CH620003 Process Modelling and Simulation

Assignment 1 **Deadline to submit: 10 Feb 2025 (before 5 PM)**

Q1: NN CORRELATION OF BOILING POINT WITH CHEMICAL PROPERTIES.

Link to the data set (excel file):
https://www.dropbox.com/scl/fi/zlkxnyaptvc48xiu76xpy/data_file.xlsx?rlkey=754ozed754fyw4dhnlugjw7fa&dl=0

The data are tabulated into rows, one for each compound, and columns that include a common name, molecular weight, critical temperature (K), acentric factor, and the normal boiling point (K). Extract the data and place it into a matrix (array) AllData to use further on.

(a) Extract the boiling points from the data and place them in a column vector. Similarly, extract the molecular weights in a second vector. Plot the normal boiling point as a function of the molecular weight of the compounds in the database. Fit a straight line through the data and find the R^2 value.

(b) While we could use all the data we have to produce a meaningful correlation, let us assume that not all of the data were available. We will select a training set, or set of data that will be used to inform our ML algorithm. Extract from AllData 100 random data compounds. Using these selected compounds, build a 100 × 3 matrix, which we call X, where each row corresponds to a training example (i.e., the data for a given compound). For each one of these rows the first column is the number 1 (corresponding to x0) and the next two columns correspond to the values of x1 and x2 (molecular weight and acentric factor). Create another column matrix y with all the corresponding expected results; i.e., each of the elements of the vector is the expected reduced boiling point (Tb/ Tc) of each training example. The resulting $\boldsymbol{y}$ vector is a 100 × 1 vector.

The "solution" of this problem can be found directly as

$$\boldsymbol{\theta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\,\boldsymbol{X}^T\,\boldsymbol{y}$$

Calculate the values of the coefficients θ_0, θ_1 and θ_2, to evaluate the quality of the correlation.

(c) From the matrix AllData retrieve two column vectors, one called InputData, which will have two columns, the MW and the acentric factor of all the data in the original set and a second matrix called TargetData which contains the reduced boiling point data.

Develop a neural network for this data, and train the network, using only 10% of the data. Present the results of the output.

You may want to explore the effect of changing the number of layers. In the above case, only a 10% of the available data is used to train the network (some 600 data points) while the rest is used for validations and testing. Explore what happens when these ratios are changed.

Q2: MULTICOMPONENT FLASH PROBLEM

A liquid mixture consisting of 100 kmol of 60 mol% benzene, 25 mol% toluene and 15 mol% o-xylene is flashed at 1 atm and 100 C. Assume ideal solutions, use vapour pressure data (from Antoine relations) to determine the K-values.

(a) Compute the component flow rates, mole fraction composition of the top and bottom products.

(b) Repeat the calculation in (a) for the same (1 atm) pressure, but different temperatures from 100 to 150 C. You need to think here before jumping on the calculations.

(c) Find the optimum temperature at which the recovery of benzene is maximum.

You need to do the numerical calculations, following the Rachford-Rice method of solution.

(d) If you recycle part of the bottom product stream, does the Benzene recovery increases? If yes, then how much?

Q3: BUBBLE POINT METHOD – MULTICOMPONENT MULTISTAGE DISTILLATION

1000 kmol/h of a saturated-liquid mixture of 60% methanol (normal boiling point 65 C), 20 mol% ethanol (normal boiling point 98 C), and 20 mol% n-propanol (normal boiling point 97 C) is fed to the middle stage of a distillation column having three equilibrium stages, a total condenser, a partial reboiler, all operated at 1 atm. The distillate rate is 600 kmol/h, and the external reflux rate is 2,000 kmol/h of saturated liquid.

(a) Performa ONE set of hand calculations for one iteration of the stage temperature.

(b) Write your own code to obtain converged solutions of the temperature profiles.

(c) Increase the number of equilibrium stages in the column to 10, and use the code (developed in part a) to determine the optimum feed location.

The *K*-values at 1 atm and the above temperatures for each component is expressed as $K = P_i^s / P$. The vapour pressure data are fitted to an extended Clausius-Clapeyron equation:
$P_s = \exp[C_1 + \frac{C_2}{T} + C_3 \ln T + C_4 T^{C_5}]$ where P_s is in Pa and T is in K. The values of the constants $C_1 - C_5$ are presented in the following table:

Component		C1	C2	C3	C4	C5
M	Methanol	81.768	-6876	-8.7078	7.1926E-6	2
E	Ethanol	74.475	-7164.3	-7.327	3.1340E-6	2
P	Propanol	88.134	-8498.6	-9.0766	8.3303E-18	6

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