

10.213 Fall 1999

Problem 23 (due Wednesday 11/17)

VLE data for methyl *tert*-butyl ether (1)/dichloromethane (2) at 308.15 K are as follows:

P/kPa	x_1	y_1		P /kPa	x_1	y_1
85.265	0.0000	0.0000		59.651	0.5036	0.3686
83.402	0.0330	0.0141		56.833	0.5749	0.4564
82.202	0.0579	0.0253		53.689	0.6736	0.5882
80.481	0.0924	0.0416		51.620	0.7676	0.7176
76.719	0.1665	0.0804		50.455	0.8476	0.8238
72.422	0.2482	0.1314		49.926	0.9093	0.9002
68.005	0.3322	0.1975		49.720	0.9529	0.9502
65.096	0.3880	0.2457		49.624	1.0000	1.0000

The data are well correlated by the three-parameter Margules equation [an extension of Eq. 11.7]:

$$\frac{G^E}{RT} = (A_{21}x_1 + A_{12}x_2 - Cx_1x_2)x_1x_2$$

Implied by this equation are the expressions:

$$\ln\gamma_1 = x_2^2 [A_{12} + 2(A_{21} - A_{12} - C)x_1 + 3C x_1^2]$$

$$\ln\gamma_2 = x_1^2 [A_{21} + 2(A_{12} - A_{21} - C)x_2 + 3C x_2^2]$$

- (a) Basing calculations on Eq. (11.1), find the values of parameters A_{12} , A_{21} , and C that provide the best fit of G^E/RT to the data.
- (b) Prepare a plot of $\ln\gamma_1$, $\ln\gamma_2$, and G^E/x_1x_2RT vs. x_1 showing both the correlation and experimental values.
- (c) Prepare a Pxy diagram (see Fig. 11.10) that compares the experimental data with the correlation determined in (a).
- (d) Prepare a consistency-test diagram like Fig. 11.12.