MATH.2360 Engineering Differential Equations Project Spring 2019

DUE DATES: FRIDAY, MARCH 22.
OPTIONAL REVISION DUE FRIDAY, APRIL 19.

No extensions will be given except in case of illness or other emergency.

General Guidelines

1. You may work in groups of up to four. Turn in just one paper for the whole group. Each member of the group will receive the same grade. **If you would like to work in a group but cannot find a group to join, please let me know no later than Friday, February 22.**

2. If you choose to turn in a revised version of your report, 90% of your grade will be based on the final version and 10% on the first version.

3. This is a major assignment, and you should plan to do some work on it every day, starting today. **DO NOT WAIT UNTIL THE LAST MINUTE. IF YOU DO, YOU WILL NOT BE ABLE TO COMPLETE THE PROJECT.**

4. The paper you turn in must be your group's work. I reserve the right to ask any or all of you for a verbal explanation of your solution.

5. I strongly encourage you to see me regularly as you work on the project to discuss your progress. If you receive any assistance from anyone other than me, of if you use our textbook or any other outside source, you must cite the source in your paper. Remember guideline number 3.

What Should You Hand In?

After you have completely solved all parts of the assigned problem, you should write a report explaining your solution. The report should contain a mixture of text, equations, and graphs, and possibly tables and diagrams. Your report should be grammatically correct, and you should use proper punctuation and spelling. If you do not type the paper, please write legibly. Your paper should contain an introduction explaining the problem and should clearly explain each step of your solution. Assume the reader knows something about differential equations but has not read the project description below. Please note that you will be graded on the quality of your presentation as well as on the mathematical content. You may find the following checklist helpful. It was adapted from a checklist developed by Dr. Annalisa Crannell of Franklin and Marshall College. Does this paper

1. clearly restate the problem to be solved?

2. clearly label diagrams, tables, and graphs?

3. define all variables used?

4. provide a paragraph explaining how the problem will be approached?

5. explain how each formula is derived or give a reference indicating where it can be found?

6. give acknowledgment where it is due?

In this paper,

7. are the spelling, grammar, and punctuation correct?

8. is the mathematics correct?

9. did you answer all the questions that were asked?

Grade Sheet

1. Derivation of equation (1) (10 points) _______

2. Explanation why $dx/dt = -dz/dt$ and $dy/dt = -dz/dt$ (10 points) _______

3. Explanation why $x + z = a$ and $y + z = b$ (10 points) _______

4. Derivation of equation (2) (5 points) _______

5. Plot of numerical solution for specified parameter values. (20 points) _______

6a. Demonstration that (2) has 2 real, distinct, positive equilibria. (10 points) _______

6b. Explanation why $z_2 > z(0)$. (10 points) _______

6c. Long-term behavior of solution to (3) (15 points) _______

7. Presentation (introduction, clarity and completeness of presentation, grammar) (10 points) _______

Total. _______

Project Description

Background Information

In this project, you will model a reversible chemical reaction. In the "forward" reaction, one molecule of substance A combines with one molecule of substance B to form one molecule of substance C; in the "reverse" reaction, one molecule of substance C dissociates into one molecule of A and one of B. This equation can be represented symbolically by the chemical equation $A+B \rightleftharpoons C$.

In order for a molecule of substance A to combine with a molecule of substance B, the two molecules must be near each other. Therefore, it is reasonable to assume that the rate of formation of C in the forward reaction is proportional to the rate at which collisions occur between molecules of A and B. Clearly, the collision rate between molecules of A and B will increase if the concentration of either A or B increases. We therefore make the further assumption that the collision rate between molecules of A and B is proportional to the product of the concentrations of substances A and B. Thus, the rate of formation of C in the forward reaction is proportional to the product of the concentrations of A and B.

For the reverse reaction, we assume that in a given time period a certain fraction of the molecules of substance C will spontaneously dissociate. Thus, the rate of decay of C in the reverse reaction is proportional to the concentration of C.

There are many questions we can ask about how the reaction proceeds. Does the forward reaction dominate, so that all of substance A and/or B is used up to form C? Does the reverse reaction dominate, so that no C remains? Does the system oscillate between these two extreme states? Does the system reach some kind of equilibrium state in which the forward and reverse reactions balance each other? In this project you will determine which, if any, of these possible behaviors is predicted by the mathematical model.

Problem Statement

The project consists of the following steps. In the remainder of this project description we let t denote time (in seconds), and we let x, y, and z denote the concentrations (in moles per liter) at time t of substances A, B, and C, respectively.

1. Assuming that

    - the rate of increase of z in the forward reaction is proportional to the product of x and y;
    - the rate of decrease of z in the reverse reaction is proportional to z; and
    - no substance is added to or removed from the vessel in which the reaction is taking place,

    explain why z must satisfy the following differential equation.

    $$\frac{dz}{dt} = k_1 xy - k_2 z \tag{1}$$

2. Explain why $dx/dt = -dz/dt$ and $dy/dt = -dz/dt$.
    Hint: Remember that the reaction you are modeling is $A+B \rightleftharpoons C$.

3. Use the result of the previous step to conclude that $x+z$ and $y+z$ are constant. Therefore, $x+z=a$ and $y+z=b$, where $a = x(0)+z(0)$ and $b = y(0)+z(0)$.

4. Use the result of the previous step and equation (1) to show that

    $$\frac{dz}{dt} = k_1 (a-z)(b-z) - k_2 z. \tag{2}$$

5. Consider a chemical reaction for which $k_1 = 1$ liter/mole/sec, $k_2 = 1$ sec^{-1}, $x(0) = 3$ moles/liter, $y(0) = 2$ moles/liter, and $z(0) = 1$ mole/liter. Use the MATLAB routine *ode45* to solve equation (2) numerically on the interval $0 \leq t \leq 3$. Plot the graphs of $x(t)$, $y(t)$, and $z(t)$ on the same set of axes. How do $x(t)$, $y(t)$, and $z(t)$ behave as t increases? (Do they oscillate, increase without bound, approach equilibrium values, ...?)

6. The purpose of this part of the project is to show that the solution of equation (2) always approaches an equilibrium no matter what the parameter values are.

   a. Show that equation (2) has two real, distinct, positive equilibria. Call these points z_1 and z_2, with $z_1 < z_2$. **Do not assign specific numerical values to the parameters a, b, k_1, or k_2.** Hints: Use the quadratic formula. Show that the quantity under the square root sign is positive, meaning that the equilibria are real and distinct. Explain why both equilibria are positive.

   b. Show that $z_2 > z(0)$. Hints: Look at the expression you found for z_2 using the quadratic formula. Look at the part of that expression before the square root sign. Remember how you defined a and b.

   c. The result of part a means that equation (2) can be rewritten as

$$\frac{dz}{dt} = k_1 (z - z_1)(z - z_2). \tag{3}$$

   Draw the phase line for equation (3) and use the phase line to show that the solution approaches z_1 as $t \to \infty$.

When writing your report, remember that your target audience does not have this project description, so you must explain the significance of what you are doing. Pretend you are trying to explain what you are doing to a friend in another section of Differential Equations.