Kinetics and Reactor Design HW1

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Assigned: January 23, 2022
Due: January 31, 2022

1 Problem Statement

1.1 P1-3$_B$ (a)

There are initially 500 rabbits (x) and 200 foxes (y) on Professor Sven Köttlov's son-in-law, Štěpán Dolež's, farm near Riça, Jofostan. Use Polymath or MATLAB to plot the concentration of foxes and rabbits as a function of time for a period of up to 500 days. The predator–prey relationships are given by the following set of coupled ordinary differential equations:

$$\frac{dx}{dt} = k_1 x - k_2 xy \tag{1}$$

$$\frac{dy}{dt} = k_3 xy - k_4 y \tag{2}$$

Constant for growth of rabbits $k_1 = 0.02/\text{day}$
Constant for death of rabbits $k_2 = 0.00004/(\text{day} \times \text{no. of foxes})$
Constant for growth of foxes after eating rabbits $k_3 = 0.0004/(\text{day} \times \text{no. of rabbits})$
Constant for death of foxes $k_4 = 0.04/\text{day}$
What do your results look like for the case of $k_3 = 0.00004/(\text{day} \times \text{no. of rabbits})$ and t final = 800 days? Also, plot the number of foxes versus the number of rabbits. Explain why the curves look the way they do.

1.2 P1-5$_A$

The reaction A + B $\rightarrow$ 2C takes place in an unsteady CSTR. The feed is only A and B in equimolar proportions. Which of the following sets of equations gives the correct set of mole balances on A, B, and C? Species A and B are disappearing and species C is being formed. Circle the correct answer where all the mole balances are correct.

1.3 P1-6$_B$ (a-c)

The reaction A $\rightarrow$ B is to be carried out isothermally in a continuous-flow reactor. The entering volumetric flow rate ν_0 is 10 dm^3/h. Calculate both the CSTR and PFR reactor volumes necessary to consume 99 percent of A (i.e., $C_A = 0.01C_{A0}$) when the entering molar flow rate is 5 mol/h, assuming the reaction rate $-r_A$ is
(a) $-r_A = k$ with $k = 0.05 \frac{mol}{h \times dm^3}$
(b) $-r_A = kC_A$ with $k = 0.0001/\text{s}$
(c) $-r_A = kC_A^2$ with $k = 300 \frac{dm^3}{h \times mol}$

1.4 P2-4$_B$ (a-e)

The exothermic reaction of stillbene (A) to form the economically important trospophene (B) and methane (C), i.e.,A $\rightarrow$ B + C was carried out adiabatically and the following data recorded:

X	0	0.2	0.4	0.45	0.5	0.6	0.8	0.9
$-r_A$ (mol/dm^3·min)	1.0	1.67	5.0	5.0	5.0	5.0	1.25	0.91

Figure 1: Reaction Data

The entering molar flow rate of A was 300 mol/min.
(a) What are the PFR and CSTR volumes necessary to achieve 40 percent conversion? (V$_{PFR}$ = 72 dm^3, V$_{CSTR}$ = 24 dm^3)
(b) Over what range of conversions would the CSTR and PFR reactor volumes be identical?
(c) What is the maximum conversion that can be achieved in a 105-dm^3 CSTR?
(d) What conversion can be achieved if a 72-dm^3 PFR is followed in series by a 24-dm^3 CSTR?
(e) What conversion can be achieved if a 24-dm^3 CSTR is followed in a series by a 72-dm^3 PFR?

1.5 P2-9$_D$

Don't calculate anything. Just go home and relax.

2 Problem Solution

2.1 P1-3$_B$ (a)

Four plots (Population and Phase Plane for initial k_3 and new k_3 respectively) are below, generated in MATLAB. The curves look the way they do for the initial problem because the (relatively) large k_3 value causes an explosion in the fox population, which then results in a very swift decrease in rabbit population. This makes the first term of the second differential equation nearly zero, and the foxes die off at a constant rate up until rabbit numbers can replenish, which repeats the cycle. For the second part of the problem, the k_3 value is smaller, which means that the fox population explosion is smaller, thus rabbit die-off is less and the cycle is slightly more frequent.

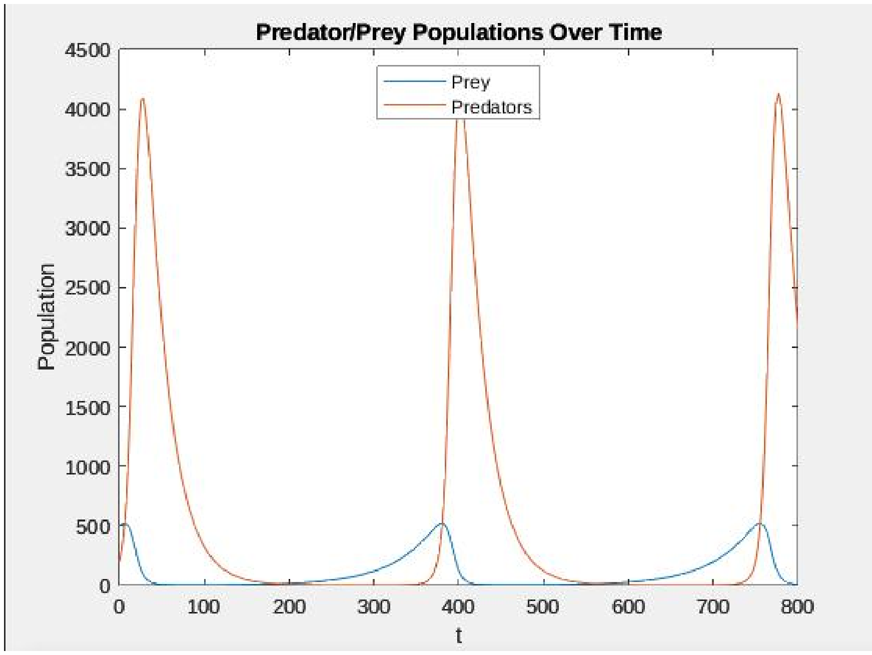

Figure 2: Predator Prey Plot 1

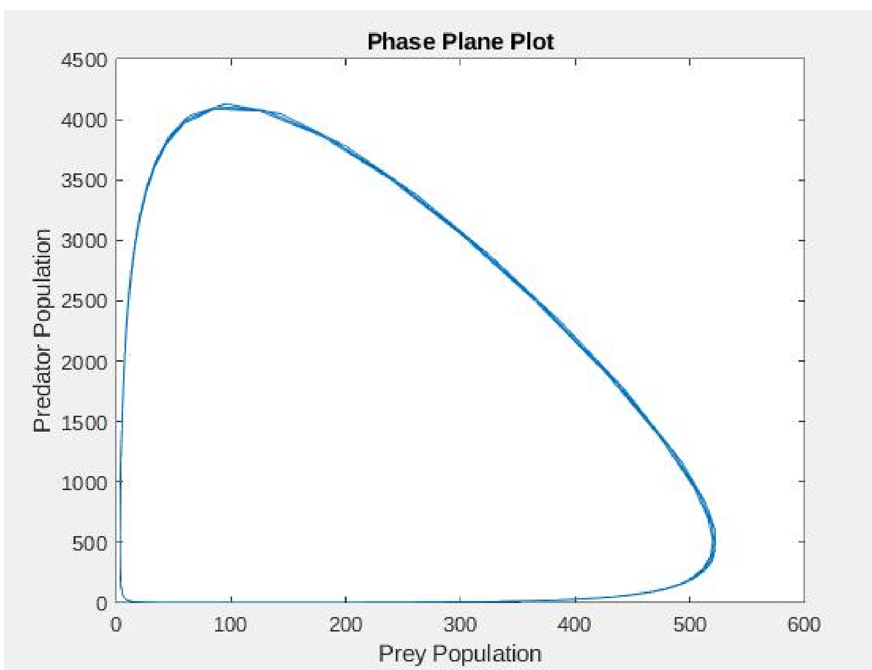

Figure 3: Predator Prey Plot 2

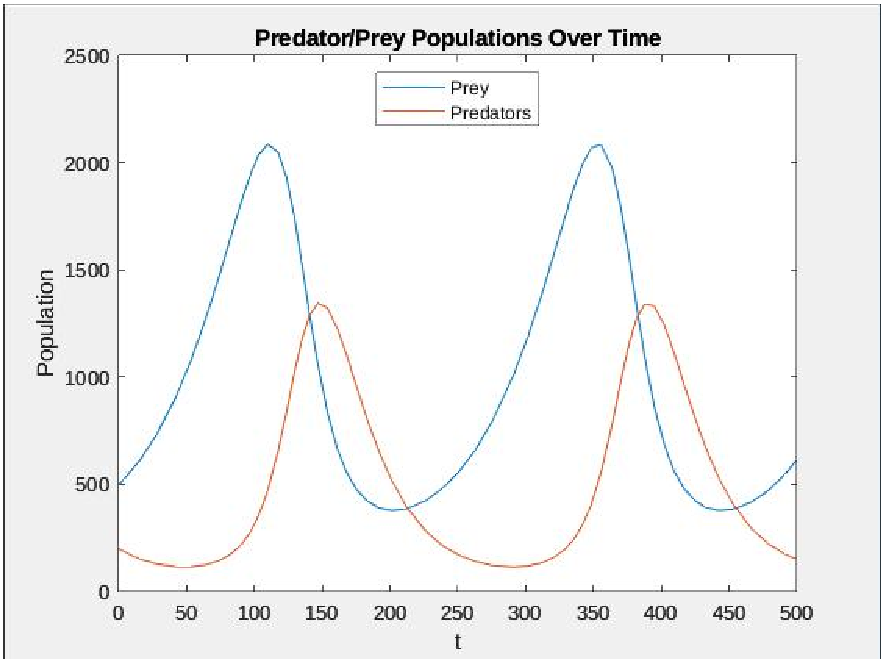

Figure 4: Predator Prey Plot 3

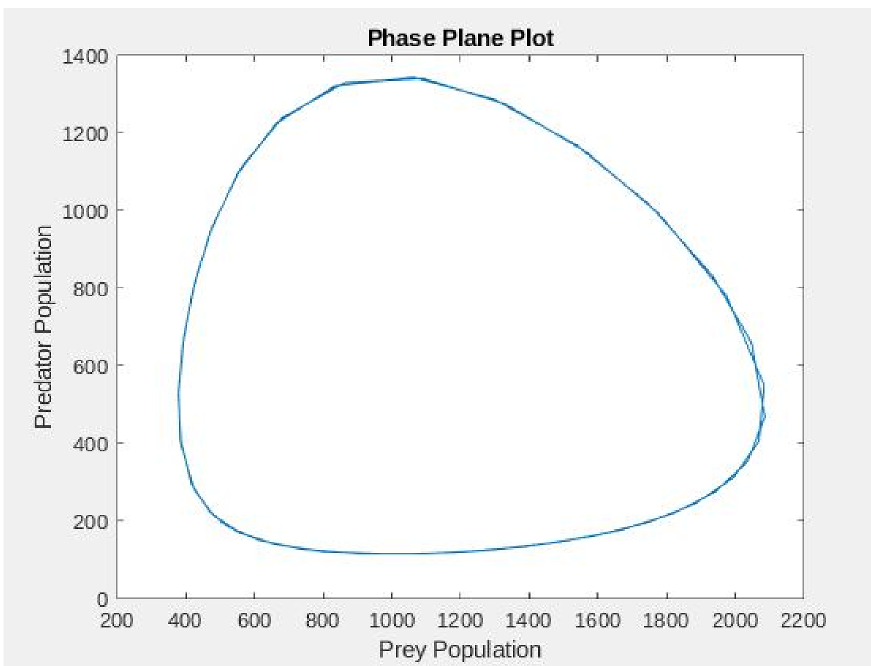

Figure 5: Predator Prey Plot 4

2.2 P1-5_A

The correct option is b.

2.3 P1-6$_B$

(a) For CSTR, we can use the second equation. We are given all the relevant values and can just plug in directly to get a volume of 99 dm^3. Since k is a constant, a PFR will also be 99 dm^3 due to the integral being that of a constant.
(b) First a conversion of k to per hour terms: k = 0.3600/hr. We can use the fact that F$_{A0}$ = $\nu_0 C_{A0}$ to find C$_{A0}$. So C$_{A0}$ is 5 mol/h divided by 10 dm^3/h, which works out to 0.5 mol/dm^3. We also know that the final concentration is 0.005 (1 percent of the initial). For CSTR now we use the following:

$$V = \frac{\nu_0 \times [C_{A0} - C_A]}{kC_A} \tag{3}$$

Therefore, V = 2750 dm^3 for a CSTR. For a PFR we know that F$_A$ = $\nu_0 C_A$ and that C$_A$ is 0.005. So F$_{A1}$ is 0.05. Now we can solve this using the following:

$$\int_{F_{A1}}^{F_{A0}} \frac{dF_A}{r_A} = V \tag{4}$$

$$\int_{C_A}^{C_{A0}} \frac{dC_A \nu_0}{-kC_A} = V \tag{5}$$

$$\frac{\nu_0}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{-C_A} = V \tag{6}$$

$$\frac{\nu_0}{k} ln \frac{C_{A0}}{C_A} = V \tag{7}$$

Plugging in all the numbers, V = 127.921 dm^3.
(c) For the CSTR, we can use equation 3 again, but use kC$_A^2$ instead of kC$_A$. This yields 660 dm^3. For the PFR we use equations 4-7 again, albeit the integration is different due to the C$_A^2$ term. This yields 6.6 dm^3.

2.4 P2-4$_B$ (a-e)

(a) For CSTR, we can use $\frac{F_{A0}X}{-r_A}$ where X is 0.4 and thus -r$_A$ is 5.0. F$_{A0}$ is given as 300 mol/min. Thus the CSTR volume is 24 dm^3. The PFR volume is determined by integrating $\frac{F_{A0}}{-r_A}dX$ from zero to X. 40 percent needs to be converted therefore X = 0.4. We can use Simpson's 1/3 rule to approximate, with Δx being 0.2 which yields 71.9 dm^3.
(b) Assuming the values between 0.4 and 0.45, 0.45 and 0.5, and 0.5 and 0.6 are constant, then a CSTR and a PFR reactor volume would be identical between X = 0.4 and X = 0.6. If a Levenspiel plot was made for this data, it would be constant and thus the integral under that portion would be rectangular, like the CSTR calculation.
The following is a 'map' to how I approached (c), (d), and (e) in Desmos.

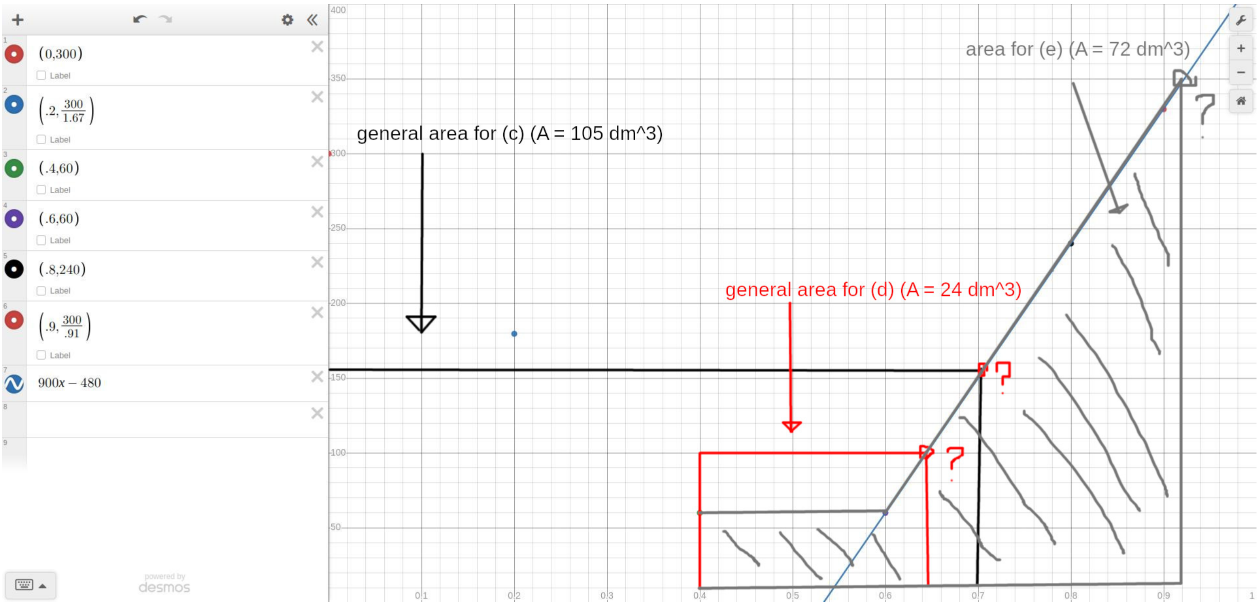

Figure 6: Approach for parts c, d, e (Black, Red, Grey respectively)

(c) Here we can work backwards. The volume is 105 dm^3.For this question as well as (d) and (e) I am making the assumption that the Levenspiel plot between X = 0.6 and 0.8 (for (e), between 0.8 and 0.9 as well) is linear. Now I can calculate the slope of the line and calculate the point at which $\frac{X}{-r_A}$ is 0.35 dm^3/mol/min. I calculated the line of $\frac{F_{A0}}{-r_A}$ between 0.6 and 0.8 to have the form $\frac{F_{A0}}{-r_A}$ = 900X - 480. Since the reactor is a CSTR, the volume will be X $\times$ $\frac{F_{A0}}{-r_A}$. We've already expressed $\frac{F_{A0}}{-r_A}$ in terms of X, so we can easily solve for the conversion: (900X-480)X = 105 dm^3. This yields X = 0.7.
(d) As we know from (a) the conversion from that PFR size would be 40 percent. Then a 24 dm^3 CSTR: we can use $\frac{F_{A0}(X_2-X_1)}{-r_A}$ = 24 dm^3. Using a similar setup to (c) (albeit with X - 0.4 instead of just X) we can solve for the conversion once again: (900X-480)(X-0.4) = 24 dm^3 yields X = 0.643.
(e) As we know from (a) the conversion from that CSTR size would be 40 percent. Then a 72 dm^3 PFR: I integrated 900X-480 from 0.6 to X such that the area under the curve would be 60 (as the sum including the flat rectangular bit in Figure 6 would be 72). I used the Desmos slider to adjust the X value until it was very close to 60. I found X to be 0.905, so the conversion with the PFR in series will be 0.905.