Laboratory and Homework Assignment 3

Reading Assignment

1. "Chapter 8: Activity Coefficient Models" from Jana, Amiya K. Chemical process modelling and computer simulation. PHI Learning Pvt. Ltd. 2011.
2. "Chapter 13: Equation of State Models" from Jana, Amiya K. Chemical process modelling and computer simulation. PHI Learning Pvt. Ltd. 2011.

Laboratory Assignment (Due after laboratory session)

1. [100 points] Regress the following Txy data using the NRTL model for activity coefficients in ASPEN. Assume that VLE is well represented by modified Raoult's law. You are given that $\alpha_{12} = 0.4973$ and the rest of the NRTL parameters needs to be determined using regression routines in ASPEN. Does the regression for these models pass consistency test? Obtain the plot of experimental *vs* estimated data. Extract the standard deviation for each model.

   NRTL equation is given by:

$$\ln \gamma_1 = x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right], \tag{1}$$

$$\ln \gamma_2 = x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right], \tag{2}$$

   where,

$$\tau_{12} = \frac{g_{12} - g_{22}}{RT}, \tag{3}$$

$$\tau_{21} = \frac{g_{21} - g_{11}}{RT}, \tag{4}$$

$$G_{12} = \exp(-\alpha_{12}\tau_{12}), \tag{5}$$

$$G_{21} = \exp(-\alpha_{21}\tau_{21}). \tag{6}$$

   g_{ij} parameter for interaction between components i and j; $g_{ij} = g_{ji}$. α_{ij} is the non-randomness parameter; $\alpha_{ij} = \alpha_{ji}$.

   Now using Matlab verify whether the data passes Redlich-Kister consistency test when NRTL equation is used to get the activity coefficients.

Experimental VLE data at P = 760 mm Hg 1-propanol/water. 1-propanol is indexed as "1" and water as "2". Taken from DECHEMA chemical data series.

T (°C)	x_1	y_1
100.00	0.0000	0.0000
95.00	0.0100	0.1100
92.00	0.0200	0.2160
90.50	0.0400	0.3200
89.30	0.0600	0.3510
88.50	0.1000	0.3720
88.10	0.2000	0.3920
87.90	0.3000	0.4040
87.80	0.4000	0.4240
87.80	0.4320	0.4320
87.90	0.5000	0.4520
88.30	0.6000	0.4920
89.00	0.7000	0.5510
90.50	0.8000	0.6410
91.50	0.8500	0.7040
92.80	0.9000	0.7780
95.00	0.9600	0.9000
97.30	1.0000	1.0000

Practice Homework Assignment

1. Regress the following Txy data in ASPEN assuming equilibrium is well represented by modified Raoult's law. Use Wilson's model to represent liquid phase activity co-efficients, and ideal behaviour for gas phase. Use Redlich-Kister consistency test assuming the measure of error is less than 12% (i.e., D-J <12%). Extract the unknown parameters from ASPEN using the following functional form for Wilson's equation. Does your regression satisfy the consistency test?

Experimental VLE data at P = 760 mm Hg water/2-chloroethanol. Water is indexed as "1" and 2-chloroethanol as "2". Taken from DECHEMA chemical data series.

T (°C)	x_1	y_1
128.6	0.0000	0.0000
111.00	0.1904	0.4866
105.00	0.3317	0.6569
101.90	0.4409	0.7283
100.40	0.5276	0.7639
99.50	0.5983	0.7926
98.90	0.6569	0.8055
98.50	0.7064	0.8171
98.30	0.7487	0.8288
98.10	0.7852	0.8371
97.90	0.8171	0.8447
97.80	0.8452	0.8515
97.90	0.8702	0.8580
98.00	0.8924	0.8649
98.20	0.9125	0.8683
98.40	0.9306	0.8771
98.60	0.9470	0.8838
98.90	0.9620	0.8991
99.20	0.9757	0.9199
99.60	0.9884	0.9501
100.00	1.0000	1.0000

The Antoine equation parameters are (Water: A = 8.07131, B = 1730.630, and C = 233.426; $1 < T < 100$°C; 2-choloroethanol: A = 6.36021, B = 1003.703, C = 160.113; $90 < T < 130$°C). The values are taken from DECHEMA chemical data series. The form of equation used is $\log_{10} P^{sat} = A - B/(T+C)$ with pressure in mmHg and temperature in °C.

Wilson's equation is given by:

$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21} x_1} \right), \tag{7}$$

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21} x_1) + x_1 \left(\frac{\Lambda_{21}}{x_2 + \Lambda_{21} x_1} - \frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} \right), \tag{8}$$

where,

$$\Lambda_{12} = \frac{v_2^L}{v_1^L} \exp\left(-\frac{A_{12}}{RT}\right) \tag{9}$$

$$\Lambda_{21} = \frac{v_1^L}{v_2^L} \exp\left(-\frac{A_{21}}{RT}\right), \tag{10}$$

where v_i^L is the molar volume of pure liquid component ith. Here take $v_1^L = 18.07$ cm^3/gmol and $v_2^L = 67.29$ cm^3/gmol.

2. Now using Matlab, write a code to obtain the Txy plot. You are also expected to plot the experimental results in the same plot. Make a separate plot for absolute error in temperatures at each x-point in the data. What is the maximum absolute error?