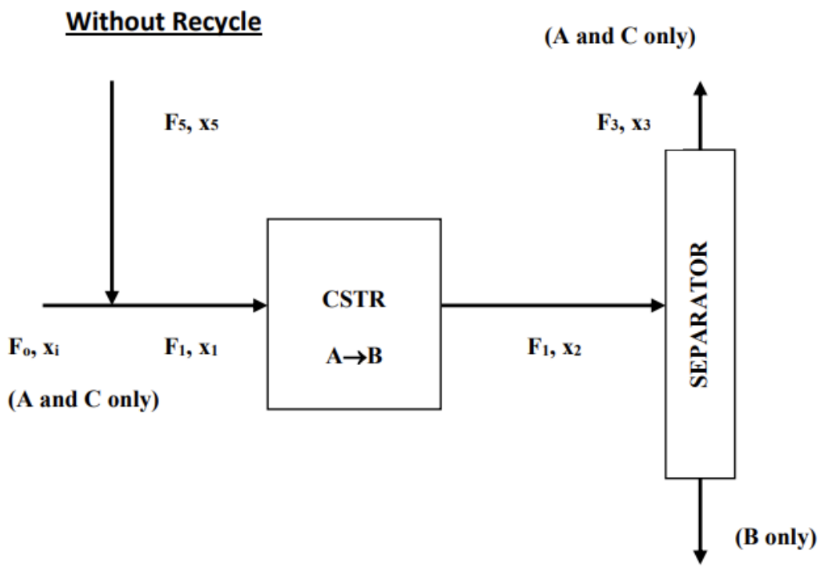
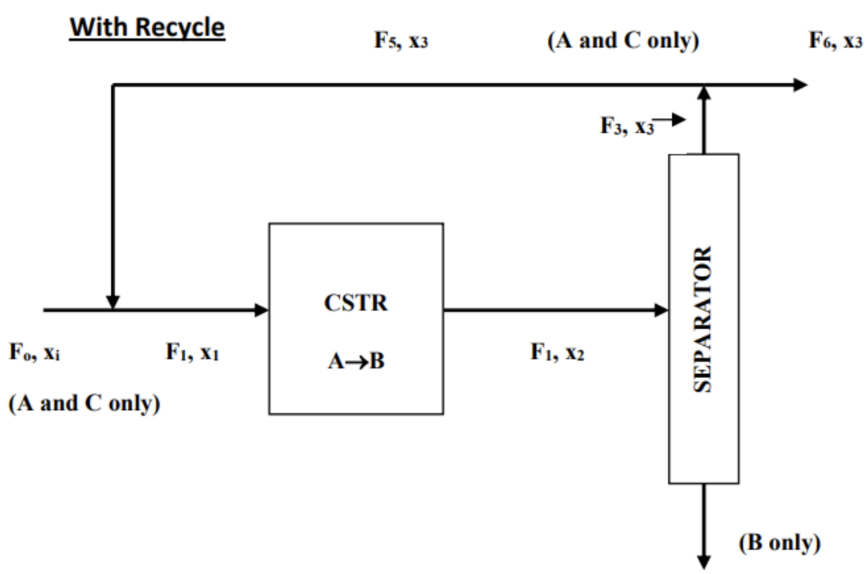
2024 CHE322 TERM PROJECT

PART-1

Consider the chemical reactor/separator systems shown below, one with a recycle stream and one without a recycle stream.





<u>Steady-State Data</u>

```
F0 = 1.0      # moles/time
F1 = 2.7      # moles/time
F3 = 1.8      # moles/time
F5 = 1.7      # moles/time
Xi_A0 = 0.95 # moles fraction
τ = 1/2.7     # time
k0 = 2.7      #  1/time
X1_A0 = 2/3  # moles fraction
X2_A0 = 1/3  # moles fraction
X3_A0 = 1/2  # moles fraction
X5_A0 = 1/2  # moles fraction
```

Assumptions

- Constant molar hold-up for CSTR.
- All molar flowrates are constant.
- Perfect separation unit with infinitely fast dynamics.
- No transportation delay between separator and fast dynamics.
- Isothermal process.

Mixing Point Subsystem

$$\begin{aligned} F_1 &= F_o + F_5 \\ F_1 x_{1,A} &= F_o x_{i,A} + F_5 x_{3,A} \end{aligned} \qquad (1)$$

Reactor Subsystem

$$\frac{d(Mx_{2,A})}{dt} = F_1 x_{1,A} - F_1 x_{2,A} - k_o x_{2,A} M$$

or

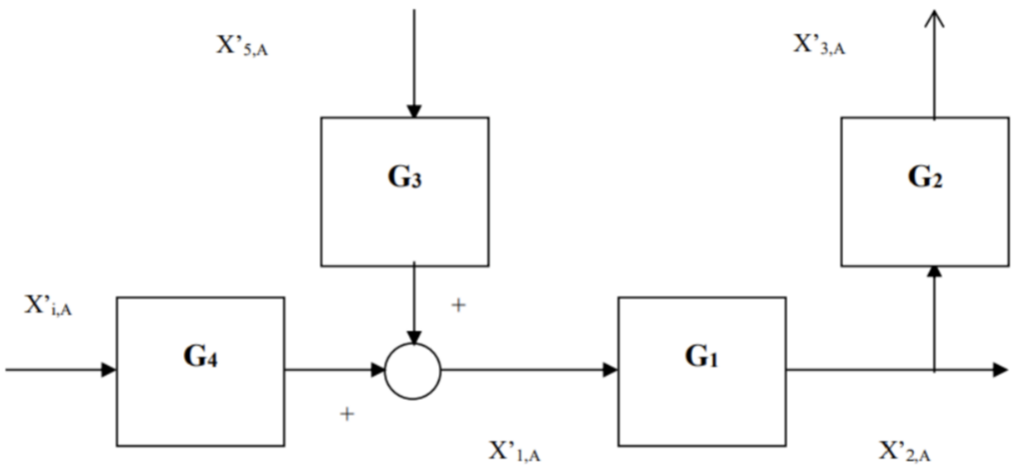
$$\frac{dx_{2,A}}{dt} = \frac{1}{\tau}(x_{1,A} - x_{2,A}) - k_o x_{2,A} \qquad (2)$$

$$\tau = \frac{M}{F_1}$$

Separator Subsystem

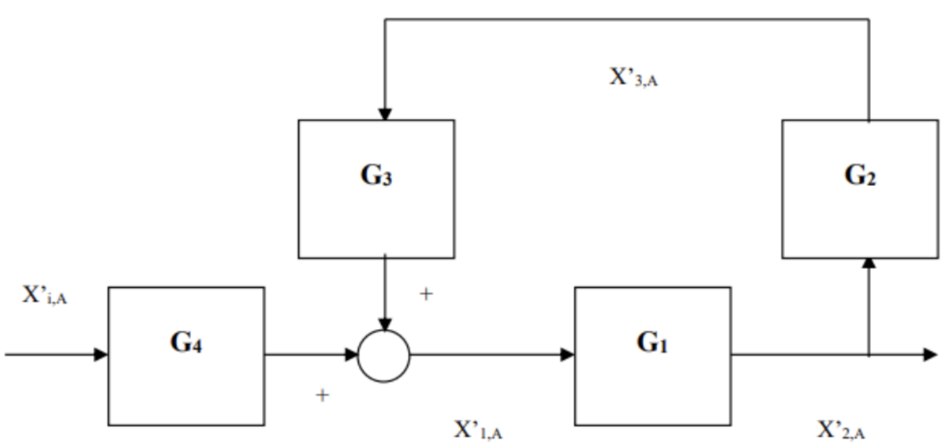
$$F_1 x_{2,A} = F_3 x_{3,A} \qquad (3)$$

Without Recycle Case



1. Develop the transfer function in the block diagram representation of the system **without recycle**. In this block diagram, the variables are deviation variables (for example, x'i,A = xi,A – xi,A_steady_state).
2. Using Python, simulate the dynamic system by using a step change in xi,A from 0.95 to 0.96 at t=2. Plot the response results of each variable in this order xi,A, x1,A, x2,A, x3,A, in a 4-by-1 subplot.
3. Using Python, fit a transfer function to the step response of x3,A and compare the key parameters with the theoretical parameters obtained in step-1.

With Recycle Case



4. Similarly, develop the transfer function in the block diagram representation of the system **with recycle**. In this block diagram, the variables are deviation variables (for example, x’i,A = xi,A – xi,A_steady_state).
5. Using Python, simulate the dynamic system by using a step change in xi,A from 0.95 to 0.96 at t=2. **Plot the results in the same plot produced in step-2** using different line types (or colors) representing each of the two cases and include a legend.
6. Using Python, fit a transfer function to the step response of x3,A and compare the key parameters with the theoretical parameters obtained in step-4.

Analysis

7. By examining the results from part 5 and based on your chemical engineering knowledge, explain the behavior observed in the plot for the two cases and state any differences observed in their behavior.
8. Derive the overall transfer function from x’i,A(s) to x’3,A(s) for the two cases. How do the overall transfer functions differ? Are these results consistent with your answer for part 7?

Report Format:

- Each tutorial group is asked to prepare a single report answering the above questions. The title page must include the names of all group members, your tutorial section (Monday or Tuesday) and your group number.
- The second page must contain a summary of each student’s contribution to the report and signatures attesting to their contribution being original work.
- You can choose to structure your report in a Q/A format or use separate headings and add content. In either case, it is expected that you answer all the questions asked in the report and highlight them.
- The page limit for the main body of the report is **10 pages**.
- Essential figures should be well integrated into the body of the report. Additional (less essential) figures may be included in the appendix (not included in the page limit). Please ensure that the content of your main body should be self-sufficient on its own.
- Use MS Word or Latex to write the report and use Python to produce your figures.
- Your report will be assessed using the following three criteria:
  - 1) clarity and cohesion
  - 2) technical correctness
  - 3) quality of report presentation.

Due Date: 15th February 2024, 11:59 PM

Deliverables: Submit one PDF file for the report and one Python (**.ipynb format only)** file including all required simulations and plotting. Submit electronically on Quercus. Please name both your files in this format: “**Group-XX_Project_Part-1"** where XX is your group number.