

Modeling Rate Eq & Diff

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$$A. \quad \frac{dA}{dt} = -k_1 A \quad ; \quad A(t=0) = A_0 .$$

$$\int_{A_0}^{A(t)} \frac{dA}{A} = -k_1 \int_0^t dt \quad \begin{aligned} A_0 + B_0 &= A(t) + B(t) \\ \frac{dB}{dt} &= k_1 A(t) \\ &= k_1 (A_0 + B_0 - B(t)) . \end{aligned}$$

$$\ln \left(\frac{A(t)}{A_0} \right) = -k_1 t$$

$$\boxed{\begin{aligned} A(t) &= A_0 e^{-k_1 t} & B(t) &= B_0 + A_0 (1 - e^{-k_1 t}) \\ A + t &= \frac{\ln 2}{k_1}, \quad A = B = \frac{A_0}{2} \end{aligned}}$$

$$B. \quad \frac{dA}{dt} = \frac{dB}{dt} = -k_2 AB$$

$$A_0 + C_0 = A(t) + C(t)$$

$$B_0 + C_0 = B(t) + C(t)$$

$$\Rightarrow A_0 - B_0 = A(t) - B(t)$$

$$\Rightarrow B(t) = B_0 + A(t) - A_0$$

$$\Rightarrow \frac{dA}{dt} = -k_2 A (B_0 - A_0 + A)$$

$$\int \frac{dA}{A(B_0 - A_0 + A)} = \int -k_2 dt$$

$$\frac{x}{A} + \frac{y}{B_0 - A_0 + A} = \frac{1}{A(B_0 - A_0 + A)}$$

$$x(B_0 - A_0 + A) + Ay = 1$$

$$A = 0 \Rightarrow x = \frac{1}{B_0 - A_0}$$

$$A = A_0 - B_0 \Rightarrow y = \frac{1}{A_0 - B_0} = \frac{-1}{B_0 - A_0}$$

$$\therefore \frac{1}{B_0 - A_0} \left[\int_{A_0}^A \frac{dA}{A} - \int_{A_0}^A \frac{dA}{B_0 - A_0 + A} \right] = -k_2 \int_0^t dt$$

$$\Rightarrow \ln\left(\frac{A}{A_0}\right) - \ln\left(\frac{B_0 - A_0 + A}{B_0}\right) = -k_2(B_0 - A_0)t$$

$$\Rightarrow \frac{B_0 A}{A_0 (B_0 - A_0 + A)} = \exp[-k_2(B_0 - A_0)t]$$

$$\text{Let } \gamma = B_0 - A_0$$

$$\Rightarrow B_0 A = A_0 (\gamma + A) \exp(-k_2 \gamma t)$$

$$\Rightarrow B_0 A + A_0 \exp(-k_2 \gamma t) A = A_0 \gamma \exp(-k_2 \gamma t)$$

$$\Rightarrow A(t) = \frac{A_0 (B_0 - A_0) \exp(-k_2 (B_0 - A_0)t)}{B_0 - A_0 \exp(-k_2 (B_0 - A_0)t)}$$

$$\Rightarrow A(t) = \frac{A_0 (A_0 - B_0)}{A_0 - B_0 \exp(-k_2 (A_0 - B_0)t)}$$

$$A(t) = \frac{A_0 - B_0}{1 - \frac{B_0}{A_0} \exp(-k_2 (A_0 - B_0)t)}$$

$$B(t) = A(t) - (A_0 - B_0)$$

$$= \frac{A_0 - B_0}{1 - \frac{B_0}{A_0} \exp(-k_2 (A_0 - B_0)t)} - (A_0 - B_0)$$

$$= (A_0 - B_0) \left[\frac{1 - \frac{B_0}{A_0} \exp(-k_2(A_0 - B_0)t)}{1 - \frac{B_0}{A_0} \exp(-k_2(A_0 - B_0)t)} - 1 \right]$$

$$= (A_0 - B_0) \left[\frac{\frac{B_0}{A_0} \exp(-k_2(A_0 - B_0)t)}{1 - \frac{B_0}{A_0} \exp(-k_2(A_0 - B_0)t)} \right]$$

$$= \frac{A_0 - B_0}{-1 + \frac{A_0}{B_0} \exp(k_2(A_0 - B_0)t)}$$

$$B(t) = \frac{B_0 - A_0}{1 - \frac{A_0}{B_0} \exp(-k_2(B_0 - A_0)t)}$$

$$C(t) = B_0 + C_0 - B(t)$$

Given $A_0 < B_0$, let $\Phi = B_0 - A_0$
be equilibrium value.

$$\begin{aligned} A(t) &= \frac{-\Phi}{1 - \frac{B_0}{A_0} \exp(k_2 \Phi t)} \\ B(t) &= \frac{\Phi}{1 - \frac{A_0}{B_0} \exp(-k_2 \Phi t)} \\ C(t) &= C_0 + \frac{A_0 [1 - \exp(-k_2 \Phi t)]}{1 - \frac{A_0}{B_0} \exp(-k_2 \Phi t)} \end{aligned}$$

$$\begin{array}{l} \lim_{t \rightarrow \infty} \quad A(t) = 0 \\ \quad \quad \quad B(t) = \Phi = B_0 - A_0 \\ \quad \quad \quad C(t) = C_0 + A_0 \end{array}$$