TITE, Applied Mathematics

Ti5417700 Modelling methodology/T. Kauranne

Exercise 21.11.2005

1. A (CSTR) tank with volume 10 m^3 is filled with dirty water, where the concentration of the impurity initially is $C(0) = 5\ kmol/m^3$, and an inflow of pure water is started with a flowrate of $2m^3/h$ (see exercise 5/22.09.05!). Write the ODE system that gives the concentration $C(t)$ for time points $t \geq 0$ and solve it numerically. How long time has the tank to be purified with this flowrate in order to reduce the impurity to the level $C = 0.1\ kmol/m^3$?

2. The chemical reaction $A \stackrel{k}{\rightarrow} B$ takes place in CSTR with volume of $1m^3$. The reaction rate is given by the expression $Re = kA$, where A denotes the concentration and k the reaction rate constant $k = 0.75$. The tank is initially filled with an inert solvent. The feed of A with a concentration A_{in} is started at time $t = 0$ using a constant flowrate so that the volume is kept constant. Derive a model for the process and solve it numerically. Check that the solution has the correct mass balance. What is an optimal flowrate, if we require that the yield of the product B should be 95% at the outlet?

3. Give an ODE model for the reaction system

$$\begin{aligned} A + B &\rightleftharpoons_{k_2}^{k_1} C \\ A + C &\stackrel{k_3}{\rightarrow} D. \end{aligned} \tag{1}$$

   Solve the system numerically in the time interval $0 \leq t \leq 9$ with $k_1 = 8.1$, $k_2 = 12.5$, $k_3 = 0.1$ when the initial amount of the components are given as $A(0) = 1$, $B(0) = 3$, $C(0) = 0$, $D(0) = 0$. Verify the mass balance of the system.