MCA for a Simple Pathway

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Consider the simplest pathway:

$$\boxed{X_1} \overset{R_1}{\longleftrightarrow} S \overset{R_2}{\longleftrightarrow} \boxed{X_2} \tag{1}$$

We assume that X_1 and X_2 are buffered external metabolites with constant concentrations (hence in boxes).
The ratelaws for the two reactions are:

$$\begin{aligned} v_1 &= k_1(X_1 - S) \\ v_2 &= k_2(S - X_2) \end{aligned} \tag{2}$$

which means we assume (1) mass action kinetics and (2) $\Delta G^0 = 0$ and hence $K_E = 1$ for both reactions (think of isomerization reactions).

At steady state, $v_1 = v_2$:

$$k_1(X_1 - S^*) = k_2(S^* - X_2) \tag{3}$$

Steady-state concentration S^* is hence the weighted average of X_1 and X_2:

$$S^* = \frac{k_1 X_1 + k_2 X_2}{k_1 + k_2} \tag{4}$$

And steady-state flux J is hence the *harmonic mean* of k_1 and k_2 times the average chemical potential difference:

$$J = k_1(X_1 - S^*) = \frac{2k_1k_2}{k_1 + k_2}\frac{X_1 - X_2}{2} \equiv H(k_1, k_2)\frac{X_1 - X_2}{2} \tag{5}$$

Elasticities for the two reactions *at steady state* are:

$$\epsilon^1 = \frac{S}{v_1}\frac{\partial v_1}{\partial S}\Big|_{S=S^*} = \frac{S^*}{k_1(X_1 - S^*)}(-k_1) = -\frac{S^*}{X_1 - S^*} \tag{6}$$

$$\epsilon^2 = \frac{S}{v_2}\frac{\partial v_2}{\partial S}\Big|_{S=S^*} = \frac{S^*}{k_2(S^* - X_2)}(k_2) = \frac{S^*}{S^* - X_2} \tag{7}$$

Flux control coefficients satisfy:

$$\begin{aligned} C_1 + C_2 &= 1 \\ C_1\epsilon^1 + C_2\epsilon^2 &= 0 \end{aligned} \tag{8}$$

And hence they are:

$$\begin{aligned} C_1 &= \frac{-\epsilon_2}{\epsilon_1 - \epsilon_2} = \frac{-\frac{S^*}{S^*-X_2}}{-\frac{S^*}{X_1-S^*} - \frac{S^*}{S^*-X_2}} = \frac{X_1 - S^*}{X_1 - X_2} = \frac{k_2}{k_1 + k_2} \\ C_2 &= \frac{\epsilon_1}{\epsilon_1 - \epsilon_2} = \frac{\frac{S^*}{X_1-S^*}}{-\frac{S^*}{X_1-S^*} - \frac{S^*}{S^*-X_2}} = \frac{S^* - X_2}{X_1 - X_2} = \frac{k_1}{k_1 + k_2} \end{aligned} \tag{9}$$