Problem 28

Chemical Reactions. A second order chemical reaction involves the interaction (collision) of one molecule of a substance P with one molecule of a substance Q to produce one molecule of a new substance X; this is denoted by $P + Q \to X$. Suppose that p and q, where $p \neq q$, are the initial concentrations of P and Q, respectively, and let $x(t)$ be the concentration of X at time t. Then $p - x(t)$ and $q - x(t)$ are the concentrations of P and Q at time t, and the rate at which the reaction occurs is given by the equation

$$dx/dt = \alpha(p - x)(q - x), \tag{i}$$

where α is a positive constant.

(a) If $x(0) = 0$, determine the limiting value of $x(t)$ as $t \to \infty$ without solving the differential equation. Then solve the initial value problem and find $x(t)$ for any t.

(b) If the substances P and Q are the same, then $p = q$ and Eq. (i) is replaced by

$$dx/dt = \alpha(p - x)^2. \tag{ii}$$

If $x(0) = 0$, determine the limiting value of $x(t)$ as $t \to \infty$ without solving the differential equation. Then solve the initial value problem and determine $x(t)$ for any t.

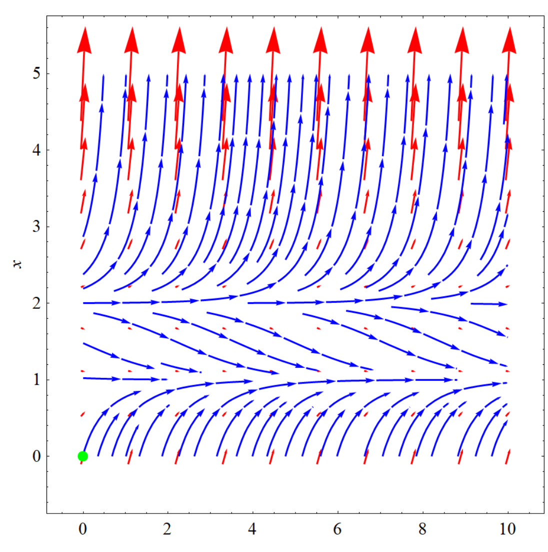
Solution

Part (a)

The chemical reaction for this problem is

$$\mathrm{P} + \mathrm{Q} \longrightarrow \mathrm{X}.$$

The (stoichiometric) coefficients of P and Q are both 1, so the molecules of P and Q combine in a one-to-one fashion. A sample direction field $\langle 1, \alpha(p - x)(q - x)\rangle$ in red is drawn below for $\alpha = 1$, $p = 1$, and $q = 2$.



In blue are solution curves, which lie tangent to the direction field vectors at every point, and the green dot represents the initial condition $x(0) = 0$. Following the blue curve that touches the green dot, we see that the solution $x(t)$ tends to 1 as $t \to \infty$. We conclude then that $x(t)$ tends to p or q, whichever of the two is smaller, as $t \to \infty$.

$$\lim_{t\to\infty} x(t) = \begin{cases} p & \text{if } p < q \\ q & \text{if } q < p \end{cases}$$

Solve the ODE now by separating variables.

$$\frac{dx}{dt} = \alpha(p - x)(q - x)$$

$$\frac{dx}{(p - x)(q - x)} = \alpha\, dt$$

Integrate both sides.

$$\int \frac{dx}{(p - x)(q - x)} = \alpha t + C$$

Use partial fraction decomposition to split up the integrand on the left.

$$\int \left(\frac{1/(q-p)}{p - x} + \frac{1/(p-q)}{q - x} \right) dx = \alpha t + C$$

$$\frac{1}{q-p} \int \frac{dx}{p - x} + \frac{1}{p-q} \int \frac{dx}{q - x} = \alpha t + C$$

$$\frac{1}{p-q} \int \frac{dx}{x - p} + \frac{1}{q-p} \int \frac{dx}{x - q} = \alpha t + C$$

$$\frac{1}{p-q} \ln|x - p| + \frac{1}{q-p} \ln|x - q| = \alpha t + C$$

$$\ln|x - p|^{1/(p-q)} + \ln|x - q|^{1/(q-p)} = \alpha t + C$$

$$-\ln|x - p|^{1/(q-p)} + \ln|x - q|^{1/(q-p)} = \alpha t + C$$

$$\ln\left|\frac{x - q}{x - p}\right|^{1/(q-p)} = \alpha t + C$$

Apply the initial condition $x(0) = 0$ now to determine C.

$$\ln\left|\frac{-q}{-p}\right|^{1/(q-p)} = C \quad \to \quad C = \ln\left(\frac{q}{p}\right)^{1/(q-p)}$$

The previous equation is then

$$\ln\left|\frac{x - q}{x - p}\right|^{1/(q-p)} = \alpha t + \ln\left(\frac{q}{p}\right)^{1/(q-p)}$$

$$\frac{1}{q-p} \ln\left|\frac{x - q}{x - p}\right| = \alpha t + \frac{1}{q-p} \ln\frac{q}{p}.$$

Multiply both sides by $q - p$.

$$\ln\left|\frac{x - q}{x - p}\right| = \alpha t(q - p) + \ln\frac{q}{p}$$

Exponentiate both sides.

$$\left|\frac{x-q}{x-p}\right| = e^{\alpha t(q-p)}\left(\frac{q}{p}\right)$$

Introduce $\pm$ on the right side to remove the absolute value sign.

$$\frac{x-q}{x-p} = \pm\frac{q}{p}e^{\alpha t(q-p)}$$

We choose the plus sign so that the initial condition remains satisfied.

$$\frac{x-q}{x-p} = \frac{q}{p}e^{\alpha t(q-p)}$$

Multiply both sides by $x-p$.

$$x - q = \frac{q}{p}e^{\alpha t(q-p)}x - qe^{\alpha t(q-p)}$$

Solve for x.

$$x\left[1 - \frac{q}{p}e^{\alpha t(q-p)}\right] = q - qe^{\alpha t(q-p)}$$

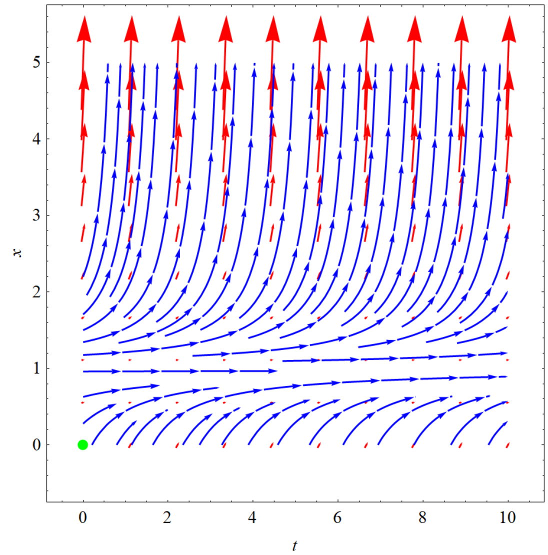
$$x(t) = \frac{q[1-e^{\alpha t(q-p)}]}{1-\frac{q}{p}e^{\alpha t(q-p)}}$$

Therefore,

$$x(t) = \frac{pq[1-e^{\alpha t(q-p)}]}{p-qe^{\alpha t(q-p)}}.$$

Part (b)

A sample direction field $\langle 1, \alpha(p-x)^2\rangle$ in red is drawn below for $\alpha = 1$ and $p = 1$.



In blue are solution curves, which lie tangent to the direction field vectors at every point, and the green dot represents the initial condition $x(0) = 0$. Following the blue curve that touches the green dot, we see that the solution $x(t)$ tends to 1 as $t \to \infty$. We conclude then that $x(t)$ tends to p as $t \to \infty$.

$$\lim_{t\to\infty} x(t) = p$$

Solve the ODE now by separating variables.

$$\frac{dx}{dt} = \alpha(p - x)^2$$

$$\frac{dx}{(p - x)^2} = \alpha\, dt$$

Integrate both sides.

$$\int \frac{dx}{(p - x)^2} = \alpha t + C_1$$

$$\int \frac{dx}{(x - p)^2} = \alpha t + C_1$$

$$-\frac{1}{(x - p)} = \alpha t + C_1$$

Apply the initial condition $x(0) = 0$ now to determine C_1.

$$-\frac{1}{-p} = C_1 \quad \rightarrow \quad C_1 = \frac{1}{p}$$

As a result, the previous equation becomes

$$-\frac{1}{(x - p)} = \alpha t + \frac{1}{p}.$$

Solve for x.

$$-(x - p) = \frac{1}{\alpha t + \frac{1}{p}}$$

$$x - p = -\frac{1}{\alpha t + \frac{1}{p}}$$

$$\begin{aligned} x(t) &= p - \frac{1}{\alpha t + \frac{1}{p}} \\ &= p - \frac{p}{\alpha p t + 1} \\ &= \frac{\alpha p^2 t + p - p}{\alpha p t + 1} \end{aligned}$$

Therefore,

$$x(t) = \frac{\alpha p^2 t}{\alpha p t + 1}.$$