

There are 5 reactions and 4 species in the OMM model.

The stoichiometric matrix is $S =$

$$\begin{array}{ccccc} -1 & 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 \\ 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{array}$$

The vector of reaction velocities is v , where

$$\begin{aligned} v(1) &= k_1 x_1 x_2 \\ v(2) &= k_2 x_3 \\ v(3) &= k_3 x_3 \\ v(4) &= k_4 \\ v(5) &= k_5 x_4 \end{aligned}$$

The vector of mass balance equations is $\dot{x} = S \cdot v$, where

$$\begin{aligned} \dot{x}(1) &= k_2 x_3 + k_3 x_3 - k_1 x_1 x_2 \\ \dot{x}(2) &= k_4 + k_2 x_3 - k_1 x_1 x_2 \\ \dot{x}(3) &= k_1 x_1 x_2 - k_3 x_3 - k_2 x_3 \\ \dot{x}(4) &= k_3 x_3 - k_5 x_4 \end{aligned}$$

Let the map ψ_p be given by

$$\begin{array}{l|l} k_1 & \rightarrow y_1 \\ k_2 & \rightarrow y_2 \\ k_3 & \rightarrow y_3 \\ k_4 & \rightarrow y_4 \\ k_5 & \rightarrow y_5 \\ x_1 & \rightarrow p_1 \\ x_2 & \rightarrow p_2 \\ x_3 & \rightarrow p_3 \\ x_4 & \rightarrow p_4 \end{array}$$

This results in a linear velocity vector $\psi_p(v)$, where

$$\begin{aligned} \psi_p(v(1)) &= p_1 p_2 y_1 \\ \psi_p(v(2)) &= p_3 y_2 \\ \psi_p(v(3)) &= p_3 y_3 \\ \psi_p(v(4)) &= y_4 \\ \psi_p(v(5)) &= p_4 y_5 \end{aligned}$$

We can express $\psi_p(v)$ as the product $P \cdot y$, where y is the vector $[y_1, \dots, y_5]^T$ and $P =$

$$\begin{array}{ccccc} p_1 p_2 & 0 & 0 & 0 & 0 \\ 0 & p_3 & 0 & 0 & 0 \\ 0 & 0 & p_3 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & p_4 \end{array}$$

From this we calculate the coefficient matrix, $C = S \cdot P =$

$$\begin{array}{ccccc} -p_1 p_2 & p_3 & p_3 & 0 & 0 \\ -p_1 p_2 & p_3 & 0 & 1 & 0 \\ p_1 p_2 & -p_3 & -p_3 & 0 & 0 \\ 0 & 0 & p_3 & 0 & -p_4 \end{array}$$

C is row equivalent to the reduced matrix $C_{\text{rref}} =$

$$\begin{array}{ccccc} 1 & -p_3/(p_1 p_2) & 0 & 0 & -p_4/(p_1 p_2) \\ 0 & 0 & 1 & 0 & -p_4/p_3 \\ 0 & 0 & 0 & 1 & -p_4 \\ 0 & 0 & 0 & 0 & 0 \end{array}$$

The null space of C is spanned by the columns of $N =$

$$\begin{array}{cc} p3/(p1*p2) & p4/(p1*p2) \\ 1 & 0 \\ 0 & p4/p3 \\ 0 & p4 \\ 0 & 1 \end{array}$$

Let $\bar{y} = N*q$, where q is given by

$$\begin{array}{l} q(1) = q1 \\ q(2) = q2 \end{array}$$

This gives

$$\begin{array}{l} \bar{y}(1) = (p3*q1 + p4*q2)/(p1*p2) \\ \bar{y}(2) = q1 \\ \bar{y}(3) = (p4*q2)/p3 \\ \bar{y}(4) = p4*q2 \\ \bar{y}(5) = q2 \end{array}$$

From \bar{y} we construct the composite forward map ψ_{py} :

$$\begin{array}{ll} k1 & \mapsto (p3*q1 + p4*q2)/(p1*p2) \\ k2 & \mapsto q1 \\ k3 & \mapsto (p4*q2)/p3 \\ k4 & \mapsto p4*q2 \\ k5 & \mapsto q2 \\ x1 & \mapsto p1 \\ x2 & \mapsto p2 \\ x3 & \mapsto p3 \\ x4 & \mapsto p4 \end{array}$$

The steady state reaction velocity vector \bar{v} is given by $\psi_{py}(v)$, where

$$\begin{array}{l} \bar{v}(1) = p3*q1 + p4*q2 \\ \bar{v}(2) = p3*q1 \\ \bar{v}(3) = p4*q2 \\ \bar{v}(4) = p4*q2 \\ \bar{v}(5) = p4*q2 \end{array}$$

The mapping function ψ_q^{-1} is given by

$$\begin{array}{ll} q1 & \mapsto y2 \\ q2 & \mapsto y5 \end{array}$$

The composite inverse map ψ_{qp}^{-1} :

$$\begin{array}{ll} p1 & \mapsto x1 \\ p2 & \mapsto x2 \\ p3 & \mapsto x3 \\ p4 & \mapsto x4 \\ q1 & \mapsto k2 \\ q2 & \mapsto k5 \end{array}$$

The complete steady state map ψ_{ss} is therefore

$$\begin{array}{ll} k1 & \mapsto (k2*x3 + k5*x4)/(x1*x2) \\ k2 & \mapsto k2 \\ k3 & \mapsto (k5*x4)/x3 \\ k4 & \mapsto k5*x4 \\ k5 & \mapsto k5 \\ x1 & \mapsto x1 \\ x2 & \mapsto x2 \\ x3 & \mapsto x3 \\ x4 & \mapsto x4 \end{array}$$

The unsubstituted steady state reaction velocity vector $\bar{v} = \psi_{ss}(v)$ is

given by

$$\begin{aligned} \text{vbar}(1) &= k_2 x_3 + k_5 x_4 \\ \text{vbar}(2) &= k_2 x_3 \\ \text{vbar}(3) &= k_5 x_4 \\ \text{vbar}(4) &= k_5 x_4 \\ \text{vbar}(5) &= k_5 x_4 \end{aligned}$$

Verify steady state. $\dot{x} = S * \text{vbar}$, where

$$\begin{aligned} \dot{x}(1) &= 0 \\ \dot{x}(2) &= 0 \\ \dot{x}(3) &= 0 \\ \dot{x}(4) &= 0 \end{aligned}$$