```
SetDirectory[NotebookDirectory[]]
```

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

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} C \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} D \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} E \overset{k_5}{\longrightarrow} P$$
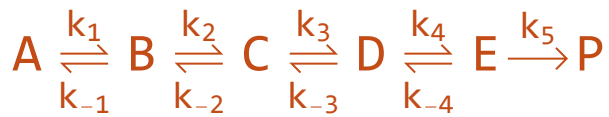
Solve differential equation like

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

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

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

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

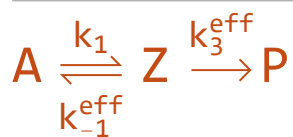$(eq\ 5)\quad \dfrac{d[E]}{dt} = k_4[D] - (k_5 + k_{-4})[E]$

```
eq1 = -k₁ * xA + k₋₁ * xB;
eq2 = k₁ * xA + k₋₂ * xC - (k₂ + k₋₁) * xB;
eq3 = k₂ * xB + k₋₃ * xD - (k₃ + k₋₂) * xC;
eq4 = k₃ * xC + k₋₄ * xE - (k₄ + k₋₃) * xE;
eq5 = k₄ * xD - (k₅ + k₋₄) * xE;
```

$$A \underset{k_{-1}^{eff}}{\overset{k_1}{\rightleftharpoons}} Z \overset{k_3^{eff}}{\longrightarrow} P$$

```
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
```

$\big\{\big\{xA \to -\big(\big(xZ\,\big(-\big(k_{-2}\,k_{-1} + \big(k_{-1} + k_2\big)\,k_3\big)\,k_4^2 + k_{-4}\,\big(k_{-3}\,\big(k_{-1} + k_2\big)\,k_3 + \big(k_{-2}\,k_{-1} + \big(k_{-1} + k_2\big)\,k_3\big)\,k_4\big) -$

$\qquad k_{-3}\,\big(k_{-2}\,k_{-1}\,k_4 + \big(k_{-1} + k_2\big)\,k_3\,\big(k_4 - k_5\big)\big)\big)\big) \big/$

$\qquad \big(k_1\,\big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 - k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) +$

$\qquad k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big)\big)\big),$

$\quad xB \to \big(xZ\,\big(\big(k_{-2} + k_3\big)\,k_4^2 - k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4\big) + k_{-3}\,\big(k_{-2}\,k_4 + k_3\,\big(k_4 - k_5\big)\big)\big)\big) \big/$

$\qquad \big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 - k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) +$

$\qquad k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big),$

$\quad xC \to \dfrac{xZ\,k_2\,\big(k_{-4} - k_{-3} - k_4\big)\,k_4}{-k_2\,k_3\,k_4 + \big(k_{-2} + k_2 + k_3\big)\,\big(k_{-4} - k_{-3} - k_4\big)\,k_4 + \big(k_{-3} - k_2\big)\,k_3\,\big(k_{-4} + k_5\big)},$

$\quad xD \to$

$\qquad \big(xZ\,k_2\,k_3\,\big(k_{-4} + k_5\big)\big) \big/ \big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 -$

$\qquad k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) + k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big),$

$\quad xE \to \big(xZ\,k_2\,k_3\,k_4\big) \big/ \big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 - k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) +$

$\qquad k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big)\big\}\big\}$

```
xB = xB /. soln[[1, 2]];
xC = xC /. soln[[1, 3]];
xD = xD /. soln[[1, 4]];
xE = xE /. soln[[1, 5]]
xB
xC
xD
xE
```

$\big(xZ\,k_2\,k_3\,k_4\big) \big/ \big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 -$

$\quad k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) + k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big)$

$\big(xZ\,\big(\big(k_{-2} + k_3\big)\,k_4^2 - k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4\big) + k_{-3}\,\big(k_{-2}\,k_4 + k_3\,\big(k_4 - k_5\big)\big)\big)\big) \big/$

$\quad \big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 -$

$\quad k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) + k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big)$

$\big(xZ\,k_2\,\big(k_{-4} - k_{-3} - k_4\big)\,k_4\big) \big/ \big(-k_2\,k_3\,k_4 + \big(k_{-2} + k_2 + k_3\big)\,\big(k_{-4} - k_{-3} - k_4\big)\,k_4 + \big(k_{-3} - k_2\big)\,k_3\,\big(k_{-4} + k_5\big)\big)$

$\big(xZ\,k_2\,k_3\,\big(k_{-4} + k_5\big)\big) \big/ \big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 -$

$\quad k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) + k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big)$

$\big(xZ\,k_2\,k_3\,k_4\big) \big/ \big(k_2\,k_3\,k_4 + k_{-2}\,k_4^2 + k_2\,k_4^2 + k_3\,k_4^2 -$

$\quad k_{-4}\,\big(k_{-3}\,k_3 + \big(k_{-2} + k_3\big)\,k_4 + k_2\,\big(-k_3 + k_4\big)\big) + k_{-3}\,\big(k_{-2}\,k_4 + k_2\,k_4 + k_3\,\big(k_4 - k_5\big)\big) + k_2\,k_3\,k_5\big)$

Rate Constant of Z

$\left(k_{-1} * xB + k_5 * xE\right) / xZ$ // **Simplify**

$\left(-k_{-4} k_{-1} \left(k_{-3} k_3 + \left(k_{-2} + k_3\right) k_4\right) + k_{-3} k_{-1} \left(k_{-2} k_4 + k_3 \left(k_4 - k_5\right)\right) + k_4 \left(k_{-2} k_{-1} k_4 + k_3 \left(k_{-1} k_4 + k_2 k_5\right)\right)\right) /$
$\left(k_2 k_3 k_4 + k_{-2} k_4^2 + k_2 k_4^2 + k_3 k_4^2 - k_{-4} \left(k_{-3} k_3 + \left(k_{-2} + k_3\right) k_4 + k_2 \left(-k_3 + k_4\right)\right) + k_{-3} \left(k_{-2} k_4 + k_2 k_4 + k_3 \left(k_4 - k_5\right)\right) + k_2 k_3 k_5\right)$

Branching Ratios

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

$k_{-1} \left(\left(k_{-2} + k_3\right) k_4^2 - k_{-4} \left(k_{-3} k_3 + \left(k_{-2} + k_3\right) k_4\right) + k_{-3} \left(k_{-2} k_4 + k_3 \left(k_4 - k_5\right)\right)\right)$

$\Gamma_P = $ **Numerator[xE]** $* k_5 / xZ$ // **Simplify**

$k_2 k_3 k_4 k_5$

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

$\left(k_{-1} \left(\left(k_{-2} + k_3\right) k_4^2 - k_{-4} \left(k_{-3} k_3 + \left(k_{-2} + k_3\right) k_4\right) + k_{-3} \left(k_{-2} k_4 + k_3 \left(k_4 - k_5\right)\right)\right)\right) /$
$\left(k_{-1} \left(\left(k_{-2} + k_3\right) k_4^2 - k_{-4} \left(k_{-3} k_3 + \left(k_{-2} + k_3\right) k_4\right) + k_{-3} \left(k_{-2} k_4 + k_3 \left(k_4 - k_5\right)\right)\right) + k_2 k_3 k_4 k_5\right)$

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

$\left(k_2 k_3 k_4 k_5\right) / \left(k_{-1} \left(\left(k_{-2} + k_3\right) k_4^2 - k_{-4} \left(k_{-3} k_3 + \left(k_{-2} + k_3\right) k_4\right) + k_{-3} \left(k_{-2} k_4 + k_3 \left(k_4 - k_5\right)\right)\right) + k_2 k_3 k_4 k_5\right)$