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

$S \underset{k_{-S}}{\overset{k_S}{\rightleftharpoons}} A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_B} P$

Solve differential equation like

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

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

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

```
eq1 = -kS * xS + k-S * xA;
eq2 = kS * xS + k-1 * xB - (k1 + k-S) * xA;
eq3 = k1 * xA - (kB + k-1) * xB;
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
```

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

```
xA = xA /. soln[[1, 2]]; xB = xB /. soln[[1, 3]];
```

Rate Constant of Z

```
(k-S * xA + kB * xB) / xZ // Simplify
```

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

Branching Ratios

```
ΓS = Numerator[xA] * k-S / xZ // Simplify
```

$$\left(k_{-1} + k_B\right) k_{-S}$$

```
ΓP = Numerator[xB] * kB / xZ // Simplify
```

$$k_1 k_B$$

$\Gamma_S / (\Gamma_S + \Gamma_P)$

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

$\Gamma_P / (\Gamma_S + \Gamma_P)$

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