```
SetDirectory[NotebookDirectory[]]
D:\VS_workspace\CPlusPlus\SOHR\projects\catalytic_cycle\theory\SSA
```

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} C \xrightarrow{k_3} P$$

Solve differential equation like

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

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

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

```
eq1 = -k1 * xA + k-1 * xB;
eq2 = k1 * xA + k-2 * xC - (k2 + k-1) * xB;
eq3 = k2 * xB - (k3 + k-2) * xC;
```

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

```
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
```

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

```
xB = xB /. soln[[1, 2]]; xC = xC /. 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 + k₃ * xC) / xZ // Simplify
```

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

Branching Ratios

```
ΓA = Numerator[xB] * k₋₁ / xZ // Simplify
```

$$k_{-1} \left(k_{-2} + k_3\right)$$

```
ΓP = Numerator[xC] * k₃ / xZ // Simplify
```

$$k_2\, k_3$$

```
ΓA / (ΓA + ΓP)
```

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

```
ΓP / (ΓA + ΓP)
```

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