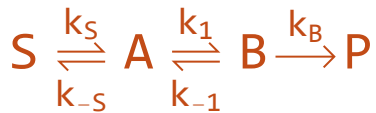


SetDirectory[NotebookDirectory[]]

D:\Github\SOHR\projects\catalytic\_cycle\theory\SSA



Solve differential equation like

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

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

$$(\text{eq } 3) \quad \frac{d[B]}{dt} = k_1 [A] - (k_B + k_{-1}) [B]$$

$$\text{eq1} = -k_S * xS + k_{-S} * xA;$$

$$\text{eq2} = k_S * xS + k_{-1} * xB - (k_1 + k_{-S}) * xA;$$

$$\text{eq3} = k_1 * xA - (k_B + k_{-1}) * xB;$$

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

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

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

$$\left\{ \left\{ xS \rightarrow \frac{xZ (k_1 k_B + (k_{-1} + k_B) k_{-S})}{(k_{-1} + k_1 + k_B) k_S}, xA \rightarrow \frac{xZ (k_{-1} + k_B)}{k_{-1} + k_1 + k_B}, xB \rightarrow \frac{xZ k_1}{k_{-1} + k_1 + k_B} \right\} \right\}$$

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

Rate Constant of Z

$$(k_{-S} * xA + k_B * xB) / xZ // \text{Simplify}$$

$$\frac{k_1 k_B + (k_{-1} + k_B) k_{-S}}{k_{-1} + k_1 + k_B}$$

Branching Ratios

$$\Gamma_S = \text{Numerator}[xA] * k_{-S} / xZ // \text{Simplify}$$

$$(k_{-1} + k_B) k_{-S}$$

$$\Gamma_P = \text{Numerator}[xB] * k_B / xZ // \text{Simplify}$$

$$k_1 k_B$$

$$\frac{\Gamma_S / (\Gamma_S + \Gamma_P)}{k_1 k_B + (k_{-1} + k_B) k_{-S}}$$

$$\frac{\Gamma_P / (\Gamma_S + \Gamma_P)}{k_1 k_B + (k_{-1} + k_B) k_{-S}}$$