CHE F418 (Modeling and Simulation in Chemical Engineering)

Marks: 90 **Time: 2- 3:30 PM** **Date: 14/03/2023**

Time: 90 minutes

Note:

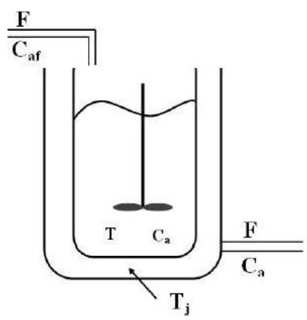
- **After completion, send the file with extension ".R" files to 'modsim418@gmail.com'.**
- **Marks would be awarded based on the approach and simulation results.**

Part-A

1. (a) What is difference between lumped and distributed parameter model. Explain by giving classical example of chemical engineering in form of mathematical expressions.

(b) What do you understand with ANOVA analysis in data-modeling. Describe the significance of the p-value, t-value, MAPE and RMSE of the model.

(c) Carry out the mass and energy balance for a non-isothermal continuously stirred tank reactor (CSTR) system of volume V as depicted below. Based on derived ODEs, carry out the degree of freedom (DOF) analysis and justify your statement. The reaction scheme for the given system is, a $\longrightarrow$ b, rate = -kCa.



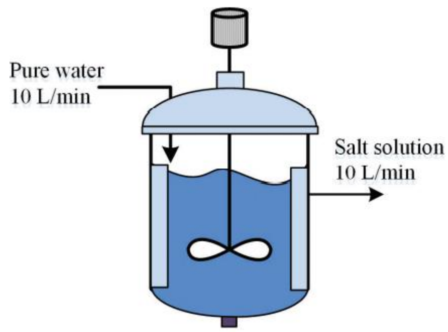
2. The Clausius–Clapyron equation relates the latent heat of vaporization to temperature and vapor pressure according to the following equation,

$$\ln(p) = -\frac{\Delta H_v}{RT} + k$$

The effects of temperature on vapor pressure is given in the datasheet. Build a linear regression model using R-programming and calculate the heat of vaporization (ΔH_v) in kJ/mol and *k*.

1/T	ln(P)
0.002755	6.2649
0.002740	6.3404
0.002725	6.4149
0.002710	6.4886
0.002695	6.5615
0.002681	6.6333

3. Pure water turns into a well-mixed tank filled with 100 L of brine. Water flows at a constant volumetric feed rate of 10 L/min. Initially, the brine has 7.0 kg of salt dissolved in the 100 L of water. The salt solution flows out of the tank at the same inlet volumetric flow rate of water. After 15 min of operation, calculate the amount of salt remaining in the tank. Plot the concentration of the salt versus time using R-ode solver.



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Part-B:

1. The excess molar enthalpy for a binary system (ethanol and water) is given in table below. x_1 and x_2 is the mole fraction of component 1 (ethanol) and component 2 (water).
   (a) Estimate the model parameter of the model equation as given below (a, b and c) using R-optimizer.
   (b) Predict the value for excess molar enthalpy of the binary system at 0.65 & 0.85 mole fraction of ethanol.

x_1	H^E /J·mol^{-1}
0.0426	−23.3
0.0817	−45.7
0.1177	−66.5
0.1510	−86.6
0.2107	−118.2
0.2624	−144.6
0.3472	−176.6
0.4158	−195.7

$$H^E = x_1 x_2 \left(a + b x_1 + c x_1^2\right)$$

2. Three tanks in series are used to heat oil. Each tank is initially filled with 1000 kg of oil at 20°C. Saturated steam at 250°C condenses within the coils immersed in each tank. Oil is fed into first tank at a rate of 2 kg/s and overflows into the second and third tank at the same flow rate. The temperature of oil fed to the first tank is 20°C. The tanks are well mixed so that the temperature if the oil fed to the first tank is 20°C. The tanks are well mixed so that temperature inside the tank is uniform and the outlet stream temperature is the temperature within the tank. The heat capacity (Cp) of the oil is 2000 J/kg.K. The rate of heat transferred to the oil from the steam us given by Q= UA (T_s-T), where A is outside area of the coil of the tank, A= 1 m^2 and the overall heat transfer coefficient is based on the outside area of the coil, U= 100 $W/m^2.K$.
   Show the control volume for the system and carry out the energy balance across the control volume. Determine the steady state temperature in all the three tanks. What time is required for tank three, T_3 to reach the 99% of the steady state value.