Model formulation - exercises 2019

TBMT37 / TBMT19

1. Consider the following model

$$[\dot{A}] = -k1[A] + k2[B] \qquad [A](0) = 1 \qquad \hat{y} = ky[A]$$
$$[\dot{B}] = -k2[B] + k1[A] \qquad [B](0) = 0$$

(a) List all model states

(b) List all model parameters?

(c) List all reaction rates

(d) What can be measured? Explain in words.

2. Consider the following reactions

$$A \rightarrow B \tag{1}$$
$$B \rightarrow C \tag{2}$$
$$C \rightarrow \varnothing \tag{3}$$

(a) Write down the differential equations that corresponds to these reactions. Assume mass action kinetics for reaction 1 and 2 and assume that reaction 3 is saturated with respect to the concentration of C. Introduce parameters and initial conditions with values of your choice.

(b) Add a measurement equation that states that you can measure the sum of the concentration of B and C.

3. Consider the following model

$$\begin{aligned} [\dot{A}] &= -k1[A] + k3[C] & \qquad [A](0) &= 1 \\ [\dot{B}] &= -k2[B] + k1[A] & \qquad [B](0) &= 0 \\ [\dot{C}] &= -k3[C] + k2[B] & \qquad [C](0) &= 0 \end{aligned}$$

(a) Which are the reactions?

(b) Choose one of the reactions and change the kinetics so that the reaction rates is saturated and give the new equations.

4. Consider the following reactions

$$\begin{aligned} A &\rightarrow B \\ A &\rightarrow \varnothing \\ B &\rightarrow \varnothing \end{aligned}$$

(a) Write down the differential equations that corresponds to these reactions. Assume mass action kinetics. Introduce parameters and initial conditions with values of your choice.

(b) Add a measurement equation that states that you can measure something that is proportional to the rate of the reaction $A \rightarrow B$.

5. Consider the following model

$$\begin{aligned} [\dot{A}] &= -k1[A][B] - k2[A] + u & \qquad [A](0) &= 1 \\ [\dot{B}] &= -k1[A][B] & \qquad [B](0) &= 0 \\ [\dot{C}] &= k2[A] & \qquad [C](0) &= 0 \end{aligned}$$

(a) Which are the reactions?

Answers

1.

(a) $[A], [B]$

(b) $k1, k2, ky, [A](0), [B](0)$

(c) $k1[A], k2[B]$

(d) The measurement equation, $\hat{y} = ky[A]$ shows that we can measure something that is proportional the concentrations of A.

2.

(a)

$$
\begin{aligned}
&[\dot{A}] = -k1[A] && [A](0) = 1 \\
&[\dot{B}] = -k2[B] + k1[A] && [B](0) = 2 \\
&[\dot{C}] = \frac{-Vmax[C]}{(Km + [C])} + k2[B] && [C](0) = 0 \\
&k1 = 3, k2 = 1, Vmax = 0.5, Km = 1
\end{aligned}
$$

(b) $\hat{y} = [C] + [B]$

3.

(a)

$$A \rightarrow B \tag{4}$$

$$B \rightarrow C \tag{5}$$

$$C \rightarrow A \tag{6}$$

4.

(a)

$$
\begin{aligned}
&[\dot{A}] = -k1[A] - k2[A] && [A](0) = 1 \\
&[\dot{B}] = k1[A] - k3[B] && [B](0) = 2 \\
&k1 = 3, k2 = 1, k3 = 0.1
\end{aligned}
$$

(b) $\hat{y} = ky * k1[A]$

5.

(a)

$$
\begin{aligned}
A + B &\rightarrow \varnothing \\
A &\rightarrow C \\
\varnothing &\rightarrow A
\end{aligned}
$$