Supporting Information

A simple correlation to fit Type I Liquid-Liquid Equilibrium (LLE) data

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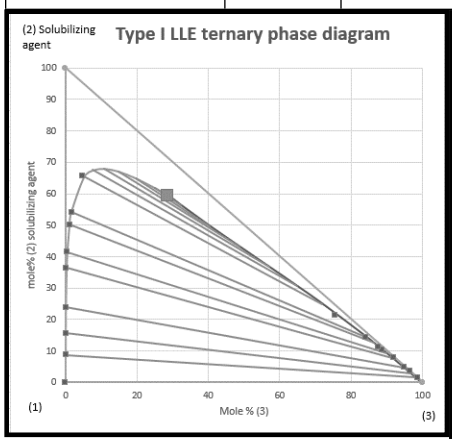
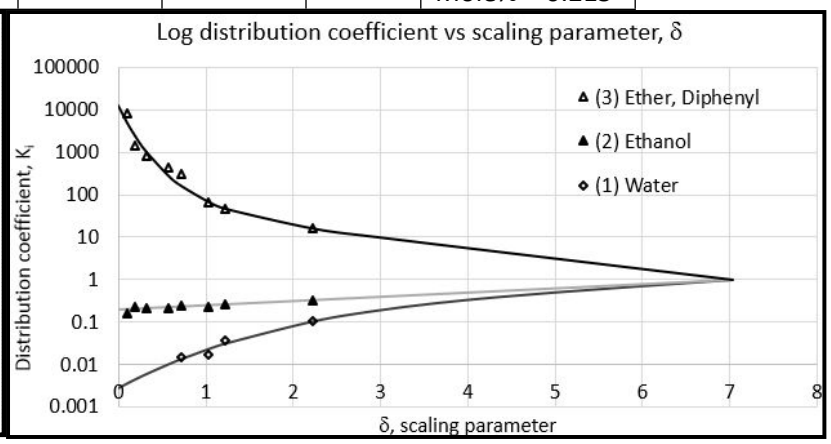
Abstract

A simple correlation to fit type I liquid-liquid equilibria (LLE) data is presented. Like the Hand plot (1) and the correlation by Rod (2), it correlates the distribution coefficients for the three components as a function of a scaling parameter that is a measure of the distance along the binodal from the binary end point to the plait point. It can be used to estimate the composition of the plait point and to interpolate and extrapolate data. It is also useful for estimating distribution coefficients for additional trace components (impurities that may build up in recycle around an extraction operation) when there is limited data. This correlation provides a fit that is comparable to or better than the fit obtained using liquid activity coefficient models.

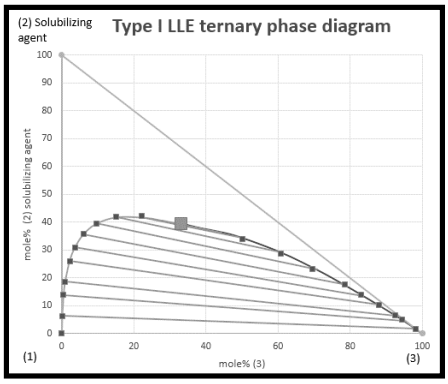
Appendix – systems fitted

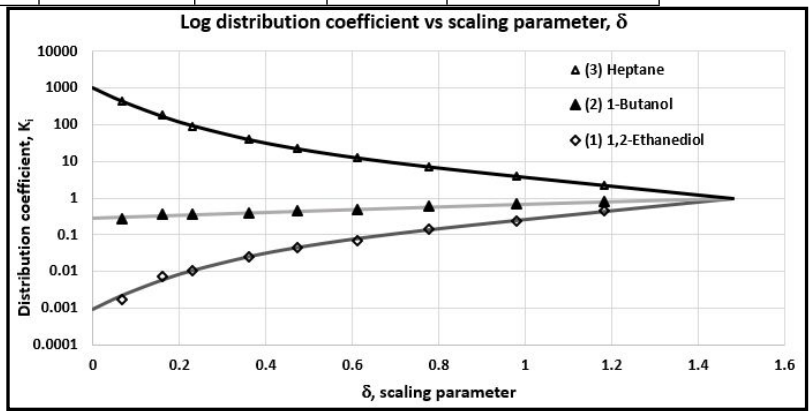
System δ_o, plait point = 7.03	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Water	0.1	0.328	0.00284	-0.00074	4.35	6 pg 392, 10
(2) Ethanol	0.194	0.233	0.194	0	1	
(3) Ether, Diphenyl	52.8	-0.564	12260	4.92E-10	11.9	Mean deviation Mole% = 0.215



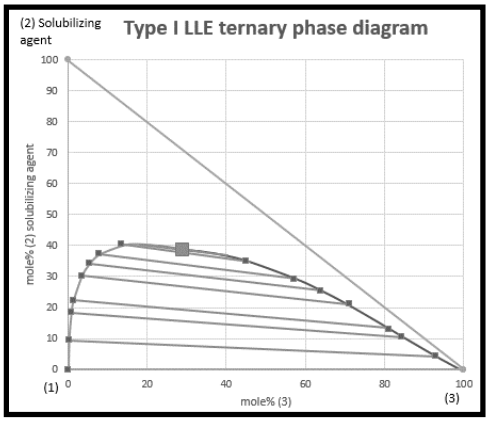


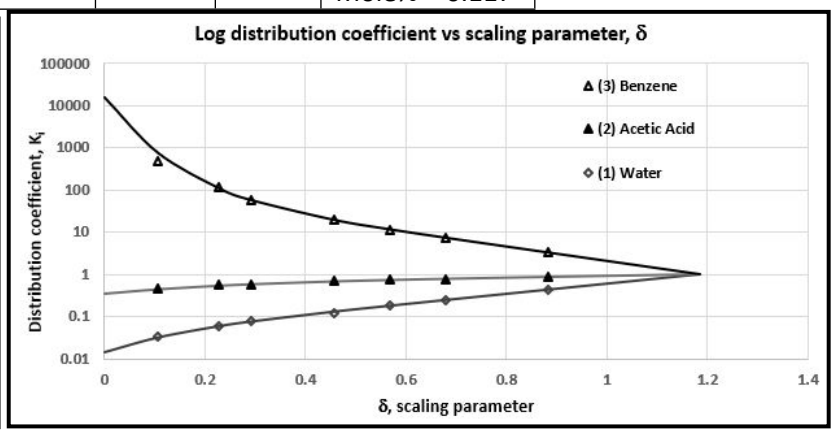
System δ_o, plait point = 1.48	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) 1,2-Ethanediol	0.0174	2.73	0.000946	-0.307	5.71	6 pg 419, 11
(2) 1-Butanol	1.10	-0.0625	0.288	-0.870	1.09	
(3) Heptane	58.3	-2.74	1007	0.324	5.52	Mean deviation Mole% = 0.136



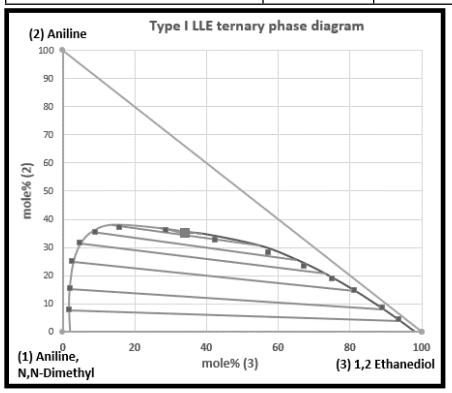


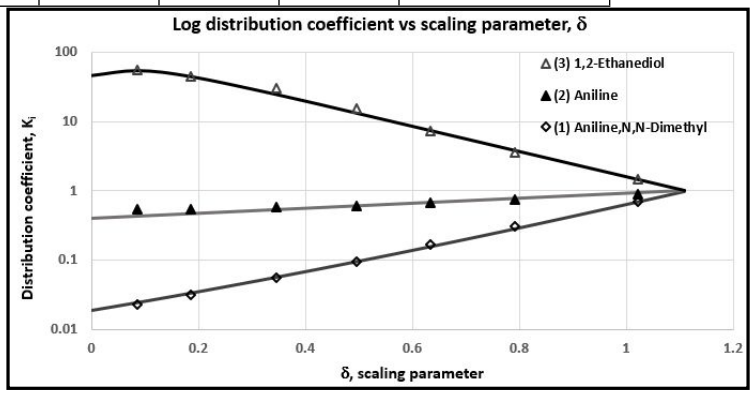
System δ_o, plait point = 1.19	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Water	0.0384	2.75	0.0147	-0.246	7.95	6 pg 251, 12
(2) Acetic Acid	0.577	0.464	0.359	-0.200	5.03	
(3) Benzene	105	-3.92	15652	1.306	7.86	Mean deviation Mole% = 0.117



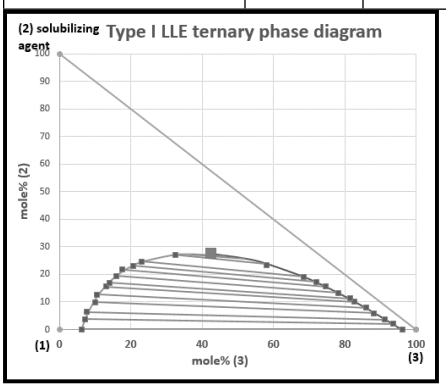


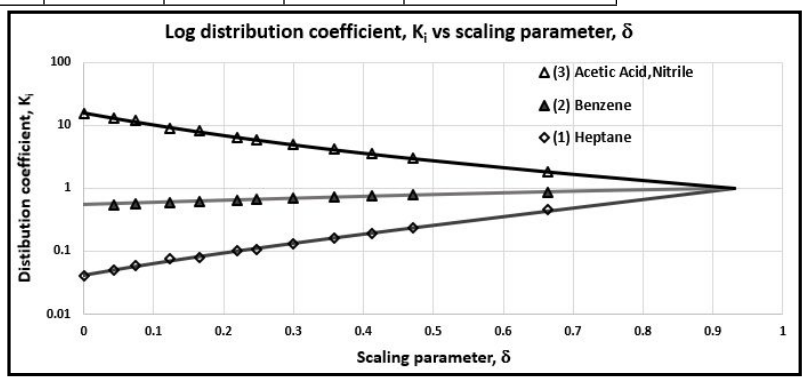
System δ_o, plait point = 1.11	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Aniline,N,N-Dimethyl	0.0116	4.02	0.0189	0.386	2.3	6 pg 427, 13
(2) Aniline	0.407	0.810	0.407	0	1.0	
(3) 1,2-Ethanediol	108	-4.22	47.1	-0.226	12.4	Mean deviation Mole% = 0.390



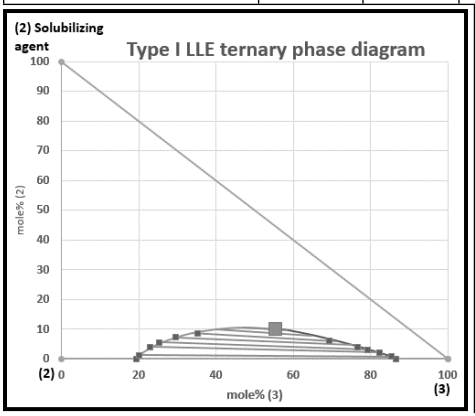


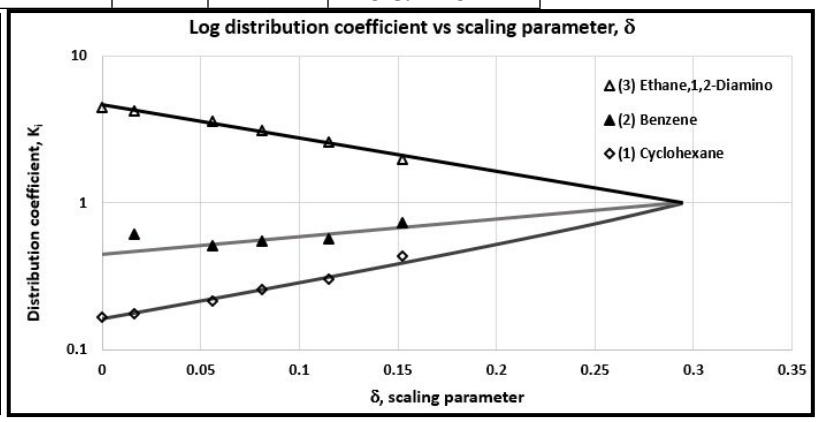
System δ_o, plait point = 0.931	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Heptane	0.0531	3.15	0.0406	-0.385	5.01	6 pg 180, 14
(2) Benzene	1.07	-0.0770	0.543	-0.744	1.23	
(3) Acetic Acid,Nitrile	7.78	-2.20	15.8	0.889	3.26	Mean deviation Mole% = 0.122



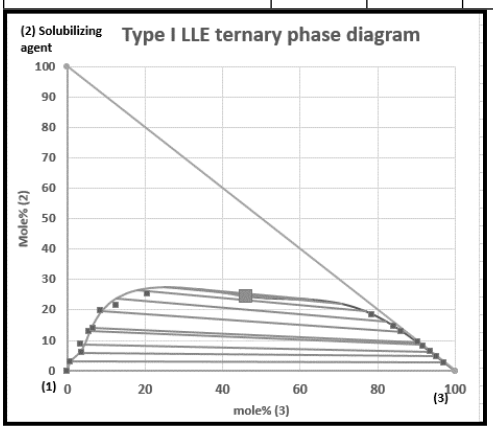


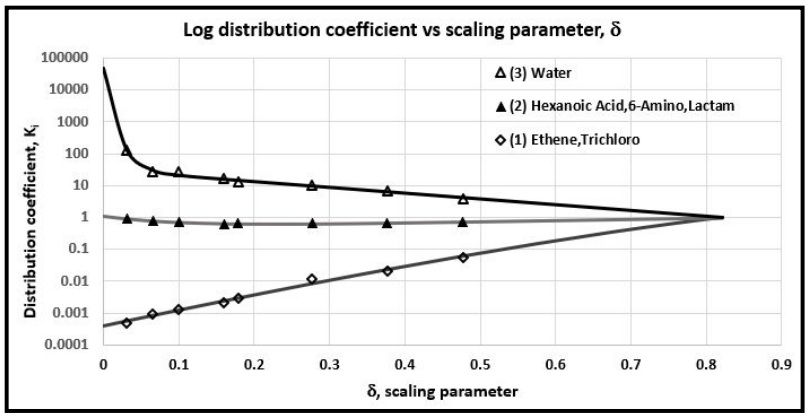
System δ_o, plait point = 0.295	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Cyclohexane	0.01	15.6	0.163	10.3	1.06	6 pg 444, 15
(2) Benzene	0.448	2.72	0.448	0.0	1	
(3) Ethane,1,2-Diamino	4.65	-5.21	4.65	0.0	1	Mean deviation Mole% = 0.427



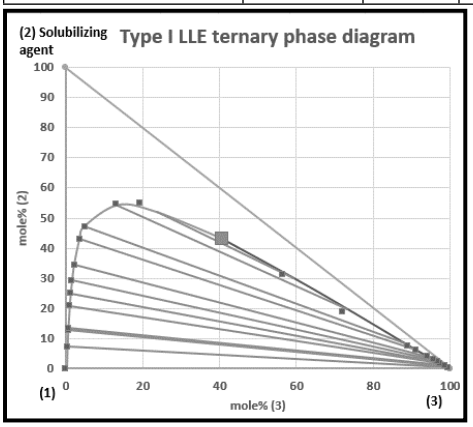


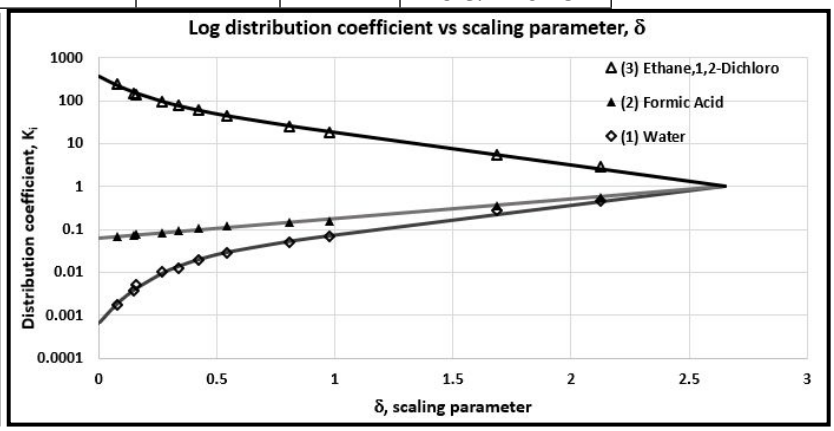
System δ_o, plait point = 0.828	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Ethene,Trichloro	0.01	5.59	0.0038	-4.37	1.55	6 pg 160, 16
(2) Hexanoic Acid,6-Amino,Lactam	0.493	0.863	1.13	3.98	8.13	
(3) Water	30.6	-4.16	41100	17700	39.9	Mean deviation Mole% = 0.499



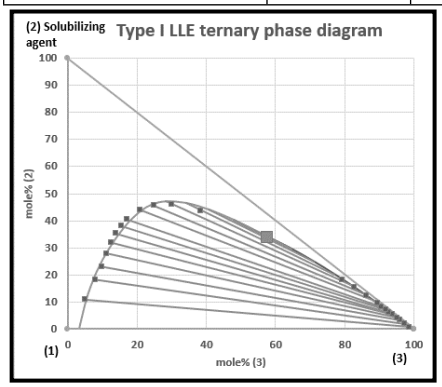


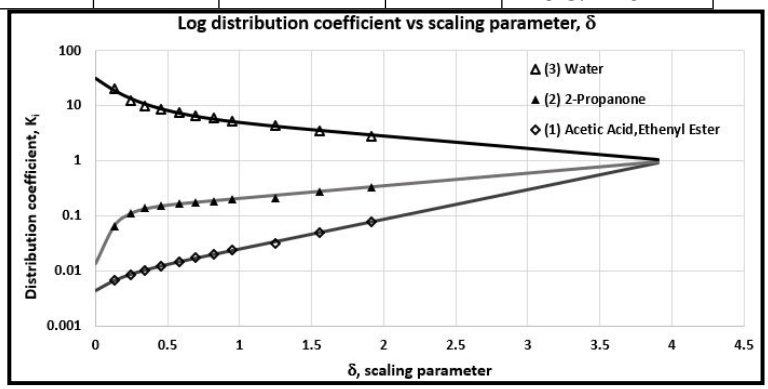
System δ_o, plait point = 2.66	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Water	0.0153	1.57	0.000657	-3.39E-05	11.7	6 pg 46, 17
(2) Formic Acid	0.0637	1.04	0.0637	0	1	
(3) Ethane, 1,2-Dichloro	101	-1.74	6160363	2.77E-05	11.0	Mean deviation Mole% = 0.152



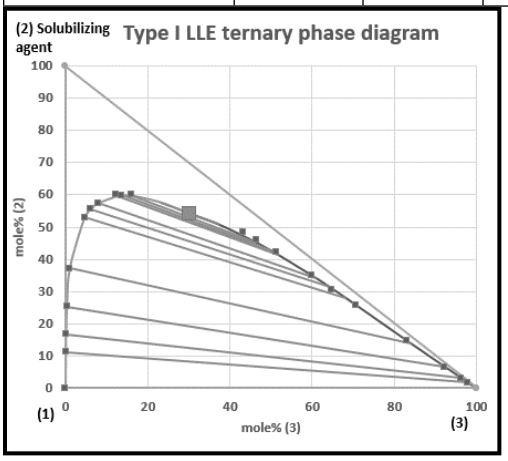


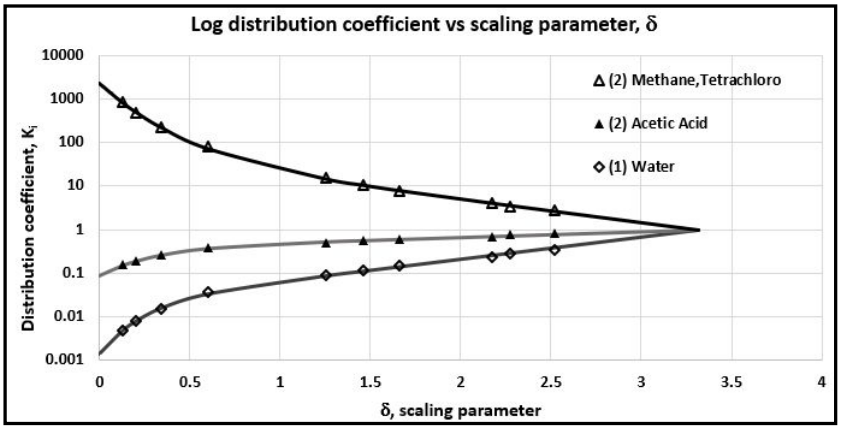
System δ_o, plait point = 3.98	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Acetic Acid,Ethenyl Ester	0.00722	1.24	0.00440	-3.13E-14	22	6 pg 465, 18
(2) 2-Propanone	0.122	0.529	0.0135	-2.2E-21	35	
(3) Water	7.82	-0.517	30.7	1.41E-07	11.6	Mean deviation Mole% = 0.214



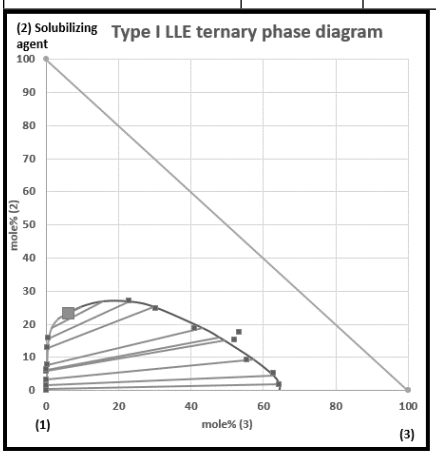


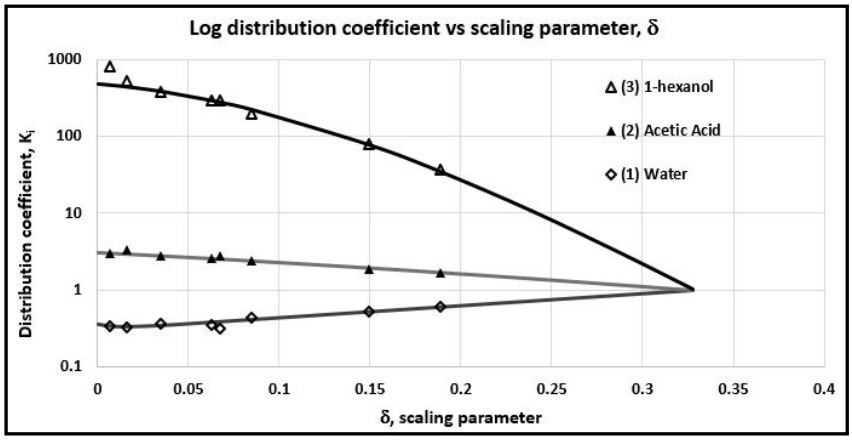
System δ_o, plait point = 3.32	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Water	0.0204	1.17	0.00142	-4.5eE-07	13.0	6 pg 4, 19
(2) Acetic Acid	0.368	0.302	0.0892	-3.6E-06	10.7	
(3) Methane, Tetrachloro	59.3	-1.23	2225	0.00105	6.79	Mean deviation Mole% = 0.358



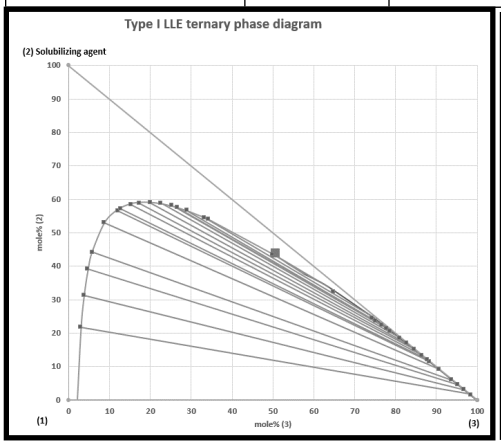


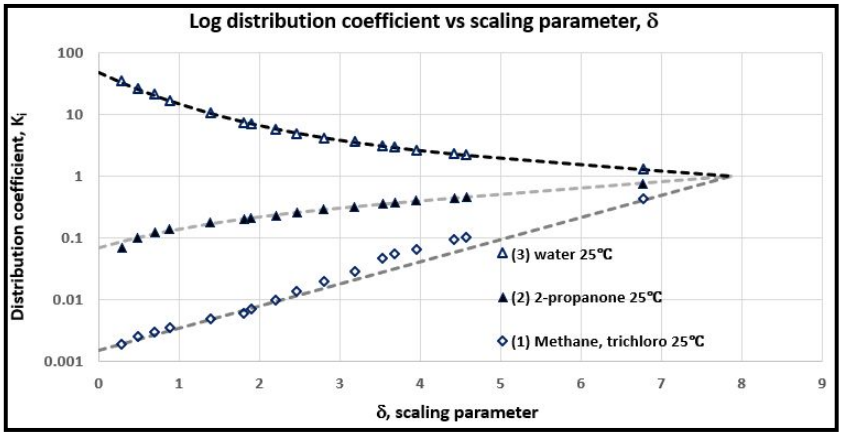
System δ_o, plait point = 0.329	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) Water	0.302	3.64	0.357	1.39E+14	30.9	7
(2) Acetic Acid	3.69	-3.98	3.07	-2.39	2.30	
(3) 1-Hexanol	8304	-27.5	484	-54.7	2.66	Mean deviation Mole% = 0.657



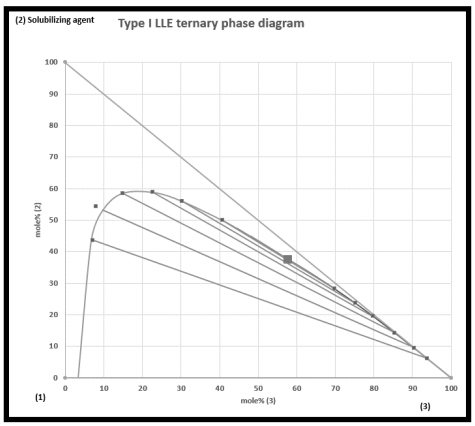


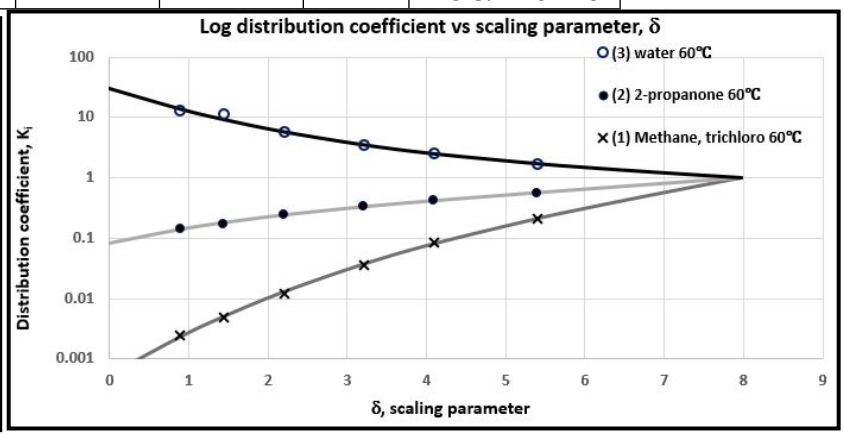
System @25°C δ_o, plait point = 7.87	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) methane, trichloro	0.00153	0.824	0.00153	0	1	6 pg 27, 20
(2) 2-propanone	0.158	0.234	0.0699	-2.8E-06	6.10	
(3) water	5.72	-0.222	47.1	0.000245	4.39	Mean deviation Mole% = 0.209





System @60°C δ_o, plait point = 7.97	K_{io} Eq. 4	a_i Eq. 4	K_{ioo} Eq. 6	b_i Eq. 4	n_i power Eq. 4	References
(1) methane, trichloro	0.0100	0.578	0.00530	-0.00335	3.26	6 pg 28, 20
(2) 2-propanone	0.174	0.219	0.0832	-2.6E-05	4.93	
(3) water	4.55	-0.190	30.1	0.00208	3.28	Mean deviation Mole% = 0.146





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