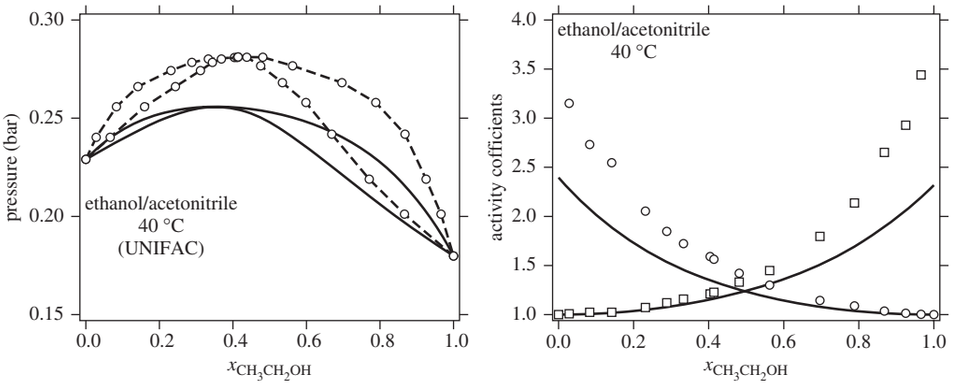

Figure 12-12: *Pxy* graph and activity coefficients for the system ethanol/acetonitrile at 50 °C calculated from UNIFAC.

Finally, the activity coefficients are

$$\gamma_1 = 2.01244,$$
$$\gamma_2 = 1.00918.$$

The *Pxy* graph is obtained by repeating this calculation at various liquid compositions in the range $x_1 = 0$ to $x_1 = 1$. The results are shown in Figure 12-12.

Comments The agreement with the experimental data is not very good. UNIFAC indeed predicts an azeotrope at $x_1 = 0.33$ (compared to $x_1 = 0.275$ from the experimental data) but its pressure is under-predicted by about 0.1 bar. We must note, however, that as a predictive model, UNIFAC has no adjustable parameters. The next example demonstrates a case in which UNIFAC produces a much better prediction of phase behavior.

Example 12.12: Using UNIFAC (2)
Use UNIFAC to calculate the *Pxy* graph for the system n-pentane/1-butanol at 30 °C.

Solution N-pentane contains ~~one~~ two "CH_3" and three "CH_2" subgroups. 1-butanol contains ~~one~~ one "CH_3", ~~two~~ three "CH_2" and one "OH". The R and Q parameters are summarized below.

Subgroup	k	$R^{(k)}$	$Q^{(k)}$	$\nu_1^{(k)}$	$\nu_2^{(k)}$
CH_3	1	0.9011	0.848	2	1
CH_2	2	0.6744	0.540	3	3
OH	14	1	1.200	0	1