P2: Time-Optimal Control of a Diafiltration Process

Diafiltration is a membrane filtration process which is designed to concentrate a valuable (high molecular weight) component in the solution from the initial concentration to the required final one. Simultaneously, impurities (low molecular weight components) are required to be diluted (decreased in concentration) from the initial concentration to the desired final one. The schematic diagram of the process is shown in Figure 1.

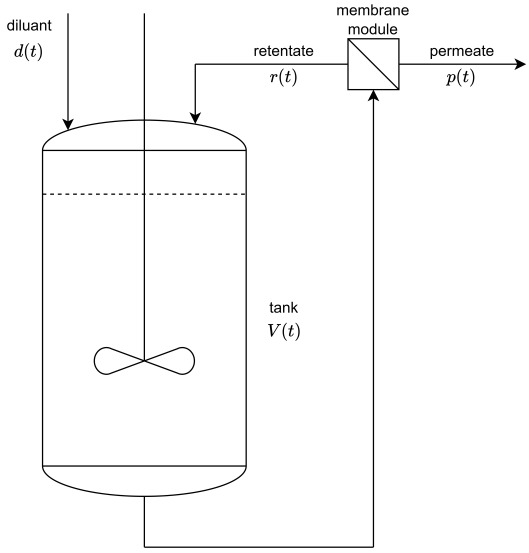

Figure 1: Diafiltration process.

Process description

At the beginning of the operation, the solution to be concentrated is loaded in the feed tank. From here, the solution is circulated continuously through the membrane module, where a portion of the fluid is filtered and leaves the system in the permeate stream with flowrate $p(t)$. This flowrate is dependent on the actual concentrations of the species in the solution. The portion of the fluid which is retained by the membrane (retentate) is returned to the feed tank and the whole filtration cycle is repeated.

Since the permeation properties of the membrane are influenced by the actual concentrations of the species in the system, we can control this process by adding a pure (solute-free) solvent into the feed tank with flowrate $d(t)$. A good choice for the control variable is then the ratio of the inlet flowrate of solvent to the flowrate of the permeate stream $u(t) = d(t)/p(t)$ with $0 \leq u(t) \leq 1$.

In this particular example, the goal is to process 100 liters of a solution which contains proteins (valuable compounds) and lactose (impurity) dissolved in water. The initial concentration of lactose and proteins are $c_{\mathrm{L},0} = 150\,\mathrm{mol\,m^{-3}}$ and $c_{\mathrm{P},0} = 10\,\mathrm{mol\,m^{-3}}$. The final solution must have a concentration of lactose and protein of $c_{\mathrm{L,f}} \leq 15\,\mathrm{mol\,m^{-3}}$ and $c_{\mathrm{P,f}} = 100\,\mathrm{mol\,m^{-3}}$. During the process, a maximum lactose concentration of $c_{\mathrm{L,max}} = 570\,\mathrm{mol\,m^{-3}}$ must be ensured to avoid lactose crystallization.

Only lactose passes through the membrane, while proteins are completely retained. The permeate flow depends on the protein concentration, and is found by the following equation

$$p(t) = kA \ln\left(\frac{c_g}{c_{\mathrm{P}}(t)}\right) \tag{1}$$

where the permeation coefficient k is equal to $4.79 \times 10^{-6}\,\mathrm{m\,s^{-2}}$, the membrane area A is $1\,\mathrm{m^2}$ and the gel concentration c_g equals to $319\,\mathrm{mol\,m^{-3}}$. The ratio between the concentrations of lactose in the

permeate and inlet streams of the membrane module is given by

$$\frac{c_{\mathrm{L},p}(t)}{c_{\mathrm{L}}(t)} = \frac{\alpha}{1 + (\alpha - 1)\exp\left(\frac{p(t)}{k_{M,\mathrm{L}} A}\right)} \tag{2}$$

with $k_{M,\mathrm{L}} = 1.6 \times 10^{-5}\,\mathrm{m\,s^{-1}}$ the mass transfer coefficient of lactose in the membrane and $\alpha = 1.3$ the partition function of lactose at the membrane interface.

Mandatory Tasks

Important: Please use only the Python packages that have been referenced in this task description. Through the entire project you are allowed to use: **CasADi**, **NumPy**, and **Matplotlib**. We have referenced additional packages that are allowed in specific subtasks. If you want to use a different package, please contact your supervisor.

The following tasks **have to be completed** in order to pass the project.

- Develop a continuous ODE model for the diafiltration process. Which states need to be considered? Is the model linear or nonlinear? Justify your answer.
- Simulate the process for 6 hours for different values of the control variable u (e.g. $u = 0.5, u = 0.6, u = 0.7$) and plot the resulting state trajectories for the different control inputs. Discuss your observations. How can optimization help to improve the process performance?
- The overall goal is to design an MPC that minimizes the batch time and satisfies the terminal product specifications. As a first step, the following objective function, which aims at tracking the terminal specifications, is investigated

$$J = \sum_{k=0}^{N} \left(c_{\mathrm{L},k} - c_{\mathrm{L,f}}\right)^2 + \left(c_{\mathrm{P},k} - c_{\mathrm{P,f}}\right)^2 . \tag{3}$$

  Implement and MPC with the objective function above, using a suitable discretization method of your choice with $\Delta t = 10\,\mathrm{min}$. Investigate the influence of the prediction horizon by considering a length of $N = 5, 20, 50$ steps. Make sure that the constraints at the end of the batch are satisfied. Investigate how your controller performs compared to the following policy

$$u(t) = \begin{cases} 0 & \text{if } c_{\mathrm{P}} < 55\,\mathrm{mol\,m^{-3}}, \\ 0.86 & \text{if } c_{\mathrm{P}} \geq 55\,\mathrm{mol\,m^{-3}}. \end{cases} \tag{4}$$

  Plot the closed loop trajectories. Discuss the results with respect to the influence of the length of the prediction horizon, how well the control goal is achieved, and why the objective function may be unsuited.
- Investigate different objective functions that aim at reflecting time optimality. How can you achieve a better performance than the policy above? Discuss how your choice of objective function resolves the issue from the previous task. **Hint:** The objective function does not need to be quadratic.
- Consider your best MPC from the task above. Investigate the performance of your MPC for the scenario that the filter cake (the layer of proteins on the filter membrane) tears for a short amount of time. If the filter cake tears, it means that the amount of fluent that passes through the membrane, increases rapidly. The investigated scenario can be modelled via an increased permeate flow $\hat{p}(t)$, which is adapted in the simulated system only. Consider that $\hat{p}(t)$ follows

$$\hat{p}(t) = \begin{cases} 2p(t) & \text{if } 30\,\mathrm{mol\,m^{-3}} \leq c_{\mathrm{P}}(t) \leq 60\,\mathrm{mol\,m^{-3}}, \\ p(t) & \text{else.} \end{cases} \tag{5}$$

  How does your best MPC perform compared to the policy from (4) for the scenario above? What is the advantage of a well tuned MPC?

Additional tasks

Below are **suggested** additional tasks to obtain an excellent grades for the project. We want to emphasize that students are encouraged to come up with their own ideas for additional investigations and not all of the suggestions below must be included for an excellent grade.

- Consider the scenario of parametric plant-model mismatch. For this, assume that $k_{M,\mathrm{L}}$ is estimated poorly. Investigate the performance of your best MPC with the estimated $k_{M,\mathrm{L}}$ for a plant with the true $k_{M,\mathrm{L,true}} = 0.75k_{M,\mathrm{L}}, 0.5k_{M,\mathrm{L}}, 0.25k_{M,\mathrm{L}}$. What happens to the lactose concentration? Can the constraints still be satisfied? How does your best MPC with plant-model mismatch perform compared to an MPC with the true plant parameters? Investigate how the MPC with plant-model mismatch can be robustified and investigate that performance.
- Consider the scenario of structural plant-model mismatch. In the description above, it is assumed that the membrane retains the proteins completely, leading to a concentration of proteins on the permeate side of $c_{\mathrm{P,p}}(t) = 0$. However, in reality some protein could still pass through the membrane, which can be modelled analogously to the lactose concentration on the permeate side, so

$$\frac{c_{\mathrm{P},p}(t)}{c_{\mathrm{P}}(t)} = \frac{\beta}{1 + (\beta - 1)\exp\left(\frac{p(t)}{k_{M,\mathrm{P}}A}\right)} \tag{6}$$