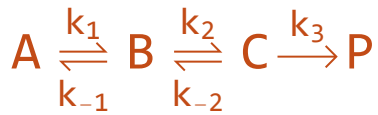


SetDirectory[NotebookDirectory[]]

D:\VS_workspace\CPlusPlus\SOHR\projects\catalytic_cycle\theory\SSA



Solve differential equation like

$$(\text{eq } 1) \quad \frac{d[A]}{dt} = -k_1 [A] + k_{-1} [B]$$

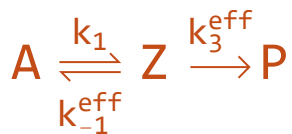
$$(\text{eq } 2) \quad \frac{d[B]}{dt} = k_1 [A] + k_{-2} [C] - (k_2 + k_{-1}) [B]$$

$$(\text{eq } 3) \quad \frac{d[C]}{dt} = k_2 [B] - (k_3 + k_{-2}) [C]$$

$$\text{eq1} = -k_1 * xA + k_{-1} * xB;$$

$$\text{eq2} = k_1 * xA + k_{-2} * xC - (k_2 + k_{-1}) * xB;$$

$$\text{eq3} = k_2 * xB - (k_3 + k_{-2}) * xC;$$



$$\text{eq4} = xZ - (xB + xC);$$

Make a Steady State Approximation (SSA), let (eq 2) = 0 and (eq 3) = 0

Clear[soln]; soln = Solve[eq2 == 0 && eq3 == 0 && eq4 == 0, {xA, xB, xC}] // Simplify

$$\left\{ \left\{ xA \rightarrow \frac{xZ (k_{-2} k_{-1} + (k_{-1} + k_2) k_3)}{k_1 (k_{-2} + k_2 + k_3)}, xB \rightarrow \frac{xZ (k_{-2} + k_3)}{k_{-2} + k_2 + k_3}, xC \rightarrow \frac{xZ k_2}{k_{-2} + k_2 + k_3} \right\} \right\}$$

$$xB = xB /. \text{soln}[[1, 2]]; xC = xC /. \text{soln}[[1, 3]];$$

xB

xC

$$\frac{xZ (k_{-2} + k_3)}{k_{-2} + k_2 + k_3}$$

$$\frac{xZ k_2}{k_{-2} + k_2 + k_3}$$

Rate Constant of Z

$(k_{-1} * xB + k_3 * xC) / xZ //$ Simplify

$$\frac{k_{-2} k_{-1} + (k_{-1} + k_2) k_3}{k_{-2} + k_2 + k_3}$$

Branching Ratios

$\Gamma_A = \text{Numerator}[xB] * k_{-1} / xZ //$ Simplify

$$k_{-1} (k_{-2} + k_3)$$

$\Gamma_P = \text{Numerator}[xC] * k_3 / xZ //$ Simplify

$$k_2 k_3$$

$\Gamma_A / (\Gamma_A + \Gamma_P)$

$$\frac{k_{-1} (k_{-2} + k_3)}{k_2 k_3 + k_{-1} (k_{-2} + k_3)}$$

$\Gamma_P / (\Gamma_A + \Gamma_P)$

$$\frac{k_2 k_3}{k_2 k_3 + k_{-1} (k_{-2} + k_3)}$$