

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

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

Let the map  $\psi_p$  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

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

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

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

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

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

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

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

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

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

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

$$q[1] = 1/p_5*q_1$$

This gives

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

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

$$\begin{array}{l|l} k_1 & \rightarrow p_2 \\ k_2 & \rightarrow p_3 \\ k_3 & \rightarrow p_4 \\ k_4 & \rightarrow q_1 \\ k_5 & \rightarrow p_5 \\ x_1 & \rightarrow (p_3 + p_4)/p_4/p_2/p_1*q_1 \\ x_2 & \rightarrow p_1 \\ x_3 & \rightarrow 1/p_4*q_1 \\ x_4 & \rightarrow 1/p_5*q_1 \end{array}$$

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

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

The mapping function  $\psi_q^{-1}$  is given by

$$q_1 \rightarrow y_4$$

The composite inverse map  $\psi_{qp}^{-1}$ :

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

The complete steady state map  $\psi_{ss}$  is therefore

$$\begin{array}{l|l} k_1 & \rightarrow k_1 \\ k_2 & \rightarrow k_2 \\ k_3 & \rightarrow k_3 \\ k_4 & \rightarrow k_4 \\ k_5 & \rightarrow k_5 \\ x_1 & \rightarrow (k_2 + k_3)/k_3/k_1/x_2*k_4 \\ x_2 & \rightarrow x_2 \\ x_3 & \rightarrow 1/k_3*k_4 \\ x_4 & \rightarrow 1/k_5*k_4 \end{array}$$

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

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

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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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