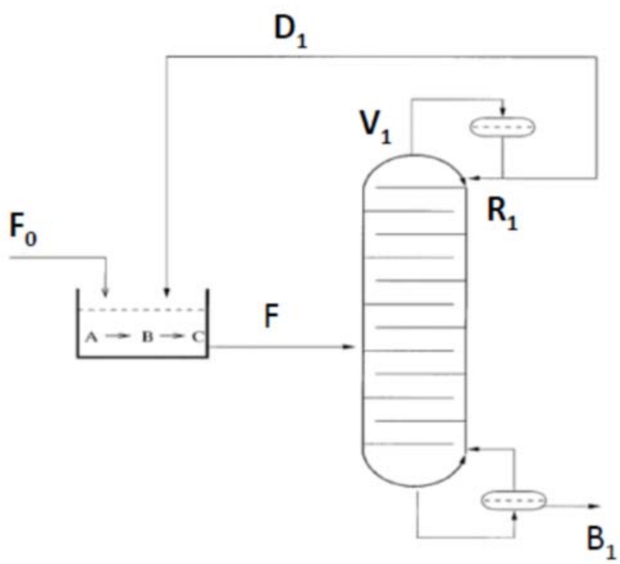
Department of Chemical Engineering, IIT Kharagpur

CH49019: CAPE Laboratory Autumn 2021

Group Assignment: Due on November 10, 2021

Email Your Report (pdf only) and MATLAB code to dsarkar@che.iitkgp.ac.in

Consider the recycle network of a continuously stirred tank reactor (CSTR) and a distillation column.



Reactant A is fed at a molar flowrate F_0 to the CSTR, where the first-order irreversible reactions

$$A \rightarrow B \rightarrow C$$

produce the desired product B and the undesired byproduct C, with reactions rate constants $k_1 = k_2$. The outlet stream from the reactor, which is a mixture of the unconverted reactant A and the products B and C, is fed to the distillation column with N trays (numbered from top to bottom) on tray f at a flowrate F. The light unconverted reactant A is distilled at the top of the column and recycled completely to the reactor at a flowrate D_1, while the heavier product B and byproduct C are withdrawn at the bottom from the reboiler at a flowrate B_1.

Let us assume isothermal operation of the reactor, constant molar overflow and relative volatilities $\alpha_A > \alpha_B > \alpha_C = 1$ and equal latent heat of vaporization for all components. Under these assumptions, the following dynamic model of the reactor-distillation column system can be derived. It consists of the material balance for the overall molar holdups in the reactor, condenser and the reboiler, and the components A and B in the reactor, condenser, reboiler and the internal trays in the column, i.e. (2N + 9) differential equations.

Reactor:

$$\dot{M}_R = F_0 + D_1 - F$$

$$\dot{x}_{A,R} = \frac{F_0(1 - x_{A,R}) + D_1(x_{A1,D} - x_{A,R})}{M_R} - k_1 x_{A,R}$$

$$\dot{x}_{B,R} = \frac{-F_0 x_{B,R} + D_1(x_{B1,D} - x_{B,R})}{M_R} + k_1 x_{A,R} - k_2 x_{B,R}$$

Condenser:

$$\dot{M}_{1,D} = V_1 - R_1 - D_1$$

$$\dot{x}_{A1,D} = \frac{V_1(y_{A1,1} - x_{A1,D})}{M_{1,D}}$$

$$\dot{x}_{B1,D} = \frac{V_1(y_{B1,1} - x_{B1,D})}{M_{1,D}}$$

<u>**Tray**</u> ***i*, 1 ≤ *i* < *f*** :

$$\left.\begin{aligned}
\dot{x}_{A1,i} &= \frac{1}{M_{1,i}}\left[V_1\left(y_{A1,i+1} - y_{A1,i}\right) + R_1\left(x_{A1,i-1} - x_{A1,i}\right)\right] \\
\dot{x}_{B1,i} &= \frac{1}{M_{1,i}}\left[V_1\left(y_{B1,i+1} - y_{B1,i}\right) + R_1\left(x_{B1,i-1} - x_{B1i}\right)\right],
\end{aligned}\right\}$$

<u>**Tray *i***</u>**:**

$$\left.\begin{aligned}
\dot{x}_{A1,f} &= \frac{1}{M_{1,f}}\left[V_1\left(y_{A1,f+1} - y_{A1,f}\right) + F\left(x_{A,R} - x_{A1,f}\right)\right. \\
&\quad \left. + R_1\left(x_{A1,f-1} - x_{A1,f}\right)\right] \\
\dot{x}_{B1,f} &= \frac{1}{M_{1,f}}\left[V_1\left(y_{B1,f+1} - y_{B1,f}\right) + F\left(x_{B,R} - x_{B1,f}\right)\right. \\
&\quad \left. + R_1\left(x_{B1,f-1} - x_{B1,f}\right)\right]
\end{aligned}\right\}$$

<u>**Tray**</u> ***i*, *f* < *i* ≤ *N*:**

$$\left.\begin{aligned}
\dot{x}_{A1,i} &= \frac{1}{M_{1,i}}\left[V_1\left(y_{A1,i+1} - y_{A1,i}\right)\right. \\
&\quad \left. + (R_1 + F)\left(x_{A1,i-1} - x_{A1,i}\right)\right] \\
\dot{x}_{B1,i} &= \frac{1}{M_{1,i}}\left[V_1\left(y_{B1,i+1} - y_{B1,i}\right)\right. \\
&\quad \left. + (R_1 + F)\left(x_{B1,i-1} - x_{B1,i}\right)\right],
\end{aligned}\right\}$$

Reboiler:

$$\dot{M}_{1,B} = R_1 + F - V_1 - B_1$$

$$\dot{x}_{A1,B} = \frac{1}{M_{1,B}}\left[(R_1 + F)\left(x_{A1,N} - x_{A1,B}\right) - V_1\left(y_{A1,B} - x_{A1,B}\right)\right]$$

$$\dot{x}_{B1,B} = \frac{1}{M_{1,B}}\left[(R_1 + F)\left(x_{B1,N} - x_{B1,B}\right) - V_1\left(y_{B1,B} - x_{B1,B}\right)\right]$$

Here M_R, M_D, M_B, M_i denote the molar liquid holdups in the reactor, condenser, reboiler and trays *i*.

$x_{A1,i}$, $x_{B1,i}$ denote the corresponding mole fractions of A and B, and $y_{A1,i}$,, $y_{B1,i}$ denote the vapor phase mole fractions given by the following relations.

$$y_{A1,i} = \frac{\alpha_A x_{A1,i}}{1 + (\alpha_A - 1)x_{A1,i} + (\alpha_B - 1)x_{B1,i}}$$

$$y_{B1,i} = \frac{\alpha_B x_{B1,i}}{1 + (\alpha_A - 1)x_{A1,i} + (\alpha_B - 1)x_{B1,i}}$$

<u>Your Work</u>:

A high conversion of the reactant A and high product selectivity for B can be achieved by keeping the single-pass conversion in the reactor low, and using a recycle flowrate D_1 much larger than the fresh reactant feed flowrate F_0. Note that a large recycle flowrate D_1 implies that the flowrates F and V_1 are also equally large, while the flowrates R_1 and B_1 are comparable to F_0. To simulate a condition where recycle flowrate is much larger than the feed flowrate ($D_1 >> F_0$), consider the following flow-rates (all molar follow rates) and process parameters.

$k_1 = 1$	$k_2 = 1$
$\alpha_A = 4$	$\alpha_B = 2$
Number of Trays, N = 15	Feed enters at Tray 4 (from top, f)
$F_0 = 100$	F = 1880
$D_1 = 1780$	$R_1 = 290$
$V_1 = 2070$	$B_1 = 100$

Write a MATLAB code (use built-in functions for solution of ODE etc.) to simulate the system for above conditions. Integrate the system equations for long time (until all compositions reach steady states). Plot how the compositions of top product and bottom product varies with time. Also, report the values of all state variables in a Table. **Make suitable assumption (or literature search) for any missing information.**

<u>Your Deliverables</u>:

You will work as a group (see the attached file to know your Group Members) and you will submit only one report per group. You will submit the following:

1. No more than two-page Report indicating results and plot as mentioned in previous section. **Include a paragraph to indicate contribution of each Group Member.**

2. Your MATLAB code. Put comments and make the code as general as possible. Put all the relevant functions/codes in one folder, zip it, and email to **dsarkar@che.iitkgp.ac.in** along with your Report. Include one Read Me file in the folder.

3. **If I run your code, I must get your results as reported.**

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