**Theory:**

The figure below, shows the schematic of the process:

A diagram of a flowchart

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The first reactor is adiabatic. T9 = T1, and stream 9 consists of pure CO2. The CO conversion is: XCO = 0.9XCOAD, EQ. The inlet mole fraction of CO2 for the second reactor equals 15%. The second reactor exchanges heat with surroundings. The pressure of outlet stream from second reactor decreases from 70 bar to 10 bar by a throttle valve. The pressure of Flash unit has been set to 10 bar and the recovery rate of Methanol in liquid phase (RRL) equals 70%.

***Assumptions:*** Ideal Gas – Ideal Liquid Mixture – NO POYNTING

**Demands:**

1. T4, y4
2. State 6,

**Resolutions:**

***1. T4, y4***

We want to solve stream “4”, so we need a suitable basis of calculation. If we plot conversion versus temperature, it will have a shape like this:

A graph on a chalkboard

Description automatically generated

The trendline represents *Energy Balance*, and the main curve represents the equilibrium equation. With the assigned conversion, we can find the corresponding temperature (T4). So, with respect to XCO = 0.9XCOAD, EQ, we can find the inlet temperature, and recalculate the process. First of all, we have to find the interception point of two curves.

The first approximation is there is not any CO2 in water.

Stream “1” is too complex to solve. Hence, we take a look at stream “2.”

Basis of Calculation: Stream “2” = 100 mol/s

The main reaction of first reactor is:

Using second session of practical, we have:

Then, we conduct a material balance:

The energy balance is:

The reference state is: Elementary species as ideal gas @ 298K.

***2.***

At node “b”, entering flows are 3,4,9 and exiting flow is 5. We can form a table like this:

|  |  |  |  |
| --- | --- | --- | --- |
| Stream | F | y | T |
| 3 | 1 unknown | known | known |
| 4 | known | known | known |
| 9 | 1 unknown | known | known |
| 5 | 1 unknown | NC unknown | known |

Write a global material balance:

Then, we can write material balance for each species:

In continue, we can write an energy balance for the system:

To simplifying the system, we compute yCO2,5 using this balance:

Therefore, we can couple these equations:

In Microsoft Excel, we have to guess F3 and F9. Then, using the goal seeking option, we solve the equations!

***For the second reactor***, T5 and y5 are known. Also, we have thermodynamic equilibrium in the outlet.

The occurred reactions are:

The material balance between stream 4 and 6 is:

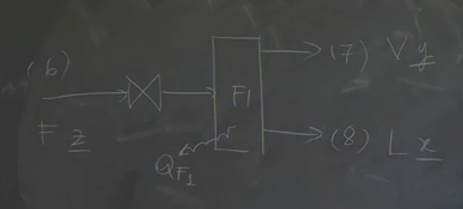
The energy balance is written as follows:

Conditions: Q>0 (removed) – same reference conditions as first reactor

Before going to separation section, we can calculate the overall conversion:

***Separation System:***

Inlet stream is stream 6, and outlet streams are stream 7 and 8.



The requests of problem are , TF1, x, y, and QF2. Stream no. 8 consists of water and Methanol only!

The flash pressure quals to 10 bar, and recovery rate of liquid for Methanol (RRL) equals 70%.

We can conduct a general material balance in separation unit:

Then, we impose VLE for the system:

*Assumptions:* Ideal Gas – Ideal liquid mixture – Negligible Poynting

For the condensable species:

For the non-condensable species, .

If we solve the equation for yi, the equation is changed to:

After that, we conduct a component material balance:

The stochiometric equation will be written as:

Ki is a function of Ki,0, which is a function of flash temperature.

We have to couple the equation above with Rachford-Rice equation in order to calculate

The control Volume is “F1” and QF1 > 0 (Removed heat) and the reference temperature as same as previous units. *The feed phase is vapor and has T6 temperature*.

A blackboard with white chalk on it

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