

$$P(\text{vector}) : nr * (ns+4) + 1.$$

n Species $\xrightarrow{n \text{ Reactions}}$ n Species.

for Reaction #1:

$$\begin{aligned} \text{rate} &= [S_1]^{v_1} [S_2]^{v_2} \dots [S_{n_s}]^{v_{n_s}} \cdot A T^b e^{-\frac{E_a}{RT}} \\ &= \exp \left\{ \underbrace{v_1}_{\substack{\cdot \\ S_i = v_i \text{ rate}}} \ln S_1 + \dots + \underbrace{v_{n_s}} \ln S_{n_s} + \ln A + \underbrace{b}_{(b)} \ln T - \underbrace{\frac{E_a}{RT}} \right\} \end{aligned}$$

① $1 \sim nr \text{ (nr } \uparrow)$: $w_b \sim \ln A$ ~~E_a~~ ? $\left\{ \begin{array}{l} * \text{ slope } * 10 \\ \text{clamp } (0, 50). \end{array} \right.$

② $nr+1 \sim nr(ns+1)$: $w_{out} \sim v_{ij}$ $\left\{ \begin{array}{l} \text{1st species: clamp } (-3, 0) \\ \text{last species: clamp } (0, 3) \end{array} \right.$
($nr \neq ns \uparrow$)

③ $nr(ns+1)+1 \sim nr(ns+2)$: $w_{in-E_a} \sim E_a$ clamp $(0, 300)$
($nr \uparrow$)

④ $nr(ns+2)+1 \sim nr(ns+3)$: w_{in-b}
($nr \uparrow$)

⑤ 氧浓度: ~~忽略~~. ($nr \uparrow$).

$$\begin{array}{c}
 (nr) \\
 (ln)(r_1, \dots, r_{nr}) =
 \end{array}
 \begin{array}{c}
 W_{in} \\
 (nr, ns+3) \text{ reaction \#1} \\
 \left[\begin{array}{cccc}
 v_{11} & \dots & v_{1,ns} & E_{a(1)} & b_{(1)} \\
 v_{21} & \dots & v_{2,ns} & E_{a(2)} & b_{(2)} \\
 \vdots & & \vdots & \vdots & \vdots \\
 v_{nr1} & \dots & v_{nr,ns} & E_{a(nr)} & b_{(nr)}
 \end{array} \right]
 \begin{array}{c}
 \ln S_1 \\
 \vdots \\
 \ln S_{ns} \\
 R/T \\
 \ln T
 \end{array}
 \end{array}
 \begin{array}{c}
 (ns+3)
 \end{array}$$

$$\begin{aligned}
 r_1 &= v_{11} \ln S_1 + \dots + v_{1,ns} \ln S_{ns} \\
 &+ \frac{R}{T} \cdot E_a + b \ln T.
 \end{aligned}$$

$$\begin{array}{c}
 (\dot{S}_1, \dot{S}_2, \dots, \dot{S}_{ns}) \\
 (ns)
 \end{array}
 =
 \begin{array}{c}
 \left[\begin{array}{ccc}
 v_{11} & \dots & \\
 \vdots & & \vdots \\
 \vdots & & \vdots
 \end{array} \right]
 \begin{array}{c}
 \ln r_1 + \ln A_1 \\
 \vdots \\
 \ln r_{nr} + \ln A_{nr}
 \end{array}
 \end{array}
 \begin{array}{c}
 (ns \times nr) \quad (nr \times 1)
 \end{array}$$

$$(\dot{S}_1, \dot{S}_2, \dots, \dot{S}_{ns}) = CRNN(S_1, \dots, S_{ns}; P)$$