

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

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

We would like to define a map  $\psi_p$  such that  $\psi_p(k_4)$  is in  $P$ . To do so we introduce a pseudospecies  $x_5_{\text{hat}}=1$  and let  $v(4) = k_4 x_5_{\text{hat}}$ . This gives

$$\begin{aligned} v(1) &= k_1 x_1 x_2 \\ v(2) &= k_2 x_3 \\ v(3) &= k_3 x_3 \\ v(4) &= k_4 x_5_{\text{hat}} \\ v(5) &= k_5 x_4 \end{aligned}$$

Let the map  $\psi_p$  be given by

$$\begin{array}{l|l} k_1 & \rightarrow y_1 \\ k_2 & \rightarrow y_2 \\ k_3 & \rightarrow y_3 \\ k_4 & \rightarrow p_5 \\ k_5 & \rightarrow y_4 \\ x_1 & \rightarrow p_1 \\ x_2 & \rightarrow p_2 \\ x_3 & \rightarrow p_3 \\ x_4 & \rightarrow p_4 \\ x_5_{\text{hat}} & \rightarrow y_5 \end{array}$$

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

$$\begin{aligned} \psi_p(v(1)) &= p_1 p_2 y_1 \\ \psi_p(v(2)) &= p_3 y_2 \\ \psi_p(v(3)) &= p_3 y_3 \\ \psi_p(v(4)) &= p_5 y_5 \\ \psi_p(v(5)) &= p_4 y_4 \end{aligned}$$

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

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

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

$$\begin{array}{ccccc} -p_1 p_2 & p_3 & p_3 & 0 & 0 \\ -p_1 p_2 & p_3 & 0 & 0 & p_5 \end{array}$$

$$\begin{array}{ccccc} p1*p2 & -p3 & -p3 & 0 & 0 \\ 0 & 0 & p3 & -p4 & 0 \end{array}$$

C is row equivalent to the reduced matrix Crref =

$$\begin{array}{ccccc} 1 & -p3/(p1*p2) & 0 & 0 & -p5/(p1*p2) \\ 0 & 0 & 1 & 0 & -p5/p3 \\ 0 & 0 & 0 & 1 & -p5/p4 \\ 0 & 0 & 0 & 0 & 0 \end{array}$$

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

$$\begin{array}{cc} p3/(p1*p2) & p5/(p1*p2) \\ 1 & 0 \\ 0 & p5/p3 \\ 0 & p5/p4 \\ 0 & 1 \end{array}$$

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

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

This gives

$$\begin{array}{l} \bar{y}(1) = (p3*q1 + p5*q2)/(p1*p2) \\ \bar{y}(2) = q1 \\ \bar{y}(3) = (p5*q2)/p3 \\ \bar{y}(4) = (p5*q2)/p4 \\ \bar{y}(5) = q2 \end{array}$$

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

$$\begin{array}{ll} k1 & \mapsto (p3*q1 + p5*q2)/(p1*p2) \\ k2 & \mapsto q1 \\ k3 & \mapsto (p5*q2)/p3 \\ k4 & \mapsto p5 \\ k5 & \mapsto (p5*q2)/p4 \\ x1 & \mapsto p1 \\ x2 & \mapsto p2 \\ x3 & \mapsto p3 \\ x4 & \mapsto p4 \\ x5\_hat & \mapsto q2 \end{array}$$

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

$$\begin{array}{l} \bar{v}(1) = p3*q1 + p5*q2 \\ \bar{v}(2) = p3*q1 \\ \bar{v}(3) = p5*q2 \\ \bar{v}(4) = p5*q2 \\ \bar{v}(5) = p5*q2 \end{array}$$

To resolve the pseudospecies we require that  $\psi_{py}(x5\_hat)=1$ . In other words,  $q2=1$ . This gives

$$\begin{array}{ll} k1 & \mapsto (p5 + p3*q1)/(p1*p2) \\ k2 & \mapsto q1 \\ k3 & \mapsto p5/p3 \\ k4 & \mapsto p5 \\ k5 & \mapsto p5/p4 \\ x1 & \mapsto p1 \\ x2 & \mapsto p2 \\ x3 & \mapsto p3 \\ x4 & \mapsto p4 \\ x5\_hat & \mapsto 1 \end{array}$$

and

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vbar(1) = p5 + p3*q1
vbar(2) = p3*q1
vbar(3) = p5
vbar(4) = p5
vbar(5) = p5

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We may now proceed with the inverse substitution.

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

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q1  |-->  y2

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

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p1  |-->  x1
p2  |-->  x2
p3  |-->  x3
p4  |-->  x4
p5  |-->  k4
q1  |-->  k2

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

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k1      |-->  (k4 + k2*x3)/(x1*x2)
k2      |-->  k2
k3      |-->  k4/x3
k4      |-->  k4
k5      |-->  k4/x4
x1      |-->  x1
x2      |-->  x2
x3      |-->  x3
x4      |-->  x4
x5_hat  |-->  1

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

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vbar(1) = k4 + k2*x3
vbar(2) = k2*x3
vbar(3) = k4
vbar(4) = k4
vbar(5) = k4

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Verify steady state.  $\mathbf{xdot} = \mathbf{S} * \mathbf{vbar}$ , where

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

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