

Course 28451: Optimizing Plantwide Operation

Exercise 3: Real-time optimisation of chemical reactors

In the previous exercises, we have introduced some tools aimed at keeping the controlled variables of a process at their set points. This exercise deals precisely with the determination of those set points by optimisation (maximisation) of the operating profit, determined as the product value minus the operating costs. You will tackle first the optimisation problem as a design problem, therefore keeping the values of the optimised variables constant throughout all the simulation. This approach will be compared with a real time optimisation, where the optimiser is launched at regular intervals in order to react to changes in the market (e.g. price of the product, of the utilities, etc.).

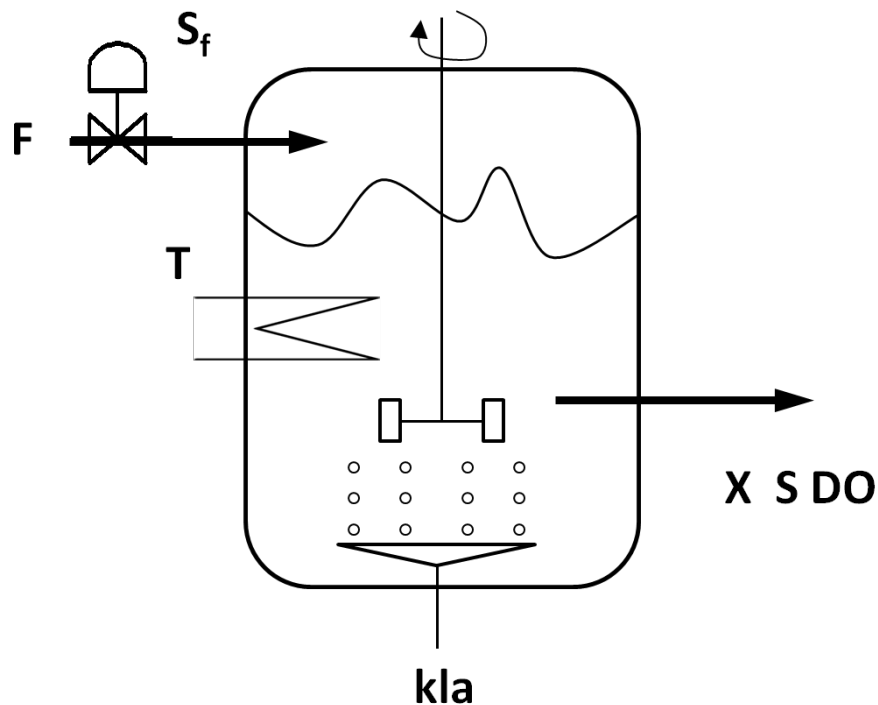


Figure 1: Continuous fermentation bioreactor (details in ex. 3A)

Model description

The model was described earlier in exercise 1 and you can use your model implementation here to perform the optimisation studies.

$$0 = \mu \cdot X - \frac{F}{V} \cdot X$$

$$0 = \frac{F}{V} \cdot (S_f - S) - \frac{1}{Y_{XS}} \mu \cdot X$$

$$0 = \frac{F}{V} \cdot (O_f - O) - \left(\frac{1}{Y_{XS}} - 1 \right) \mu \cdot X + k_l a \cdot (O^{sat} - O)$$

Problem statement

For the continuous bioreactor already presented in the previous exercises, the operating profit can be approximated by the following equation:

$$P = V F X - C k_l a$$

where P is the operating profit (DKK/h)

V (DKK/g) is the value of the biomass product at a concentration between 3-5 g/L

F is the flow of product (L/h)

X is the biomass concentration in the outlet (g/L)

C is the cost of the electricity for aeration (DKK)

$k_l a$ represents the aeration intensity (h^{-1})

The price of the biomass product varies daily around 12 000 DKK/g (as a uniform distribution between 11 400 and 12 600 DKK/g). The contract between the electricity supplier and the company running the process establishes two periods of pricing. The value of C varies as follows:

- From 0 to 8h am. C = 60 DKK
- From 8h am. to 12h pm. C=100 DKK

Given the following constraints

$$\begin{array}{lll} F: 0 \leq F \leq 1 \text{ L/h} & T: 288.5 \leq T \leq 318.5 \text{ K} & k_l a: 0 \leq k_l a \leq 1000 \text{ h}^{-1} \\ X: 0.1 \leq X \leq 10 \text{ g/L} & S: 0 \leq S \leq 10 \text{ g/L} & DO: 0 \leq DO \leq O_{\text{sat}} \end{array}$$

and using a numerical search algorithm, maximize the operating profit (P) for the following scenarios :

- a. Find the optimal value of F, T and $k_l a$ that provides the maximum operating profit considering the steady state optimisation of the operation, $V = 12\,000$ DKK/g of biomass and the weighted average value of $C = 86.7$ DKK. Determine the operating profit over a long period. Perform open loop simulation for a week with this operating point i.e. Initial values for the states and values for the inputs.

Matlab hint 1: In order to solve the optimization problem in a robust and time effective way, it is important to provide a good initial guess for the optimization and response variable. Therefore, it is advisable to use the values of F , T , kla , X , S , DO as $[0.5 \ 298 \ 250 \ 4 \ 0.01 \ 0.0024]$.

- b. Now, consider that the price of the product (V) varies daily, according to a uniform distribution with upper and lower bound corresponding to $\pm 5\%$ of the mean value (12 000 DKK); and that the price of the electricity is 60 DKK from 12 pm to 8 am and 100 from 8 am to 12 pm.

Find the optimal value of F , T and kla that provides the maximum operating profit for 8h intervals, and simulate the system for a period of one week starting from the steady state in question a). Determine the average operating profit for the week and compare with the one obtained previously. What is the profit associated to the real time optimisation and how much has it improved compared to not updating the RTO as in question a)?

Matlab hint 2: Use the matlab command `rand` to generate the (uniform) random variation of product price. In the optimisation problem, consider a moving window with an 8h optimisation horizon, which means basically you solve the optimisation problem every 8 hrs, record the data. Then analyse and plot the recorded data.

- c. Numerical algorithms for optimisation may fail to provide a solution if a *hot-start* (an initial guess close to the solution) is not provided, or if the number of optimisation variables is too large. **Contour plots** are useful in order to provide an approximation to the solution, or an initial guess to be used in a numerical method. However, its visualization can be cumbersome if a large number of parameters are involved. Setting one of the optimising variables (F , T or kla), illustrate the variation of the objective function by one or several contour plots and comment on them. Note this is a simulation task (not optimisation).

Matlab hint 3: Use your system understanding from question a) and b) in order to propose which variables and in which intervals the investigation of the cost function by contour plots is interesting. It may be difficult to get the solution to converge for each grid point so you can use a converged solution in a neighbouring point for the initial guess on the solution. If your results is not a smooth surface you most likely have an issue that not all solutions have converged.

A written report about the results, interpretation and discussion of the exercises is to be handed in on DTU Learn as a single pdf file.

The report should contain a problem statement (you may rephrase the exercise), the results and interpretation / discussion of the results. The following is suggested for the documentation:

- A few representative plots (with appropriate titles and labels), in particular to illustrate the operation of the bioreactor with constant inputs and when the real time optimiser is online.
- A description of the solution procedure.
- Answers to the specific questions in the problem.