Introductory Chemical Engineering Thermodynamics

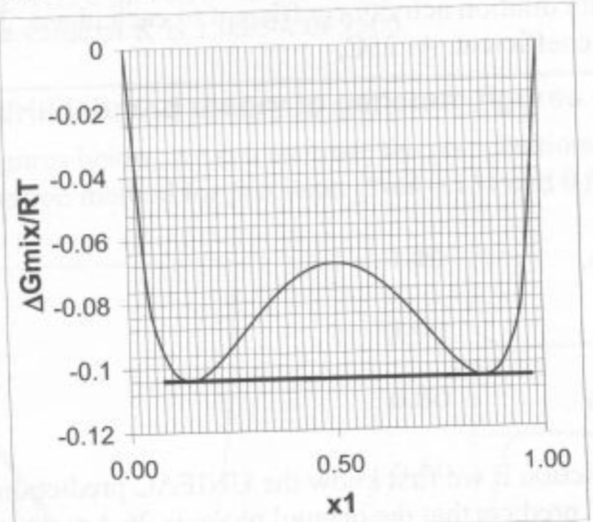
SOLUTIONS FOR HOMEWORK PROBLEMS: Chapter 14

(14.01) Suppose the (1) + (2) system exhibits liquid-liquid …

SOLUTION: a)

0.05 G1/RT 0.1 G2/RT 0.3

x1	x2	ΔGmix/RT
1.00E-11	1.00E+00	-2.4E-10
5.00E-02	9.50E-01	-0.07977
1.00E-01	9.00E-01	-0.10008
1.50E-01	8.50E-01	-0.10396
2.00E-01	8.00E-01	-0.1004
2.50E-01	7.50E-01	-0.09359
3.00E-01	7.00E-01	-0.08586
3.50E-01	6.50E-01	-0.0787
4.00E-01	6.00E-01	-0.07301
4.50E-01	5.50E-01	-0.06939
5.00E-01	5.00E-01	-0.06815
5.50E-01	4.50E-01	-0.06939
6.00E-01	4.00E-01	-0.07301
6.50E-01	3.50E-01	-0.0787
7.00E-01	3.00E-01	-0.08586
7.50E-01	2.50E-01	-0.09359
8.00E-01	2.00E-01	-0.1004
8.50E-01	1.50E-01	-0.10396
9.00E-01	1.00E-01	-0.10008
9.50E-01	5.00E-02	-0.07977
1.00E+00	1.00E-11	-2.2E-10



b) At the phase split, $x_1^{\alpha} = 0.145$, $x_1^{\beta} = 0.855$ (Most systems with liquid-liquid immiscibility must be modeled with a more complex formula for excess gibbs energy. The humps on the diagram are usually off center as in Figure 14.3 in the text. The simple model used for the calculations here results in the symmetrical diagram.

(c).When a mixture splits into two phases, the overall fractions (of total moles) of the two phases are found by the lever rule along the composition coordinate. Suppose 0.6 moles of (1) and 0.4 moles of (2) are mixed. Use the lever rule to calculate the total number of moles which would be found in each phase of the actual system.((0.6-0.145)/0.855-0.145)*100%=64% β)

(d). What is the value of the hypothetical Gibbs energy (expressed as G/RT) of a mixture of 0.6 mols of (1) and 0.4 moles of (2) if the mixture were to remain as one phase? Calculate the Gibbs energy (expressed as G/RT) of the total system considering the phase split into two phases, and show that the Gibbs energy is less than the Gibbs energy of the single phase system?

One phase system:

$G/RT = -0.073+0.6*0.1+0.4*0.3 = 0.107$

Two-phase system:

$G/RT = 0.6*G_1/RT + 0.4G_2/RT + 0.36*\Delta G^{\alpha}_{mix}/RT + 0.64*\Delta G^{\beta}_{mix}/RT = 0.60(0.1) + 0.4*(0.3) + 0.36(-0.104) + 0.64(-0.104) = 0.076$ which is less than staying as single phase. (For this simple system, $\Delta G^{\alpha}_{mix} = \Delta G^{\beta}_{mix}/RT$, but that will not generally apply.)

(14.02) Assume solvents A and B are virtually insoluble in each other at 298K

Component C is soluble in both.

(a). $K = \gamma^L/\gamma^U = \exp[\ln\gamma - \ln\gamma] = \exp\{(1.0)^2 * (9.8\text{-}10.4)^2 - (1.0)^2 * (9.8\text{-}5.8)^2]/1.987/298\} = 0.0$

(b). $K=0.0713 \rightarrow x_c^B = 1.4\% \rightarrow K=0.0711$ close enough

(c). (NO: C partitions favorably into B)

(14.03) A new drug is to have the formula para-CH3CH2ΦCH2COOH …

Solution:

This is a ternary LLE problem. This soln uses UNIFAC LLE

We can get an approximate answer by assuming that water and octanol are totally immiscible and calculating the infinite dilution activity coefficient in each phase. Then using eq. 14.4 we can estimate the distribution coefficient. At 25C,

$\gamma^{\infty}_{\text{Drug in water}} = 15413$

$\gamma^{\infty}_{\text{Drug in octanol}} = 1.164$

$K = 15413/1.164 = 13241$

at 37C, body temperature,

$\gamma^{\infty}_{\text{Drug in water}} = 13930$

$\gamma^{\infty}_{\text{Drug in octanol}} = 1.189$

$K = 13930/1.189 = 11716$

We can give a better prediction if we first know the UNIFAC prediction for mutual solubility for water + octanol. UNIFAC predicts that the octanol phase is 26.4 mol% water, while the water phase is essentially pure. Therefore the infinite dilution values for the organic phase will change, but the values for the aqueous phase should be the same:

At 25C,

$\gamma^{\infty}_{\text{Drug in octanol rich phase}} = 1.379$

$K = 15413/1.379 = 11177$

At 37C,

$\gamma^{\infty}_{\text{Drug in octanol rich phase}} = 1.429$

$K = 13930/1.429 = 9748$

(Note: the octanol phase is assumed to be 26.4 mol% at both temperatures.)

A rigorous calculation models all three components with just a trace of drug. By adapting the method from section 14.9, the results are:

The drug is made of CH3 + CH2 + 4(ACH) + 2(ACCH2) + COOH

At 25C

1	2	3
Water	Octanol	Drug
0.264	0.735	0.001

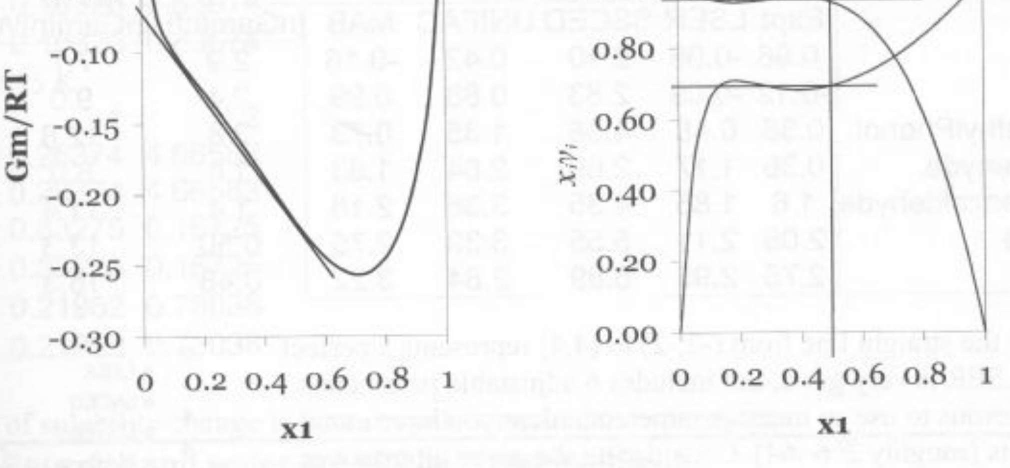
3.780	1.042	1.378
Water	Octanol	Drug
1.000	0.000	0.000
1.000	4479.783	15146.972

	1	2	3
$K_{i,old}$	3.78018	0.00023	0.00009
$K_{i,new}$	3.78018	0.00023	0.00009
$x^{\alpha}_{i,old}$	0.26449	0.73451	0.00100
$x^{\alpha}_{i,new}$	0.26449	0.73451	0.00100
$x^{\beta}_{i,old}$	0.99983	0.00017	0.00000
$x^{\beta}_{i,new}$	0.99983	0.00017	0.00000
			10989.54

The K value for the drug is 9.1E-6 or 10,989 depending on which phase is numerator. Octanol is highly favored. At 37C the value of K is 1.05E-4 or 9566.

(14.04) Use Scatchard/Hildebrand theory to generate figures of activity vs. ...

Solution: Based on the Figures below, we can estimate the compositions to be ~ 0.13 and 0.50. Following the K-value iteration method for precision gives 0.131 and 0.4888.



(14.05) The bubble point of a liquid mixture of n-butanol and water

Solution: Use modified Raoult's law,

1.013 bar = 0.04*0.383*γ + 0.96*0.776*1.0 → γ = 17.5 ;
y = 0.04*0.383*17.5/1.013 = 0.265
UNIFAC VLE gives: γ = 16.9, y = 0.28 (P = 1.04 bars)

Now, from UNIFAC VLE, if we insert xw = 0.96 and xb = 0.04, we obtain γ_b = 16.99 and γ_w = 1.02 at 92.7 C, the bubble pressure is 1.02 bar and y = 0.26, the estimation is fairly close.

Although the problem statement doesn't say anything, this mixture is at the experimental liquid solubility limit of butanol in water. UNIFAC LLE at xw = 0.96 and xb = 0.04, gives γ_b = 15.97 and γ_w = 1.02. If we use UNIFAC LLE at 92.7°C, we find (water(1) + n-butanol(2))the model gives 3 mol% instead of 4 mol% for the water phase.

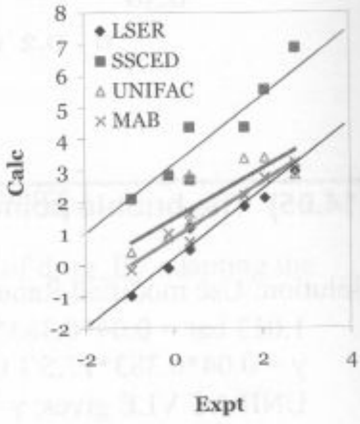
	1	2
$K_{i,old}$	0.58172	14.34023
$K_{i,new}$	0.58172	14.34023
$x^{\alpha}_{i,old}$	0.96960	0.03040
$x^{\alpha}_{i,new}$	0.96960	0.03040
$x^{\beta}_{i,old}$	0.56403	0.43597
$x^{\beta}_{i,new}$	0.56403	0.43597

(14.06) Shulte et al discuss plot for LSER and (ii) SSCED vs. $K_{H/W}$ at 298K……

Errata: Printings 1-3 show α and β switched in Table 14.2.
It suffices to create a parity plot. Assume pollutants are dilute: $K_{HW} = \gamma_i^{\infty,W} / \gamma_i^{\infty,H}$.
(ii) For n-hexane: $\delta = \delta' = 14.87$, $V = 130.6$, $\alpha = \beta = 0$;
For water: $\delta = 47.9 \Rightarrow \delta' = 28.01$; $\alpha = 50.13$, $\beta = 15.06$
For solutes, we can estimate $V_i = 88.8*v/0.536$, as can be checked for phenol, benzene, toluene.
For SSCED and MAB, simplified expressions for γ^{∞} can be typed in.
E.g. for SSCED with nHexane as solvent, $\ln\gamma^{\infty} = V_i((\delta_i'-14.87)^2 + (\alpha_i-0)(\beta_i-0)/2)/(8.314*298.15)$

	logKH/W					SSCED	
	Expt	LSER	SSCED	UNIFAC	MAB	lnGamInfH	lnGamInfW
phenol	-0.96	-0.96	2.10	0.42	-0.16	2.9	7.7
mcresol	-0.12	-0.09	2.83	0.88	0.99	2.4	9.0
2,4DiMethylPhenol	0.36	0.48	4.36	1.35	0.73	2.8	12.8
benzaldehyde	0.36	1.17	2.69	2.84	1.63	1.8	8.0
chlorobenzaldehyde	1.6	1.85	4.35	3.36	2.18	1.4	11.4
benzene	2.06	2.11	5.55	3.39	2.75	0.50	13.3
toluene	2.75	2.95	6.89	2.84	3.22	0.48	16.3

Note that the straight line from (-2,-2) to (4,4) represents a perfect fit. The LSER is very good, but includes 6 adjustable parameters. It is dangerous to use so many parameters unless you have many data points (roughly 2^6=64). Considering the given alternatives, the simple MAB model is arguably the best for this particular data set, but UNIFAC is close and reliable in many more situations so that would probably be the best recommendation. The SSCED model would require a systematic shift of 1000x to be reasonable but at least its trendline is parallel to the data.



(14.07) Use UNIFAC to predict the compositions of the ...

Using UNIFAC LLE,
methanol (1) + cyclohexane (2)

	1	2
$K_{i,old}$	0.22561	5.26303
$K_{i,new}$	0.22561	5.26303
$x^{\alpha}_{i,old}$	0.84627	0.15373
$x^{\alpha}_{i,new}$	0.84627	0.15373
$x^{\beta}_{i,old}$	0.19093	0.80907
$x^{\beta}_{i,new}$	0.19093	0.80907

(14.08) Use UNIFAC to predict the compositions (at 285.15 and 310.15 K)...

Using UNIFAC LLE, methanol (1) + cyclohexane (2)
α – meth. rich β -- cyclohexane
At 285.15 K

	1	2
$K_{i,old}$	0.19009	5.92918
$K_{i,new}$	0.19009	5.92918
$x^{\alpha}_{i,old}$	0.85888	0.14112
$x^{\alpha}_{i,new}$	0.85888	0.14112
$x^{\beta}_{i,old}$	0.16326	0.83674
$x^{\beta}_{i,new}$	0.16326	0.83674

At 310.15 K

	1	2
$K_{i,old}$	0.26374	4.66583
$K_{i,new}$	0.26374	4.66583
$x^{\alpha}_{i,old}$	0.83275	0.16725
$x^{\alpha}_{i,new}$	0.83275	0.16725
$x^{\beta}_{i,old}$	0.21962	0.78038
$x^{\beta}_{i,new}$	0.21962	0.78038

T-dep of solubility change is far too weak compared to experiment.

(14.09) Benzene and water are virtually immiscible...

$P = P^{sat} + P^{sat} = 648 + 288 = 936$ mmHg

(14.10) Water + hexane and water + benzene are immischible pairs...

(a) The vapor pressures at 69.4°C are $P_w^{sat} = 227$ mmHg and $P_b^{sat} = 540.2$ mmHg. If the bubble pressure is 760 mmHg at 69.4°C, then
$760 = x_w\gamma_w P_w^{sat} + x_b\gamma_b P_b^{sat} = 1(1)227 + 1.6\text{E-}4(\gamma_b)540.2 \Rightarrow \gamma_h = 6167$

(b) The vapor pressure of hexane is 776 mmHg. If the overall mixture is equimolar and all the organics are in one phase and all the water is in the other phase, then the composition of the water phase will be 100% water, and the composition of the organic phase will be 50% of each organic.

We will use UNIFAC VLE. The bubble pressure at 18.85°C is

$P = x_w^{\text{water}}\gamma_w^{\text{water}}P_w^{\text{sat}} + x_h^{\text{organic}}\gamma_h^{\text{organic}}P_h^{\text{sat}} + x_b^{\text{organic}}\gamma_b^{\text{organic}}P_b^{\text{sat}}$

$= 1(1)16.3 + 0.5(1)115 + 0.5(1)71.1 = 109$ mmHg

The vapor composition is

$y_w = 16.3/109 = 0.15$, $y_h = 0.5(115)/109 = 0.53$, $y_b = 1\text{-}0.15 - 0.53 = 0.32$

(c) very much like part (b). Keeping the assumption that the water and organics are totally immiscible, and introducing the UNIFAC VLE activity coefficients at 18.85°C

$\gamma_h^{\text{organic}} = 1.12$, $\gamma_b^{\text{organic}} = 1.18$

$P = x_w^{\text{water}}\gamma_w^{\text{water}}P_w^{\text{sat}} + x_h^{\text{organic}}\gamma_h^{\text{organic}}P_h^{\text{sat}} + x_b^{\text{organic}}\gamma_b^{\text{organic}}P_b^{\text{sat}}$

$= 1(1)16.3 + 0.5(1.12)115 + 0.5(1.18)71.1 = 122.6$ mmHg

The vapor composition is

$y_w = 16.3/122.6 = 0.13$, $y_h = 0.5(1.12)(115)/122.6 = 0.53$, $y_b = 1\text{-}0.13 - 0.53 = 0.34$

(14.11) Consider the system water(1) + MEK(2) at 299.85 K…

	1	2
$K_{i,\text{old}}$	2.689267	0.115105
$K_{i,\text{new}}$	2.689267	0.115105
$x^{\alpha}_{i,\text{old}}$	0.924463	0.075537
$x^{\alpha}_{i,\text{new}}$	0.924463	0.075537
$x^{\beta}_{i,\text{old}}$	0.34376	0.65624
$x^{\beta}_{i,\text{new}}$	0.34376	0.65624

The experimental mol fractions of water in each phase are 92.7 mol% and 36.3 mol%.

(14.12) For a binary system, iterations…

a) $K_i = \dfrac{x_i^{\beta}}{x_i^{\alpha}} = \dfrac{\gamma_i^{\alpha}}{\gamma_i^{\beta}}$ $\alpha, \beta \rightarrow$ phases

$i \rightarrow$ component

$$x_i^{\beta} = K_i x_i^{\alpha}$$

$$\sum x_i^{\beta} = 1 = K_1 x_1^{\alpha} + K_2 x_2^{\alpha} + K_3 x_3^{\alpha}$$

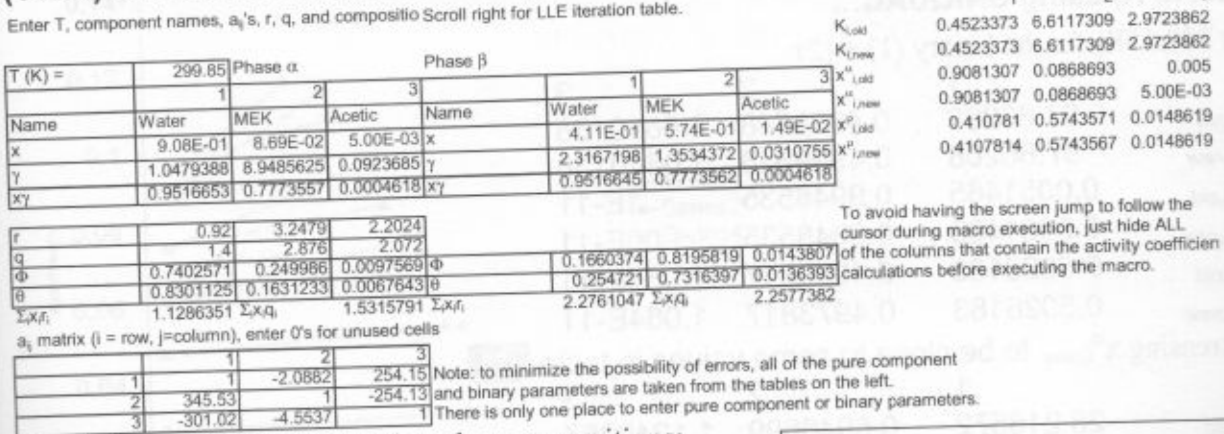
$$= K_1 x_1^{\alpha} + K_3 x_3^{\alpha} + K_2(1 - x_1^{\alpha} - x_3^{\alpha})$$

Rearranging,

$$x_1^{\alpha}(K_1 - K_2) = 1 - K_2 - x_3^{\alpha}(K_3 - K_2)$$

$$x_1^{\alpha} = \frac{\left[1 - x_3^{\alpha}(K_3 - K_2) - K_2\right]}{(K_1 - K_2)}$$

(14.13) Consider the system water(1) + MEK(2) + acetic acid(3)…



Enter T, component names, a_{ij}'s, r, q, and compositio Scroll right for LLE iteration table.

T (K) =	299.85	Phase α		Phase β			
	1	2	3		1	2	3
Name	Water	MEK	Acetic	Name	Water	MEK	Acetic
x	9.08E-01	8.69E-02	5.00E-03	x	4.11E-01	5.74E-01	1.49E-02
γ	1.0479388	8.9485625	0.0923685	γ	2.3167198	1.3534372	0.0310755
xγ	0.9516653	0.7773557	0.0004618	xγ	0.9516645	0.7773562	0.0004618

	1	2	3
$K_{i,old}$	0.4523373	6.6117309	2.9723862
$K_{i,new}$	0.4523373	6.6117309	2.9723862
$x^{\alpha}_{i,old}$	0.9081307	0.0868693	0.005
$x^{\alpha}_{i,new}$	0.9081307	0.0868693	5.00E-03
$x^{\beta}_{i,old}$	0.410781	0.5743571	0.0148619
$x^{\beta}_{i,new}$	0.4107814	0.5743567	0.0148619

r	0.92	3.2479	2.2024				
q	1.4	2.876	2.072				
Φ	0.7402571	0.249986	0.0097569	Φ	0.1660374	0.8195819	0.0143807
θ	0.8301125	0.1631233	0.0067643	θ	0.254721	0.7316397	0.0136393
$\Sigma_i x_i r_i$	1.1286351	$\Sigma_i x_i q_i$	1.5315791	$\Sigma_i x_i r_i$	2.2761047	$\Sigma_i x_i q_i$	2.2577382

To avoid having the screen jump to follow the cursor during macro execution, just hide ALL of the columns that contain the activity coefficien calculations before executing the macro.

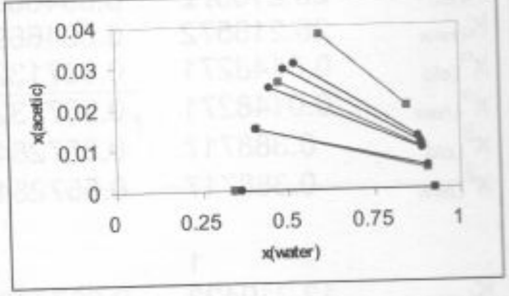
a_{ij} matrix (i = row, j=column), enter 0's for unused cells

	1	2	3
1	1	-2.0882	254.15
2	345.53	1	-254.13
3	-301.02	-4.5537	1

Note: to minimize the possibility of errors, all of the pure component and binary parameters are taken from the tables on the left. There is only one place to enter pure component or binary parameters.

Tabulating, and repeating at the other compositions:

Alpha phase			Beta phase		
1	2	3	1	2	3
0.924	0.076	0	0.344	0.656	0
0.908	0.087	0.005	0.411	0.574	0.015
0.890	0.100	0.01	0.477	0.497	0.026
0.849	0.131	0.02	0.597	0.365	0.038



Plot: squares are calcs, circles are expt, compare well.

(14.14) Calculate the LLE in the system nPentane (1) + acetone (2) + methanol(3) + water(4) at 298.15 K, using SSCED. The feed is PAMW{0.75, 0.13, 0.11, 0.01}+W{1}

1st Iteration		Guess	Guess			Flash=>	L/F	0.533
	zi	x_i^{Lo}	x_i^{Up}	γ^{Lo}	γ^{Up}	K	x_i^{Lo}	x_i^{Up}
npentane	0.375	0.0001	0.75	2.78E+11	1.06	2.62E+11	3.06E-12	8.03E-01
acetone	0.065	0.0001	0.13	135.29	1.67	81.0289	0.0017	0.1373
methanol	0.055	0.0001	0.11	3.99	7.49	0.5333	0.0703	0.0375
water	0.505	0.9997	0.01	1.00	36.13	0.0277	0.9250	0.0256
						rmsd	0.04857	1.00E+00

4th Iteration		Guess	Guess			Flash=>	L/F	0.544
	zi	x_i^{Lo}	x_i^{Up}	γ^{Lo}	γ^{Up}	K	x_i^{Lo}	x_i^{Up}
npentane	0.375	2.01E-10	0.8224	3.58E+09	1.03	3.49E+09	2.36E-10	8.22E-01
acetone	0.065	0.006	0.1356	41.35	1.86	22.1859	0.0061	0.1353
methanol	0.055	0.081	0.0238	2.48	8.63	0.2868	0.0815	0.0234
water	0.505	0.910	0.0225	1.02	41.59	0.0246	0.9096	0.0224
						RMSD =	0.000264	1.00E+00

(14.15) Calculate the LLE in the system 1-butanol(1) + water(2) + methanol(3) at 288.15 K, using UNIQUAC...

At 288.15K, for the binary (1) + (2):

	1	2	3
$K_{i,old}$	97.66208	0.4999548	1.0640138
$K_{i,new}$	97.66208	0.4999548	1.0640138
$x^{\alpha}_{i,old}$	0.0051465	0.9948535	1E-11
$x^{\alpha}_{i,new}$	0.0051465	0.9948535	1.00E-11
$x^{\beta}_{i,old}$	0.5026183	0.4973817	1.064E-11
$x^{\beta}_{i,new}$	0.5026183	0.4973817	1.064E-11

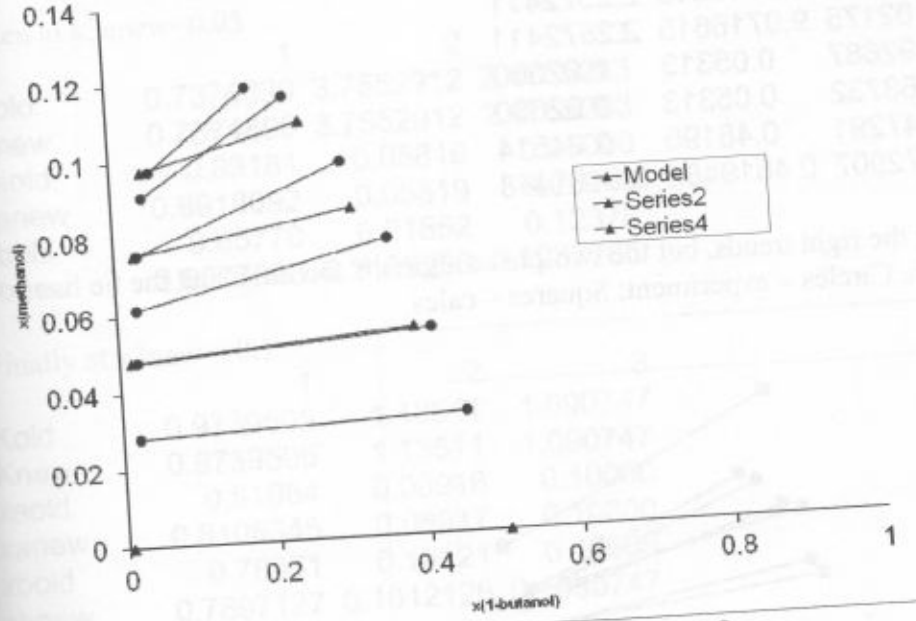
Increasing $x^{\alpha}_{i,new}$ to be close to some values in table 14.4:

	1	2	3
$K_{i,old}$	26.216572	0.5946699	1.1240267
$K_{i,new}$	26.216572	0.5946699	1.1240267
$x^{\alpha}_{i,old}$	0.0148271	0.9371329	0.04804
$x^{\alpha}_{i,new}$	0.0148271	0.9371329	4.80E-02
$x^{\beta}_{i,old}$	0.388717	0.5572847	0.0539982
$x^{\beta}_{i,new}$	0.388717	0.5572847	0.0539982

	1	2	3
$K_{i,old}$	12.219423	0.6678774	1.1313047
$K_{i,new}$	12.219423	0.6678774	1.1313047
$x^{\alpha}_{i,old}$	0.0257128	0.8985472	0.07574
$x^{\alpha}_{i,new}$	0.0257128	0.8985472	7.57E-02
$x^{\beta}_{i,old}$	0.3141956	0.6001194	0.085685
$x^{\beta}_{i,new}$	0.3141956	0.6001194	0.085685

	1	2	3
$K_{i,old}$	6.3204389	0.7416343	1.1157144
$K_{i,new}$	6.3204389	0.7416343	1.1157144
$x^{\alpha}_{i,old}$	0.0397837	0.8628563	0.09736
$x^{\alpha}_{i,new}$	0.0397837	0.8628563	9.74E-02
$x^{\beta}_{i,old}$	0.2514502	0.6399239	0.1086259
$x^{\beta}_{i,new}$	0.2514502	0.6399239	0.1086259

The model looks good at low methanol concentrations, but the modeled tie line slopes are not steep enough at higher methanol concentrations.



(14.16) Solve problem 14.13, except use UNIFAC…

At 26.7C, starting with x3anew = 1e-11

	1	2	3
Kold	0.3648545	15.50485	2.5080709
Knew	0.3648545	15.50485	2.5080709
xaold	0.95805	0.04195	0.00000
xanew	0.9580485	0.04195	0.00000
xbold	0.34955	0.65045	0.00000
xbnew	0.3495483	0.6504517	2.508E-11

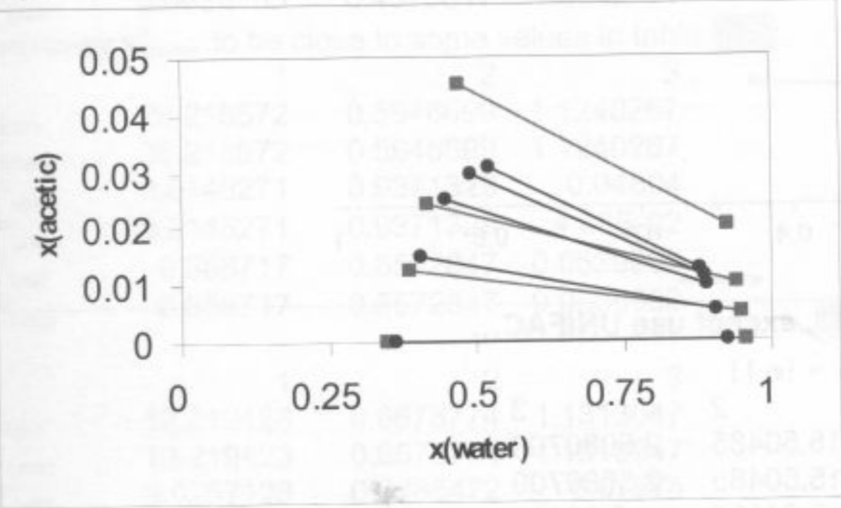
Then at x3anew = 0.005

	1	2	3
Kold	0.4066955	13.487525	2.4702498
Knew	0.4066955	13.487525	2.4702498
xaold	0.95043	0.04457	0.00500
xanew	0.950432	0.04457	0.00500
xbold	0.38654	0.60111	0.01235
xbnew	0.3865364	0.6011124	0.0123512

x3anew = 0.01	1	2	3
Kold	0.4441831	11.781921	2.4103711
Knew	0.4441831	11.781921	2.4103711
xaold	0.94271	0.04729	0.01000
xanew	0.9427106	0.04729	0.01000
xbold	0.41874	0.55716	0.02410
xbnew	0.4187361	0.5571601	0.0241037

x3anew=0.02	1	2	3
Kold	0.5102175	9.0716615	2.2572411
Knew	0.5102175	9.0716615	2.2572411
xaold	0.92687	0.05313	0.02000
xanew	0.9268732	0.05313	0.02000
xbold	0.47291	0.48195	0.04514
xbnew	0.472907	0.4819482	0.0451448

UNIFAC LLE is getting the right trends, but the two-phase region is too large and the tie line slope is not steep enough. Circles – experiment; Squares – calcs.



(14.17) Consider the system water(1) + methylethylketone(2) + propionic acid...

Results using UNIFAC(LLE)

First enter the formulas for a ternary system, but set x3alphanew to 1e-11. Initialize by starting each phase at infinite dilution. In this solution, the alpha phase was initially assumed to be pure water with a trace of MEK and the MEK phase was assumed to have a trace of water.

	1	2	3
Kold	0.3690424	15.473207	5.5621608
Knew	0.3690424	15.473207	5.5621608
xaold	0.95823	0.04177	0.00000
xanew	0.9582262	0.04177	0.00000
xbold	0.35363	0.64637	0.00000
xbnew	0.3536261	0.6463739	5.562E-11

From this result, we can change x3anew to 0.01 and start iterating again. The result is:

	1	2	3
Kold	0.4984339	10.621894	4.80201
Knew	0.4984339	10.621894	4.80201
xaold	0.94471	0.04529	0.01000
xanew	0.9447062	0.04529	0.01000
xbold	0.47087	0.48111	0.04802
xbnew	0.4708736	0.4811063	0.0480201

Then at x3anew=0.05

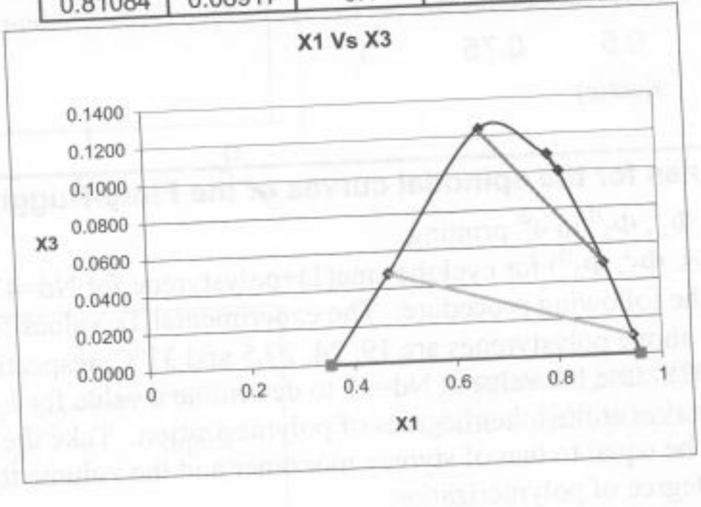
```
              1          2          3
Kold    0.7374899  3.7552912  2.4755293
Knew    0.7374899  3.7552912  2.4755293
xaold     0.89181    0.05819    0.05000
xanew   0.8918092    0.05819    0.05000
xbold     0.65770    0.21852    0.12378
xbnew   0.6577003  0.2185233  0.1237765
```

Finally at x3new = 0.1

```
              1          2          3
Kold    0.9739505    1.13511   1.090747
Knew    0.9739505    1.13511   1.090747
xaold     0.81084    0.08916    0.10000
xanew   0.8108345    0.08917    0.10000
xbold     0.78971    0.10121    0.10908
xbnew   0.7897127  0.1012126  0.1090747
```

Overall Summary

α phase			β phase		
water	MEK	PA	water	MEK	PA
0.958226	0.04177	1.00E-11	0.353626	0.646374	5.56E-11
0.944706	0.04529	0.01	0.470874	0.481106	0.04802
0.891809	0.05819	0.05	0.6577	0.218523	0.123777
0.81084	0.08917	0.1	0.789713	0.101213	0.109075

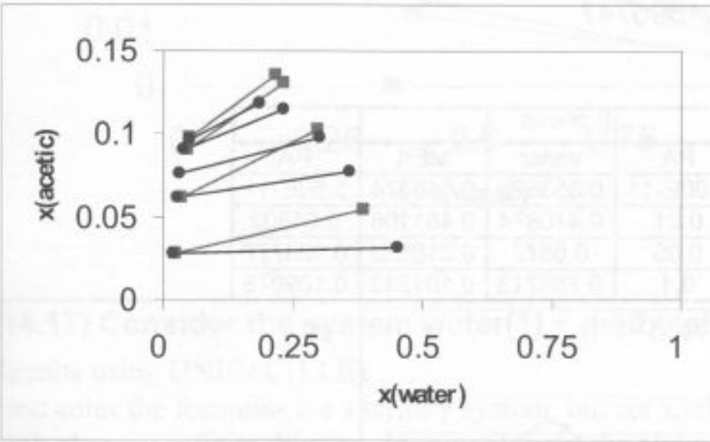


It would be interesting to compare with experiment.

(14.18) Solve problem 14.15 except use UNIFAC…

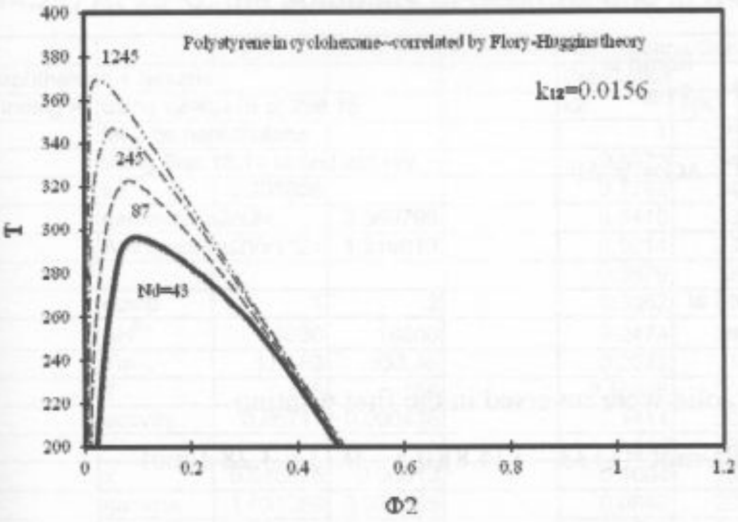
Using UNIFAC LLE, Calculated tie line sets at 288.15 K. (Circles – expt, Squares – calc, tie slopes are wrong, but location and size of three phase region isn't too bad.

	1 butanol	2 water	3 methanol
α	0.0232	0.9488	0.028
β	0.38623	0.55921	0.05456
α	0.03387	0.90463	0.0615
β	0.2997	0.59774	0.10257
α	0.04793	0.86127	0.0908
β	0.23269	0.63619	0.13112
α	0.05208	0.85052	0.0974
β	0.21827	0.64588	0.13585



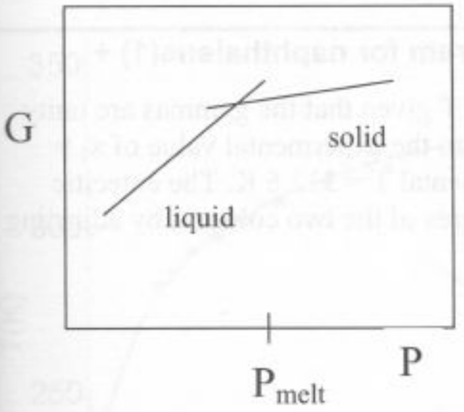
(14.19) Derive the formulas for the spinodal curves of the Flory-Huggins model…

Erratum: x_2^{I}, x_2^{II} changed to Φ_2^{I}, Φ_2^{II} in 4th printing.
Develop a spinodal plot (*T* vs. Φ_2^{I}, Φ_2^{II}) for cyclohexane(1)+polystyrene for Nd=43, 87, 245, 1245 of the polystyrene by the following procedure. The experimental Tc values for cyclohexane mixed with the above polystyrenes are 19, 24, 27.5 and 31°C, respectively (Schultz and Flory, 1952, JCP 74:4762). Use the value at Nd=43 to determine a value for k_{ij} then predict the Tc values and spinodal curves at the other degrees of polymerization. Take the solubility parameter for polystyrene to be equal to that of styrene monomer and the volume to be that of styrene monomer times the degree of polymerization.
Solution:
For Nd1=1, $1=(1-r)\,\Phi_1 + 2\Phi_1(1-\Phi_1)\chi$. $2\Phi_1^2\chi - \Phi_1\,(2\chi+1-r) + 1 = 0$
$\Rightarrow \Phi_1 = \{(2\chi+1-r) \pm \sqrt{[(2\chi+1-r)^2 - 8\chi]}\}/[4\chi]$
Vstyrene = 104/0.906 = 115 ; VC6 = 84/.7786 = 107
$\delta_{PS}=9.3 \quad \delta_{C6} = 8.2$
$Tc = [107^{-1/2} + (Nd_{PS}*115)^{-1/2}\,]^{-2}\, 2*(1.1^2 + 2k_{ij}\, 8.2*9.3)/1.987 = 292 \Rightarrow k_{ij} = 0.0156$
$\Rightarrow$ Tc(max) = 387



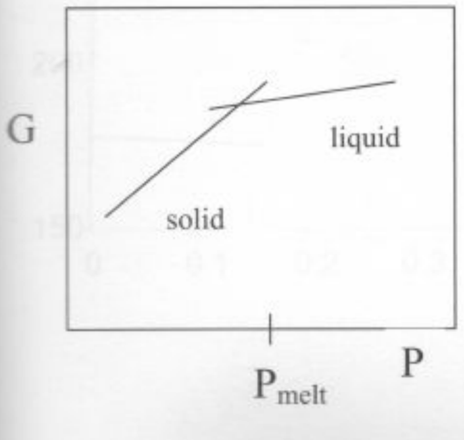
(14.20) In the treatment of solid-liquid equilibria, the effects of pressure on melting…

(a)



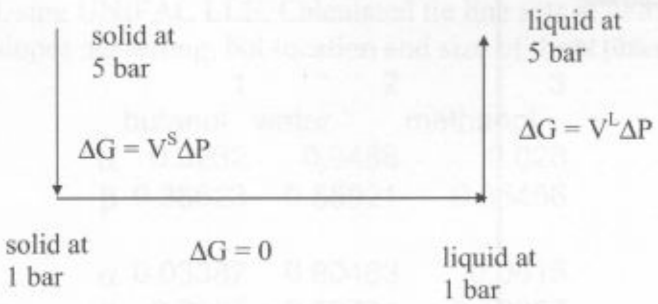
dG = VdP, $V^S < V^L$, so slope will be positive, and slope of solid will be less than slope of liquid. Pressure will make liquid freeze.

(b)



For water, increasing pressure will cause the solid to melt.

(c)



Note: the molar volumes of liquid and solid were reversed in the first printing

$$\Delta G = (V^L - V^S)(0.5 - 0.1)\text{cm}^3\text{MPa/mol} = (133 - 124.8)(0.5 - 0.1) = 3.28 \text{ J/mol}$$

(d) The Gibbs energy is given by Eqn 14.22,

$\Delta G = \Delta H^{fus}(1 - T/T_m) = 18800*(1 - 351.15/353.35) = 117.05$ J/mol

The temperature effect is much greater than the pressure effect.

(14.21) Generate a solid-liquid equilibrium T-x diagram for naphthalene(1) +

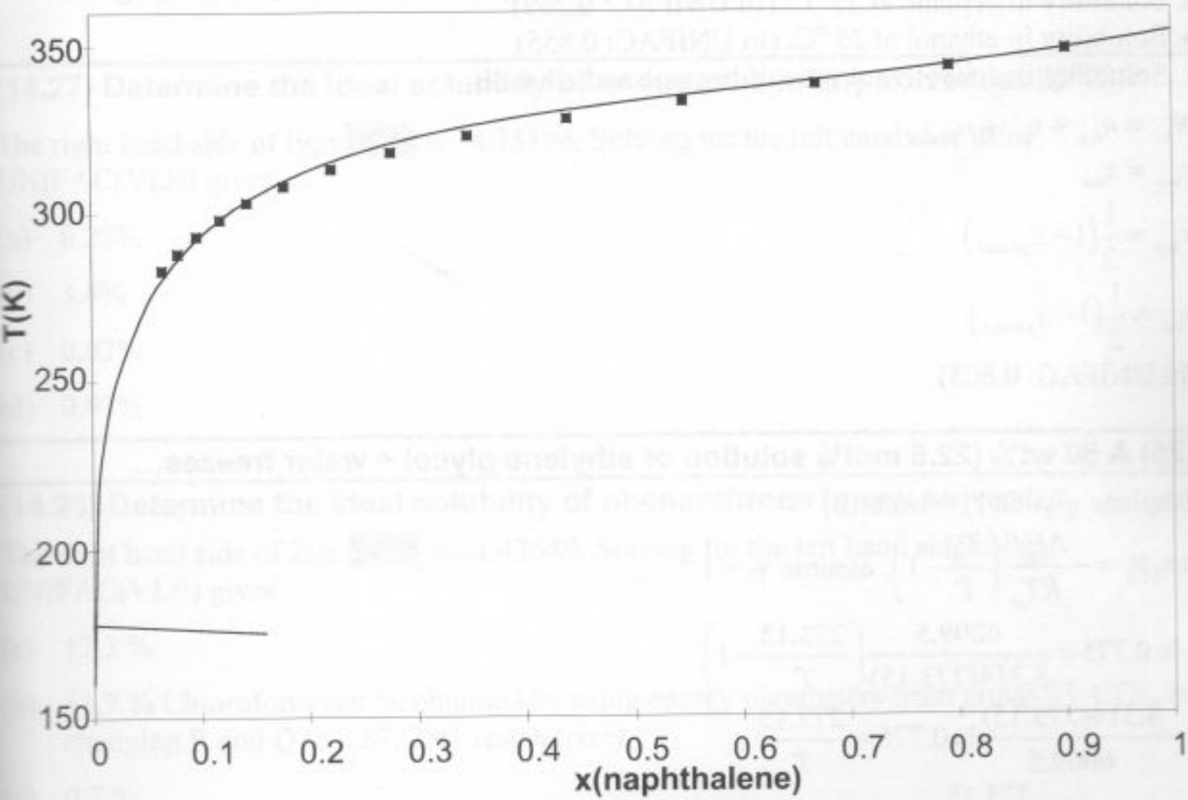
The solution is found by rearranging Eqn 14.23 or 14.24 for T given that the gammas are unity for an ideal solution. The eutectic composition is very close to the expermental value of $x_1 = 0.445$ and the temperature is within about 1K of the experimental T = 312.6 K. The eutecitic point is found by minimizing the difference in the temperatures of the two columns by adjusting x_1.

	Biphenyl(2) curve	Napthalene(1) curve	
	342.35	353.35	Tm(K)
	18.58	18.8	Hfus(kJ/mol)
x1	T(K)	T(K)	
0	342.35		
0.1	336.9121		
0.2	331.034		
0.3	324.6133	297.398393	
0.4	317.504	309.0932	obj
0.447041	313.8632	313.863372	-0.00012165
0.5	309.4873	318.817725	
0.6	300.2101	327.22945	
0.7		334.695658	
0.8		341.444127	
0.9		347.626677	
1		353.35	

(14.22) At 25°C, the solubility of naphthalene in n-hexane is 11.9 mol%...

naphthalene + hexane			
Finding A	using x2=0.119 at 298.15		
	let 2 be naphthalene		
	using Eqn 13.11 to find activity		
	a2	0.305806	
	gamma2=a2/x2=		2.569796
	A=ln(gamma2)/x1^2=		1.216019
	comp	1	2
	ΔH^{fus}	13030	18800
	Tm	177.83	353.35
	T	175	160
	activity	0.86717	0.000438
	x	0.840876	0.00013
	gamma	1.031269	3.372665
	act	0.86717	0.000438
	obj	9.67E-09	-1.2E-08

Naphthalene Curve			Hexane Curve	
Calculated		Expt	Calculated	
x2	T(K)	x2	x2	T
1	353.35		0	177.8
0.8972	348.15	0.902	0.0982	176
0.7792	343.15	0.794	0.1591	175
0.6415	338.15	0.67		
0.5014	333.15	0.547		
0.3879	328.15	0.44		
0.3062	323.15	0.348		
0.2474	318.15	0.277		
0.2032	313.15	0.222		
0.16886	308.15	0.178		
0.1414	303.15	0.144		
0.119	298.15	0.119		
0.1004	293.15	0.0973		
0.0849	288.15	0.0798		
0.0717	283.15	0.065		
0.0511	273.15			
0.022188	250			
0.0098	230			
0.00488	215			
0.00013	160			



(14.23) Phenanthrene and anthracene are structurally similar…

If we assume that they behave similarly in the liquid phase, their very different melting temperatures are indicative of more stable structure in the solid phase for anthracene.

$$\ln x_2 = -\frac{\Delta H_2}{RT_m}\left(\frac{T_m}{T}-1\right)$$

$\Delta H_{Ph}^{fus} = 16460$ J/mol $\qquad T_m = 96.0$

$\Delta H_{An}^{fus} = 28860$ J/mol $\qquad T_m = 216.0$

at 298.15 (assuming ideal solution) $x_{Ph} = 0.279 \;\; x_{An} = 0.01$

using UNIFAC(VLE), the answers aren't much different, $x_{Ph} = 0.286$, $x_{An} = 0.012$

The differences occur because anthracene can pack more efficiently in the solid phase. It's fugacity (as can be measured by the vapor pressure) will be lower than phenanthrene's.

(14.24) Use UNIFAC to determine the solubility (in mole fraction) of phenol…

Use UNIFAC to determine the solubility (in mole fraction) of phenol in the following conditions.

For phenol, $\Delta H^{fus} = 11.43$ kJ/mol, $T_m = 314.05$ K.

a. Solubility in heptane at 25 °C. (In UNIFAC: 0.269)
b. Solubility in ethanol at 25 °C. (In UNIFAC: 0.855)
c. Solubility in a 50/50 mol ratio of heptane and ethanol.

$$N_{tot} = n_{hep} + n_{eth} + n_{phenol}$$

$$x_{hep} = x_{eth}$$

$$x_{hep} = \frac{1}{2}\left(1 - x_{phenol}\right)$$

$$x_{eth} = \frac{1}{2}\left(1 - x_{phenol}\right)$$

(In UNIFAC: 0.805)

(14.25) A 50 wt% (22.5 mol% solution of ethylene glycol + water freezes…

Ethylene glycol(1) + water(2)

a) $\ln x_2\gamma_2 = -\frac{\Delta H^f}{RT_m}\left(\frac{T_m}{T}-1\right)$, assume $\gamma_2 = 1$

$$-\ln 0.775 = \frac{6009.5}{8.314(273.15)}\left(\frac{273.15}{T}-1\right)$$

$$1 - \frac{8.314(273.15)}{6009.5}\ln 0.775 = \frac{273.15}{T}$$

$$T = \frac{273.15}{1 - \frac{8.314(273.15)}{6009.5}\ln 0.775}$$

$T = 249$ K if ideal solution

b) System has $\gamma_2 < 1$ since water freezes at a lower T than ideal solution.

(14.26) Determine the ideal solubility of naphthalene in any solvent...

The right hand side of Eqn 13.11 is –0.82152. Solving for the left hand side using UNIFAC(VLE) gives:

(a) 4.8%

(b) 4.4%

(c) 6.8%

(d) 6.8%

(e) 9.1%

(f) 25.9%

(g) 15.5%

(h) 12.5%

(i) 35.8%

(j) 48.6% Chloroform can be obtained by using energy parameters from group 23, CCl_3, but changing R and Q to 2.87, 2.41 respectively.

(14.27) Determine the ideal solubility of anthracene in any solvent at 20°C...

The right hand side of Eqn 14.24 is –4.75196. Solving for the left hand side using UNIFAC(VLE) gives:

(a) 0.25%

(b) 3.4%

(c) 0.02%

(d) 0.03%

(14.28) Determine the ideal solubility of phenanthrene in any solvent...

The right hand side of Eqn 14.24 is –1.43649. Solving for the left hand side using UNIFAC(VLE) gives

(a) 12.3 %

(b) 31.7 % Chloroform can be obtained by using energy parameters from group 23, CCl_3, but changing R and Q to 2.87, 2.41 respectively.

(c) 0.7 %

(d) 3.0%

(e) 1.1%

(14.29) Determine the solubility curve for naphthalene in the specified solvent...

Some portions of the solubility curves are calculated by entering the solvent structure in UNIFAC(VLE), and after entering x, adjusting the T using Solver until the two sides of Eqn 14.24 are equal. Some portions are obtained by entering T and adjusting x.

(a) acetic

x_{naph}	T(C)
0.95	77.6
0.9	75.3
0.8	71.4
0.7	68.4
0.6	65.8
0.5	63.5
0.4	60.9
0.3	57.2
0.2	50.4
0.15	44.3
0.1	34.5 (made a big jump, continue by choosing T's)
0.084	30
0.070	25
0.059	20
0.049	15

(b) n-hexane

x_{naph}	T
0.9	74.7
0.8	69.4
0.7	64
0.6	58.5
0.5	52.7
0.4	46.2
0.3	38.2
0.2	27.3
0.15	19.5
0.1	8.5
0.08	2.5

(c) cyclohexanol

x_{naph}	T	x_{naph}	T
0.95	77.7	0.2	46.6
0.9	75.6	0.15	39.1
0.8	72.4	0.1	27.9
0.7	69.9	0.07	17.9
0.6	67.6	0.05	8.5
0.5	65.0	0.03	-5.3
0.4	61.5		
0.3	56.0		

(d) acetone

x_{naph}	T
0.9	74.6
0.8	68.9
0.7	62.9
0.6	56.8
0.5	50.3
0.4	43.2
0.3	35.2
0.2	24.9
0.1	8.1
0.05	-8.3

(e) Chloroform can be obtained by using energy parameters from group 23, CCl_3, but changing R and Q to 2.87, 2.41 respectively.

x_{naph}	T
0.9	74.4
0.8	67.8
0.7	60.3
0.6	51.7
0.5	41.3
0.4	28.6
0.3	12.1
0.2	-11.2

(f) methanol

x_{naph}	T
0.95	77.8
0.85	74.5
0.75	72.7
0.5	71.8
0.2	69.0
0.1	58.3
0.07	50.0
0.058	45.0
0.041	35.0
0.035	30.6
0.03	26.1
0.02	13.7
0.01	-6.8

(g) n-butanol

x_{naph}	T
0.9	75.7
0.8	72.9
0.7	71.3

0.6	70.2
0.5	69.4
0.3	65.2
0.2	58.8
0.15	52.7
0.1	42.6
0.07	32.8
0.05	23.3
0.03	9.0
0.02	-2.1

(h) ethanol

x_{naph}	T
0.9	75.7
0.85	74.1
0.8	72.8
0.7	71.3
0.5	71.0
0.3	72.1
0.2	70.4
0.15	67.3
0.1	60.4
0.075	54.0
0.05	43.6
0.035	33.6
0.025	24.0
0.015	9.5
0.01	-1.6

(i) n-propanol

x_{naph}	T
0.9	75.7
0.8	72.9
0.7	71.3
0.6	70.5
0.5	70.1
0.4	69.7
0.3	68.4
0.2	63.9
0.15	59.0
0.1	50.
0.075	42.7
0.05	31.6
0.035	21.5
0.025	12.0
0.015	-2.0

(j) 2-propanol

x_{naph}	T
0.9	75.7
0.8	72.9
0.7	71.2
0.6	70.4
0.5	70.1
0.4	69.7
0.3	66.2
0.2	63.8
0.15	58.8
0.1	49.8
0.075	42.5
0.05	31.4
0.035	21.3
0.025	11.8
0.015	-2.1

(14.30) The gas condensate from a new gas well in Prudoe Bay Alaska...

Use procedure of Example 14.12

#Carbons	Wt%	Mol Wt.	moles	mole frct.	density	densityCorr	zi wax	T fusion	H fusion	K-values	XiS
4	0	58	0	0	0.666	0.666	0	28.22	975.78		
5	1	72	0.0139	0.0535	0.6800	0.6800	0.0535	96.2	4129	43.625	0.0012
10	4	142	0.0282	0.1086	0.7260	0.7260	0.1086	236.2	19989	32.123	0.0034
15	7	212	0.0330	0.1272	0.7530	0.7530	0.1272	284.9	36001	22.471	0.0057
20	10	282	0.0355	0.1367	0.7720	0.7720	0.1367	310.3	52167	14.932	0.0092
25	12	352	0.0341	0.1314	0.7870	0.7870	0.1314	326.4	68485	9.426	0.0139
30	12	422	0.0284	0.1096	0.8000	0.8000	0.1096	337.7	84956	5.653	0.0194
35	12	492	0.0244	0.0940	0.8100	0.8100	0.0940	346.4	101580	3.220	0.0292
40	12	562	0.0214	0.0823	0.8190	0.8190	0.0823	353.3	118357	1.743	0.0472
45	8	632	0.0127	0.0488	0.8270	0.8270	0.0488	359.1	135287	0.896	0.0544
50	8	702	0.0114	0.0439	0.8340	0.8340	0.0439	364.1	152369	0.438	0.1004
60	14	842	0.0166	0.0641	0.8460	0.8460	0.0641	372.6	186993	0.089	0.7161
Sums			0.2594	1			0.83792				1

T (K) =
358.2536

(14.31) Generate a SLE phase diagram for Phenol (1) + cylcohexane (2)...

ideal solution

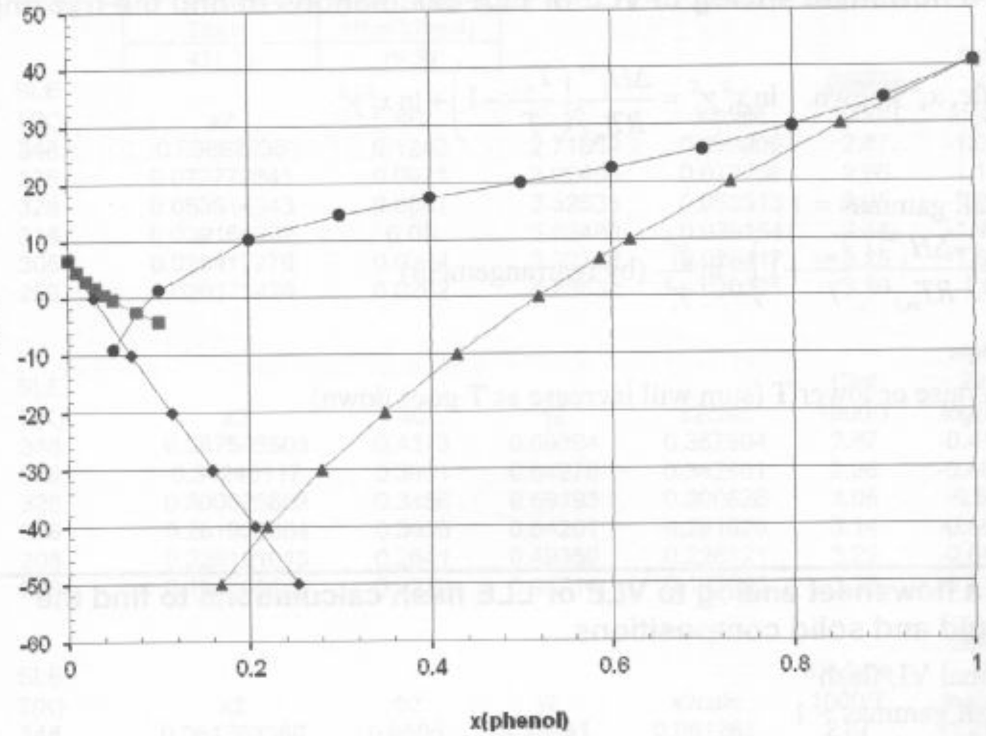
The values assume gamma = 1 for both components. The freezing curve can be found either by adjusting x at a given T, or T at a given x. In this case, the T will be chosen and x_{phenol} will be varied using solver. The objective function is a_{calc} - a_{SLE} where a_{SLE} is calculated from the heat of fusion and pure component melting temperature.

T(C)	x(phenol) phenol freezing	x(phenol) cyclo freezing	T(C)	x(phenol) phenol freezing	x(phenol) cyclo freezing
40.9	1		-10	0.429	0.07
30	0.854		-20	0.349	0.114
20	0.732		-30	0.279	0.159
10	0.620		-40	0.219	0.206
6.7		1	-50	0.168	0.253
0	0.519	0.028			

(b) The phenol concentration will be used to tabulate the freezing points. The column labeled T_{phenol} is the temperature where phenol freezes. The column labeled T_{chclo} is the temperature where cyclohexane freezes. The eutectic point is found by simultaneously solving for one objective function subject to the constraint that the other is simultaneously zero. The objective function is a_{calc} - a_{SLE} where a_{SLE} is calculated from the heat of fusion and pure component melting temperature.

x_{phenol}	T_{phenol}	T_{cyclo}	x_{phenol}	T_{phenol}	T_{cyclo}
1	40.9		0.1	1.4	-4.2
0.9	34.5		0.076 (eutectic)	-2.5	-2.5
0.8	29.6		0.05	-9.0	-0.3
0.7	25.7		0.04		0.6
0.6	22.6		0.03		1.7
0.5	19.98		0.02		3.0
0.4	17.51		0.01		4.6
0.3	14.6		0		6.7
0.2	10.3				

c) The phenol has a larger activity coefficient in cyclohexane since the phenol solubility curve is at higher temperatures.



(14.32) Create a flowsheet analog to VLE or LLE calculations to find the melting temperature…

(a) analog to bubble calc, x_i^S known. $\ln x_i^L = \dfrac{-\Delta H_i^{fus}}{RT_{m,i}}\left(\dfrac{T_{m,i}}{T}-1\right)+\ln x_i^S$

guess T til $\sum_i x_i^L = 1$

(b) analog to bubble calc, x_i^S known. $\ln x_i^L\gamma_i^L = \dfrac{-\Delta H_i^{fus}}{RT_{m,i}}\left(\dfrac{T_{m,i}}{T}-1\right)+\ln x_i^S\gamma_i^S$

1. guess T
2. assume ideal, all gammas = 1
3. $\ln K_i = \ln\dfrac{x_i^L}{x_i^S} = \dfrac{-\Delta H_i^{fus}}{RT_{m,i}}\left(\dfrac{T_{m,i}}{T}-1\right)-\ln\dfrac{\gamma_i^L}{\gamma_i^S}$ (by rearrangement)
4. $x_i^L = K_i x_i^S$

if $\sum_i x_i^L \neq 1$, then raise or lower T (sum will increase as T goes up)

5. normalize x_i^L
6. calc γ_i^L, γ_i^S
7. go to 3

(14.33) Create a flowsheet analog to VLE or LLE calculations to find the freezing temperature…

analog to dew calc, x_i^L known. $\ln x_i^S \gamma_i^S = \dfrac{\Delta H_i^{fus}}{RT_{m,i}}\left(\dfrac{T_{m,i}}{T}-1\right)+\ln x_i^L \gamma_i^L$

1. guess T
2. assume ideal, all gammas = 1
3. $\ln K_i = \ln\dfrac{x_i^L}{x_i^S} = \dfrac{-\Delta H_i^{fus}}{RT_{m,i}}\left(\dfrac{T_{m,i}}{T}-1\right)-\ln\dfrac{\gamma_i^L}{\gamma_i^S}$ (by rearrangement)
4. $x_i^S = K_i/x_i^L$

if $\sum_i x_i^S \neq 1$, then raise or lower T (sum will increase as T goes down)

5. normalize x_i^S
6. calc γ_i^L, γ_i^S
7. go to 3

(14.34) Create a flowsheet analog to VLE or LLE flash calculations to find the coexisiting liquid and solid compositions…

analog to isothermal VL flash

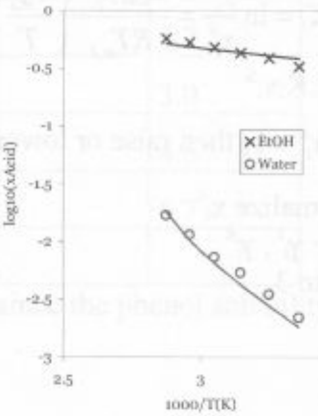
1. assume ideal, all gammas = 1
2. $\ln K_i = \ln\dfrac{x_i^L}{x_i^S} = \dfrac{-\Delta H_i^{fus}}{RT_{m,i}}\left(\dfrac{T_{m,i}}{T}-1\right)-\ln\dfrac{\gamma_i^L}{\gamma_i^S}$ (by rearrangement)
3. $\sum_i \dfrac{z_i(1-K_i)}{K_i+(S/F)(1-K_i)} = 0$, adjust S/F until sum is zero
4. $x_i^S = \dfrac{z_i}{K_i+(S/F)(1-K_i)}$, $x_i^L = K_i x_i^S$
5. if x_i^L or x_i^S changed, calc γ_i^L, γ_i^S go to 3

(14.35) Salicylic acid is similar in structure to aspirin…

Characterizing the acidity of salicylic acid. From DIPPR: Mw=131.1, ρ=1.155, δ=24.21, Tm … Iterate on α to minimize rmsd for water. Then $\alpha^{opt} \approx 41.1$. Predict SLE for E+acid => not bad!

Tm(K)	Hfus(kJ/mol)
431.75	19.59

						alpha	rmsd
SLE					water	41.1	0.00099
T(K)	x2	Φ2	γ2	x2calc	1000/T	log(x2)	x2expt
348	0.01855	0.1115	14.50	0.018549	2.87	-1.7317	0.0171
338	0.01049	0.0657	20.98	0.010489	2.96	-1.9793	0.0116
328	0.00658	0.0421	27.03	0.006583	3.05	-2.1815	0.0074
318	0.00427	0.0277	33.25	0.00427	3.14	-2.3696	0.0054
308	0.00279	0.0182	39.98	0.002792	3.25	-2.5541	0.0035
298	0.00182	0.0119	47.52	0.001817	3.36	-2.7407	0.0022
						alpha	rmsd
SLE					ethanol	41.1	0.03823
T(K)	x2	Φ2	γ2	x2calc	1000/T	log(x2)	x2expt
348	0.515	0.6853	0.52169	0.515	2.874	-0.2878	0.5698
338	0.485	0.6584	0.45415	0.485	2.959	-0.3146	0.5252
328	0.456	0.6326	0.39026	0.456	3.049	-0.3411	0.4779
318	0.430	0.6074	0.33013	0.430	3.145	-0.3665	0.4274
308	0.406	0.5831	0.27525	0.405	3.247	-0.392	0.3851
298	0.383	0.5595	0.2257	0.383	3.356	-0.4173	0.3254



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FYI: alpha can be optimized vs other data too. 41.1 is fortuitously good for ethanol.

Tm(K)	Hfus(kJ/mol)
431.75	19.59

SLE						alpha	rmsd
					vinylAc	0	0.04469
T(K)	x2	Φ2	γ2	x2calc	1000/T	log(x2)	x2expt
348	0.09892935	0.1242	2.71869	0.098909	2.87	-1.0048	0.025
338	0.072772841	0.0921	3.02455	0.072768	2.96	-1.1381	0.018
328	0.053514343	0.0681	3.32533	0.053513	3.05	-1.2715	0.0126
318	0.039164682	0.05	3.62489	0.039164	3.14	-1.4071	0.0077
308	0.028417276	0.0364	3.92758	0.028417	3.25	-1.5464	0.0049
298	0.020371426	0.0262	4.23832	0.020371	3.36	-1.691	0.003

SLE						alpha	rmsd
					Ctet	229	0.01
T(K)	x2	Φ2	γ2	x2calc	1000/T	log(x2)	x2expt
348	0.387503503	0.4373	0.69394	0.387504	2.87	-0.4117	0.3692
338	0.34240117	0.3901	0.64278	0.342401	2.96	-0.4655	0.3347
328	0.300625688	0.3456	0.59193	0.300626	3.05	-0.522	0.301
318	0.261925384	0.3036	0.54201	0.261925	3.14	-0.5818	0.2692
308	0.226121015	0.2641	0.49359	0.226121	3.25	-0.6457	0.2358
298	0.193093156	0.2272	0.44714	0.193093	3.36	-0.7142	0.2008

SLE						alpha	rmsd
					pXylene	0	0.00629
T(K)	x2	Φ2	γ2	x2calc	1000/T	log(x2)	x2expt
348	0.061262389	0.0595	4.38941	0.061262	2.87	-1.2128	0.0578
338	0.045678289	0.0443	4.81825	0.045678	2.96	-1.3403	0.0401
328	0.033850691	0.0328	5.25687	0.033851	3.05	-1.4704	0.027
318	0.02484863	0.0241	5.71325	0.024849	3.14	-1.6047	0.0175
308	0.018013307	0.0175	6.19602	0.018013	3.25	-1.7444	0.011
298	0.012857852	0.0125	6.71501	0.012858	3.36	-1.8908	0.0062

(14.36) Using the result from 14.35 for α^{acid}, estimate the amount of ethanol required to achieve 10wt%salicylic acid in water.

$\ln(\gamma_A x_A)=(-Hfus/R)(1/T-1/Tm)$ Eqn. 14.24

$RT\ln(\gamma_A) = V_A [(\delta'_A-<\delta'>)^2 + 2<k_{2m}>\delta_A - <<k_{mm}>>]$ Eqn. 12.54

Since Mwacid ~ 5*MwH2O, guess xacid ~ 0.02. $x_A^{is} = 0.05$ => γA ~ 3.

Use multicomponent SSCED xls to "guess" ethanol amount until $\gamma_A \sim 3$ => x_E~0.05, x_W~0.93

Further refining xA => xA ~ 0.016 to get wA = 0.10. Then eqn. 14.24 => γA = 5.5.

MultiSSCED => xE = 0.0417, xW = 0.9427, xA = 0.0156, γA = 5.55, wA = 10.2% close enough.

FYI, on final iteration: <δ'> = 26.70; <k2m> = 0.7279; <<kmm>> = 0.131

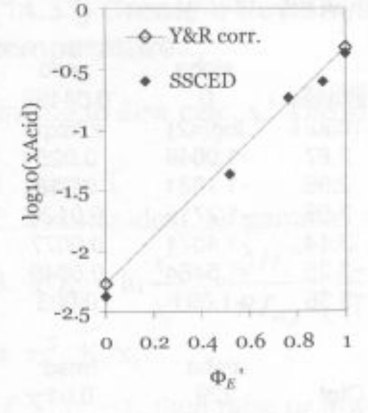
(14.37) Estimate the solubility of salicylic acid…

Estimate the solubility of salicylic acid in a mixture of ethanol and water. Plot log10(xAcid) vs. ΦE' where ΦE' = ΦE/(ΦE+ΦW) using points for these estimates. Also include the experimental results with a straight line indicating the empirical rule. Use multicomponent SSCED xls.

SalicylicAcid in a mixed solvent of ethanol+water at 318K

Tm(K)	Hfus(kJ/mol)
431.75	19.59

	SLE						alpha		
							41.1		
Φ_E	Φ_W	Φ_E'	x_A^{guess}	Φ_A	γ_A	x_A^{calc}	$\log(x_A^{calc})$	x_A^{expt}	$\log(x_A^{expt})$
0.3926	0	1	0.43	0.607405	0.330134	0.430026	-0.3665	0.4779	-0.32066
0.4964	0.0511	0.9067	0.25	0.4525	0.569	0.249502	-0.60293		
0.4476	0.1383	0.7640	0.184	0.4141	0.7724	0.183799	-0.73566		
0.436	0.404	0.51905	0.0429	0.16	3.31	0.04289	-1.36764		
0	0.9723	0	0.00427	0.0277	33.2498	0.00427	-2.36957	0.0054	-2.26761


0
-0.5
-1
-1.5
-2
-2.5
log10(xAcid)
Y&R corr.
SSCED
0
0.2
0.4
0.6
0.8
1
Φ_E'