# EXERCISES TO THE LECTURE POLYMER REACTION & COLLOID ENGINEERING

# SERIES 2

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## Optimal design of CSTRs in series

The enzymatic conversion of sucrose has to be carried out in a chemical reactor. This reaction follows the Michaelis-Menten mechanism where it is possible to assume constant activity of the biocatalyst in the reactor. The reaction mechanism for this reaction is reported in the following expression:

$$E + S \underset{k_{-1}}{\overset{k_{+1}}{\rightleftharpoons}} ES \overset{k_2}{\rightarrow} E + P \tag{1}$$

The reaction rate according to the Michaelis-Menten kinetic for the enzymatic conversion of the subtrate is given by:

$$R = \frac{V_{Max} * [S]}{K_m + [S]} \tag{2}$$

a) Consider a Batch reactor and solve the balance for the substrate according to the Michaelis-Menten mechanism. Plot the profile of the concentration of the substrate as a function of the reaction time. Evaluate the reaction time needed to achieve a conversion of the substrate equal to 80%.

b) Consider a cascade of 3 CSTRs with the total residence time equal to the reaction time derived in point a) of the exercise. Assume equal residence time in each CSTR reactor. Solve the balance for each CSTR and compute the achieved conversion after each of them. Is the obtained conversion higher or lower than the one in point a) of the exercise? Which configuration would you implement in an industrial process?

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c) In the previous point of the exercise it was assumed equal residence time distribution in each reactor. As you can imagine, this assumption is not necessarily the optimal solution for a given cascade of CSTRs, where each reactor can have a different residence time. In this point of the exercise, it is asked to derive a simple analytical expression for the optimal design of CSTRs in series. It is possible to define the optimum as the smallest total reactor size (*i.e.*, residence time) to achieve a specific conversion. Consider N CSTRs in series with an inlet substrate concentration of $S_0$. Derive an expression for the residence time of the ith reactor, $\tau_i$ in terms of $S_{i-1}$, the substrate concentration entering the reactor i, $S_i$ the substrate concentration leaving the reactor i, and the enzyme kinetic parameters. Rewrite this equation in dimensionless form by introducing the following parameters:

$$\alpha_i = S_i/S_0 \quad \kappa = K_m/S_0 \quad \theta_i = (\tau_i V_{Max})/S_0$$

Where $\alpha_i$ is the dimensionless concentration of the substrate and $\theta_i$ the dimensionless residence time in the ith CSTR. Now we have to find the intermediate $\theta_i$ values (or equivalently the intermediate $\alpha_i$ values), which correspond to the minimum total residence time. Mathematically, these values must satisfy the following equation:

$$\frac{[\sum_{j=1}^{N} \theta_j]}{d\alpha_i} = 0, \qquad i = 1, 2, ..., N-1 \tag{3}$$

Show that this equation reduces to the following simple result:

$$\alpha_i^2 = \alpha_{i-1}\alpha_{i+1}, \qquad i = 1, 2, ..., N-1 \tag{4}$$

Which can be rearranged by expliciting the terms for each reactor and using a bottom up approach to:

$$\alpha_i = \alpha_{i+1}^{i/(i+1)}, \qquad i = 1, 2, ..., N-1 \tag{5}$$

d) Use the obtained expression to compute the conversion and the optimal residence time distribution in each reactor of the CSTR cascade in point b). Is the obtained total residence time lower than the one resulting from point b) of the exercise?

**Additional information:**

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|---|---|---|
| $K_m =$ | 8 | $mol/m^3$ |
| $V_{Max} =$ | $4.45 \times 10^{-3}$ | $mol/m^3/s$ |
| $S_0 =$ | 100 | $mol/m^3$ |