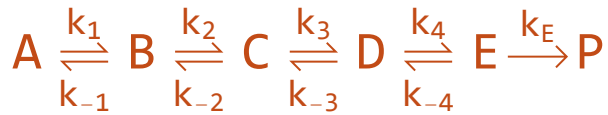


SetDirectory[NotebookDirectory[]]

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



Solve differential equation like

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

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

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

$$(\text{eq } 4) \quad \frac{d[D]}{dt} = k_3 [C] + k_{-4} [E] - (k_4 + k_{-3}) [D]$$

$$(\text{eq } 5) \quad \frac{d[E]}{dt} = k_4 [D] - (k_E + k_{-4}) [E]$$

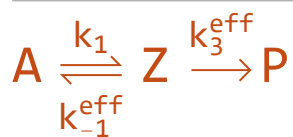
$$\text{eq1} = -k_1 * xA + k_{-1} * xB;$$

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

$$\text{eq3} = k_2 * xB + k_{-3} * xD - (k_3 + k_{-2}) * xC;$$

$$\text{eq4} = k_3 * xC + k_{-4} * xE - (k_4 + k_{-3}) * xD;$$

$$\text{eq5} = k_4 * xD - (k_E + k_{-4}) * xE;$$



$$\text{eqz} = xZ - (xB + xC + xD + xE);$$

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

Clear[soln];

soln = Solve[eq2 == 0 && eq3 == 0 && eq4 == 0 && eq5 == 0 && eqz == 0, {xA, xB, xC, xD, xE}] // Simplify

$$\left\{ \begin{aligned} xA &\rightarrow \frac{xZ \left(k_{-4} k_{-3} k_{-2} k_{-1} + (k_{-3} k_{-2} k_{-1} + (k_{-2} k_{-1} + (k_{-1} + k_2) k_3) k_4) k_e \right)}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)}, \\ xB &\rightarrow \frac{xZ \left(k_{-4} k_{-3} k_{-2} + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e \right)}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)}, \\ xC &\rightarrow \frac{xZ k_2 \left(k_{-4} k_{-3} + (k_{-3} + k_4) k_e \right)}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)}, \\ xD &\rightarrow \frac{xZ k_2 k_3 \left(k_{-4} + k_e \right)}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)}, \\ xE &\rightarrow \frac{xZ k_2 k_3 k_4}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)} \end{aligned} \right\}$$

xB = xB /. soln[[1, 2]];

xC = xC /. soln[[1, 3]];

xD = xD /. soln[[1, 4]];

xE = xE /. soln[[1, 5]]

xB

xC

xD

xE

$$\begin{aligned} &\frac{(xZ k_2 k_3 k_4)}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)} \\ &\frac{(xZ \left(k_{-4} k_{-3} k_{-2} + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e \right))}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)} \\ &\frac{(xZ k_2 \left(k_{-4} k_{-3} + (k_{-3} + k_4) k_e \right))}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)} \\ &\frac{(xZ k_2 k_3 \left(k_{-4} + k_e \right))}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)} \\ &\frac{(xZ k_2 k_3 k_4)}{k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right)} \end{aligned}$$

Rate Constant of Z

(k₋₁ * xB + k_E * xE) / xZ // Simplify

$$\frac{(k_{-4} k_{-3} k_{-2} k_{-1} + (k_{-3} k_{-2} k_{-1} + (k_{-2} k_{-1} + (k_{-1} + k_2) k_3) k_4) k_e)}{(k_{-4} \left(k_{-3} (k_{-2} + k_2) + k_2 k_3 \right) + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e + k_2 \left((k_{-3} + k_4) k_e + k_3 (k_4 + k_e) \right))}$$

Branching Ratios

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

$$k_{-1} (k_{-4} k_{-3} k_{-2} + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e)$$

$\Gamma_P = \text{Numerator}[xE] * k_E / xZ //$ **Simplify**

$$k_2 k_3 k_4 k_e$$

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

$$\frac{(k_{-1} (k_{-4} k_{-3} k_{-2} + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e))}{(k_2 k_3 k_4 k_e + k_{-1} (k_{-4} k_{-3} k_{-2} + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e))}$$

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

$$\frac{(k_2 k_3 k_4 k_e)}{(k_2 k_3 k_4 k_e + k_{-1} (k_{-4} k_{-3} k_{-2} + (k_{-3} k_{-2} + (k_{-2} + k_3) k_4) k_e))}$$