

# Model formulation - exercises 2019

TBMT37 / TBMT19

1. Consider the following model

$$\begin{aligned}\dot{[A]} &= -k_1[A] + k_2[B] & [A](0) &= 1 & \hat{y} &= ky[A] \\ \dot{[B]} &= -k_2[B] + k_1[A] & [B](0) &= 0\end{aligned}$$

- (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



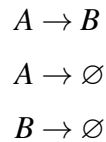
- (a) Write down the differential equations that corresponds to these reactions. Assume mass action kinetics for reaction 1 and 2 and assume that reaction 3 is saturated with respect to the concentration of C. Introduce parameters and initial conditions with values of your choice.
- (b) Add a measurement equation that states that you can measure the sum of the concentration of B and C.

3. Consider the following model

$$\begin{aligned}\dot{[A]} &= -k_1[A] + k_3[C] & [A](0) &= 1 \\ \dot{[B]} &= -k_2[B] + k_1[A] & [B](0) &= 0 \\ \dot{[C]} &= -k_3[C] + k_2[B] & [C](0) &= 0\end{aligned}$$

- (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



- (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

$$\begin{aligned}\dot{[A]} &= -k_1[A][B] - k_2[A] + u & [A](0) &= 1 \\ \dot{[B]} &= -k_1[A][B] & [B](0) &= 0 \\ \dot{[C]} &= k_2[A] & [C](0) &= 0\end{aligned}$$

- (a) Which are the reactions?

## Answers

1.

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

(b)  $k_1, k_2, k_y, [A](0), [B](0)$

(c)  $k_1[A], k_2[B]$

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

2.

(a)

$$[\dot{A}] = -k_1[A]$$

$$[A](0) = 1$$

$$[\dot{B}] = -k_2[B] + k_1[A]$$

$$[B](0) = 2$$

$$[\dot{C}] = \frac{-V_{max}[C]}{(K_m + [C])} + k_2[B]$$

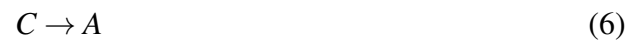
$$[C](0) = 0$$

$$k_1 = 3, k_2 = 1, V_{max} = 0.5, K_m = 1$$

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

3.

(a)



4.

(a)

$$\begin{aligned}\dot{[A]} &= -k_1[A] - k_2[A] & [A](0) &= 1 \\ \dot{[B]} &= k_1[A] - k_3[B] & [B](0) &= 2 \\ k_1 &= 3, k_2 = 1, k_3 = 0.1\end{aligned}$$

(b)  $\hat{y} = ky * k_1[A]$

5.

(a)

