Exercise 40

In an elementary chemical reaction, single molecules of two reactants A and B form a molecule of the product C: $\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C}$. The law of mass action states that the rate of reaction is proportional to the product of the concentrations of A and B:

$$\frac{d[\mathrm{C}]}{dt} = k[\mathrm{A}][\mathrm{B}]$$

(See Example 3.7.4.) Thus, if the initial concentrations are $[\mathrm{A}] = a$ moles/L and we write $x = [\mathrm{C}]$, then we have

$$\frac{dx}{dt} = k(a - x)(b - x)$$

(a) Assuming that $a \neq b$, find x as a function of t. Use the fact that the initial concentration of C is 0.

(b) Find $x(t)$ assuming that $a = b$. How does this expression simplify for $x(t)$ simplify if it is known that $[\mathrm{C}] = \frac{1}{2}a$ after 20 seconds?

Solution

Part (a)

Assume that $a \neq b$. Since the differential equation is separable, we can solve for $x(t)$ by bringing all terms with x to the left side and all constants and terms with t to the right side and then integrating both sides.

$$\begin{aligned} \frac{dx}{dt} &= k(a - x)(b - x) \\ dx &= k(a - x)(b - x)\, dt \\ \frac{dx}{(a - x)(b - x)} &= k\, dt \\ \int \frac{dx}{(a - x)(b - x)} &= \int k\, dt \end{aligned}$$

To integrate the left side, we have to split it up using partial fraction decomposition. Because the denominator is a product of linear factors, the integrand can be written as follows.

$$\frac{1}{(a - x)(b - x)} = \frac{D_1}{a - x} + \frac{D_2}{b - x}$$

Multiply both sides by $(a - x)(b - x)$.

$$1 = D_1(b - x) + D_2(a - x)$$

Setting $x = a$ and $x = b$ gives

$$\begin{aligned} x = a: &\quad 1 = D_1(b - a) \quad \rightarrow \quad D_1 = \frac{1}{b - a} \\ x = b: &\quad 1 = D_2(a - b) \quad \rightarrow \quad D_2 = -\frac{1}{b - a}. \end{aligned}$$

So

$$\begin{aligned}\int\left(\frac{1}{b-a}\frac{1}{a-x}-\frac{1}{b-a}\frac{1}{b-x}\right)dx &= \int k\,dt\\ \int\frac{dx}{a-x}-\int\frac{dx}{b-x} &= \int k(b-a)\,dt.\end{aligned}$$

$$\begin{aligned}\text{Let } u = a-x \quad &\text{and} \quad v = b-x\\ du = -dx \quad &\text{and} \quad dv = -dx\end{aligned}$$

$$\begin{aligned}\int\frac{-du}{u}-\int\frac{-dv}{v} &= \int k(b-a)\,dt\\ -\ln|u|+\ln|v| &= k(b-a)t+D_3\\ \ln\left|\frac{v}{u}\right| &= k(b-a)t+D_3\end{aligned}$$

Now exponentiate both sides.

$$\begin{aligned}\left|\frac{b-x}{a-x}\right| &= e^{k(b-a)t+D_3} = e^{k(b-a)t}e^{D_3}\\ \frac{b-x}{a-x} &= \pm e^{D_3}e^{k(b-a)t}\end{aligned}$$

Let $D_4 = \pm e^{D_3}$.

$$\begin{aligned}b-x &= D_4(a-x)e^{k(b-a)t}\\ b-x &= D_4ae^{k(b-a)t}-D_4xe^{k(b-a)t}\\ b-D_4ae^{k(b-a)t} &= x-D_4xe^{k(b-a)t}\\ b-D_4ae^{k(b-a)t} &= x\left(1-D_4e^{k(b-a)t}\right)\end{aligned}$$

$$x(t) = \frac{b-D_4ae^{k(b-a)t}}{1-D_4e^{k(b-a)t}}$$

We're not done yet. The initial concentration of C is 0, so x(t = 0) = 0. We can use this to determine D_4.

$$\begin{aligned}x(0) = \frac{b-D_4ae^0}{1-D_4e^0} &= 0\\ b-D_4a &= 0\\ D_4 &= \frac{b}{a}\end{aligned}$$

$$x(t) = \frac{b-\frac{b}{a}ae^{k(b-a)t}}{1-\frac{b}{a}e^{k(b-a)t}}\cdot\frac{a}{a}$$

$$x(t) = \frac{ab\left[1-e^{k(b-a)t}\right]}{a-be^{k(b-a)t}}, \quad a\neq b$$

Part (b)

Now assume that $a = b$. The differential equation that needs to be solved is

$$\frac{dx}{dt} = k(a-x)^2.$$

This is still a separable equation, so we can solve it as we did before by bringing the terms with x to the left and the constants and terms with t to the right and then integrating both sides.

$$dx = k(a-x)^2\,dt$$

$$\frac{dx}{(a-x)^2} = k\,dt$$

$$\int \frac{dx}{(a-x)^2} = \int k\,dt$$

$$\text{Let } u = a - x$$

$$du = -dx$$

$$\int \frac{-du}{u^2} = \int k\,dt$$

$$u^{-1} = kt + D_5$$

$$\frac{1}{a-x} = kt + D_5$$

$$\frac{1}{kt + D_5} = a - x$$

$$x(t) = a - \frac{1}{kt + D_5}$$

If [C] $= \frac{1}{2}a$ after 20 seconds, then $x(t = 20) = \frac{1}{2}a$. We can use this information to determine D_5.

$$x(20) = a - \frac{1}{k(20) + D_5} = \frac{1}{2}a$$

$$\frac{1}{2}a = \frac{1}{20k + D_5}$$

$$a(20k + D_5) = 2$$

$$20k + D_5 = \frac{2}{a}$$

$$D_5 = \frac{2}{a} - 20k$$

$$x(t) = a - \frac{1}{kt + \frac{2}{a} - 20k} \cdot \frac{a}{a}$$

$$x(t) = a - \frac{a}{ak(t-20) + 2}$$

$$x(t) = a\left[1 - \frac{1}{ak(t-20)+2}\right], \quad a = b$$