MATH 271, Homework 3, *Solutions*

Problem 1. Write down the equations for each of the reactants and products for the following reactions.

(a) $A + 3B + C \xrightarrow{k} 2D + 2E$.

(b) $A \xrightarrow{k_1} B + C \xrightarrow{k_2} D$.

Solution 1. (a) We have the equations

$$\begin{aligned}
[A]' &= -k[A][B]^3[C] \\
[B]' &= -3k[A][B]^3[C] \\
[C]' &= -k[A][B]^3[C] \\
[D]' &= 2k[A][B]^3[C] \\
[E]' &= 2k[A][B]^3[C].
\end{aligned}$$

(b) The equations are

$$\begin{aligned}
[A]' &= -k_1[A] \\
[B]' &= k_1[A] - k_2[B][C] \\
[C]' &= k_1[A] - k_2[B][C] \\
[D]' &= k_2[B][C].
\end{aligned}$$

Problem 2. Consider the following reaction

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C.$$

For the following parts, use the link: `https://www.desmos.com/calculator/srrpeadlou`.

(a) Compare and contrast the reactions that take place given the three different scenarios for initial conditions. Explain why what the graph displays makes sense and include your graphs.

- $[A]_0 = 1$, $[B]_0 = 0$, and $[C]_0 = 0$.
- $[A]_0 = 0$, $[B]_0 = 1$, and $[C]_0 = 0$.
- $[A]_0 = 0$, $[B]_0 = 0$, and $[C]_0 = 1$.

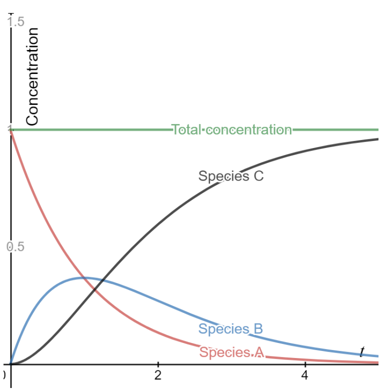
(b) For the initial conditions $[A]_0 = 1$, $[B]_0 = 0$, and $[C]_0 = 0$, explain what happens when you let

- $k_1 = 0$ and $k_2 = 1$,
- $k_1 = 1$ and $k_2 = 0$.

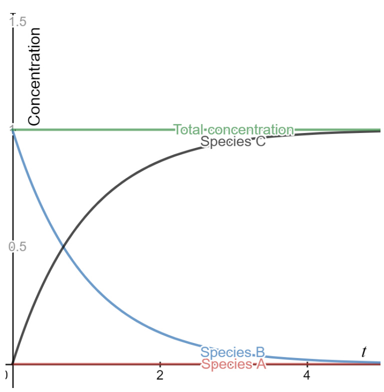
Include plots for these cases as well.

(c) Consider the initial conditions $[A]_0 = 1$, $[B]_0 = 0$, and $[C]_0 = 0$ and rate constants $k_1 = 1$ and $k_2 = 2$. Then, choose initial conditions of your own and compare your plots with the other initial conditions. Why do yours behave the way they do? Include your plots.

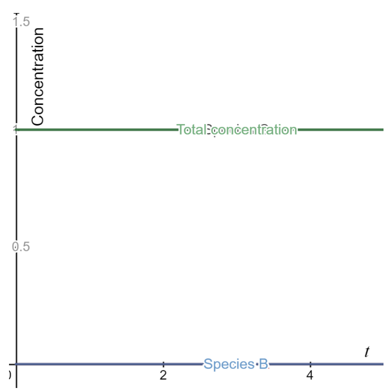
Solution 2. (a) Here are the graphs for the given initial conditions.



(a) Curves for $[A]_0 = 1$, $[B]_0 = 0$, and $[C]_0 = 0$.



(b) Curves for $[A]_0 = 0$, $[B]_0 = 1$, and $[C]_0 = 0$.

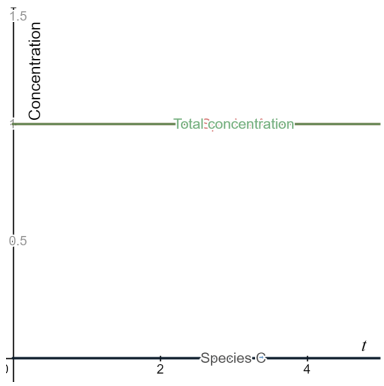


(c) Curves for $[A]_0 = 0$, $[B]_0 = 0$, and $[C]_0 = 1$.

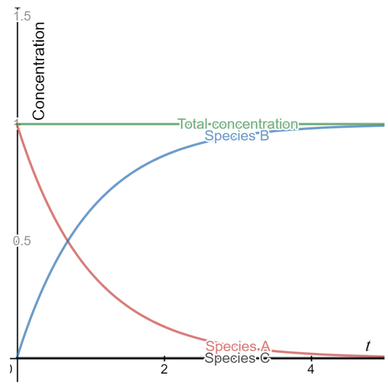
Let's now think about these graphs.

- The first sees exponential decay of species A and initially a quick growth of species B. But, as species B reacts and creates species C, we start to see a plateau and then decline in the concentration of species B. Ultimately, the concentration of species C seems to grow consistently. In the beginning, the concentration of species C increases more slowly since there is less of B to react, and it grows more slowly towards the end of the reaction for a similar reason.
- Now, species A has no role in the reaction. We simply see exponential decay of species B as it produces C.
- There is no reaction taking place since we have removed A and B from the system entirely. All we have left is the stable species C.

(b) Here are the graphs for the different k values.



(a) Curves for $k_1 = 0$ and $k_2 = 1$ with initial concentrations $[A]_0 = 1$, $[B]_0 = 0$, and $[C]_0 = 0$.

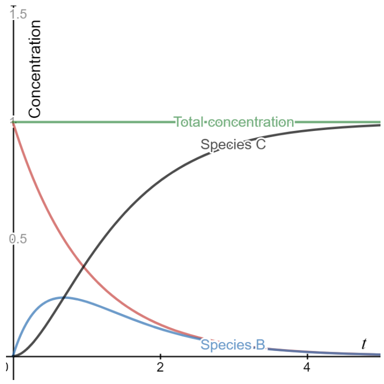


(b) Curves for $k_1 = 1$ and $k_2 = 0$ with initial concentrations $[A]_0 = 1$, $[B]_0 = 0$, and $[C]_0 = 0$.

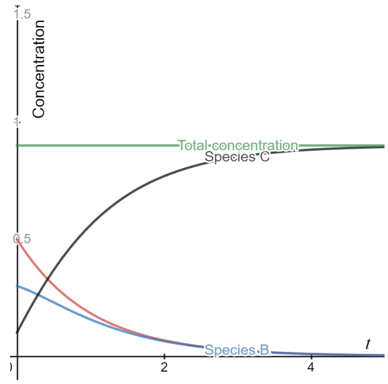
Let's now think about these graphs.

- Here, if $k_1 = 0$, then the first reaction never takes place. So, none of species A can react to form species B. Since there is no initial concentration for B or C, there are never any of these products produced. We simply see $[A]$ remain constant. This is similar to what we see in the third case in the previous part of this problem.
- By taking $k_2 = 0$ we have essentially removed the second reaction. Now, A converts to B and B never converts to C. Thus, we see exponential decay of A which produces B. This is similar to what we see in the second case in the previous part of this problem.

(c) Plots for (c) below.



(a) Curves for $k_1 = 1$ and $k_2 = 2$ with initial concentrations $[A]_0 = 1$, $[B]_0 = 0$, and $[C]_0 = 0$.



(b) Curves for $k_1 = 1$ and $k_2 = 0$ with initial concentrations $[A]_0 = 0.5$, $[B]_0 = 0.3$, and $[C]_0 = 0.1$.

I chose these other initial conditions because we never see an increase in the amount of species B. To me, this is a bit interesting. The rate of reaction k_2 being larger means that we do not always see a build up of species B.

Problem 3. Consider the second order chemical reaction given by

$$A + B \xrightarrow{k} \text{Products.}$$

(a) Write a *system* of differential equations to describe the concentration of the reactants A and B (this means write one for each).

(b) The concentrations of A and B can be related to each other in the following way: Let $A = A_0 - x$ and $B = B_0 - x$. Here, we think of x as the amount of each chemical that has reacted, and note that it depends on time t. Use this change of variables to rewrite the differential equation for chemical A in terms of x and t.

(c) Solve the differential equation in (b) with the initial condition $x(0) = 0$.You will need to use *partial fraction decomposition* to evaluate the integral.

Solution 3.

(a) The system of equations we will get is

$$\begin{aligned} \frac{d[A]}{dt} &= -k[A][B] \\ \frac{d[B]}{dt} &= -k[A][B]. \end{aligned}$$

(b) Now, let $[A] = [A]_0 - x$ and $[B] = [A]_0 - x$ and, since $[A]_0$ and $[B]_0$ are constant, we get the equation for $[A]$,

$$-\frac{dx}{dt} = k([A]_0 - x)([B]_0 - x).$$

It turns out $[B]$ has the same equation (which you should double check yourself).

(c) This is a separable equation, so we can find the solution by

$$\begin{aligned} -\frac{dx}{dt} &= k([A]_0 - x)([B]_0 - x) \\ \int \frac{dx}{([A]_0 - x)([B]_0 - x)} &= -k \int dt. \end{aligned}$$

Here, we can use the partial fraction decomposition to get

$$\frac{1}{[A]_0 - [B]_0} \ln\left(\frac{x - [A]_0}{x - [B]_0}\right) = -kt + C.$$

Then we can find

$$\frac{x - [A]_0}{x - [B]_0} = e^{-kt+C}$$

With $x(0) = 0$ we have

$$\frac{-[A]_0}{-[B]_0} = e^{-kt}e^{C}$$

and so $e^C = \frac{[A]_0}{[B]_0}$. We can rewrite this in terms of $[A]$ and $[B]$ as

$$\frac{[A]}{[B]} = \frac{[A]_0}{[B]_0} e^{-kt}.$$

This is as simplified as I would take the expression. What we can see here is that the ratio of $[A]$ to $[B]$ will change exponentially over time.

Problem 4. If $x_1(t)$ and $x_2(t)$ are solutions to the differential equation

$$x'' + bx' + cx = 0$$

is $x = x_1 + x_2 + k$ for a constant k always a solution? Is the function $y = tx_1$ a solution?

Solution 4. x and y are *not* solutions. Let's see why. We note that x_1 and x_2 are solutions and thus

$$x_i'' + bx_i' + cx_i = 0 \qquad \text{for } i = 1, 2.$$

Now, we check if x is a solution by plugging into the left hand side

$$\begin{aligned} x'' + bx' + cx &= (x_1 + x_2 + k)'' + b(x_1 + x_2 + k)' + c(x_1 + x_2 + k) \\ &= \underbrace{x_1'' + bx_1' + cx_1}_{=0} + \underbrace{x_2'' + bx_2' + cx_2}_{=0} + ck \\ &= ck \neq 0. \end{aligned}$$

So this x is not a solution.

Similarly, we take $y = tx_1$ and plug it into the left hand side and find

$$\begin{aligned} y'' + by' + cy &= (tx_1)'' + b(tx_1)' + c(tx_1) \\ &= tx_1'' + 2x_1' + b(tx_1' + x_1) + c(tx_1) \\ &= t\underbrace{(x_1'' + bx_1' + cx_1)}_{=0} + 2x_1' + bx_1 \\ &= 2x_1' + bx_1, \end{aligned}$$

which is not in general a solution unless $x_1 = 0$.

Problem 5. Consider the following initial value problem:

$$x'' + 4x' + 3x = 0$$

with initial data $x(0) = 1$, $x'(0) = 0$.

(a) Find the solution.

(b) Sketch a plot of the solution.

(c) Explain in words what is happening to the solution as time goes on. What happens as $t \to \infty$?

Solution 5.

(a) We can solve this homogeneous second order linear equation with constant coefficients by finding roots to its characteristic polynomial. In this case, that amounts to

$$\begin{aligned} \lambda^2 + 4\lambda + 3 &= 0 \\ \iff (\lambda + 3)(\lambda + 1) &= 0, \end{aligned}$$

so the roots are $\lambda_1 = -1$ and $\lambda_2 = -3$. Thus our general solution is

$$x(t) = C_1 e^{\lambda_1 t} + C_2 e^{\lambda_2 t} = C_1 e^{-t} + C_2 e^{-3t}.$$

Then we use the initial conditions to find a particular solution. Namely,

$$\begin{aligned} 1 = x(0) &= C_1 e^{-0} + C_2 e^{-3\cdot 0} = C_1 + C_2 \\ 0 = x'(0) &= -C_1 e^{-0} - 3C_2 e^{-3\cdot 0} = -C_1 - 3C_2. \end{aligned}$$

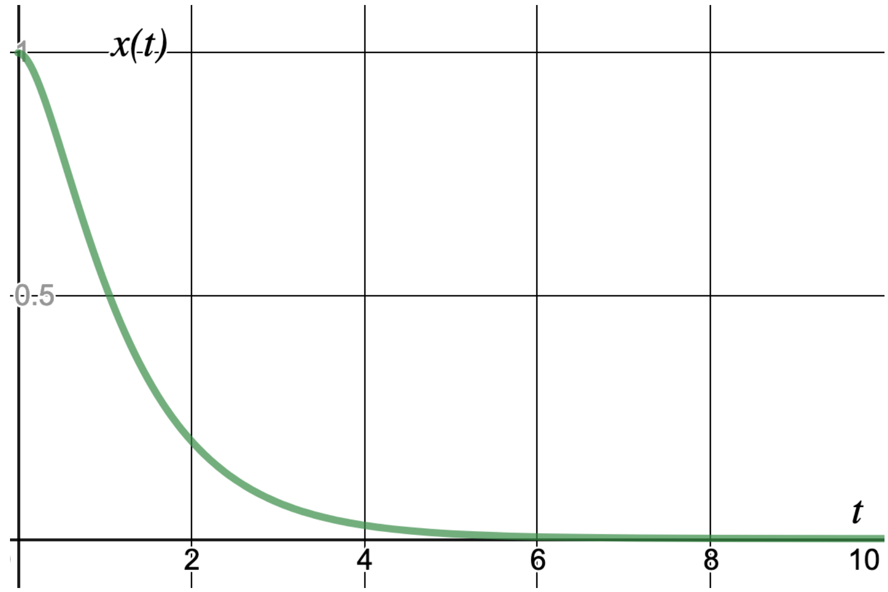
Using the second equation we get $C_1 = -3C_2$. We can plug this into the first equation to get

$$1 = -3C_2 + C_2 = -2C_2$$

meaning that $C_2 = -\frac{1}{2}$. Thus $C_2 = \frac{3}{2}$. Hence, our particular solution for this IVP is

$$x(t) = \frac{3}{2} e^{-t} - \frac{1}{2} e^{-3t}.$$

(b) Here is a plot of the particular solution from time $t = 0$ to time $t = 10$.



(c) The solution decays exponentially over time. As $t \to \infty$ our solution approaches zero.

Problem 6. Write down a homogeneous second-order linear differential equation where the system displays a decaying oscillation.

Solution 6. Since our solution should oscillate and decay, we need some form of a "spring" and some form of damping. These terms show up respectively as b and c in the equation

$$x'' + bx' + cx = 0.$$

Now, also note that (aside from one special case of two of the same real roots), our general solution has the form

$$x(t) = C_1 e^{\lambda_1 t} + C_2 e^{\lambda_2 t}$$

where λ_1 and λ_2 are roots to the characteristic polynomial

$$\lambda^2 + b\lambda + c = 0.$$

Now, the roots for the characteristic polynomial are

$$\lambda = \frac{-b \pm \sqrt{b^2 - 4c}}{2}.$$

- To have oscillation, our roots must have an imaginary part and thus

  $$b^2 - 4c < 0.$$

  In other words, $b^2 < 4c$.

- To have a decaying solution, the real part of the roots must be negative. The real part of the roots will be $\frac{-b}{2}$ and thus we need

  $$\frac{-b}{2} < 0.$$

Now, I'll choose $b = 1$ and $c = 1$ which satisfy both of these requirements. We then have

$$x'' + x' + x = 0$$

as our equation.

Note, we can also find the solution as the roots are then

$$\lambda = \frac{-1 \pm \sqrt{1-4}}{2} = \frac{-1}{2} \pm \frac{\sqrt{3}}{2}.$$

Plugging this into the form for the general solution and we get

$$x(t) = e^{-\frac{1}{2}t} \left(C_1 \sin\left(\frac{\sqrt{3}}{2}\right) + \cos\left(\frac{\sqrt{3}}{2}\right)\right)$$

Problem 7. Consider the following differential equation:

$$x'' + 2x' + x = 3e^{-t} + 2t.$$

(a) Find the homogeneous solution $x_H(t)$.

(b) Find the particular integral $x_P(t)$.

(c) Find the specific solution corresponding to the initial data $x(0) = 0$, $x'(0) = 0$.

Solution 7.

(a) The roots to characteristic polynomial satisfy

$$\lambda^2 + 2\lambda + 1 = 0$$

which can be found by factoring

$$(\lambda + 1)^2 = 0,$$

which gives us that $\lambda = -1$ is the only root. Thus, this is the special case where our general solution looks slightly different. We'll have

$$x_h(t) = C_1 e^{-t} + C_2 t e^{-t}.$$

(b) The right hand side has a e^{-t} term which is already present in our x_h. In fact, this means we have to take kt^2e^{-t} as a guess for this part of x_p. Then, we also have a $2t$ term, so our x_p should be

$$x_p = kt^2e^{-t} + a_0 + a_1 t.$$

Now we have to find the undetermined coefficients by plugging in and solving

$$\begin{aligned} x_p'' + 2x_p' + x_p &= 3e^{-t} + 2t \\ 2ke^{-t} - 4kte^{-t} + kt^2e^{-t} + 2(2kte^{-t} - kt^2e^{-t} + a_1) + kt^2e^{-t}a_1 t + a_0 &= 3e^{-t} + 2t \end{aligned}$$

which gives us that $k = \frac{3}{2}$, $a_1 = 2$, and $a_0 = -4$. So

$$x_p(t) = \frac{3}{2}t^2e^{-t} + 2t - 4.$$

(c) Now, we take it that our solution is of the form

$$x(t) = x_h + x_p = C_1e^{-t} + C_2te^{-t} + \frac{3}{2}t^2e^{-t} + 2t - 4.$$

If we take

$$0 = x(0) = C_1 - 4$$

then $C_1 = 4$, and

$$0 = x'(0) = -4 + C_2 + 2$$

so $C_2 = 2$. Thus, our specific solution is

$$x(t) = (4 + 2t)e^{-t} + \frac{3}{2}t^2e^{-t} + 2t - 4.$$