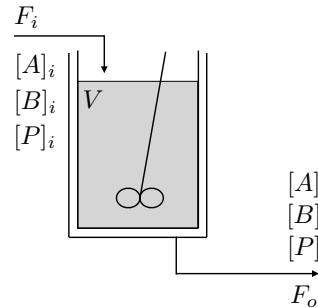


CHEM-E7190/2020: Exercise II

Task 1. Consider two chemical species A and B in a solvent feed entering a chemical reactor. The two species react to form a third one, the product component P , according to the stoichiometric equation $A + 2B \xrightarrow{k} P$. The reactor operates in liquid-phase with a hold-up V and at some constant temperature T . Assuming volumetric flowrates for $F_i(t)$ and $F_o(t)$ and assuming perfect mixing, we are interested in the concentrations $[A](t)$, $[B](t)$, and $[P](t)$ in the reactor and in the liquid volume $V(t)$, all as functions of time.



The dynamics of the system (see 04.Linearisation_example.2020.2x1.pdf) are given by the equations

$$\begin{bmatrix} \dot{V}(t) \\ [A](t) \\ [B](t) \\ [P](t) \end{bmatrix} = \begin{bmatrix} F_i(t) - F_o(t) \\ \frac{F_i(t)}{V(t)} ([A]_i(t) - [A](t)) - k[A](t)[B](t) \\ \frac{F_i(t)}{V(t)} ([B]_i(t) - [B](t)) - 2k[A](t)[B](t) \\ -\frac{F_i(t)}{V(t)} [P](t) + k[A](t)[B](t) \end{bmatrix}.$$

V , $[A]$, $[B]$ and $[P]$ are the state variables, F_i , F_o , $[A]_i$ and $[B]_i$ are the inputs and k is a model parameter.

0. Verify that the given model equations are correct;
1. Write a script (with model function) to simulate the reactor for different initial conditions and inputs;
2. Choose reasonable values for the model parameters (k), the initial conditions ($[V](0)$, $[A](0)$, $[B](0)$, $[P](0)$) and the inputs ($[F_i](t)$, $[F_o](t)$, $[A]_i(t)$, $[B]_i(t)$), for $0 \leq t \leq t_f$ and test your implementation. To verify/demonstrate the correctness of your implementation, display the evolution of all model variables.
3. For the chosen model parameters, define a set of operating conditions ($[F_i]^{SS}$, $[F_o]^{SS}$, $[A]_i^{SS}$, $[B]_i^{SS}$) of your choice to run the reactor and find the corresponding steady-states ($[V]^{SS}$, $[A]^{SS}$, $[B]^{SS}$, $[P]^{SS}$) by simulating the process for a sufficiently long time. (Avoid flooding/emptying the reactor by carefully choosing the operating conditions; Use your implementation to support you in the selection task.)
4. Linearise the model around that steady-state (again, see 04.Linearisation_example.2020.2x1.pdf),

$$\dot{x}'(t) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ -\frac{u_1(u_3 - x_2)}{x_1^2} & -\frac{u_1}{x_1} - kx_3 & -kx_2 & 0 \\ -\frac{u_1(u_4 - x_3)}{x_1^2} & -2kx_3 & -\frac{u_1}{x_1} - 2kx_2 & 0 \\ \frac{u_1x_4}{x_1^2} & k & kx_2 & -\frac{u_1}{x_1} \end{bmatrix}_{SS} x'(t) + \begin{bmatrix} 1 & -1 & 0 & 0 \\ \frac{u_3 - x_2}{x_1} & 0 & \frac{u_1}{x_1} & 0 \\ \frac{u_4 - x_3}{x_1} & 0 & 0 & \frac{u_1}{x_1} \\ -\frac{x_4}{x_1} & 0 & 0 & 0 \end{bmatrix}_{SS} u'(t),$$

implement the linearised model and compare its evolution with the nonlinear one under the same conditions defined in (2.). Do not forget to verify the correctness of the linearised model above and plot the temporal evolution of all the involved process variables, to show the correctness of your code.