CH620003 Process Modelling and Simulation

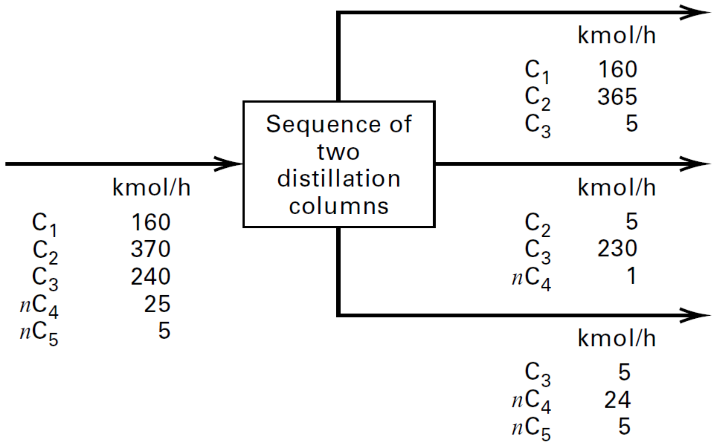
Assignment 3 Deadline to submit: **16 Mar 2025 (before 5 PM)**

Q1: SEQUENCING OF DISTILLATION COLUMN

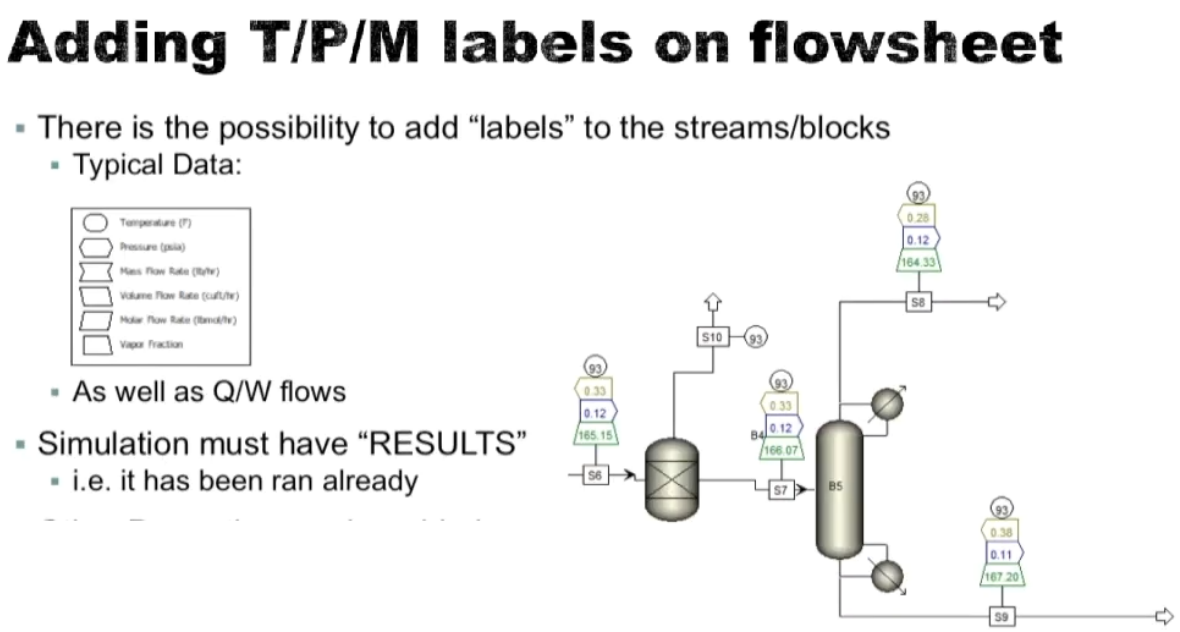
Two distillation columns are used to produce the products indicated in the Figure. Establish the type of condenser and an operating pressure for each column for the:

(a) direct sequence (C2/C3 separation first) and

(b) indirect sequence (C3/nC4 separation first).

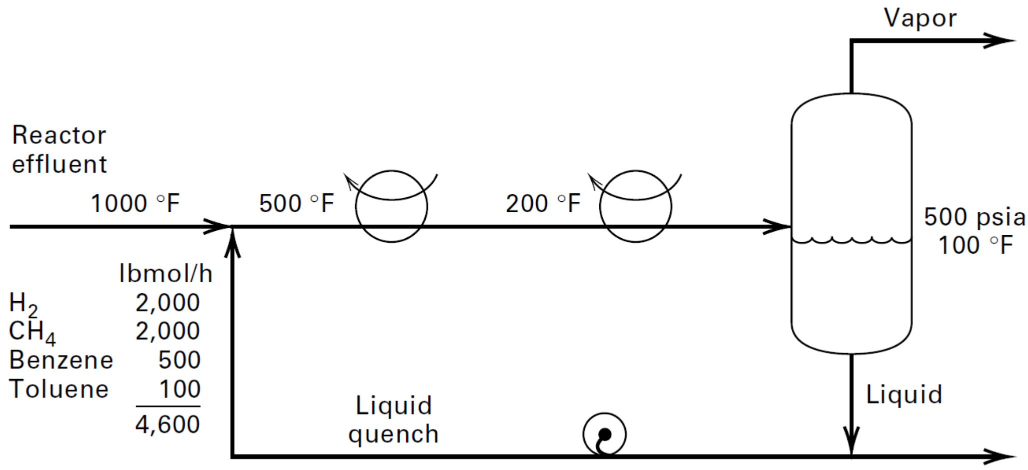


You must show the complete flowsheet for case (a) and case (b) scenarios including the process conditions (temperature, pressure and mass flow rates) of all streams embedded within the flow sheet with appropriate labelling (for reference see the illustration below).



Q2: RECYCLE STREAM

In the following figure, a system to cool reactor effluent and separate light gases from hydrocarbons is shown. K-values at 500 psia and 100 °F are:



Component	K_i
H_2	80
CH_4	10
Benzene	0.010
Toluene	0.004

(a) Calculate composition and flow rate of vapor leaving the flash drum.

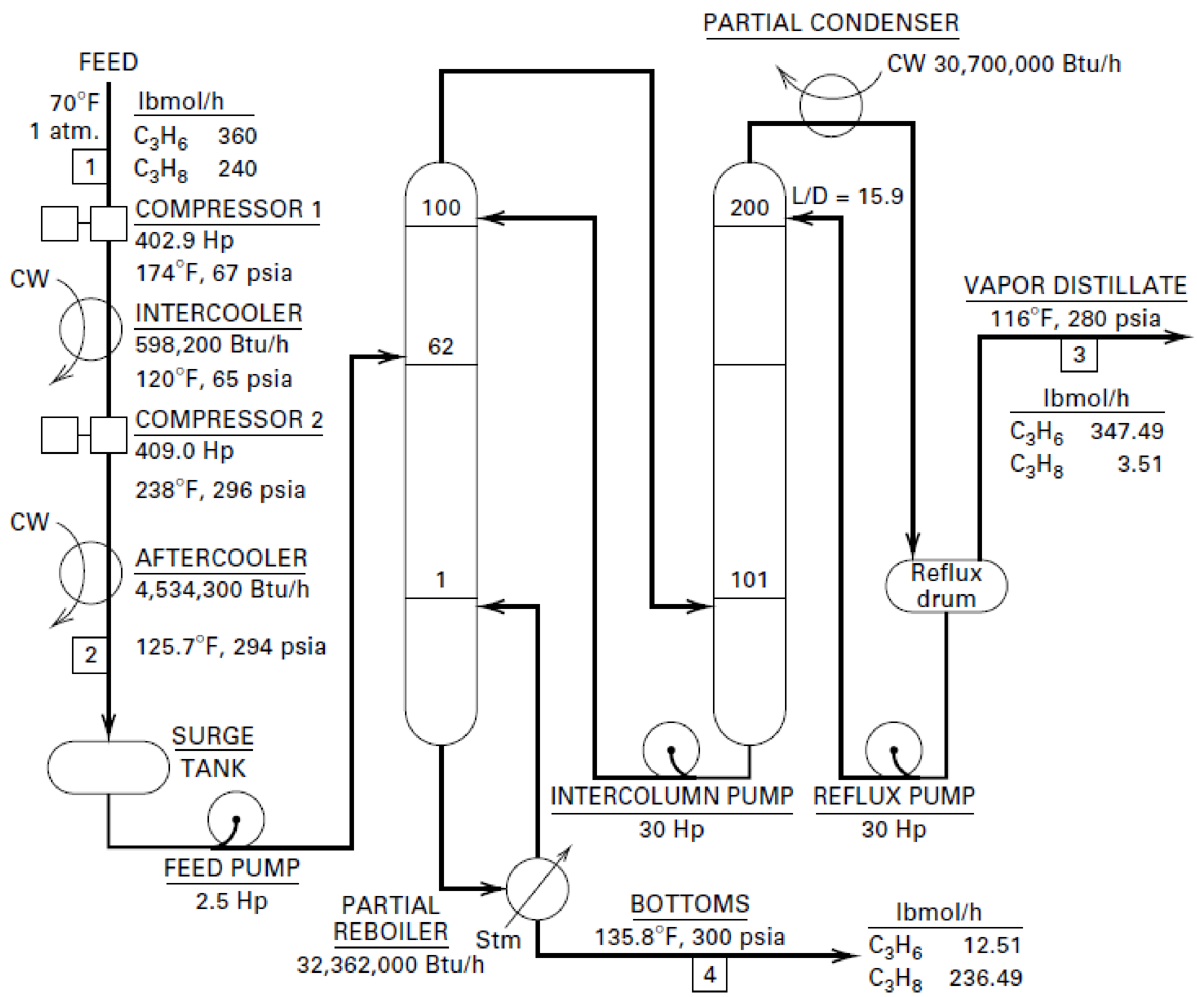
(b) Does the liquid-quench flow rate influence the result? Justify your answer.

Suggestion: Please do some background reading about quench(ing), to understand what exactly it means in this context.

You must show the complete flowsheet for case (a) and case (b) scenarios including the process conditions (temperature, pressure and mass flow rates) of all streams embedded within the flow sheet with appropriate labelling

Q3: SEPARATION OF PROPYLENE FROM PROPANE

A process for the separation of a propylene-propane mixture to produce 99 mol% propylene and 95 mol% propane is shown. Because of the high product purities and the low a, 200 stages may be required. A tray efficiency of 100% and tray spacing of 24 inches will necessitate two columns in series, because a single tower would be too tall. Assume a vapor distillate pressure of 280 psia, a pressure drop of 0.1 psi per tray, and a 2-psi drop through the condenser. The stage numbers and reflux ratio shown are only approximate. Use AspenPlus with a real gas Equation of State to determine the necessary reflux ratio for the stage numbers shown in the respective columns.

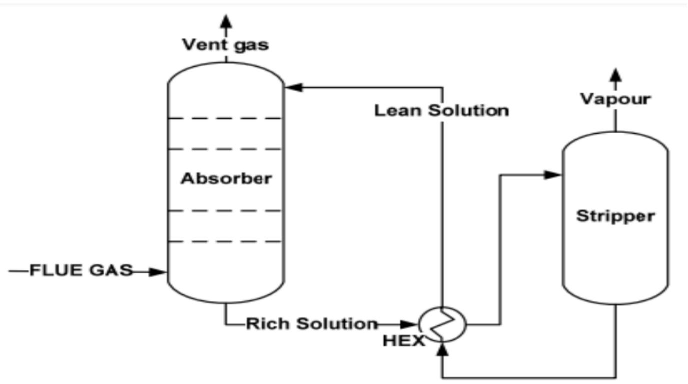


You must show the complete flowsheet including the process conditions (temperature, pressure and mass flow rates) of all streams embedded within the flow sheet with appropriate labelling

Q4: CO2 CAPTURE FROM AIR (FLUE GAS)

This is the basic operational flow diagram for amine absorption unit. The process is an exothermic, reversible reaction between a weak base (monoethanolamine, MEA) and a weak acid (CO2) that leads to the formation of dissolved salts. In the absorber, the inlet gas is treated with a lean solvent. The solvent preferentially absorbs the acid gases. The CO2-enriched solution is pre-heated before reaching the stripper, where the reaction is reversed by adding heat. The lean solvent escapes the stripper and is cooled by mixing heat with the rich solvent. The residual solvent is transferred to the absorber. A high purity CO2 is extracted from the stripper's tip.

A huge amount of heat is mandatory for the regeneration of rich solvent.



Typically, the flue gas contains around 5 – 15% CO2, by volume.

The overall forward reactions between CO2 and MEA are-

$$CO_2 + HO\,(CH_2)_2NH_2 \rightleftharpoons HO\,(CH_2)_2NHCOOH$$

$$HO(CH_2)_2NHCOOH + HO(CH_2)_2NH_2 \rightleftharpoons HO(CH_2)_2NHCOO^- + HO(CH_2)_2NH_3^+$$

The first step is rate determining and second-order. The second phase is a reaction that occurs instantly.

Develop a AspenPlus simulation model, for

(a) Cutting-off the CO2 emissions up to 85% by optimizing different parameters like MEA solvent, temperature, pressure, and reboiler duty.

(b) optimum reboiler duty by using heat of low pressure steam (waste steam) to reduce the operational cost.

You can use the ENTRL-RK or some appropriate thermodynamic method in Aspen Plus. Please do some background reading on the choice of suitable thermodynamic model for the CO2 capture application problem simulation.

You must show the complete flowsheet including the process conditions (temperature, pressure and mass flow rates) of all streams embedded within the flow sheet with appropriate labelling

Q5: DESIGN OF A MEMBRANE ELECTROLYSER FOR GREEN H2 PRODUCTION

Green hydrogen is produced by electrolyzing water, a process driven by renewable electricity sources like wind or solar power. The PEM electrolyser uses a solid polymer electrolyte to conduct protons from the anode to the cathode, where hydrogen gas is produced. This technology is favored for its rapid response times, high hydrogen purity, and compact design, making it suitable for integration with intermittent renewable energy sources. The Electrolyser simulation in Aspen Plus can be performed using the stack (applicable for part i and ii) component or the module (applicable for part iii).

(i) Perform (short-cut) simulation of the electrolyser and determine:

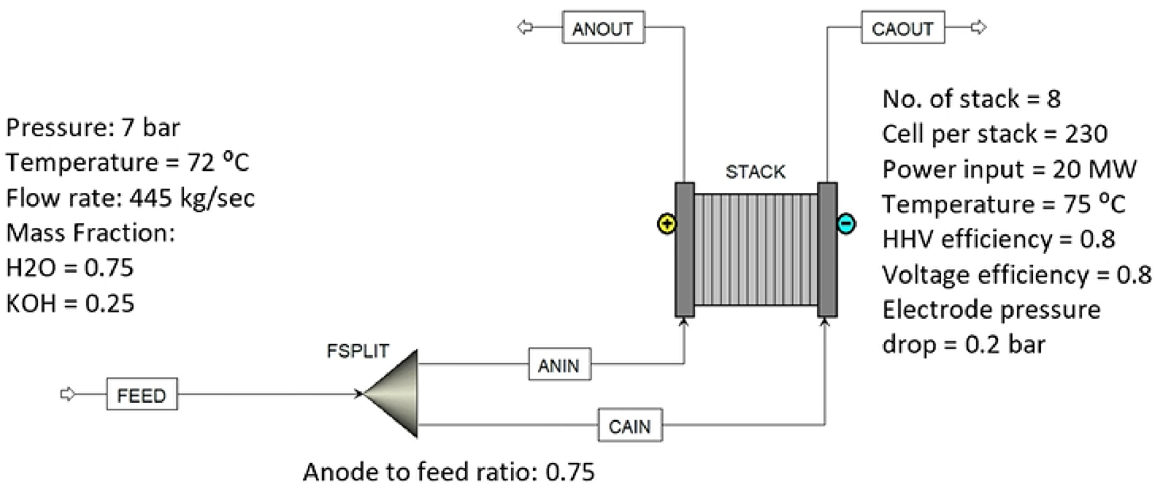
a. Rate of production of H2 and O2
b. Rate of water consumption and make-up water

(ii) Perform rigorous simulation using the geometrical parameters given below and determine:

a. Electrolyser efficiency
b. Energy requirements per unit mass of H2 production

(iii) Perform the same simulation using the electrolyser module and determine products.

a. The makeup water flow rate (consider 96% purity of H2 and O2).



Electrode Parameters for Rigorous simulation:

Parameter	Anode	Units	Cathode	Units
Active area	4	sqm	4	sqm
Width of channel	2	meter	2	meter
Length of channel	2	meter	2	meter
Separation b/w electrode and separator	1.25	mm	1.25	mm
Thickness of channel	2	cm	2	cm
Thickness of electrode	2	mm	2	mm
Bubble zone width	0.5	mm	0.5	mm
Resistivity	7.00E-08	ohm-cm	7.00E-08	ohm-cm

Membrane Parameters

Parameter	Value	Units
Active area	4	sqm
Thickness (ts)	0.5	mm