

# MS EXCEL AND VBA FOR CHEMICAL ENGINEERS

TSEC - ONLINE CERTIFICATE COURSE

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## QUESTION SET

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Date: 09 - 06 - 2024

### 1 Vapor pressure data representation by polynomials and equations

Table 1 presents data of vapor pressure versus temperature for benzene. Some design calculations require these data to be accurately correlated by various algebraic expressions which provide  $P$  in mmHg as a function of  $T$  in  $^{\circ}\text{C}$ . A simple polynomial is often used as

Temperature, $T$ ( $^{\circ}\text{C}$ )	Pressure, $P$ (mm Hg)
-36.7	1
-19.6	5
-11.5	10
-2.6	20
+7.6	40
15.4	60
26.1	100
42.2	200
60.6	400
80.1	760

Table 1: Vapour pressure of Benzene

an empirical modeling equation. This can be written in general form for this problem as

$$P = a_0 + a_1T + a_2T^2 + a_3T^3 + \cdots + a_nT^n \quad (1)$$

where  $a_0, \cdots, a_n$  are the parameters (coefficients) to be determined by regression and  $n$  is the degree of the polynomial. Typically the degree of the polynomial is selected which

gives the best data representation when using a least-squares objective function.

The Clausius–Clayperon equation which is useful for the correlation of vapor pressure data is given by

$$\log_{10}(P) = A - \frac{B}{T + 273.15} \quad (2)$$

where  $P$  is the vapor pressure in mmHg and  $T$  is the temperature in  $^{\circ}\text{C}$ . Note that the denominator is just the absolute temperature in K. Both  $A$  and  $B$  are the parameters of the equation which are typically determined by regression.

The Antoine equation which is widely used for the representation of vapor pressure data is given by

$$\log_{10}(P) = A - \frac{B}{T + C} \quad (3)$$

where typically  $P$  is the temperature in  $^{\circ}\text{C}$ . Note that this equation has parameters  $A$ ,  $B$  and  $C$  which must be determined by nonlinear regression as it is not possible to linearize this equation. The Antoine equation is equivalent to the Clausius–Clayperon equation when  $C = 273.15$

1. Regress the data with polynomials having the form of Equation 1. Determine the degree of polynomial which best represents the data.
2. Regress the data using linear regression on Equation 2
3. Regress the data using nonlinear regression on Equation 3

## 2 Steady state Material balances on a separation train

Xylene, styrene, toluene and benzene are to be separated with the array of distillation columns that is shown below where  $F$ ,  $D$ ,  $B$ ,  $D_1$ ,  $B_1$ ,  $D_2$  and  $B_2$  are the molar flow rates in mol/min.

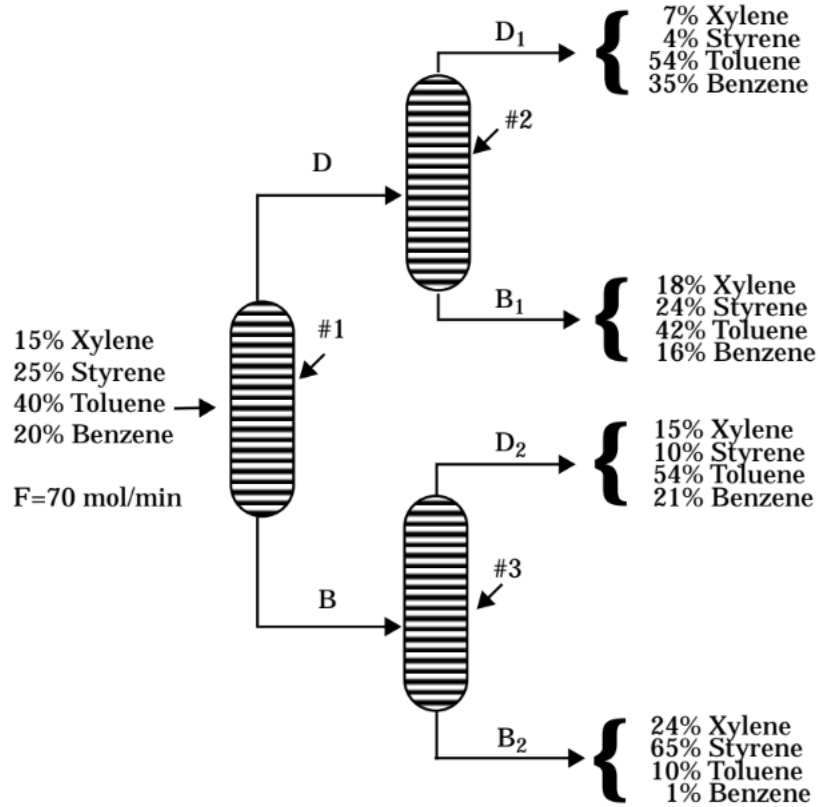


Figure 1: Separation Train

Material balances on individual components on the overall separation train yield the equation set

$$\text{Xylene : } 0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 0.15 \times 70$$

$$\text{Styrene : } 0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2 = 0.25 \times 70$$

$$\text{Toluene : } 0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2 = 0.40 \times 70$$

$$\text{Benzene : } 0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 0.20 \times 70$$

Overall balances and individual component balances on column #2 can be used to determine the molar flow rate and mole fractions from the equation of stream D from

$$\text{Molar Flow Rates : } D = D_1 + B_1$$

$$\text{Xylene : } X_{Dx}D = 0.07D_1 + 0.18B_1$$

$$\text{Styrene : } X_{Ds}D = 0.04D_1 + 0.24B_1$$

$$\text{Toluene : } X_{Dt}D = 0.54D_1 + 0.42B_1$$

$$\text{Benzene : } X_{Db}D = 0.35D_1 + 0.16B_1$$

where  $X_{Dx}$  = mole fraction of Xylene,  $X_{Ds}$  = mole fraction of Styrene,  $X_{Dt}$  = mole fraction of Toluene and  $X_{Db}$  = mole fraction of Benzene. Similarly, overall balances and individual component balances on column #3 can be used to determine the molar flow rate and mole fractions of stream B from the equation set

$$\text{Molar Flow Rates : } B = D_2 + B_2$$

$$\text{Xylene : } X_{Bx}B = 0.15D_2 + 0.24B_2$$

$$\text{Styrene : } X_{Bs}B = 0.10D_2 + 0.65B_2$$

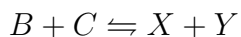
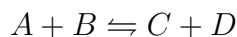
$$\text{Toluene : } X_{Bt}B = 0.54D_2 + 0.10B_2$$

$$\text{Benzene : } X_{Bb}B = 0.21D_2 + 0.01B_2$$

1. Calculate the molar flow rates of streams  $D_1$ ,  $D_2$ ,  $B_1$  and  $B_2$ .
2. Determine the molar flow rates and compositions of streams  $B$  and  $D$ .

### 3 Reaction Equilibrium for Multiple Gas Phase Reactions

The following reactions are taking place in a constant volume, gas-phase batch reactor.



A system of algebraic equations describes the equilibrium of the above reactions. The nonlinear equilibrium relationships utilize the thermodynamic equilibrium expressions, and the linear relationships have been obtained from the stoichiometry of the reactions.

$$\begin{aligned} K_{C_1} &= \frac{C_C C_D}{C_A C_B} & K_{C_2} &= \frac{C_X C_Y}{C_B C_C} & K_{C_3} &= \frac{C_Z}{C_A C_X} \\ C_A &= C_{A0} - C_D - C_Z & C_B &= C_{B0} - C_D - C_Y \\ C_C &= C_D - C_Y & C_Y &= C_X + C_Z \end{aligned}$$

In this equation set  $C_A$ ,  $C_B$ ,  $C_C$ ,  $C_D$ ,  $C_X$ ,  $C_Y$  and  $C_Z$  are concentrations of the various species at equilibrium resulting from initial concentrations of only  $C_{A0}$  and  $C_{B0}$ . The equilibrium constants  $K_{C_1}$ ,  $K_{C_2}$  and  $K_{C_3}$  have known values.

Solve this system of equations when  $C_{A0} = C_{B0} = 1.5$ ,  $K_{C_1} = 1.06$ ,  $K_{C_2} = 2.63$  and  $K_{C_3} = 5$  starting from three sets of initial estimates

1.  $C_D = C_X = C_Z = 0$
2.  $C_D = C_X = C_Z = 1$
3.  $C_D = C_X = C_Z = 10$

## 4 Chemical reaction in a perfectly stirred tank

Suppose chemical A is in solution in a perfectly stirred tank and its concentration is  $C_A^\circ$  (g/L) . The constant volumetric flow into and out of the tank is  $F$  (L/min) and the tank volume is  $V$ (L). A mass balance on component A leads to

$$V \frac{dC_A}{dt} = -FC_A \quad (4)$$

The analytical solution is

$$C_A = C_A^\circ e^{-tF/V} \quad (5)$$

The calculations for the fourth-order RK method are shown below

$$\begin{aligned} k_1 &= dt f(C_{A,n}, t_n) \\ k_2 &= dt f(C_{A,n} + \frac{k_1}{2}, t_n + \frac{dt}{2}) \\ k_3 &= dt f(C_{A,n} + \frac{k_2}{2}, t_n + \frac{dt}{2}) \\ k_4 &= dt f(C_{A,n} + k_3, t_n + dt) \\ C_{A,n+1} &= C_{A,n} + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \end{aligned}$$

Use  $dt = 0.1$  min and  $\tau = V/F = 0.5$  min. Compare with the analytical solution.

## 5 Heat Exchange in a series of tanks

Three tanks in series are used to preheat a multi-component oil solution before it is fed to a distillation column for separation as shown in Figure 2. Each tank is initially filled with 1000 kg of oil at 20 C. Saturated steam at a temperature of 250 C condenses within coils immersed in each tank. The oil is fed into the first tank at the rate of 100 kg/min and overflows into the second and the third tanks at the same flow rate. The temperature of the oil fed to the first tank is 20 C. The tanks are well mixed so that the temperature inside the tanks is uniform, and the outlet stream temperature is the temperature within the tank. The heat capacity,  $C_p$ , of the oil is 2.0 KJ/kg. For a particular tank, the rate at which heat is transferred to the oil from the steam coil is given by the expression

$$Q = UA(T_{steam} - T) \quad (6)$$

where  $UA = 10$  kJ/min-C is the product of the heat transfer coefficient and the area of the coil for each tank,  $T$  = temperature of the oil tank in C, and  $Q$  = rate of heat transferred in kJ/min. Energy balances can be made on each of the individual tanks. In these balances, the mass flow rate to each tank will remain at the same fixed value. Thus  $W = W_1 = W_2 = W_3$ . The mass in each tank will be assumed constant as the tank volume and oil density are assumed to be constant. Thus  $M = M_1 = M_2 = M_3$ . For the first tank, the energy balance can be expressed by

$$\text{Accumulation} = \text{Input} - \text{Output}$$

$$MC_p \frac{dT_1}{dt} = WC_p T_0 + UA(T_{steam} - T_1) - WC_p T_1 \quad (7)$$

Note that the unsteady state mass balance is not needed for tank 1 or any other tanks since the mass in each tank does not change with time. The above differential equation can be rearranged and explicitly solved for the derivative which is the usual format for

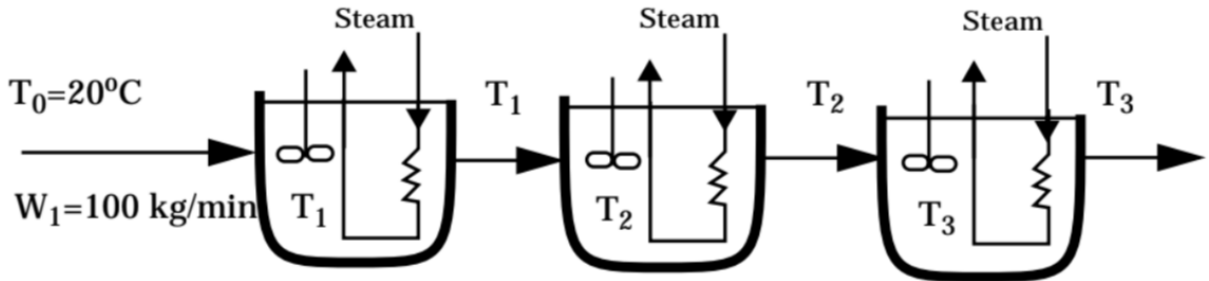


Figure 2: Series of Tanks for Oil Heating

numerical solution.

$$\frac{dT_1}{dt} = \frac{WC_p(T_0 - T_1) + UA(T_{steam} - T_1)}{MC_p} \quad (8)$$

Similarly for the second tank

$$\frac{dT_2}{dt} = \frac{WC_p(T_1 - T_2) + UA(T_{steam} - T_2)}{MC_p} \quad (9)$$

For the third tank

$$\frac{dT_3}{dt} = \frac{WC_p(T_2 - T_3) + UA(T_{steam} - T_3)}{MC_p} \quad (10)$$

Determine the steady state temperatures in all three tanks. What time interval will be required for  $T_3$  to reach 99% of this steady state value during startup?