UNIVERSITI TEKNOLOGI PETRONAS

FINAL EXAMINATION
JANUARY 2025 SEMESTER

COURSE	**:**	**CFB2083 - PROCESS MODELLING & SIMULATION**
DATE	**:**	**19 APRIL 2025 (SATURDAY)**
TIME	**:**	**9.00 AM - 12.00 NOON (3 HOURS)**

INSTRUCTIONS TO CANDIDATES

1. Answer **ALL** questions in the Answer Booklet.
2. Begin **EACH** answer on a new page in the Answer Booklet.
3. Indicate clearly answers that are cancelled, if any.
4. Where applicable, show clearly steps taken in arriving at the solutions and indicate **ALL** assumptions, if any.
5. **DO NOT** open this Question Booklet until instructed.

Note :

i. There are **TEN (10)** pages in this Question Booklet including the cover page and appendix.

ii. **DOUBLE-SIDED** Question Booklet.

1. Given that a stirred tank with volumetric holdup, V [m^3], is used to blend two streams of components A and B, as shown in **FIGURE Q1.**

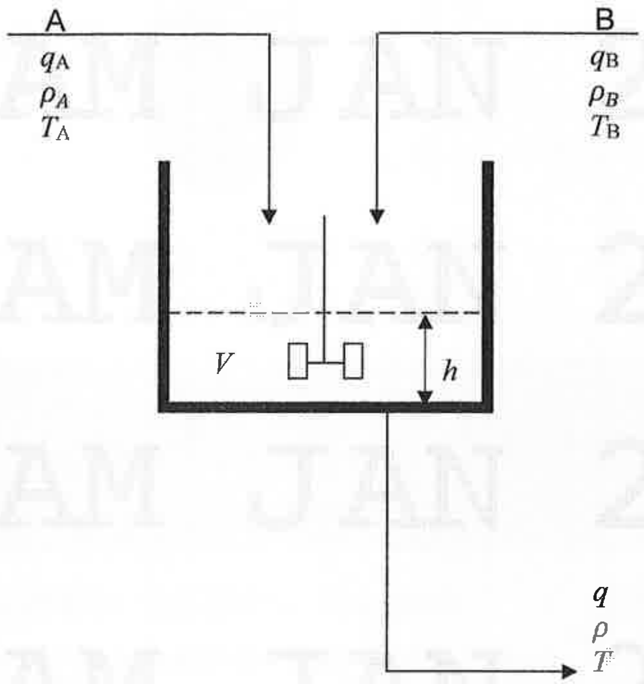

FIGURE Q1: A stirred tank to blend components A and B

The tank is filled with components A and B at volumetric flow rates [m^3/s] of q_A and q_B, densities [kg/m^3] of ρ_A and ρ_B, and temperatures [K] of T_A and T_B. The volumetric flow rate [m^3/s], density [kg/m^3] and temperature [K] of the stream flowing out from the tank are q, ρ and T.

Density, ρ [kg/m^3], is reported to be independent on species concentration but dependent on temperature, T, with the following relation based on measurement from plant data:

$$\rho = \alpha T + \beta$$

In which α [kg/(K.m^3)] and β [kg/m^3] are coefficients of the model.

It is given that the tank has a cross-sectional area of A_c [m^2]. Additionally, the dynamic equation that quantifies the change of temperature in the tank is given by the following equation:

$$\frac{dT}{dt} = \frac{\rho_A q_A (T_A - T) + \rho_B q_B (T_B - T)}{\rho V}$$

As a process engineer working in the plant, you are tasked to develop a dynamic equation for the liquid height in the tank [m], h, to ensure no overspill occurs during the blending process.

a. Identify and elaborate the system, surroundings and boundaries properly associated with the modelling objective. In addition, support the classification of system, surroundings and boundaries with sketch.

[9 marks]

b. Classify the types of process model that can be developed based on the listed criteria with suitable justification.

i. Behaviour of intensive property with position in the tank
ii. Time
iii. Equations involved in the models (e.g., first-principle, empirical and hybrid)

[6 marks]

c. Examine the suitable dynamic equation for the liquid height in the tank, h, by making at least **TWO (2)** assumptions. Show full steps from fundamental equation. Simplify the process model whenever possible.

[10 marks]

2. Consider a semi-batch stirred tank reactor with constant volumetric liquid holdup, V [m^3], as shown in **FIGURE Q2**.

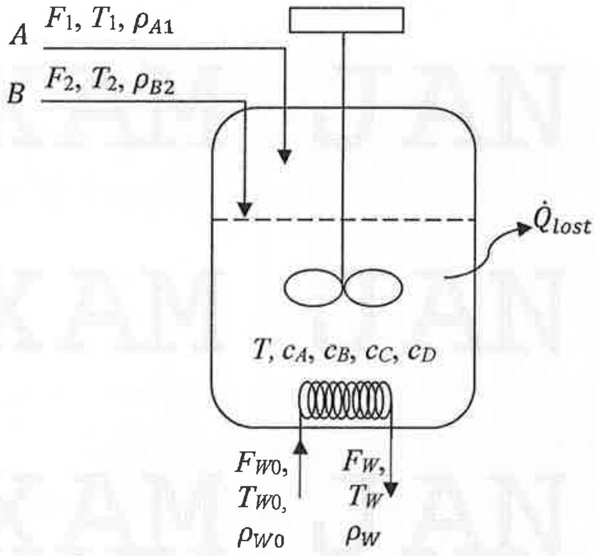

FIGURE Q2: A stirred tank reactor under semi-batch operation

Notations:

c_i = concentration of species i [kmol/m^3]

F_j = volumetric flow rate for stream j [m^3/s]

ρ_{ij} = density of species i for stream j [kg/m^3]

T_j = temperature for stream j [K]

MW_i = molecular weight of component i [kg/kmol]

It is given that specific heat capacities, c_p, are independent of species and temperature [kJ/kg.K]. On the other hand, density is reported to be an intensive property that depends on the species concentration.

Consider that the following elementary reactions take place in the reactor:

Reaction 1: 2A → 7B + 5C : $-r_A = k_1 c_A{}^2$ [kmol/(s·m^3)]

Reaction 2: A+B → 3C : $r_C = k_2 c_A c_B$ [kmol/(s·m^3)]

The reactor is heated with a coil of constant volumetric holdup, V_W [m^3], in which water is flowing in at temperature T_{W0} [K], volumetric flowrate F_{W0} [m^3/s] and density ρ_{W0} [kg/m^3], while flowing out with a temperature T_W [K], volumetric flowrate F_W [m^3/s] and density ρ_W [kg/m^3]. Given that hot water is passed through the coil as heating medium. Additionally, heat of reaction for Reaction 1 and Reaction 2 are ΔH_1 [kJ/kmol of C produced] and ΔH_2 [kJ/kmol of C produced], respectively, in which both reactions are endothermic in nature. U_c is the overall heat transfer coefficient [kW/(m^2·K)] and A_c is the surface area of the coil [m^2]. Moreover, $\dot{Q}_{lost}$ [kJ/s] is the amount of energy that is lost to the environment and has been reported to be significant.

a. Identify any **THREE (3)** variables and **THREE (3)** parameters from the problem statement.

[3 marks]

b. Identify any **THREE (3)** ongoing processes within the system of interest.

[3 marks]

c. Develop dynamic mathematical model for the following intensive property inside the reactor by making **TWO (2)** assumptions for each model in (i) and (ii). Show full steps from fundamental equation. Simplify the model whenever possible.

i. Concentration of species B (c_B).

[7 marks]

ii. Temperature of the reaction mixture (T).

[12 marks]

3. A flash separator in a chemical plant is used to separate a binary feed that contains water and ethanol as shown in **FIGURE Q3**.

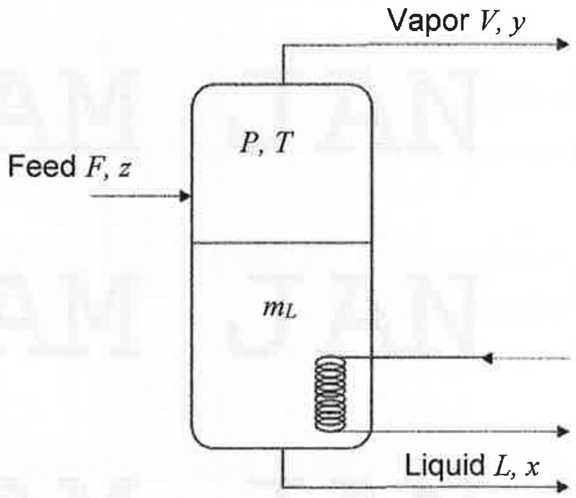

FIGURE Q3: A flash separator

The flash separator is operated with a total pressure of 101.325 kPa. It is fed with a saturated liquid with mass flow rate F = 100 kg/s and mass fraction of z = 0.5 for ethanol. Ethanol is the more volatile component with vapor mass fraction y and liquid mass fraction x in the overhead and bottom streams, respectively. Additionally, it has been reported by the plant operator that liquid holdup [kg], m_L, of the flash separator is constant.

a. Determine the steady state models for the overall mass and component balances of the flash separator. State all assumptions made and constitutive relations used.

[7 marks]

b. Properties of ethanol and water have been summarized in **TABLE Q3b**. Saturated vapor pressure of species i, P_{vi}, is given by Antoine equation, whereby P_{vi} is in kPa and T is in °C:

$$log_{10}(P_{vi}) = A_i - \frac{B_i}{C_i + T}$$

TABLE Q3b: Coefficients for Antoine Equation

Species i	Coefficients for Antoine Equation			T_B
	A	B	C	(°C)
Water	16.4	3885.7	230.2	100.0
Ethanol	16.9	3795.2	231.0	78.2

Using Secant method, estimate the bubble point temperature of the flash separator under steady state operation when x = 0.45. Show full steps hand calculation up until **THREE (3)** iterations. From the estimated bubble point temperature, calculate the vapor phase composition, y, vapor mass flow rate, V, and liquid mass flowrate, L, of the flash separator under steady state operation.

[18 marks]

4. A parallel reaction occurs in a plug flow reactor with properties at time t as shown in **FIGURE Q4**. The variables along the length of the reactor are given by concentration of species j [kmol/m^3], c_j, temperature [K], T, and velocity [m/s], v. At inlet position z = 0 m, the concentration of species A is c_{Ai} [kmol/m^3], temperature is T_i [K] while velocity is v_i [m/s]. On the other hand, at outlet position z = L m, the concentration of species A, B and C [kmol/m^3] are c_{Ao}, c_{Bo} and c_{Co}, temperature is T_o [K] and velocity is v_o [m/s].

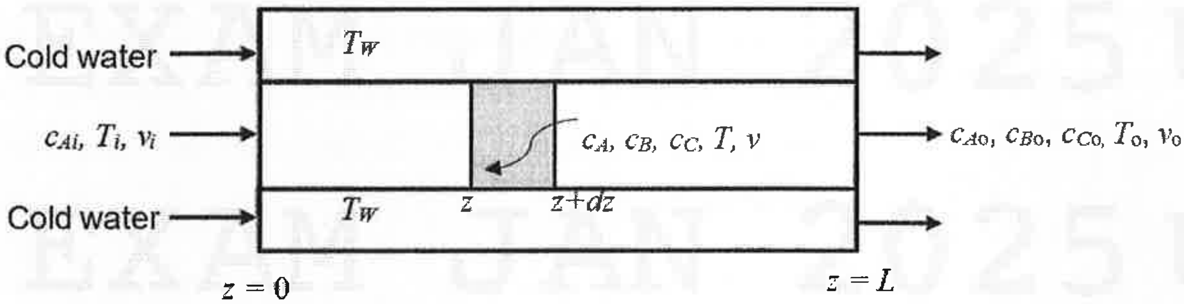

FIGURE Q4: A plug flow reactor with parallel reactions

The plug flow reactor has constant tube side diameter D_T [m]. Consider that the following exothermic reactions take place in the reactor:

2A → 5B + C	: $-r_A = k_1 c_A^2$ [kmol/(s·m^3)]	: ΔH_1 [kJ/kmol A reacted]
A + 2B → 3C	: $-r_A = k_2 c_A c_B^2$ [kmol/(s·m^3)]	: ΔH_2 [kJ/kmol B reacted]

The reactor is cooled with cold water flowing within the shell in a concurrent direction with respect to the tube side at constant temperature T_w [K]. The overall heat transfer coefficient between the shell and tube sides is U_C [kW/(m^2·K]. Properties in the tube side can change as the fluid flows along the axial or z direction. There are no radial gradients in all properties, but axial gradients may exist. It is given that specific heat capacity [kJ/kg.K], c_p, is independent of species and temperature. On the other hand, density [kg/m^3], ρ, has been reported to be dependent on species concentration.

a. Develop the following mathematical models in the plug flow reactor using suitable fundamental relations and assumptions.

   i. Mass balance

   [5 marks]

   ii. Component balance for species A, B and C

   [9 marks]

   iii. Energy balance

   [8 marks]

b. Comment on how the resulting model equation can be solved using suitable numerical methodology and boundary or initial conditions.

   [3 marks]

-END OF PAPER-

APPENDIX

Secant method

$$x_{i+1} = x_i - \frac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)}$$

Overall mass balance

$$\frac{dm}{dt} = \sum_{j=1}^{N_{in}} \dot{m}_{in,j} - \sum_{j=1}^{N_{out}} \dot{m}_{out,j}$$

Component balance for species *i* in molar basis

$$\frac{dN_i}{dt} = \sum_{j=1}^{N_{in}} \dot{N}_{in,i,j} - \sum_{j=1}^{N_{out}} \dot{N}_{out,i,j} + \sum_{j=1}^{N_r} r_{ij} V$$

Energy balance

$$\frac{d(m.h)}{dt} = \dot{m}_{in} h_{in} - \dot{m}_{out} h_{out} + V \sum_{j=1}^{N_r} -\Delta \widehat{H_{r,j}} | r_{gen,ij} | + \Delta \dot{Q} + \Delta \dot{W}$$