1. Recall that the reactions

   $$\mathrm{A} + \mathrm{B} \underset{b}{\overset{f}{\rightleftharpoons}} \mathrm{C} \xrightarrow{k} \mathrm{D}.$$

   give the following differential equation for C

   $$\frac{dC}{dt} = fAB - bC - kC.$$

   Convert the following set of differential equations into a `.psc` file for `StochPy`:

   $$\begin{aligned} \frac{dX}{dt} &= k_x - d_x X - fXY \\ \frac{dY}{dt} &= k_y - d_y Y - fXY \\ \frac{dZ}{dt} &= fXY - d_z Z \end{aligned}$$

2. An enzyme obeys the Michaelis-Menten equation

   $$\mathrm{E} + \mathrm{S} \underset{b}{\overset{f}{\rightleftharpoons}} \mathrm{C} \xrightarrow{k} \mathrm{E} + \mathrm{P}.$$

   with $f = 10^8$ M^{-1} s^{-1}, $b = 0.03$ s^{-1}, and $k = 0.8$ s^{-1}. If the concentration of enzyme is 0.01 mM in *Escherichia coli* and the initial concentration of substrate is 10 mM, convert this system into a stochastic model – a `.psc` file – for `StochPy`. Remember that the rate constants need to be transformed into their mesoscopic values (Section 2.1 of the lecture notes).

Solution

1. There is one reaction for each rate constant in the set of equations:

```
# Reactions
R1:
     $pool > X
     kx
R2:
     X > $pool
     dx*X
R3:
     X + Y > Z
     f*X*Y
R4:
     $pool > Y
     ky
R5:
     Y > $pool
     dy*Y
R6:
     Z > $pool
     dz*Z
```

2. Although the mesoscopic and macroscopic rates for first-order reactions are the same, we should use the formula $f = \tilde{f} n_A V$ to find the mesoscopic rate $\tilde{f}$ for the second-order reaction. Using that the volume of *E coli* is 10^{-15} ℓ (Section 2.1.3), then

$$\tilde{f} = \frac{10^8}{6 \times 10^{23} \times 10^{-15}} = 0.17\,\mathrm{s}^{-1}.$$

We also need to convert the concentrations into numbers of molecules:

$$N_E = 0.01 \times 10^{-6} \times 6 \times 10^{23} \times 10^{-15} = 6$$
$$N_S = 10 \times 10^{-6} \times 6 \times 10^{23} \times 10^{-15} = 6000$$

Hence

```
# Reactions
R1:
     E + S > C
     f*E*S
R2:
     C > E + S
     b*C
R3:
     C > E + P
     k*C
```

```
# Variable species
E= 6
S= 6000
C= 0
P= 0

# Parameters
f= 0.17
b= 0.03
k= 0.8
```