Laboratory and Homework Assignment 4

Reading Assignment

1. "Chapter 12: Equilibrium Flash Vaporization" from Jana, Amiya K. Chemical process modelling and computer simulation. PHI Learning Pvt. Ltd. 2011.

Laboratory Assignment (Due after laboratory session)

1. A stream containing 30 kmol/h of vinylacetate and 50 kmol/hr toluene at $T = 25°$C and 1 atm pressure is heated to $T = 75°$C and sent to a flash drum. The outlet liquid and vapor streams are in equilibrium with each other. Assume that the vapor-liquid equilibria is adequately represented by Raoult's law. The Antoine's parameters can be obtained from NIST database.

   (a) [30 points] Does a unique root exits for $f(\phi)$? Plot Rachford-Rice function ($f(\phi)$) vs ϕ to verify this.

   (b) [60 points] Solve the Rachford-Rice equations to obtain the liquid and vapor fractions leaving the flash drum. You need to do this first using Matlab and then using ASPEN.

   (c) [10 points] Does a single-stage flash provide good separation? Explain your results for part a) using T-x-y diagram in ASPEN.

Practice Homework Assignment

1. A stream containing 80 kmol/h of 1,3-butadiene and 20 kmol/h of styrene is to be flashed at 20°C and 1 atm pressure.

   (a) [20 points] Solve the flash equations to obtain the molar flow rate of vapour leaving the flash drum. As a first guess, assume Raoult's law adequately represents the VLE for the mixture. Obtain Antione's coefficient from the NIST database. Does Raoult's law do a good job in representing VLE data for this mixture? Verify this by plotting T-x-y and y-x diagrams and comparing them with the data from DECHEMA chemistry data series (given below). This exercise is to be done in Matlab only.

   (b) [80 points] Again solve this problem, now using modified Raoult's law. For Matlab, use NRTL equation for estimating the activity coefficients. For ASPEN do this exercise first using NRTL equation for estimating activity coefficient. Now add vapor phase non-idealities using UNIQUAC fugacity coefficient model. The NRTL equation parameters are given below along with the experimental data. Use 'VLE-LIT' as the source in ASPEN for getting UNIQUAC parameters for estimating activity coefficients. Pen down UNIQUAC equation along with all the values of parameters obtained from ASPEN.

   Do you notice a marked improvement in the estimation of flash outlet compositions? If yes why and if no why?

   If 1,3-butadiene is indexed as '1' and styrene is indexed as '2', the NRTL's equation parameters are: $g_{12} - g_{22} = -457.6701$ cal/gmol, $g_{21} - g_{11} = 1177.2226$ cal/gmol, and $\alpha_{12} = 0.2984$.

Table 1: **Experimental VLE data for 1,3-butadiene and styrene at P = 1.013 bar. Taken from DECHEMA chemical data series.**

T (K)	x_1	y_1
363.15	0.0255	0.829
353.15	0.035	0.887
338.15	0.0577	0.94
323.15	0.102	0.971
298.15	0.253	0.994
273.15	0.811	0.9995