1R Model Equations

The one-reaction model (1R) is described by the following differential equations:

$$
\begin{aligned}
\frac{dX_1}{dt} &= r_1 - DX_1 \\
\frac{dS_1}{dt} &= k_1 r_1 + D(S_{1,\text{in}} - S_1) \\
q_m &= k_3 r_1
\end{aligned}
$$

The reaction rate r_1 using Moser kinetics is given by:

$$
r_1 = \mu_{\max} \frac{S_1}{k_s + S_1} X_1
$$

2R Model Equations

The two-reaction model (2R) is described by the following differential equations:

$$
\begin{aligned}
\frac{d\xi}{dt} &= Kr(\xi) + D(\xi_{\text{in}} - \xi) \\
q_m &= k_6 r_2
\end{aligned}
$$

where $\xi = \begin{bmatrix} X_1 & X_2 & S_1 & S_2 & C & N & Z \end{bmatrix}^T$ and $r(\xi) = \begin{bmatrix} r_1(\xi) & r_2(\xi) \end{bmatrix}^T$. The reaction rates r_1 and r_2 are given by:

$$
\begin{aligned}
r_1 &= \mu_{1,\max} \frac{S_1}{k_{s1} X_1 + S_1} X_1 \\
r_2 &= \mu_{2,\max} \frac{S_2}{k_{s2} + S_2 + \frac{S_2^2}{k_i}} X_2 I_N
\end{aligned}
$$

The inhibition factor for ammonia I_N is:

$$
I_N = \frac{1}{1 + \frac{N}{k_{i,N}}}
$$

The stoichiometric matrix K for the 2R model is:

$$
K = \begin{bmatrix}
1 & 0 \\
0 & 1 \\
-k_1 & 0 \\
k_2 & -k_3 \\
k_4 & k_5 \\
k_n k_1 & 0 \\
0 & 0
\end{bmatrix}
$$

3R Model Equations

The three-reaction model (3R) is described by the following differential equations:

$$\frac{d\xi}{dt} = Kr(\xi) + D(\xi_{\text{in}} - \xi)$$
$$q_m = k_{11} r_3$$

where $\xi = \begin{bmatrix} X_{1a} & X_{1b} & X_2 & S_{1a} & S_{1b} & S_2 & C & N & Z \end{bmatrix}^T$ and $r(\xi) = \begin{bmatrix} r_{1a}(\xi) & r_{1b}(\xi) & r_2(\xi) \end{bmatrix}^T$. The reaction rates r_{1a}, r_{1b}, and r_2 are given by:

$$r_{1a} = \mu_{1a,\max} \frac{S_{1a}}{k_{s1a} X_{1a} + S_{1a}} X_{1a}$$
$$r_{1b} = \mu_{1b,\max} \frac{S_{1b}}{k_{s1b} X_{1b} + S_{1b}} X_{1b}$$
$$r_2 = \mu_{2,\max} \frac{S_2}{k_{s2} + S_2 + \frac{S_2^2}{k_i}} X_2 I_N$$

The inhibition factor for ammonia I_N is:

$$I_N = \frac{1}{1 + \frac{N}{k_{i,N}}}$$

The stoichiometric matrix K for the 3R model is:

$$K = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -k_1 & 0 & 0 \\ 0 & -k_5 & 0 \\ k_3 & k_6 & -k_9 \\ k_4 & k_8 & k_{12} \\ -k_2 & k_7 & k_{10} \\ 0 & 0 & 0 \end{bmatrix}$$