
0.3644	0.3908	0.2448	0.9902	0.0095	0.0002	0.2410	0.4650	0.2940	0.9884	0.0114	0.0002
0.4177	0.3987	0.1836	0.9896	0.0102	0.0002	0.3196	0.4647	0.2157	0.9879	0.0118	0.0002
0.5140	0.3906	0.0954	0.9882	0.0116	0.0002	0.4655	0.4292	0.1054	0.9870	0.0128	0.0002
T = 313.15K											
0.0935	0.1838	0.7227	0.9914	0.0083	0.0002	0.0288	0.1969	0.7742	0.9920	0.0077	0.0002
0.1675	0.2706	0.5619	0.9901	0.0097	0.0003	0.0632	0.3031	0.6337	0.9894	0.0103	0.0002
0.2246	0.3185	0.4569	0.9894	0.0103	0.0003	0.1037	0.3661	0.5302	0.9879	0.0118	0.0003
0.3027	0.3631	0.3342	0.9885	0.0112	0.0003	0.1833	0.4232	0.3935	0.9865	0.0132	0.0003
0.3818	0.3869	0.2313	0.9875	0.0123	0.0003	0.2887	0.4436	0.2677	0.9857	0.0141	0.0002
0.4646	0.3904	0.1450	0.9861	0.0136	0.0002	0.4099	0.4295	0.1605	0.9849	0.0148	0.0002
0.5604	0.3690	0.0706	0.9842	0.0156	0.0002	0.5428	0.3836	0.0736	0.9837	0.0161	0.0002
Average absolute difference											
0.0334	0.0191	0.0142	0.0391	0.0021	0.0001	0.0589	0.0269	0.0320	0.0014	0.0014	0.0001

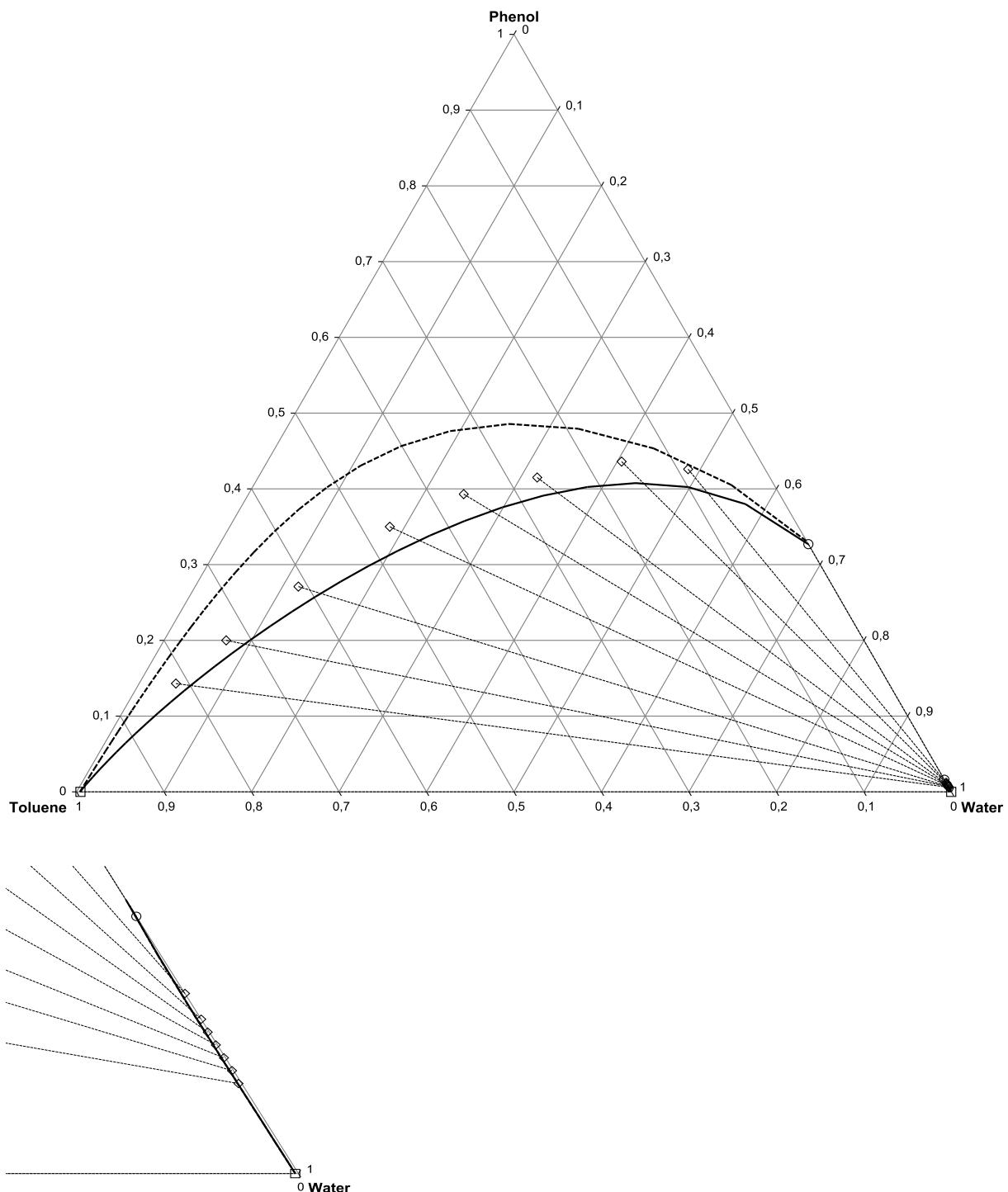


Figure 34: Ternary diagram for water – phenol - toluene system LLE at 293.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [11], (◊): experimental data [20], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

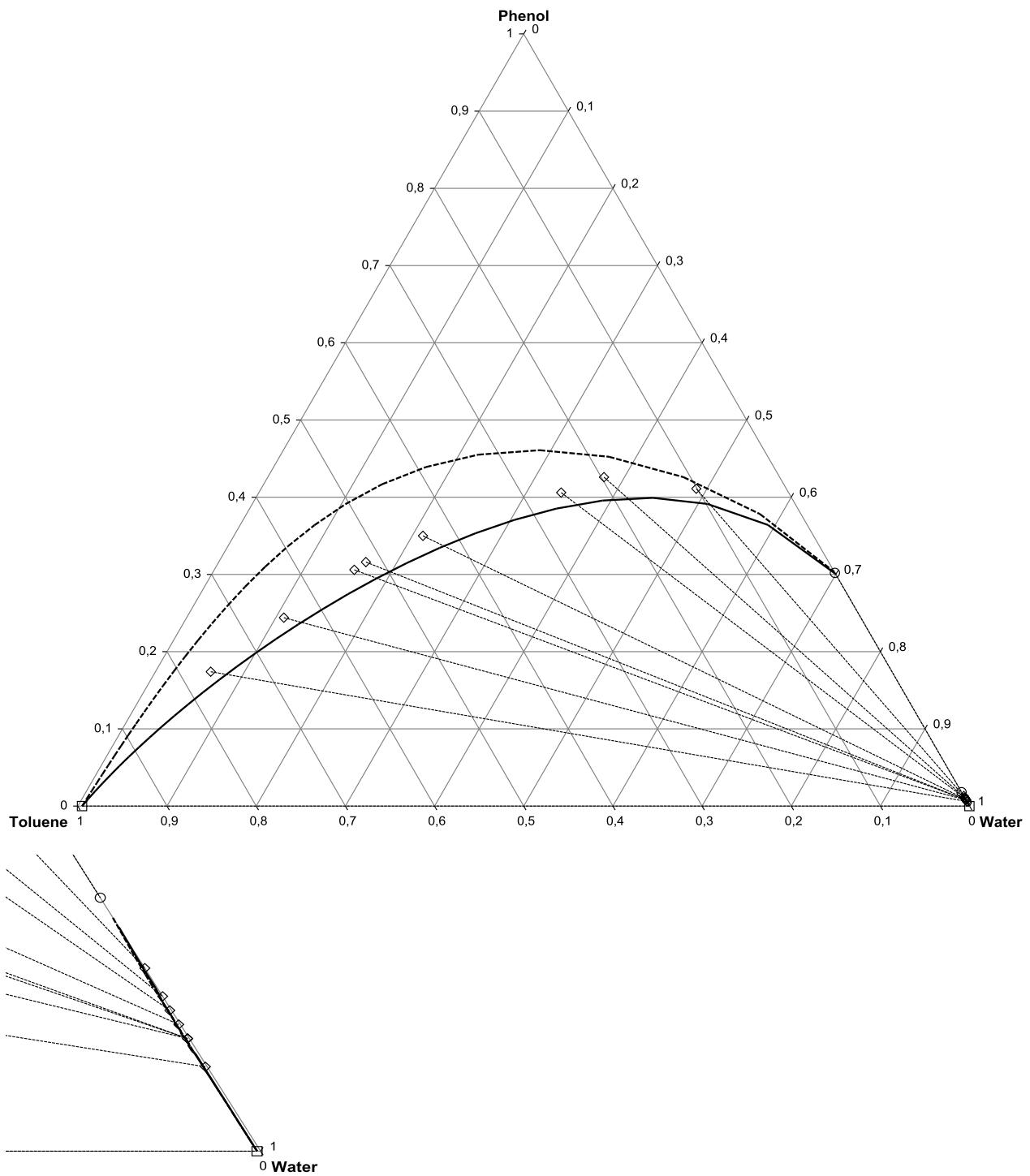


Figure 35: Ternary diagram for water – phenol - toluene system LLE at 303.15K and atmospheric pressure, (\square): experimental data [14], (\circ): experimental data [11], (\diamond): experimental data [20], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

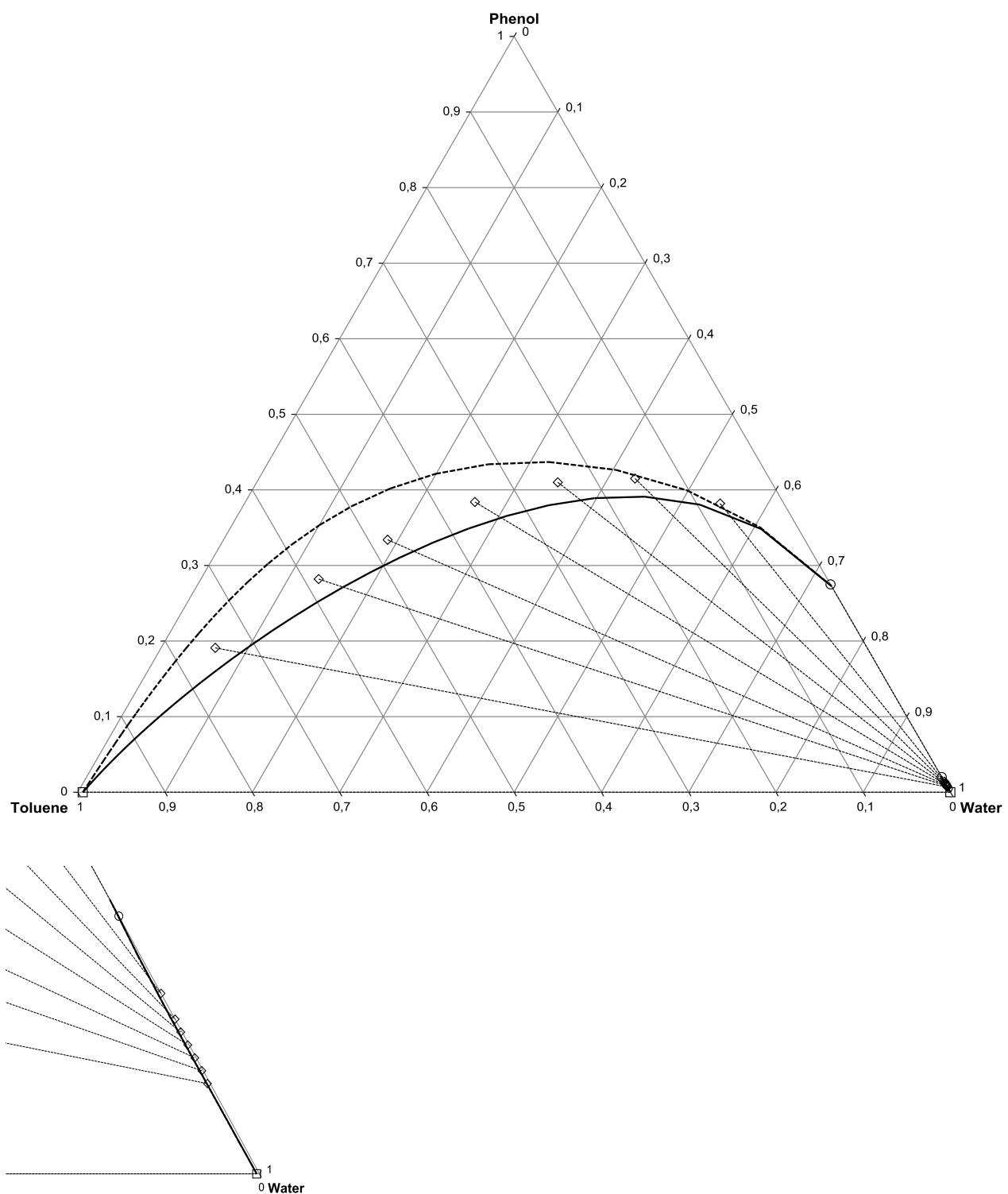


Figure 36: Ternary diagram for water – phenol - toluene system LLE at 313.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [11], (◊): experimental data [20], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

Both models have significant deviations from experimental data. NRTL model is more accurate than UNIQUAC model.

Table 27: Calculation of Ternary LLE data for water (1) – propanal (2) - toluene (3) system at atmospheric pressure using UNIQUAC and NRTL activity coefficient model, with average absolute deviations calculated based on the experimental data (this work).

UNIQUAC						NRTL					
Organic phase			Aqueous phase			Organic phase			Aqueous phase		
x1	x2	x3	x1	x2	x3	x1	x2	x3	x1	x2	x3
T = 298.15K											
0.0073	0.0999	0.8928	0.9919	0.0079	0.0002	0.0069	0.0998	0.8933	0.9917	0.0080	0.0002
0.0130	0.2278	0.7592	0.9810	0.0188	0.0002	0.0121	0.2275	0.7604	0.9803	0.0194	0.0002
0.0274	0.4123	0.5603	0.9630	0.0368	0.0003	0.0262	0.4117	0.5621	0.9610	0.0387	0.0003
0.0613	0.6041	0.3346	0.9385	0.0612	0.0003	0.0604	0.6030	0.3365	0.9346	0.0651	0.0003
0.1151	0.7129	0.1720	0.9150	0.0847	0.0003	0.1154	0.7115	0.1732	0.9098	0.0898	0.0003
T = 323.15K											
0.0088	0.0843	0.9069	0.9943	0.0055	0.0002	0.0082	0.0847	0.9070	0.9948	0.0050	0.0002
0.0164	0.2348	0.7488	0.9840	0.0158	0.0002	0.0147	0.2359	0.7494	0.9849	0.0149	0.0002
0.0337	0.4269	0.5393	0.9691	0.0306	0.0002	0.0303	0.4291	0.5406	0.9704	0.0294	0.0002
0.0714	0.6162	0.3124	0.9505	0.0492	0.0002	0.0655	0.6206	0.3139	0.9521	0.0477	0.0002
0.1250	0.7174	0.1576	0.9343	0.0655	0.0002	0.1162	0.7249	0.1589	0.9365	0.0633	0.0002
Average absolute difference											
0.0172	0.0081	0.0095	0.0027	0.0027	0.0001	0.0168	0.0078	0.0092	0.0030	0.0031	0.0001

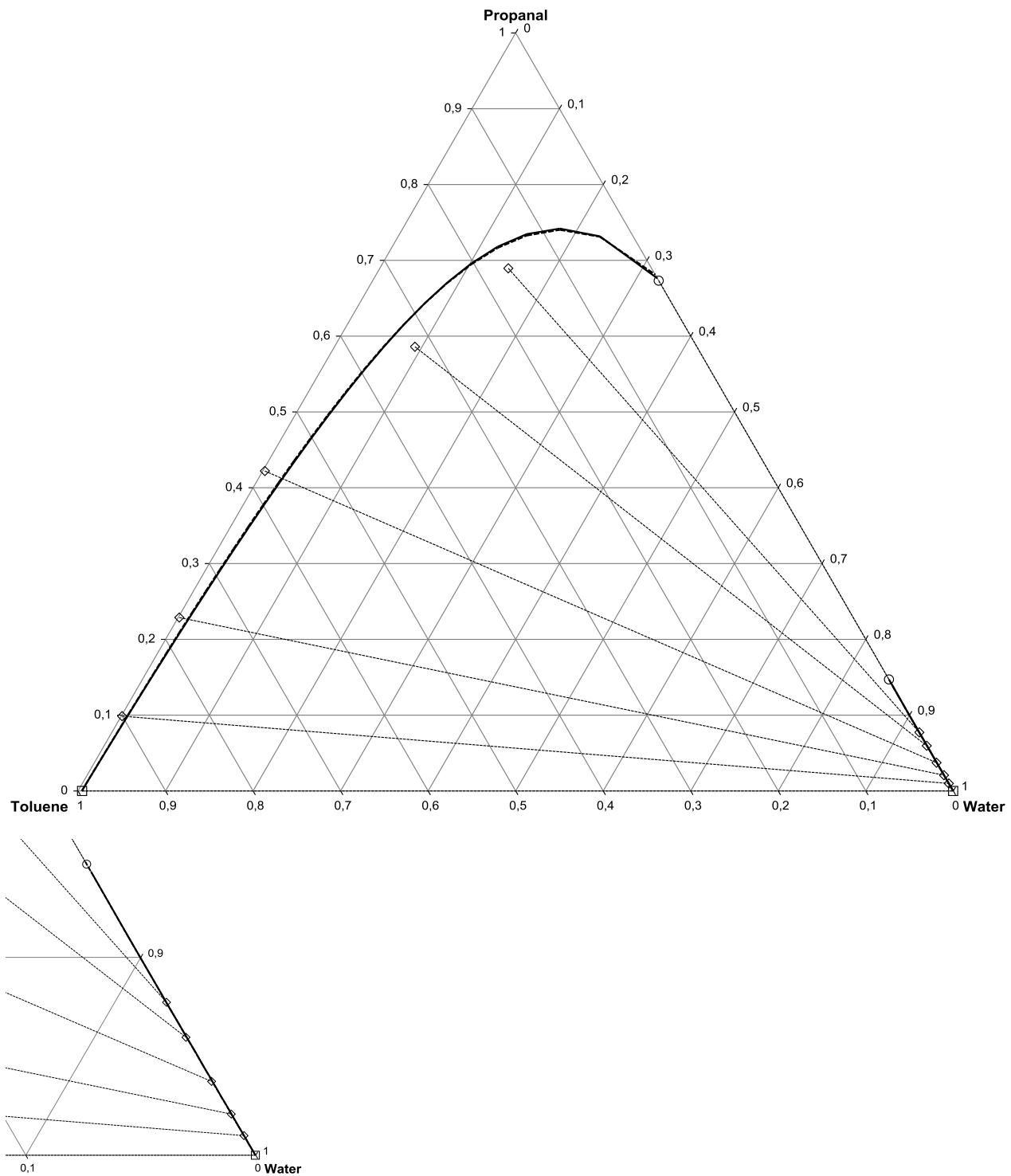


Figure 37: Ternary diagram for water – propanal - toluene system LLE at 298.15K and atmospheric pressure, (\square): experimental data [14], (\circ): experimental data [12], (\diamond): experimental data [this work], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

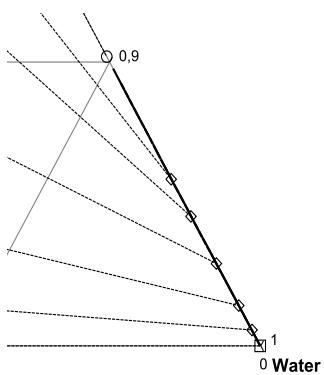
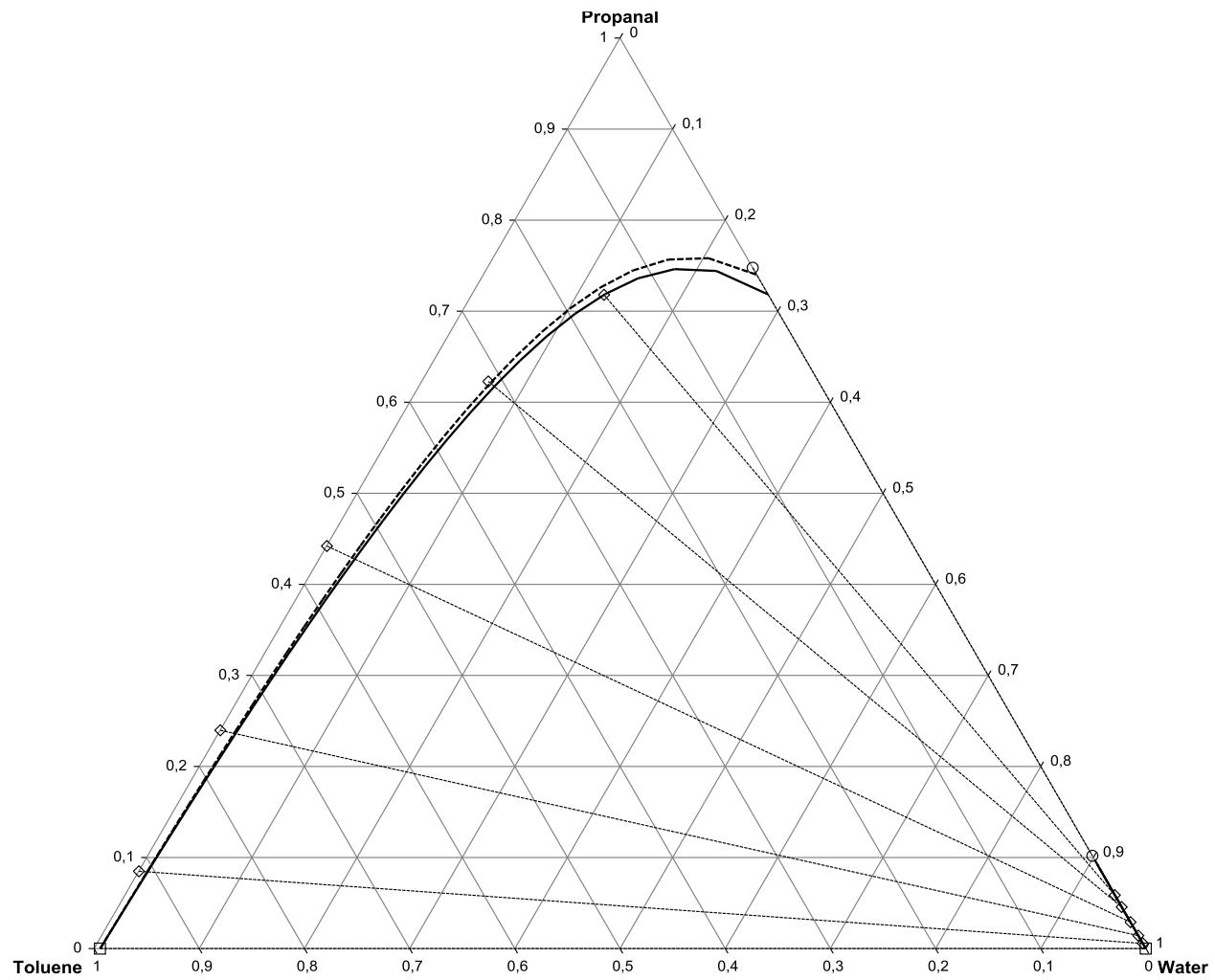


Figure 38: Ternary diagram for water – phenol - toluene system LLE at 313.15K and atmospheric pressure, (□): experimental data [14], (○): experimental data [12], (◇): experimental data [this work], (—): UNIQUAC model, (---): NRTL model; zoom on the aqueous phase data

Accurate representation of the data for both NRTL and UNIQUAC models

Parity charts of partition coefficients

Figures 40 to 65 present the parity charts of partition coefficients (K_i). The calculated values of K_i with the models are on X axis and the experimental values of K_i are on Y axis. The first bisector is drawn on the graphs in order to compare experimental and calculated data. In dotted line a 20% range is shown as an information and as a supplementary tool of comparison between calculated and experimental data.

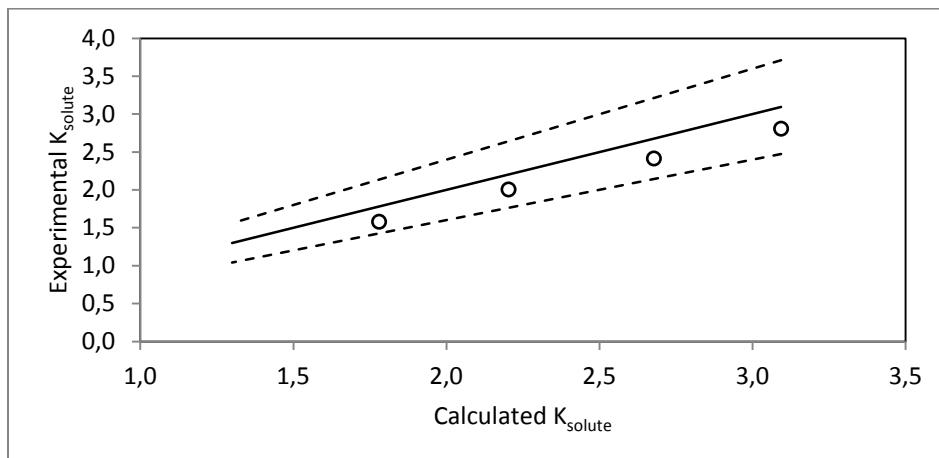


Figure 39: Parity chart of experimental [15] and calculated partition coefficient of acetic acid between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 297.75 K. (—): first bisector. (---): +/- 20%

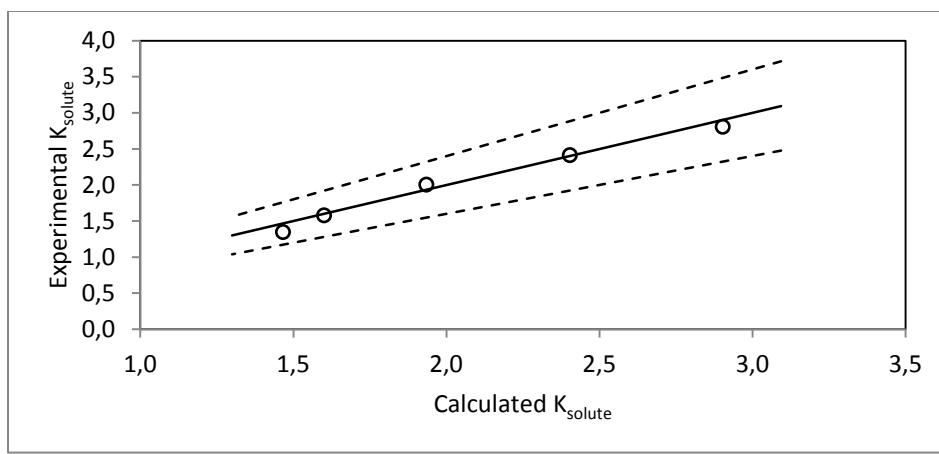


Figure 40: Parity chart of experimental [15] and calculated partition coefficient of acetic acid between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 297.75 K. (—): first bisector. (---): +/- 20%

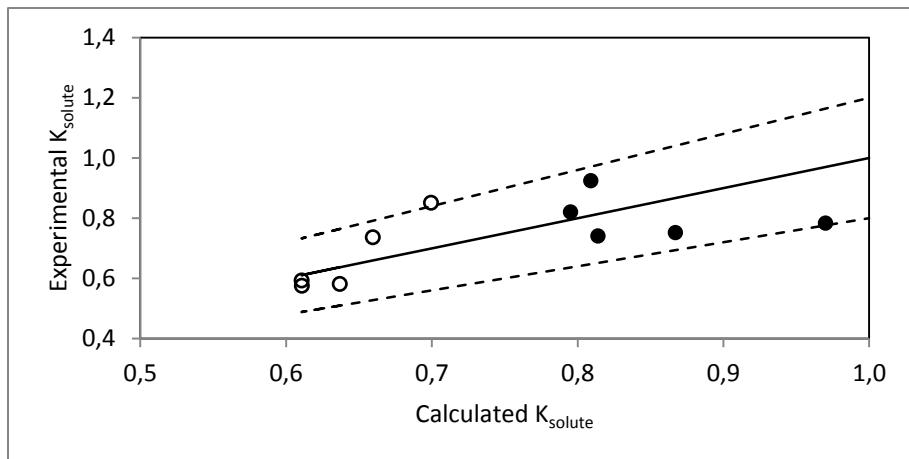


Figure 41: Parity chart of experimental [this work] and calculated partition coefficient of acetol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (○): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

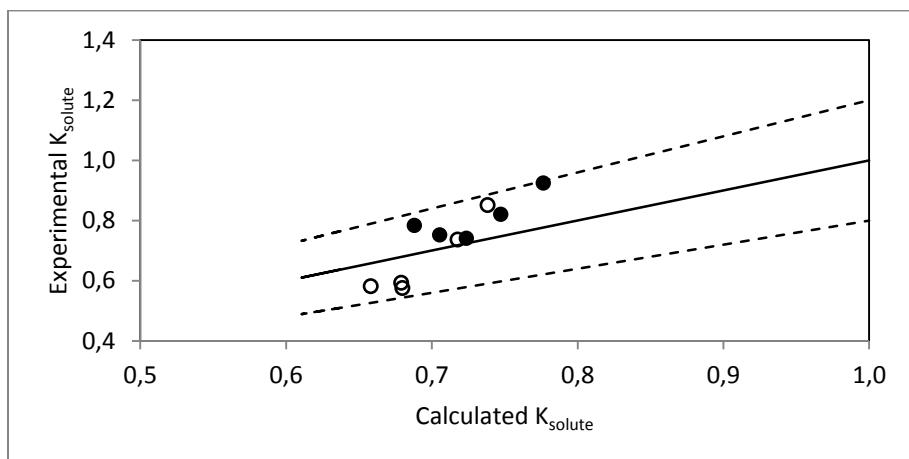


Figure 42: Parity chart of experimental [this work] and calculated partition coefficient of acetol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using NRTL (○): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

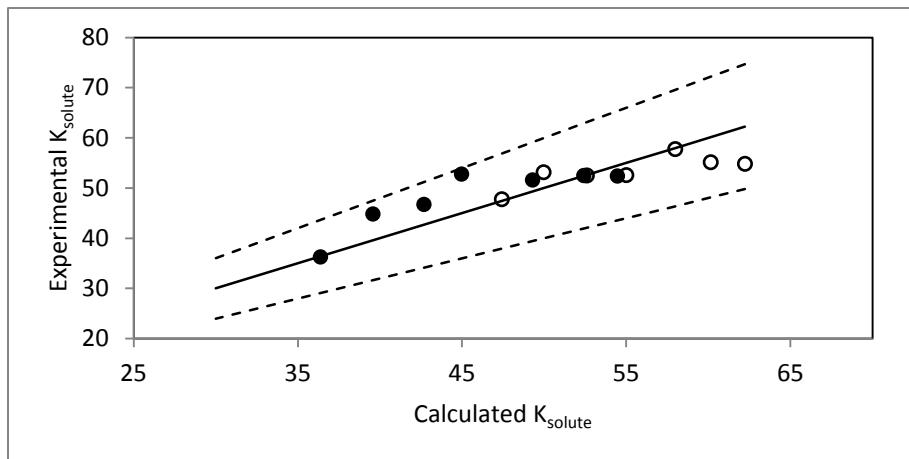


Figure 43: Parity chart of experimental [this work] and calculated partition coefficient of furfural between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

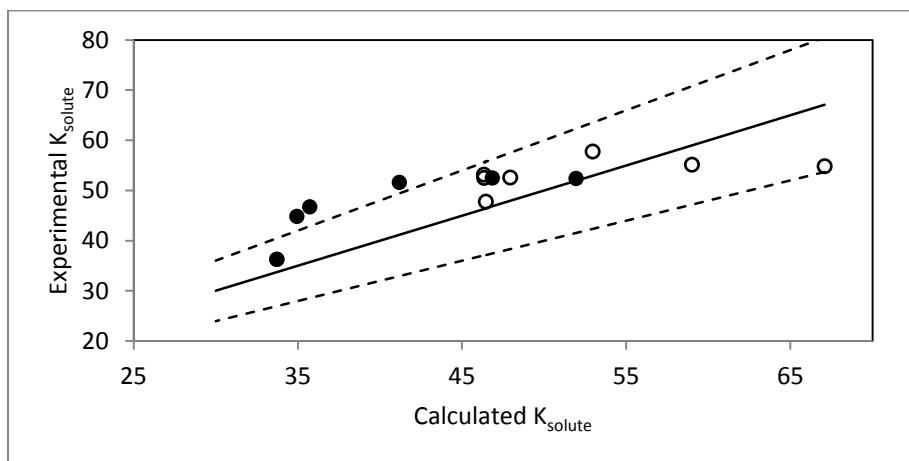


Figure 44: Parity chart of experimental [this work] and calculated partition coefficient of furfural between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

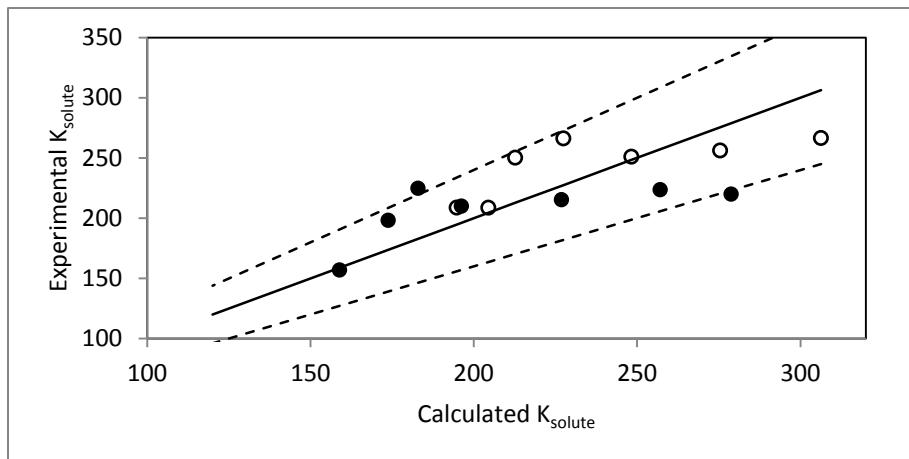


Figure 45: Parity chart of experimental [this work] and calculated partition coefficient of guaiacol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

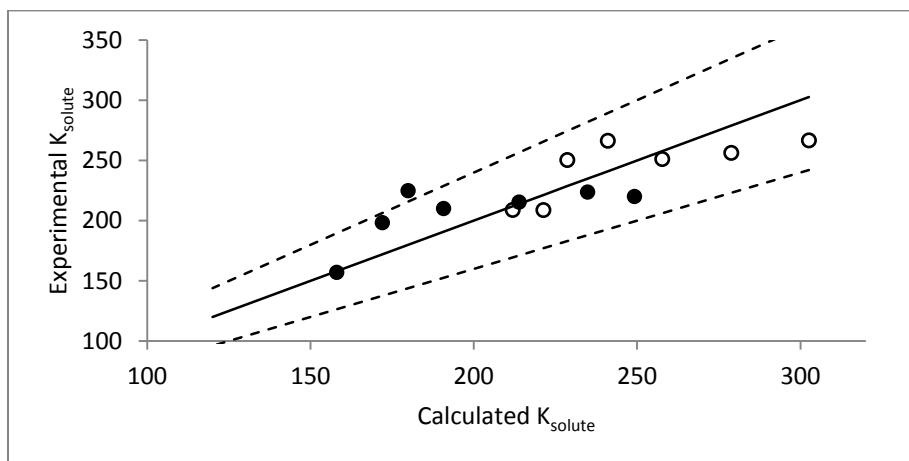


Figure 46: Parity chart of experimental [this work] and calculated partition coefficient of guaiacol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

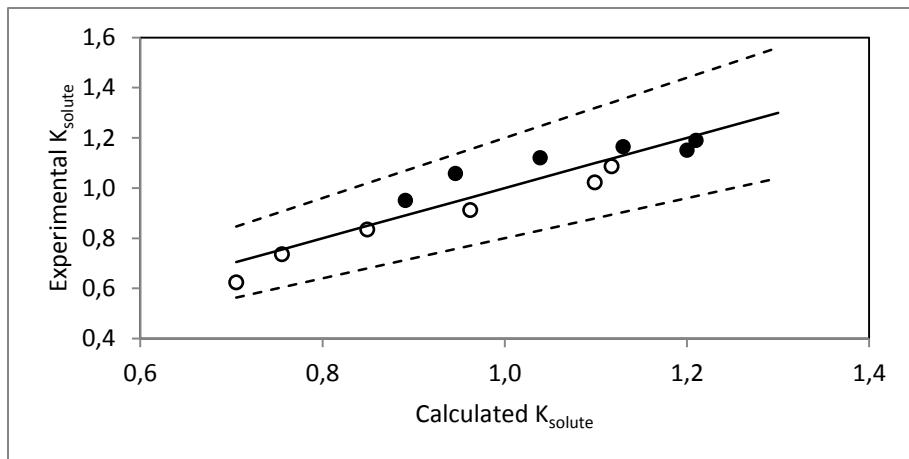


Figure 47: Parity chart of experimental [this work] and calculated partition coefficient of methanol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

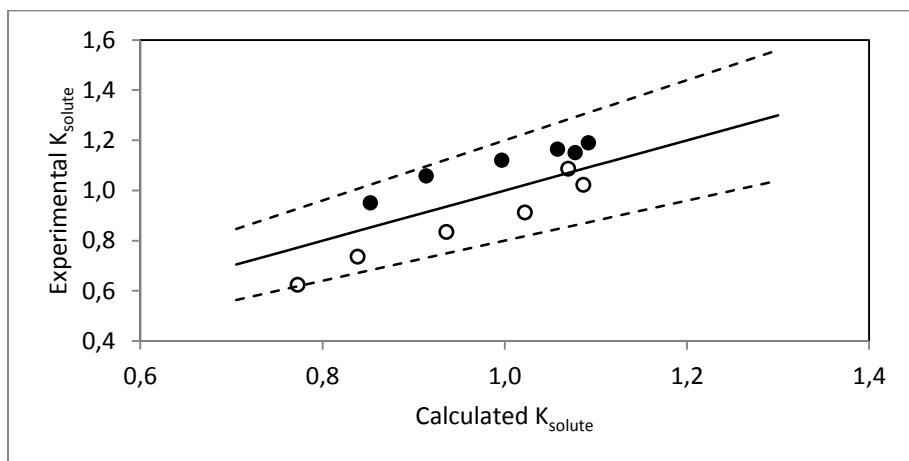


Figure 48: Parity chart of experimental [this work] and calculated partition coefficient of methanol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

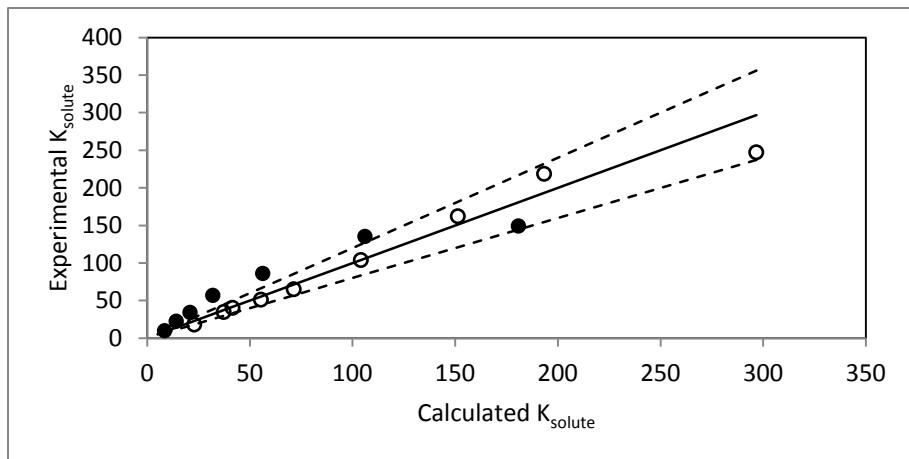


Figure 49: Parity chart of experimental [this work], [16], and calculated partition coefficient of phenol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

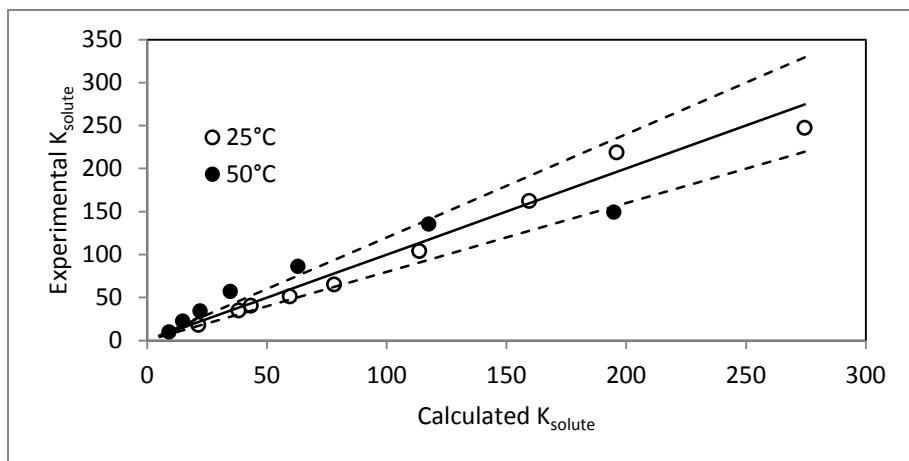


Figure 50: Parity chart of experimental [this work], [16], and calculated partition coefficient of phenol between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 323.15 K. (—): first bisector. (---): +/- 20%

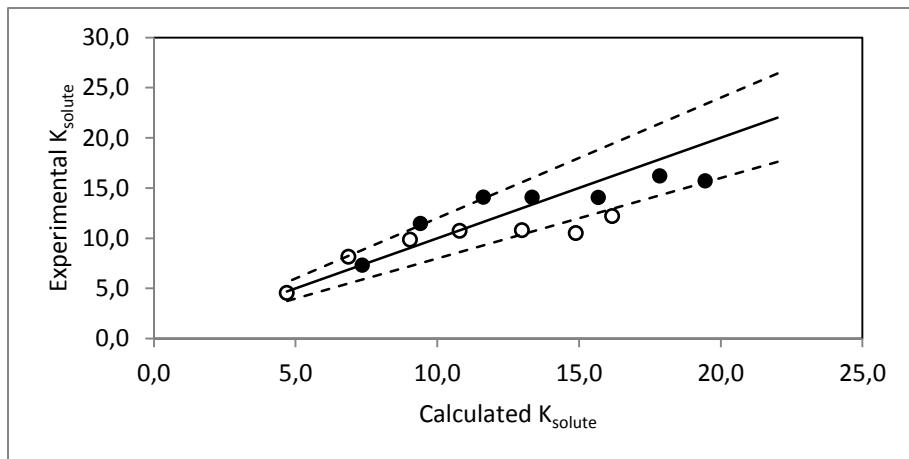


Figure 51: Parity chart of experimental [this work] and calculated partition coefficient of propanal between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

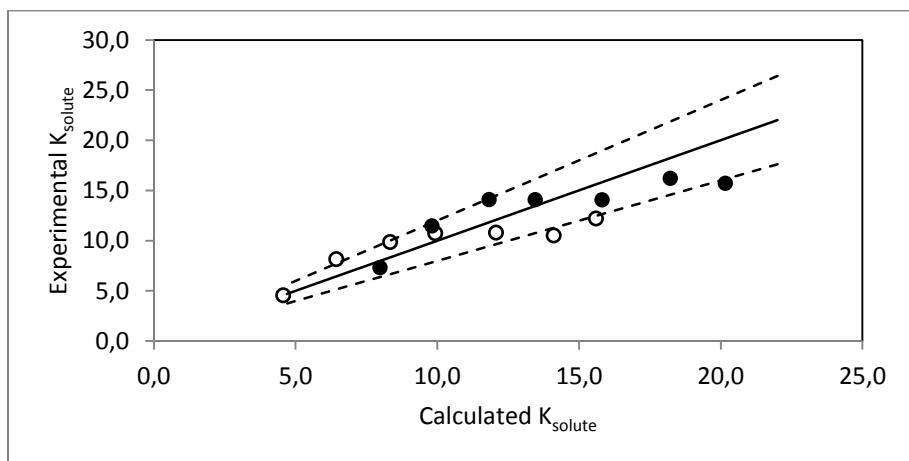


Figure 52: Parity chart of experimental [this work] and calculated partition coefficient of propanal between isopropyl acetate-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

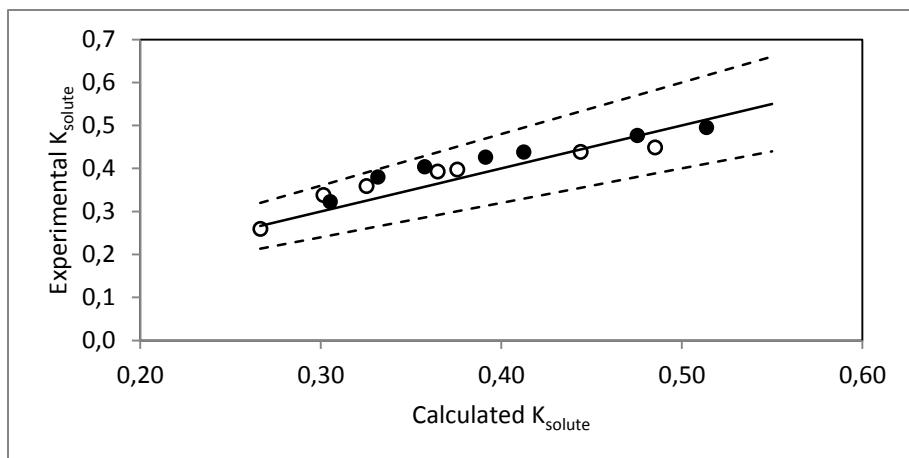


Figure 53: Parity chart of experimental [17] and calculated partition coefficient of acetic acid between toluene-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

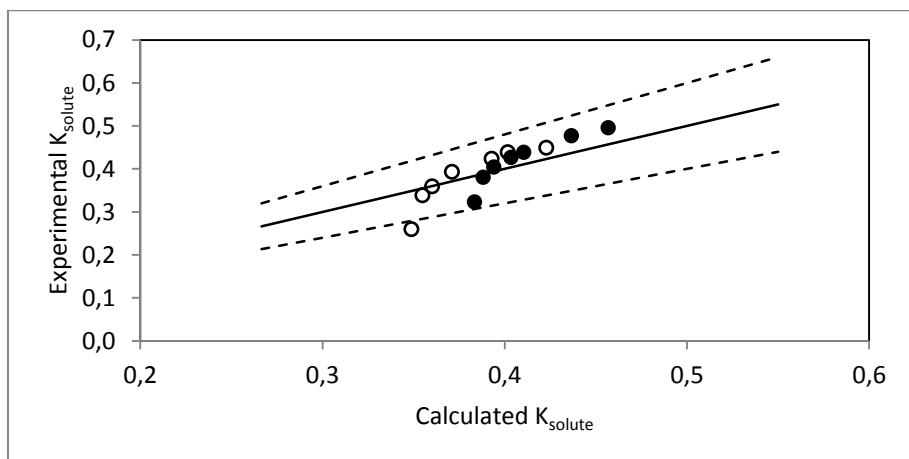


Figure 54: Parity chart of experimental [17] and calculated partition coefficient of acetic acid between toluene-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

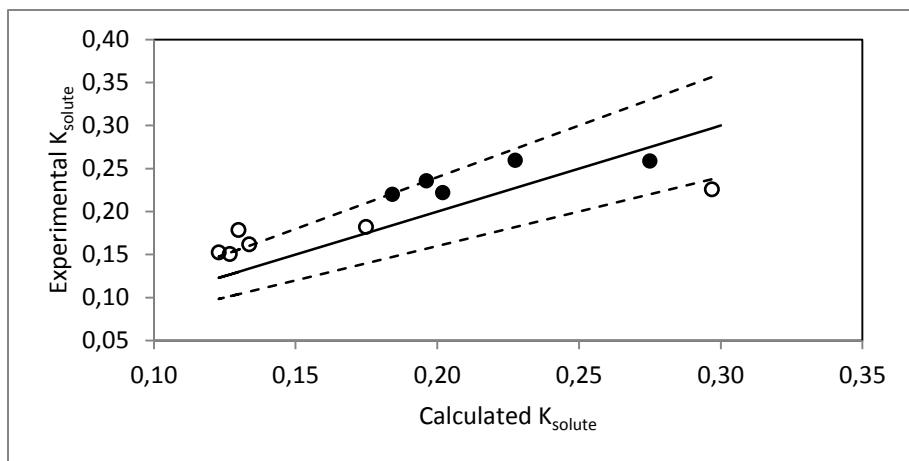


Figure 55: Parity chart of experimental [this work] and calculated partition coefficient of acetol between toluene-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

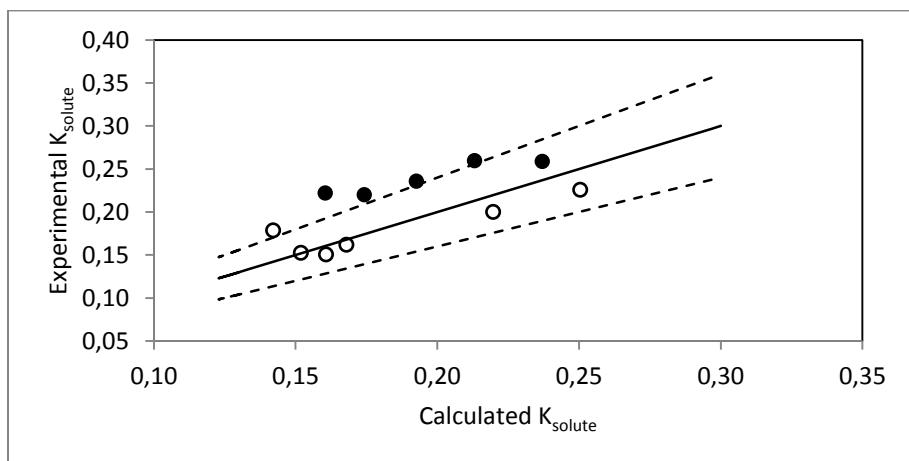


Figure 56: Parity chart of experimental [this work] and calculated partition coefficient of acetol between toluene-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

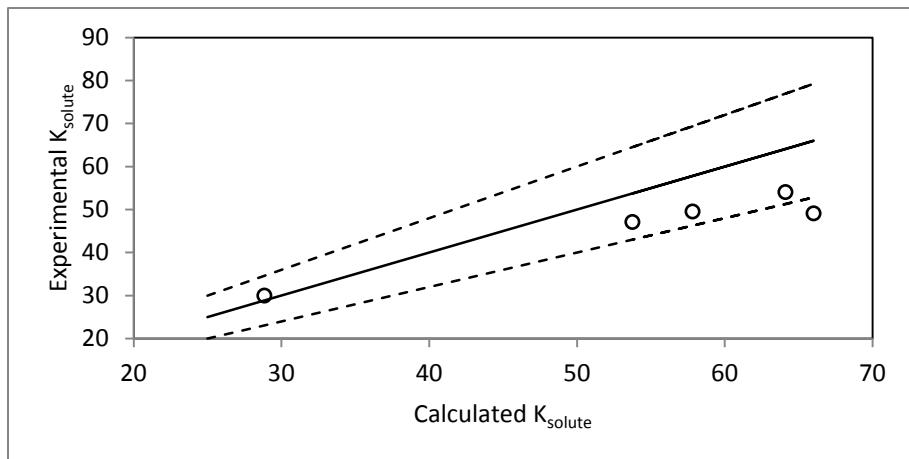


Figure 57: Parity chart of experimental [18] and calculated partition coefficient of furfural between toluene-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 303.15 K. (—): first bisector. (---): +/- 20%

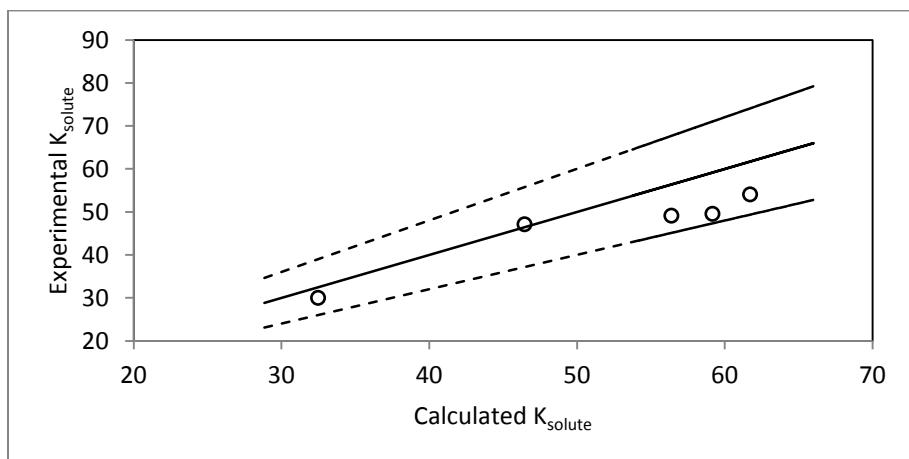


Figure 58: Parity chart of experimental [18] and calculated partition coefficient of furfural between toluene-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 303.15 K. (—): first bisector. (---): +/- 20%

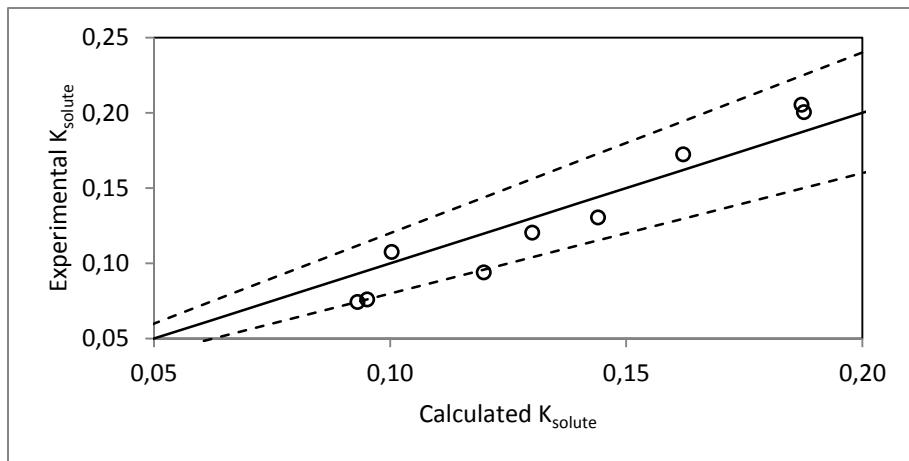


Figure 59: Parity chart of experimental [19] and calculated partition coefficient of methanol between toluene-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. (—): first bisector. (---): +/- 20%

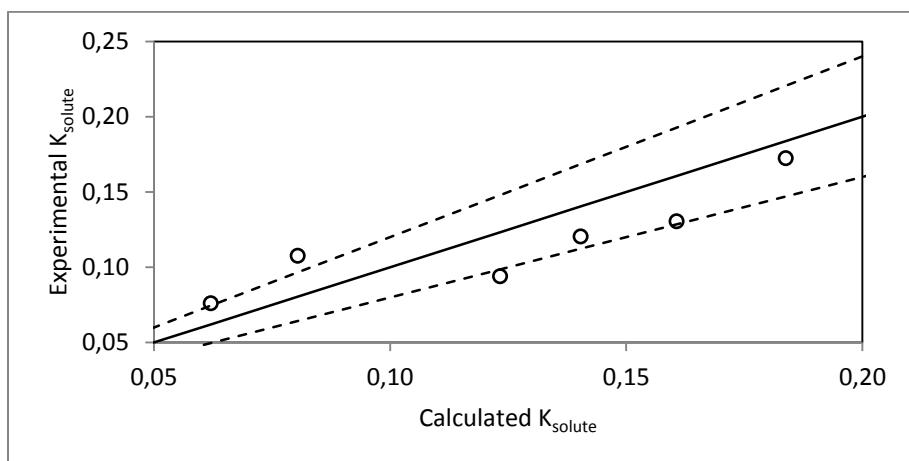


Figure 60: Parity chart of experimental [19] and calculated partition coefficient of methanol between toluene-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. (—): first bisector. (---): +/- 20%

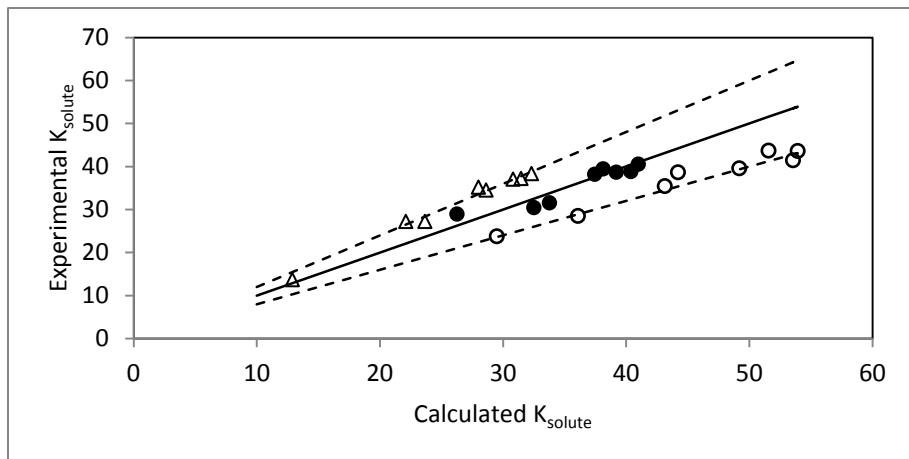


Figure 61: Parity chart of experimental [20] and calculated partition coefficient of phenol between toluene-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 293.15 K. and (●): 303.15 K. (Δ): 313.15 K. (—): first bisector. (---): +/- 20%

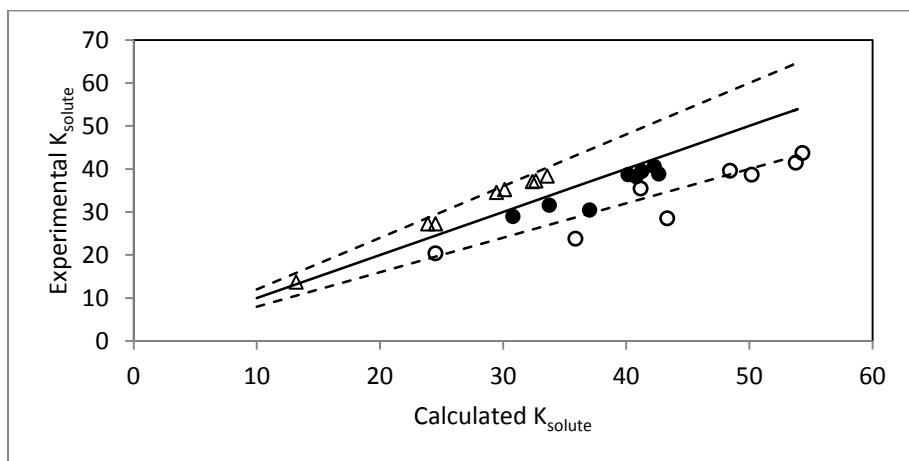


Figure 62: Parity chart of experimental [20] and calculated partition coefficient of phenol between toluene-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 293.15 K. and (●): 303.15 K. (Δ): 313.15 K. (—): first bisector. (---): +/- 20%

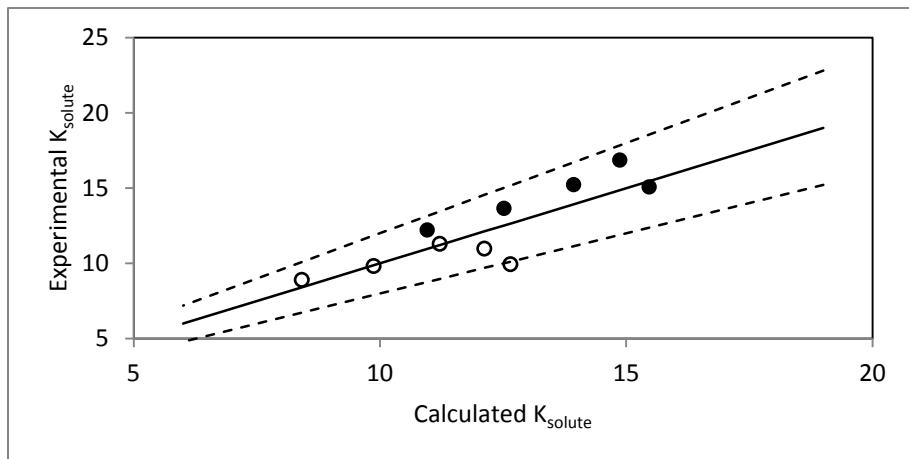


Figure 63: Parity chart of experimental [this work] and calculated partition coefficient of propanal between toluene-rich phase and water-rich phase at atmospheric pressure using UNIQUAC (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

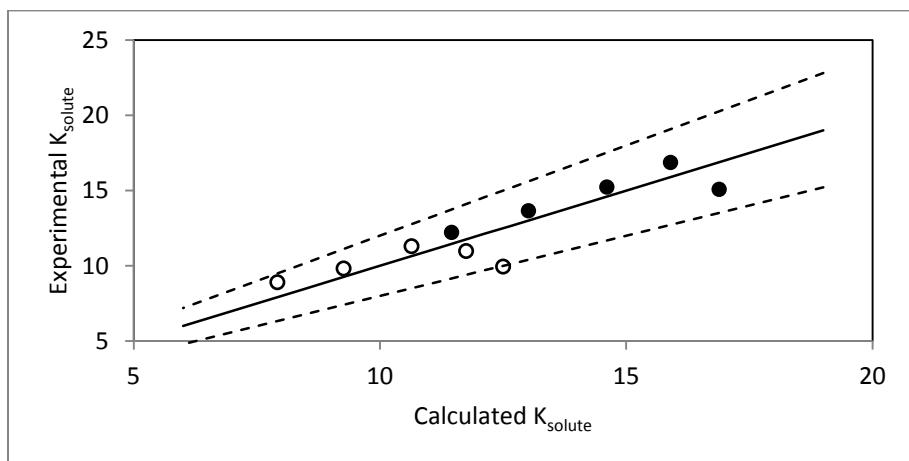


Figure 64: Parity chart of experimental [this work] and calculated partition coefficient of propanal between toluene-rich phase and water-rich phase at atmospheric pressure using NRTL (o): 298.15 K. and (●): 313.15 K. (—): first bisector. (---): +/- 20%

According to these charts, NRTL and UNIQUAC models have similar accuracy for the representation of partition coefficients. Most of the calculated values have less than 20% deviation with the experimental data.