Assignment 1: Model development and equations

Question 1: The "Living" Ice

Derivation of K_{m2}

$$v = \frac{V_{max} S_1 S_2}{K_{m1} S_2 + K_{m2} S_1 + S_1 S_2} \tag{1}$$

$$v(K_{m1} S_2 + K_{m2} S_1 + S_1 S_2) = V_{max} S_1 S_2 \tag{2}$$

$$K_{m1} S_2 + K_{m2} S_1 + S_1 S_2 = \frac{V_{max} S_1 S_2}{v} \tag{3}$$

$$K_{m2} S_1 = \frac{V_{max} S_1 S_2}{v} - K_{m1} S_2 - S_1 S_2 \tag{4}$$

$$K_{m2} = \frac{V_{max} S_2}{v} - \frac{K_{m1} S_2}{S_1} - S_2 \tag{5}$$

Conversion to mM

$$[S_{1,initial}]_{mM} = \frac{[S_{1,initial}]_{g/L}}{MW_{g/mol}} \times 1000$$

$$[S_{1,limit}]_{mM} = \frac{[S_{1,limit}]_{g/L}}{MW_{g/mol}} \times 1000$$

Question 2: The Case of the possible Biomass

$$N = \begin{array}{c} \\ CIT \\ ICT \\ AKG \\ SCA \\ SUC \\ FUM \\ MAL \\ OAA \\ X \end{array} \begin{array}{c} \begin{matrix} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 \end{matrix} \\ \begin{bmatrix} 2 & -1 & & & & & & & \\ & 1 & -1 & & & & & & \\ & & 1 & -1 & & & & & \\ & & & 1 & -1 & & & & \\ & & & & 1 & -1 & & & \\ & & & & & 1 & -1 & & \\ & & & & & & 1 & -1 & \\ -1 & & & & & & & 1 & -1 \\ & & & & & & & & 1 \end{bmatrix} \end{array}$$

Steady state assumption $Nv = 0$ gives:

$$C\dot{I}T = 2v_1 - v_2 = 0$$

$$I\dot{C}T = v_2 - v_3 = 0$$

$$A\dot{K}G = v_3 - v_4 = 0$$

$$S\dot{C}A = v_4 - v_5 = 0$$

$$S\dot{U}C = v_5 - v_6 = 0$$

$$F\dot{U}M = v_6 - v_7 = 0$$

$$M\dot{A}L = v_7 - v_8 = 0$$

$$O\dot{A}A = v_8 - v_1 - v_9 = 0$$

$$\dot{X} = v_9 = 0$$

From this we get:

$$v_8 = v_7 = v_6 = v_5 = v_4 = v_3 = v_2 = 2v_1$$

$$O\dot{A}A = v_6 - v_1 - v_9 = v_6 - v_1 - D = 0$$

Combining the above equations we get:

$$v_6 - v_1 - D = 2v_1 - v_1 - D = v_1 - D = 0 \implies v_1 = D$$

and hence $v_6 = 2D$.

In order to have biomass conversion to X we must have:

$$\dot{X} = v_9 = D > 0$$

We get:

$$v_6 - v_1 = D$$

Since $D > 0$

$$v_6 > v_1$$

Irrevirsibility constraint gives $v_1 \geq 0$ and MM constraints give $v_6 \leq v_{6,max}$.

$$v_6 = v_1 + D \implies v_1 + D \leq v_{6,max} \iff v_1 \leq v_{6,max} - D$$

And $v_6 > v_1$.

$$v_1 \geq 0 \implies v_1 = v_6 - D \geq 0 \iff v_6 \geq D$$

The equation for the reaction rate v_6 is given by:

$$v_6 = (V_{max}[Succ])/(K_m + [Succ]) - (V_{max}[Fum])/(K_m + [Fum])$$