[Student number] CHEM-E7140/2019: Assignment I, part 2

Exercise 1. Consider a continuous stirred tank reactor in which the reaction scheme occurs

 $\begin{array}{c|c} \hline F_i \\ \hline [A]_i \\ \hline V \\ \hline V \\ \hline C \\ \hline [C] \\ \hline [B] \\ \hline F_o \end{array} \qquad A \xrightarrow{k_1} B \xrightarrow{k_2} C \qquad (1a) \\ 2A \xrightarrow{k_3} D \qquad (1b) \end{array}$

Component B is the desired product and we assume that we can measure its composition in the reactor, [B](t). We also assume that the feed only contains component A, whose composition $[A]_i(t)$ can be set, and that density, temperature and volume in the reactor are constant.

Let $F_i(t)$ [lt min⁻¹] be the volumetric flow-rate of the inlet stream, $F_o(t)$ [lt min⁻¹] the volumetric flow-rate of the outlet stream, and let $F^{SS}/V = 4/7$ [min⁻¹] be the dilution-rate/space-velocity at a steady-state operation point, V [lt] indicates the volume. Let $[A]_i^{SS} = 10 \text{ [mol lt}^{-1}]$ be the concentration of component A in the feed at that steady-state. The rate constants are i) $k_1 = 5/6 \text{ [min}^{-1}\text{]}$; ii) $k_2 = 5/3 \text{ [min}^{-1}\text{]}$; and, iii) $k_3 = 1/6 \text{ [mol lt}^{-1} \text{ min}^{-1}\text{]}$, with $A \to B$ and $B \to C$ characterised by first-order rates of reaction per unit volume and $A + A \to D$ characterised by a second-order rate per unit volume.

- Indicate input, output and state variables. Comment on their properties (measurable, manipulable, controllable, control, disturbance, ...);
- Write the total material balance and the material balances for all of the components;
- Write the complete state-space model of this system. Use the control notation for state, input and output variables, and parameters, to replace the problem-specific quantities;
- Given the steady-state values of the dilution rate and feed composition, determine the steady-state concentration of component A, $[A]^{ss}$, and use it to determine the steady states concentrations of the components B, C and D (that is, $[B]^{SS}$, $[C]^{SS}$, and $[D]^{SS}$);
- Plot the function $[B]^{SS} = h(F^{SS}/V)$ and comment on the choice of $F^{SS}/V = 4/7 \, [\min^{-1}]$ as operating point for this reactor;
- Linearise the state-space model and compute the specific model realisation (A, B, C, D) corresponding to the steady-state operating point that you have calculated;
- Compute the eigenvalues and eigenvectors of the state matrix A and comment on the stability of the reactor under the assume linear approximation.