UNIVERSITI TEKNOLOGI PETRONAS

FINAL EXAMINATION
MAY 2024 SEMESTER

COURSE : **CEB2053/CFB2083 - PROCESS MODELLING & SIMULATION**

DATE : **2 AUGUST 2024 (FRIDAY)**

TIME : **3.00 PM - 6.00 PM (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. a. Liquid surge tanks, particularly those containing hydrocarbons, often have a gas "blanket" of nitrogen. This gas blanket is maintained to prevent the accumulation of explosive vapors above the liquid. The inert nature of nitrogen helps to reduce the risk of ignition and explosion by displacing flammable vapours that could be present. An example of a liquid surge tank is shown in **FIGURE Q1a.**

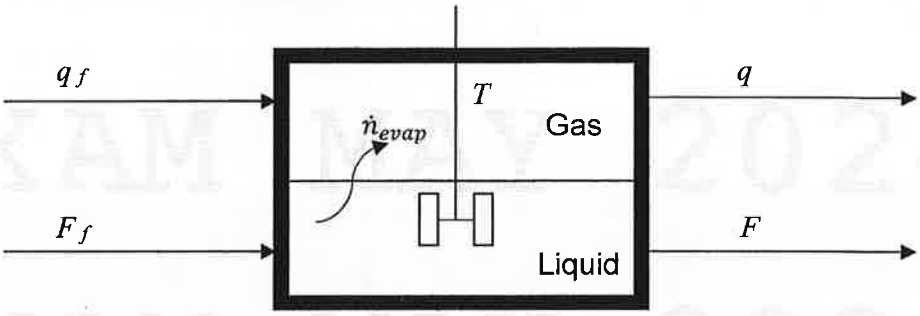


FIGURE Q1a: A liquid surge tank with gas blanket

Given that q_f and q represent the inlet and outlet gas molar flow rates (kmol/s) while F_f and F the inlet and outlet liquid molar flow rates (kmol/s). Both gas and liquid flow rates are constant with time. Additionally, V is the total volume of the surge tank (m^3), V_l is the liquid volume (m^3), P is the gas pressure (Pa) and T is the temperature inside the tank (K). $\dot{n}_{evap}$ is the rate of hydrocarbons evaporation (kmol/s) from the liquid to vapour phase that is dependent on T. Temperature of the vapor phase is equal to the liquid phase under thermal equilibrium assumption. Process models are required to monitor change in the liquid volumetric holdup, accumulation of pressure and temperature in the surge tank with time.

i. Identify and explain **THREE (3)** different types of process models that can be developed based on the behaviour of intensive property with position, time and equations.

[6 marks]

ii. Identify and elaborate the system, surroundings and boundaries properly associated with **ONE (1)** objective.

[9 marks]

b. A n-stages distillation column with a total condenser and a partial reboiler is separating a mixture containing components A and B as shown in **FIGURE Q1b**.

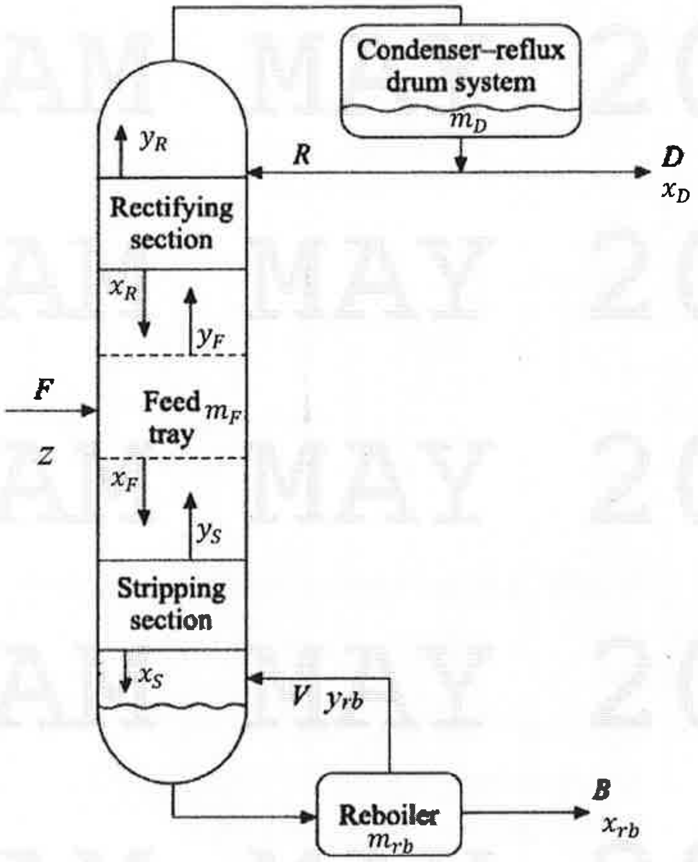


FIGURE Q1b: Distillation column to separate components A and B

A partially vaporized feed is fed to the distillation column with vapor fraction of δ. F, B, D, R and V are mass flow rates (kg/s) of the distillation column for the feed tray, column bottom, distillate, reflux and boil-up vapour, respectively. z, x and y are mass fractions for the more volatile component A. Mass fractions for vapor and liquid phases are represented by y and x, respectively. z is mass fraction for stream containing a mixture of liquid and vapor. It has been reported that liquid holdup (e.g., m_F, m_D and m_{rb}) is constant for all compartments in the distillation column. Apply mass and component balances to describe dynamic variations in liquid mass fractions of component A for the condenser and reboiler with **TWO (2)** assumptions. Simplify the model whenever possible.

[10 marks]

2. Consider a stirred tank reactor under semi-batch operation with volumetric liquid holdup, V (m^3), and liquid height, h (m) that are changing with time as shown in **FIGURE Q2**. Cross sectional area of the reactor is given by A_c (m^2).

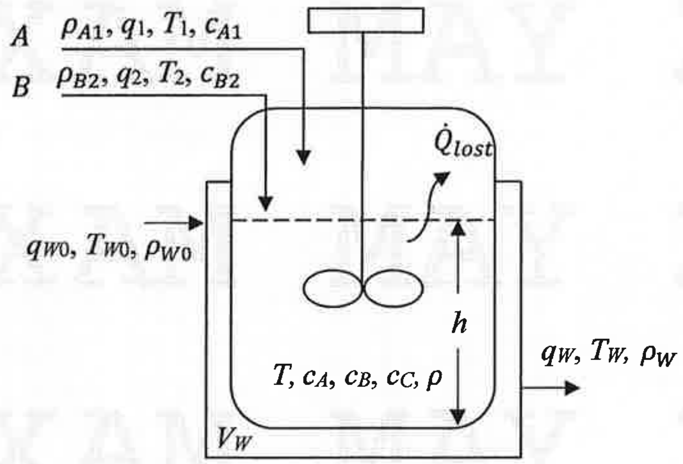


FIGURE Q2 A stirred tank reactor under semi-batch operation

Notations:

c_{ij} = concentration of species i for stream j (kmol/m^3)

q_j = volumetric flow rate for stream j (m^3/s)

ρ_j = density 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]. However, density of the reaction mixture changes with time and is reported to temperature, T, dependent:

$$\rho = \alpha T^2 + \beta T + \gamma$$

In which α, β and γ are coefficients in the empirical model.

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 wrapped with a jacket with constant volumetric holdup, V_W (m^3), in which water is flowing in at temperature T_{W0}, flowrate q_{W0} and density ρ_{W0}, while flowing out with a temperature T_W, flowrate q_W and density ρ_W . It is given that hot water is passed through the jacket 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 Reaction 1 is endothermic while Reaction 2 is exothermic in nature. U_j is the overall heat transfer coefficient (kW/(m^2·K)) and A_j is the surface area of the jacket surrounding the tank (m^2). Moreover, $\dot{Q}_{lost}$ (kJ/s) is the amount of energy that is lost to the environment.

By making at least **TWO (2)** unique assumptions for each, develop the following dynamic mathematical models to describe change of property inside the reactor. Show full steps from fundamental equation. Simplify the models whenever possible.

a. Concentration of species B.

[13 marks]

b. Temperature of the reaction mixture.

[12 marks]

3. a. A CO_2-rich stream (F_1) with 100 kmol/h is to be treated in absorption column at steady-state to remove CO_2 from the natural gas using lean solvent as shown in **FIGURE 3a**:

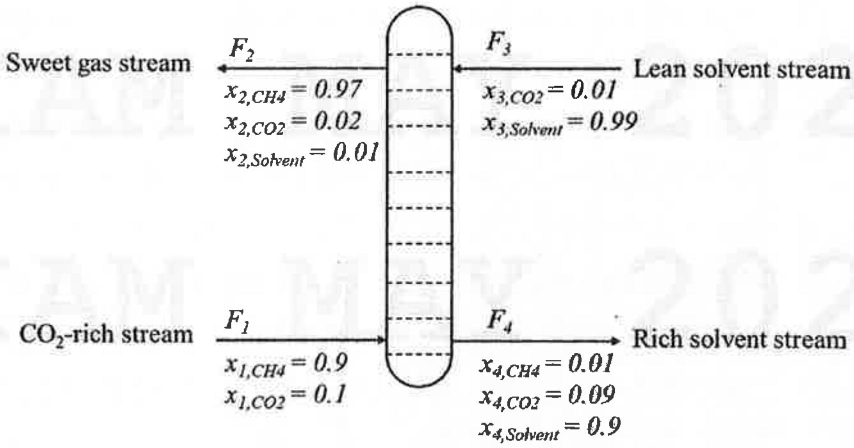


FIGURE 3a Absorption column

By using LU decomposition, determine the amount of the solvent required for the process (F_3), natural gas loss in rich solvent stream (in kmol/h), and the amount of sweet gas produced (F_2).

[15 marks]

b. An overhead vapor product of column C-101 is cooled down into liquid in heat exchanger (HX-102). The product exits the HX-102 with volumetric flowrate of F_D and enters a reflux drum (C-102). Part of the exit of C-102 is return back to the distillation column with volumetric flowrate of F_R, which controlled by valve V-101 opening of x (0 = fully closed, 1 = fully open). The remaining exit of C-102, F_P is sent to the next processes (**FIGURE 3b**).

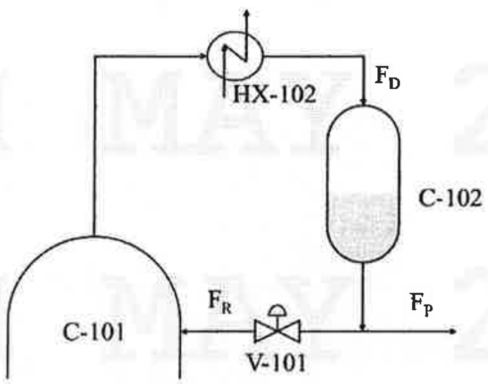


FIGURE 3b Stripping section of a distillation column

Given the change of liquid height (h) in the C-102 against time is:

$$\frac{dh}{dt} = F_D - 7.5\sqrt{h} - 6x\sqrt{h}$$

The process is now at steady-state with the valve opening is at 50% with F_D = 12 m^3/h. The valve opening suddenly increases to 70%. Sketch the liquid height profile (h) against time from t = 0 to t = 1 h, with Δt = 0.2 h.

[10 marks]

4. a. Discuss the importance of selecting the appropriate thermodynamic model in performing process simulation by providing example(s).

[5 marks]

b. Define the first-principle, empirical, and hybrid model. By providing a process example, discuss how empirical model can be useful to engineer.

[10 marks]

c. Given a wet gas stream, containing natural gas with moisture, enters a dehydration unit to remove moisture by using lean triethylene glycol (TEG) stream through absorption process (**FIGURE Q4a**).

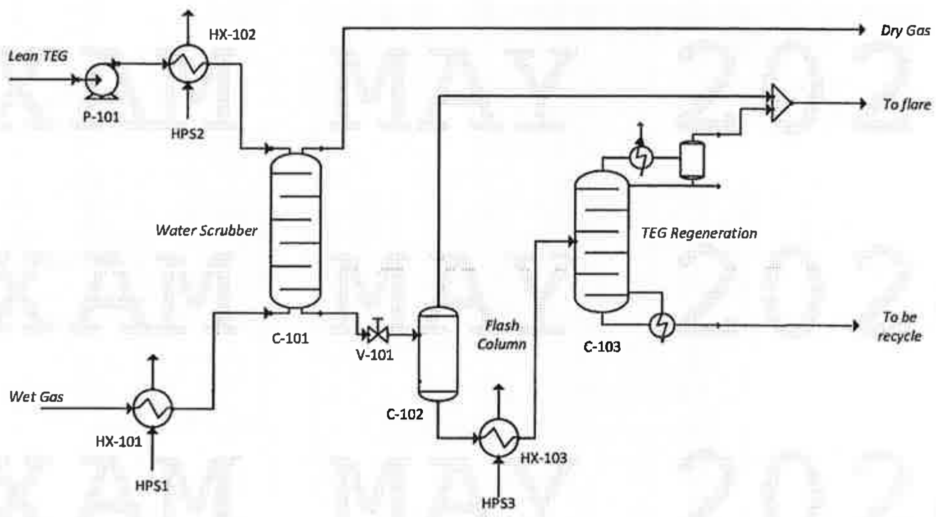


FIGURE Q4c: Process flow diagram (PFD) of dehydration unit

The process can be controlled by manipulating high pressure steam flowrates (HPS1,2 and 3), pump (P-101) outlet pressure, and valve (V-101) opening prior to the flash separator. Explain and justify the impact of **TWO (2)** variables change towards **ONE (1)** key performance of the process.

[10 marks]

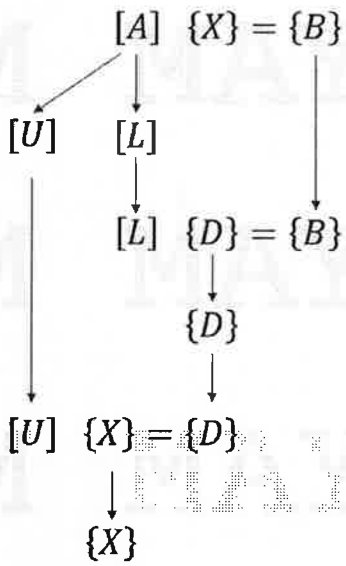
-END PAPER-

APPENDIX

Given Matrix expression of $[A] \times [X] = [b]$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

Can be solved using LU decomposition:



Where the Upper Matrix $[U]$:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \rightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \rightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & a'_{32} & a'_{33} \end{bmatrix} \rightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix}$$

with:

- $a'_{22} = a_{22} - a_{21}(a_{12}/a_{11})$
- $a'_{23} = a_{23} - a_{21}(a_{13}/a_{11})$
- $a'_{32} = a_{32} - a_{31}(a_{12}/a_{11})$
- $a'_{33} = a_{33} - a_{31}(a_{13}/a_{11})$
- $a''_{33} = a'_{33} - a'_{32}(a'_{23}/a'_{22})$

Where the Lower Matrix $[L]$:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 0 \\ f_{21} & 1 & 0 \\ f_{31} & f_{32} & 1 \end{bmatrix}$$

with:

- $f_{21} = a_{21}/a_{11}$
- $f_{31} = a_{31}/a_{11}$
- $f_{32} = a'_{32}/a'_{22}$