Question

Consider a sequential reaction

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

in which atoms of type A decay into atoms of type B, and atoms of type B decay into atoms of type C, which are stable. Let a(t), b(t), c(t) be the number of atoms at time t of type A, B, C respectively. The numbers of atoms are large, so that they may taken to vary continuously, and the processes may then be modelled by a pair of coupled first order differential equations describing the rates of the decay:

$$\frac{da}{dt} = -k_1 a, \ \frac{db}{dt} = k_1 a - k_2 b,$$

together with the information that a(t)+b(t)+c(t) is constant. Assuming that at time t = 0, $a(0) = \alpha$ and b(0) = 0 = c(0) find expressions for the number of atoms of each type which are present at any given time.

Answer

Number of atoms of type A: Solve $\frac{\partial a}{\partial t} = -K_1 a$ (Separation of variables) $a(t) = \lambda e^{-K_1 t} (\lambda \text{ constant})$ Using boundary condition, $a(0) = \alpha$ gives $\lambda = \alpha$ so $\underline{a(t) = \alpha e^{-K_1 t}}$

Number of atoms of type B:

Solve $\frac{\partial b}{\partial t} = K_1 a - K_2 b = K_1 \alpha e^{-K_1 t} - K_2 b$ (from above) This gives a first order linear differential equation

$$\frac{\partial b}{\partial t} + K_2 b = K_1 \alpha e^{-K_1 t}$$

with integrating factor: $I(t) = e^{K_2 \int dt} = e^{K_2 t}$ Multiplying equation by integrating factor gives

$$e^{K_2 t} \frac{\partial b}{\partial t} + K_2 b e^{K_2 t} = K_1 \alpha e^{(K_2 - K_1)t}$$

 \mathbf{SO}

$$\frac{\partial}{\partial t}(be^{K_2t}) = K_1 \alpha e^{(K_2 - K_1)t}.$$

Integrating gives

$$be^{K_2 t} = \frac{K_1 \alpha}{K_2 - K_1} e^{(K_2 - K_1)t} + D$$

where D is constant.

Boundary conditions b(0) = 0 gives

$$0 = \frac{K_1 \alpha}{K_2 - K_1} + D \Rightarrow D = -\frac{K_1 \alpha}{K_2 - K_1}$$

Solution is

$$\underline{b(t) = \frac{K_1 \alpha}{K_2 - K_1} \left(e^{-K_1 t} - e^{-K_2 t} \right)}$$

Number of atoms of type C: c(t) = K - a(t) - b(t) for some constant K. Using boundary conditions $a(0) = \alpha$, b(0) = 0 = c(0) we have

$$0 = K - \alpha - 0 \Rightarrow K = \alpha$$

 \mathbf{SO}

$$c(t) = \alpha - \alpha e^{-K_{1}t} - \frac{K_{1}\alpha}{K_{2} - K_{1}} \left(e^{-K_{1}t} - e^{-K_{2}t} \right)$$
$$= \alpha \left(1 + \frac{K_{2}}{K_{1} - K_{2}} e^{K_{1}t} - \frac{K_{1}}{K_{1} - K_{2}} e^{-K_{2}t} \right)$$