

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

$$\begin{array}{l|l} k_1 & \rightarrow p_2 \\ k_2 & \rightarrow p_3 \\ k_3 & \rightarrow p_4 \\ k_4 & \rightarrow y_4 \\ k_5 & \rightarrow p_5 \\ x_1 & \rightarrow y_1 \\ x_2 & \rightarrow p_1 \\ x_3 & \rightarrow y_2 \\ x_4 & \rightarrow y_3 \end{array}$$

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

$$\begin{aligned} \psi_p(v(1)) &= p_1 p_2 y_1 \\ \psi_p(v(2)) &= p_3 y_2 \\ \psi_p(v(3)) &= p_4 y_2 \\ \psi_p(v(4)) &= y_4 \\ \psi_p(v(5)) &= p_5 y_3 \end{aligned}$$

We can express $\psi_p(v)$ as the product $P \cdot y$, where y is the vector $[y_1, \dots, y_4]^T$ and $P =$

$$\begin{array}{cccc} p_1 p_2 & 0 & 0 & 0 \\ 0 & p_3 & 0 & 0 \\ 0 & p_4 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & p_5 & 0 \end{array}$$

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

$$\begin{array}{cccc} -p_1 p_2 & p_3 + p_4 & 0 & 0 \\ -p_1 p_2 & p_3 & 0 & 1 \\ p_1 p_2 & -p_3 - p_4 & 0 & 0 \\ 0 & p_4 & -p_5 & 0 \end{array}$$

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

$$\begin{array}{cccc} 1 & 0 & 0 & -(p_3 + p_4)/(p_1 p_2 p_4) \\ 0 & 1 & 0 & -1/p_4 \\ 0 & 0 & 1 & -1/p_5 \\ 0 & 0 & 0 & 0 \end{array}$$

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

$$\begin{pmatrix} (p_3 + p_4)/(p_1 p_2 p_4) \\ 1/p_4 \\ 1/p_5 \\ 1 \end{pmatrix}$$

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

$$q(1) = q_1$$

This gives

$$\begin{aligned} \bar{y}(1) &= (q_1(p_3 + p_4))/(p_1 p_2 p_4) \\ \bar{y}(2) &= q_1/p_4 \\ \bar{y}(3) &= q_1/p_5 \\ \bar{y}(4) &= q_1 \end{aligned}$$

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

$$\begin{array}{l|l} k_1 & \rightarrow p_2 \\ k_2 & \rightarrow p_3 \\ k_3 & \rightarrow p_4 \\ k_4 & \rightarrow q_1 \\ k_5 & \rightarrow p_5 \\ x_1 & \rightarrow (q_1(p_3 + p_4))/(p_1 p_2 p_4) \\ x_2 & \rightarrow p_1 \\ x_3 & \rightarrow q_1/p_4 \\ x_4 & \rightarrow q_1/p_5 \end{array}$$

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

$$\begin{aligned} \bar{v}(1) &= (q_1(p_3 + p_4))/p_4 \\ \bar{v}(2) &= (p_3 q_1)/p_4 \\ \bar{v}(3) &= q_1 \\ \bar{v}(4) &= q_1 \\ \bar{v}(5) &= q_1 \end{aligned}$$

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

$$q_1 \rightarrow y_4$$

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

$$\begin{array}{l|l} p_1 & \rightarrow x_2 \\ p_2 & \rightarrow k_1 \\ p_3 & \rightarrow k_2 \\ p_4 & \rightarrow k_3 \\ p_5 & \rightarrow k_5 \\ q_1 & \rightarrow k_4 \end{array}$$

The complete steady state map ψ_{ss} is therefore

$$\begin{array}{l|l} k_1 & \rightarrow k_1 \\ k_2 & \rightarrow k_2 \\ k_3 & \rightarrow k_3 \\ k_4 & \rightarrow k_4 \\ k_5 & \rightarrow k_5 \\ x_1 & \rightarrow (k_4(k_2 + k_3))/(k_1 k_3 x_2) \\ x_2 & \rightarrow x_2 \\ x_3 & \rightarrow k_4/k_3 \\ x_4 & \rightarrow k_4/k_5 \end{array}$$

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

$$\begin{aligned} \bar{v}(1) &= (k_4(k_2 + k_3))/k_3 \\ \bar{v}(2) &= (k_2 k_4)/k_3 \end{aligned}$$

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vbar(3) = k4  
vbar(4) = k4  
vbar(5) = k4
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Verify steady state. $\dot{x} = S * vbar$, where

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xdot(1) = 0  
xdot(2) = 0  
xdot(3) = 0  
xdot(4) = 0
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