

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

The stoichiometric matrix is  $S =$

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

In this variant of the OMM model, we assume the rate of product formation is proportional to the square of the enzyme-substrate complex:

$$v(3) = k_3 x_3^2$$

The resulting vector of reaction velocities is  $v$ , where

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

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

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

We would like to define a map  $\psi_p$  such that  $\psi_p(x_3)$  is in set  $Y$ . To do so we introduce a pseudospecies  $x_5_{\text{hat}} = x_3^2$  and let  $v(3) = k_3 x_5_{\text{hat}}$ . Now,

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

Let the map  $\psi_p$  be given by

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{array}{l} q(1) = q_1 \\ q(2) = q_2 \end{array}$$

This gives

$$\begin{array}{l} \bar{y}(1) = -(q_2 - p_1 \cdot p_2 \cdot q_1)/p_3 \\ \bar{y}(2) = q_2/p_4 \\ \bar{y}(3) = q_2/p_5 \\ \bar{y}(4) = q_1 \\ \bar{y}(5) = q_2 \end{array}$$

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

$$\begin{array}{ll} k_1 & \mapsto p_2 \\ k_2 & \mapsto p_3 \\ k_3 & \mapsto p_4 \\ k_4 & \mapsto q_2 \\ k_5 & \mapsto p_5 \\ x_1 & \mapsto q_1 \\ x_2 & \mapsto p_1 \\ x_3 & \mapsto -(q_2 - p_1 \cdot p_2 \cdot q_1)/p_3 \\ x_4 & \mapsto q_2/p_5 \\ x_5_{\text{hat}} & \mapsto q_2/p_4 \end{array}$$

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

$$\begin{array}{l} \bar{v}(1) = p_1 \cdot p_2 \cdot q_1 \\ \bar{v}(2) = p_1 \cdot p_2 \cdot q_1 - q_2 \\ \bar{v}(3) = q_2 \\ \bar{v}(4) = q_2 \\ \bar{v}(5) = q_2 \end{array}$$

To resolve the pseudospecies we require that  $\psi_{\text{py}}(x_5_{\text{hat}}) = \psi_{\text{py}}(x_3^2)$ . In other words,  $(-(q_2 - p_1 \cdot p_2 \cdot q_1)/p_3)^2 = q_2/p_4$ . This gives

$$\begin{array}{ll} k_1 & \mapsto p_2 \\ k_2 & \mapsto p_3 \\ k_3 & \mapsto p_4 \\ k_4 & \mapsto q_2 \\ k_5 & \mapsto p_5 \\ x_1 & \mapsto (q_2 + (p_3 \cdot q_2^{(1/2)})/p_4^{(1/2)})/(p_1 \cdot p_2) \\ x_2 & \mapsto p_1 \\ x_3 & \mapsto q_2^{(1/2)}/p_4^{(1/2)} \end{array}$$

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x4      |-->  q2/p5
x5_hat  |-->  q2/p4

```

and

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vbar(1) = q2 + (p3*q2^(1/2))/p4^(1/2)
vbar(2) = (p3*q2^(1/2))/p4^(1/2)
vbar(3) = q2
vbar(4) = q2
vbar(5) = q2

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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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q2  |-->  y5

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

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p1  |-->  x2
p2  |-->  k1
p3  |-->  k2
p4  |-->  k3
p5  |-->  k5
q2  |-->  k4

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

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k1      |-->  k1
k2      |-->  k2
k3      |-->  k3
k4      |-->  k4
k5      |-->  k5
x1      |-->  (k4 + (k2*k4^(1/2))/k3^(1/2))/(k1*x2)
x2      |-->  x2
x3      |-->  k4^(1/2)/k3^(1/2)
x4      |-->  k4/k5
x5_hat  |-->  k4/k3

```

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

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vbar(1) = k4 + (k2*k4^(1/2))/k3^(1/2)
vbar(2) = (k2*k4^(1/2))/k3^(1/2)
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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