

There are 12 reactions and 9 species in the fumarase model.

The stoichiometric matrix is $S =$

```

-1  0 -1  0  0  1  1  0  1  0  0 -1
 0  0  0  0  1 -1  0  0  0  0 -1  1
 1 -1  0  0  0  0 -1  1  0  0  0  0
 0  1  0  1 -1  0  0 -1  0 -1  1  0
 0  0  1 -1  0  0  0  0 -1  1  0  0
-1  0  0 -1  0  0  1  0  0  1  0  0
 0 -1 -1  0  0  0  0  1  1  0  0  0
 0  0  0  0 -1  0  0  0  0  0  1  0
 0  0  0  0  0 -1  0  0  0  0  0  1

```

The vector of reaction velocities is v , where

```

v( 1) = k1*x1*x6
v( 2) = k2*x3*x7
v( 3) = k3*x1*x7
v( 4) = k4*x5*x6
v( 5) = k5*x4*x8
v( 6) = k6*x2
v( 7) = k7*x3
v( 8) = k8*x4
v( 9) = k9*x5
v(10) = k10*x4
v(11) = k11*x2
v(12) = k12*x1*x9

```

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

```

xdot(1) = k6*x2 + k7*x3 + k9*x5 - k1*x1*x6 - k3*x1*x7 - k12*x1*x9
xdot(2) = k5*x4*x8 - k11*x2 - k6*x2 + k12*x1*x9
xdot(3) = k8*x4 - k7*x3 + k1*x1*x6 - k2*x3*x7
xdot(4) = k11*x2 - k8*x4 - k10*x4 + k2*x3*x7 + k4*x5*x6 - k5*x4*x8
xdot(5) = k10*x4 - k9*x5 + k3*x1*x7 - k4*x5*x6
xdot(6) = k7*x3 + k10*x4 - k1*x1*x6 - k4*x5*x6
xdot(7) = k8*x4 + k9*x5 - k3*x1*x7 - k2*x3*x7
xdot(8) = k11*x2 - k5*x4*x8
xdot(9) = k12*x1*x9 - k6*x2

```

To compare py-substitution with King-Altman, we assume that the substrate abundances $x_6 \dots x_9$ are constant. This gives $S_5 = S(1:5,:) =$

```

-1  0 -1  0  0  1  1  0  1  0  0 -1
 0  0  0  0  1 -1  0  0  0  0 -1  1
 1 -1  0  0  0  0 -1  1  0  0  0  0
 0  1  0  1 -1  0  0 -1  0 -1  1  0
 0  0  1 -1  0  0  0  0 -1  1  0  0

```

and $x' =$

```

x'(1) = x1
x'(2) = x2
x'(3) = x3
x'(4) = x4
x'(5) = x5

```

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%
% Solve S_5 * v = 0 by King-Altman
%

```

First substitute in the following transition rate constants.

```

kp13 = k1*x6
kp34 = k2*x7

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kp15 = k3*x7
kp54 = k4*x6
kp42 = k5*x8
kp21 = k6
kp31 = k7
kp43 = k8
kp51 = k9
kp45 = k10
kp24 = k11
kp12 = k12*x9

```

Now $S_5 * v = K * x'$, where $K = S_5 * \text{jacobian}(v, x') =$

$K(1,1)$	$kp21$	$kp31$	0	$kp51$
$kp12 - kp21 - kp24$	0	0	$kp42$	0
$kp13$	$0 - kp31 - kp34$	$kp43$	0	0
0	$kp24$	$kp34 - kp42 - kp43 - kp45$	$kp54$	$kp54$
$kp15$	0	0	$kp45 - kp51 - kp54$	

where

$$K(1,1) = -kp12 - kp13 - kp15$$

Solve $K * x' = 0$ by the King-Altman method. The resulting steady state expression for each enzyme i has the form $N_{ka}(i)/D_{ka}$, where

$$N_{ka}(1) = k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k10*k11 + k4*k6*k7*k8*x6 + k2*k6*k9*k10*x7 + k5*k6*k7*k9*x8 + k4*k7*k8*k11*x6 + k2*k9*k10*k11*x7 + k4*k5*k6*k7*x6*x8 + k2*k5*k6*k9*x7*x8 + k2*k4*k5*k6*x6*x7*x8$$

$$N_{ka}(2) = k7*k8*k9*k12*x9 + k7*k9*k10*k12*x9 + k4*k7*k8*k12*x6*x9 + k2*k9*k10*k12*x7*x9 + k5*k7*k9*k12*x8*x9 + k1*k2*k5*k9*x6*x7*x8 + k3*k4*k5*k7*x6*x7*x8 + k4*k5*k7*k12*x6*x8*x9 + k2*k5*k9*k12*x7*x8*x9 + k1*k2*k4*k5*x6^2*x7*x8 + k2*k3*k4*k5*x6*x7^2*x8 + k2*k4*k5*k12*x6*x7*x8*x9$$

$$N_{ka}(3) = k1*k6*k8*k9*x6 + k1*k6*k9*k10*x6 + k1*k8*k9*k11*x6 + k1*k9*k10*k11*x6 + k8*k9*k11*k12*x9 + k1*k4*k6*k8*x6^2 + k1*k4*k8*k11*x6^2 + k1*k4*k5*k6*x6^2*x8 + k3*k4*k6*k8*x6*x7 + k1*k5*k6*k9*x6*x8 + k3*k4*k8*k11*x6*x7 + k4*k8*k11*k12*x6*x9$$

$$N_{ka}(4) = k7*k9*k11*k12*x9 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*x7^2 + k1*k2*k4*k11*x6^2*x7 + k2*k3*k4*k11*x6*x7^2 + k1*k2*k6*k9*x6*x7 + k3*k4*k6*k7*x6*x7 + k1*k2*k9*k11*x6*x7 + k3*k4*k7*k11*x6*x7 + k4*k7*k11*k12*x6*x9 + k2*k9*k11*k12*x7*x9 + k2*k4*k11*k12*x6*x7*x9$$

$$N_{ka}(5) = k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9$$

and

$$D_{ka} = k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k10*k11 + k1*k6*k8*k9*x6 + k3*k6*k7*k8*x7 + k4*k6*k7*k8*x6 + k1*k6*k9*k10*x6 + k3*k6*k7*k10*x7 + k2*k6*k9*k10*x7 + k1*k8*k9*k11*x6 + k5*k6*k7*k9*x8 + k3*k7*k8*k11*x7 + k4*k7*k8*k11*x6 + k1*k9*k10*k11*x6 + k3*k7*k10*k11*x7 + k2*k9*k10*k11*x7 + k7*k8*k9*k12*x9 + k7*k9*k10*k12*x9 + k7*k9*k11*k12*x9 + k7*k10*k11*k12*x9 + k8*k9*k11*k12*x9 + k1*k4*k6*k8*x6^2 + k2*k3*k6*k10*x7^2 + k1*k4*k8*k11*x6^2 + k2*k3*k10*k11*x7^2 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*x7^2 + k1*k4*k5*k6*x6^2*x8 + k1*k2*k4*k11*x6^2*x7 + k2*k3*k5*k6*x7^2*x8 + k2*k3*k4*k11*x6*x7^2 + k1*k2*k6*k9*x6*x7 + k1*k2*k6*k10*x6*x7 + k3*k4*k6*k7*x6*x7 + k3*k4*k6*k8*x6*x7 + k1*k5*k6*k9*x6*x8 + k1*k2*k9*k11*x6*x7 + k3*k5*k6*k7*x7*x8 + k4*k5*k6*k7*x6*x8 + k1*k2*k10*k11*x6*x7 + k2*k5*k6*k9*x7*x8 + k3*k4*k7*k11*x6*x7 + k3*k4*k8*k11*x6*x7 + k4*k7*k8*k12*x6*x9 + k2*k9*k10*k12*x7*x9 + k4*k8*k11*k12*x6*x9 + k5*k7*k9*k11*k12*x6*x9 + k2*k9*k11*k12*x7*x9 + k4*k8*k11*k12*x6*x9 + k5*k7*k9*$$

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k12*x8*x9 + k2*k10*k11*k12*x7*x9 + k1*k2*k5*k9*x6*x7*x8 + k2*k4*k5*k6
*x6*x7*x8 + k3*k4*k5*k7*x6*x7*x8 + k2*k4*k11*k12*x6*x7*x9 + k4*k5*k7*
k12*x6*x8*x9 + k2*k5*k9*k12*x7*x8*x9 + k1*k2*k4*k5*x6^2*x7*x8 + k2*k3
*k4*k5*x6*x7^2*x8 + k2*k4*k5*k12*x6*x7*x8*x9

%
% Solve S_5 * v = 0 by py-substitution
%
```

Let the map ψ_p be given by

```

k1  |--> p1
k2  |--> p2
k3  |--> p3
k4  |--> p4
k5  |--> p5
k6  |--> p6
k7  |--> p7
k8  |--> p8
k9  |--> p9
k10 |--> p10
k11 |--> p11
k12 |--> p12
x1  |--> y1
x2  |--> y2
x3  |--> y3
x4  |--> y4
x5  |--> y5
x6  |--> p13
x7  |--> p14
x8  |--> p15
x9  |--> p16
```

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

```

psi_p(v( 1)) = p1*p13*y1
psi_p(v( 2)) = p2*p14*y3
psi_p(v( 3)) = p3*p14*y1
psi_p(v( 4)) = p4*p13*y5
psi_p(v( 5)) = p5*p15*y4
psi_p(v( 6)) = p6*y2
psi_p(v( 7)) = p7*y3
psi_p(v( 8)) = p8*y4
psi_p(v( 9)) = p9*y5
psi_p(v(10)) = p10*y4
psi_p(v(11)) = p11*y2
psi_p(v(12)) = p12*p16*y1
```

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

```

p1*p13    0    0    0    0
0    0    p2*p14    0    0
p3*p14    0    0    0    0
0    0    0    0    p4*p13
0    0    0    p5*p15    0
0    p6    0    0    0
0    0    p7    0    0
0    0    0    p8    0
0    0    0    0    p9
0    0    0    p10    0
0    p11    0    0    0
p12*p16    0    0    0    0
```

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

```

C(1,1)      p6      p7      0      p9
```

$$\begin{array}{ccccccc}
p_{12}p_{16} & - & p_6 & - & p_{11} & & 0 \\
p_1p_{13} & & 0 & - & p_7 & - & p_2p_{14} \\
0 & & p_{11} & & p_2p_{14} & - & p_8 - p_{10} - p_5p_{15} \\
p_3p_{14} & & 0 & & 0 & & p_{10} - p_9 - p_4p_{13}
\end{array}$$

where

$$C(1,1) = -p_1p_{13} - p_3p_{14} - p_{12}p_{16}$$

C is row equivalent to the reduced matrix Crref =

$$\begin{array}{cccccc}
1 & 0 & 0 & 0 & \text{Crref}(1,5) \\
0 & 1 & 0 & 0 & \text{Crref}(2,5) \\
0 & 0 & 1 & 0 & \text{Crref}(3,5) \\
0 & 0 & 0 & 1 & \text{Crref}(4,5) \\
0 & 0 & 0 & 0 & 0
\end{array}$$

where

$$\begin{aligned}
\text{Crref}(1,5) = & -(p_6p_7p_8p_9 + p_6p_7p_9p_{10} + p_7p_8p_9p_{11} + p_7p_9p_{10}p_{11} + p_4p_6p_7p_8p_{13} + p_2p_6p_9p_{10}p_{14} + p_5p_6p_7p_9p_{15} + p_4p_7p_8p_{11}p_{13} + p_2p_9p_{10}p_{11}p_{14} + p_4p_5p_6p_7p_{13}p_{15} + p_2p_5p_6p_9p_{14}p_{15} + p_2p_4p_5p_6p_{13}p_{14}p_{15}) / (p_3p_6p_7p_8p_{14} + p_3p_6p_7p_{10}p_{14} + p_3p_7p_8p_{11}p_{14} + p_3p_7p_{10}p_{11}p_{14} + p_7p_{10}p_{11}p_{12}p_{16} + p_2p_3p_6p_{10}p_{14}^2 + p_2p_3p_{10}p_{11}p_{14}^2 + p_2p_3p_5p_6p_{14}^2p_{15} + p_1p_2p_6p_{10}p_{13}p_{14} + p_3p_5p_6p_7p_{14}p_{15} + p_1p_2p_{10}p_{11}p_{13}p_{14} + p_2p_{10}p_{11}p_{12}p_{14}p_{16})
\end{aligned}$$

$$\begin{aligned}
\text{Crref}(3,5) = & -(p_1p_6p_8p_9p_{13} + p_1p_6p_9p_{10}p_{13} + p_1p_8p_9p_{11}p_{13} + p_1p_9p_{10}p_{11}p_{13} + p_8p_9p_{11}p_{12}p_{16} + p_1p_4p_6p_8p_{13}^2 + p_1p_4p_8p_{11}p_{13}^2 + p_1p_4p_5p_6p_{13}^2p_{15} + p_3p_4p_6p_8p_{13}p_{14} + p_1p_5p_6p_9p_{13}p_{15} + p_3p_4p_8p_{11}p_{13}p_{14} + p_4p_8p_{11}p_{12}p_{13}p_{16}) / (p_3p_6p_7p_8p_{14} + p_3p_6p_7p_{10}p_{14} + p_3p_7p_8p_{11}p_{14} + p_3p_7p_{10}p_{11}p_{14} + p_7p_{10}p_{11}p_{12}p_{16} + p_2p_3p_6p_{10}p_{14}^2 + p_2p_3p_{10}p_{11}p_{14}^2 + p_2p_3p_5p_6p_{14}^2p_{15} + p_1p_2p_6p_{10}p_{13}p_{14} + p_3p_5p_6p_7p_{14}p_{15} + p_1p_2p_{10}p_{11}p_{13}p_{14} + p_2p_{10}p_{11}p_{12}p_{14}p_{16})
\end{aligned}$$

$$\begin{aligned}
\text{Crref}(4,5) = & -(p_7p_9p_{11}p_{12}p_{16} + p_1p_2p_4p_6p_{13}^2p_{14} + p_2p_3p_4p_6p_{13}p_{14}^2 + p_1p_2p_4p_{11}p_{13}^2p_{14} + p_2p_3p_4p_{11}p_{13}p_{14}^2 + p_1p_2p_6p_9p_{13}p_{14} + p_3p_4p_6p_7p_{13}p_{14} + p_1p_2p_9p_{11}p_{13}p_{14} + p_3p_4p_7p_{11}p_{13}p_{14} + p_4p_7p_{11}p_{12}p_{13}p_{16} + p_2p_9p_{11}p_{12}p_{14}p_{16} + p_2p_4p_{11}p_{12}p_{13}p_{14}p_{16}) / (p_3p_6p_7p_8p_{14} + p_3p_6p_7p_{10}p_{14} + p_3p_7p_8p_{11}p_{14} + p_3p_7p_{10}p_{11}p_{14} + p_7p_{10}p_{11}p_{12}p_{16} + p_2p_3p_6p_{10}p_{14}^2 + p_2p_3p_{10}p_{11}p_{14}^2 + p_2p_3p_5p_6p_{14}^2p_{15} + p_1p_2p_6p_{10}p_{13}p_{14} + p_3p_5p_6p_7p_{14}p_{15} + p_1p_2p_{10}p_{11}p_{13}p_{14} + p_2p_{10}p_{11}p_{12}p_{14}p_{16})
\end{aligned}$$

$$\begin{aligned}
\text{Crref}(2,5) = & -(p_7p_8p_9p_{12}p_{16} + p_7p_9p_{10}p_{12}p_{16} + p_4p_7p_8p_{12}p_{13}p_{16} + p_2p_9p_{10}p_{12}p_{14}p_{16} + p_5p_7p_9p_{12}p_{15}p_{16} + p_1p_2p_5p_9p_{13}p_{14}p_{15} + p_3p_4p_5p_7p_{13}p_{14}p_{15} + p_4p_5p_7p_{12}p_{13}p_{15}p_{16} + p_2p_5p_9p_{12}p_{14}p_{15}p_{16} + p_1p_2p_4p_5p_{13}^2p_{14}p_{15} + p_2p_3p_4p_5p_{13}p_{14}^2p_{15} + p_2p_4p_5p_{12}p_{13}p_{14}p_{15}p_{16}) / (p_3p_6p_7p_8p_{14} + p_3p_6p_7p_{10}p_{14} + p_3p_7p_8p_{11}p_{14} + p_3p_7p_{10}p_{11}p_{14} + p_7p_{10}p_{11}p_{12}p_{16} + p_2p_3p_6p_{10}p_{14}^2 + p_2p_3p_{10}p_{11}p_{14}^2 + p_2p_3p_5p_6p_{14}^2p_{15} + p_1p_2p_6p_{10}p_{13}p_{14} + p_3p_5p_6p_7p_{14}p_{15} + p_1p_2p_{10}p_{11}p_{13}p_{14} + p_2p_{10}p_{11}p_{12}p_{14}p_{16})
\end{aligned}$$

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

$$\begin{array}{c}
N(1,1) \\
N(2,1) \\
N(3,1) \\
N(4,1) \\
1
\end{array}$$

where

$$N(1,1) = (p_6 p_7 p_8 p_9 + p_6 p_7 p_9 p_{10} + p_7 p_8 p_9 p_{11} + p_7 p_9 p_{10} p_{11} + p_4 p_6 p_7 p_8 p_{13} + p_2 p_6 p_9 p_{10} p_{14} + p_5 p_6 p_7 p_9 p_{15} + p_4 p_7 p_8 p_{11} p_{13} + p_2 p_9 p_{10} p_{11} p_{14} + p_4 p_5 p_6 p_7 p_{13} p_{15} + p_2 p_5 p_6 p_9 p_{14} p_{15} + p_2 p_4 p_5 p_6 p_{13} p_{14} p_{15}) / (p_3 p_6 p_7 p_8 p_{14} + p_3 p_6 p_7 p_{10} p_{14} + p_3 p_7 p_8 p_{11} p_{14} + p_3 p_7 p_{10} p_{11} p_{14} + p_7 p_{10} p_{11} p_{12} p_{16} + p_2 p_3 p_6 p_{10} p_{14}^2 + p_2 p_3 p_{10} p_{11} p_{14}^2 + p_2 p_3 p_5 p_6 p_{14}^2 p_{15} + p_1 p_2 p_6 p_{10} p_{13} p_{14} + p_3 p_5 p_6 p_7 p_{14} p_{15} + p_1 p_2 p_{10} p_{11} p_{13} p_{14} + p_2 p_{10} p_{11} p_{12} p_{14} p_{16})$$

$$N(3,1) = (p_1 p_6 p_8 p_9 p_{13} + p_1 p_6 p_9 p_{10} p_{13} + p_1 p_8 p_9 p_{11} p_{13} + p_1 p_9 p_{10} p_{11} p_{13} + p_8 p_9 p_{11} p_{12} p_{16} + p_1 p_4 p_6 p_8 p_{13}^2 + p_1 p_4 p_8 p_{11} p_{13}^2 + p_1 p_4 p_5 p_6 p_{13}^2 p_{15} + p_3 p_4 p_6 p_8 p_{13} p_{14} + p_1 p_5 p_6 p_9 p_{13} p_{15} + p_3 p_4 p_8 p_{11} p_{13} p_{14} + p_4 p_8 p_{11} p_{12} p_{13} p_{16}) / (p_3 p_6 p_7 p_8 p_{14} + p_3 p_6 p_7 p_{10} p_{14} + p_3 p_7 p_8 p_{11} p_{14} + p_3 p_7 p_{10} p_{11} p_{14} + p_7 p_{10} p_{11} p_{12} p_{16} + p_2 p_3 p_6 p_{10} p_{14}^2 + p_2 p_3 p_{10} p_{11} p_{14}^2 + p_2 p_3 p_5 p_6 p_{14}^2 p_{15} + p_1 p_2 p_6 p_{10} p_{13} p_{14} + p_3 p_5 p_6 p_7 p_{14} p_{15} + p_1 p_2 p_{10} p_{11} p_{13} p_{14} + p_2 p_{10} p_{11} p_{12} p_{14} p_{16})$$

$$N(4,1) = (p_7 p_9 p_{11} p_{12} p_{16} + p_1 p_2 p_4 p_6 p_{13}^2 p_{14} + p_2 p_3 p_4 p_6 p_{13} p_{14}^2 + p_1 p_2 p_4 p_{11} p_{13}^2 p_{14} + p_2 p_3 p_4 p_{11} p_{13} p_{14}^2 + p_1 p_2 p_6 p_9 p_{13} p_{14} + p_3 p_4 p_6 p_7 p_{13} p_{14} + p_1 p_2 p_9 p_{11} p_{13} p_{14} + p_3 p_4 p_7 p_{11} p_{13} p_{14} + p_4 p_7 p_{11} p_{12} p_{13} p_{16} + p_2 p_9 p_{11} p_{12} p_{14} p_{16} + p_2 p_4 p_{11} p_{12} p_{13} p_{14} p_{16}) / (p_3 p_6 p_7 p_8 p_{14} + p_3 p_6 p_7 p_{10} p_{14} + p_3 p_7 p_8 p_{11} p_{14} + p_3 p_7 p_{10} p_{11} p_{14} + p_7 p_{10} p_{11} p_{12} p_{16} + p_2 p_3 p_6 p_{10} p_{14}^2 + p_2 p_3 p_{10} p_{11} p_{14}^2 + p_2 p_3 p_5 p_6 p_{14}^2 p_{15} + p_1 p_2 p_6 p_{10} p_{13} p_{14} + p_3 p_5 p_6 p_7 p_{14} p_{15} + p_1 p_2 p_{10} p_{11} p_{13} p_{14} + p_2 p_{10} p_{11} p_{12} p_{14} p_{16})$$

$$N(2,1) = (p_7 p_8 p_9 p_{12} p_{16} + p_7 p_9 p_{10} p_{12} p_{16} + p_4 p_7 p_8 p_{12} p_{13} p_{16} + p_2 p_9 p_{10} p_{12} p_{14} p_{16} + p_5 p_7 p_9 p_{12} p_{15} p_{16} + p_1 p_2 p_5 p_9 p_{13} p_{14} p_{15} + p_3 p_4 p_5 p_7 p_{13} p_{14} p_{15} + p_4 p_5 p_7 p_{12} p_{13} p_{15} p_{16} + p_2 p_5 p_9 p_{12} p_{14} p_{15} p_{16} + p_1 p_2 p_4 p_5 p_{13}^2 p_{14} p_{15} + p_2 p_3 p_4 p_5 p_{13} p_{14}^2 p_{15} + p_2 p_4 p_5 p_{12} p_{13} p_{14} p_{15} p_{16}) / (p_3 p_6 p_7 p_8 p_{14} + p_3 p_6 p_7 p_{10} p_{14} + p_3 p_7 p_8 p_{11} p_{14} + p_3 p_7 p_{10} p_{11} p_{14} + p_7 p_{10} p_{11} p_{12} p_{16} + p_2 p_3 p_6 p_{10} p_{14}^2 + p_2 p_3 p_{10} p_{11} p_{14}^2 + p_2 p_3 p_5 p_6 p_{14}^2 p_{15} + p_1 p_2 p_6 p_{10} p_{13} p_{14} + p_3 p_5 p_6 p_7 p_{14} p_{15} + p_1 p_2 p_{10} p_{11} p_{13} p_{14} + p_2 p_{10} p_{11} p_{12} p_{14} p_{16})$$

Let q be a linear combination of null space basis vectors, where $q = [q_1]$.
Let $ybar = N \cdot q$. This gives

$$ybar(1) = (q_1 (p_6 p_7 p_8 p_9 + p_6 p_7 p_9 p_{10} + p_7 p_8 p_9 p_{11} + p_7 p_9 p_{10} p_{11} + p_4 p_6 p_7 p_8 p_{13} + p_5 p_6 p_7 p_9 p_{15} + p_4 p_7 p_8 p_{11} p_{13} + p_4 p_5 p_6 p_7 p_{13} p_{15}) + p_{14} q_1 (p_2 p_6 p_9 p_{10} + p_2 p_9 p_{10} p_{11} + p_2 p_5 p_6 p_9 p_{15} + p_2 p_4 p_5 p_6 p_{13} p_{15})) / (p_3 p_6 p_7 p_8 p_{14} + p_3 p_6 p_7 p_{10} p_{14} + p_3 p_7 p_8 p_{11} p_{14} + p_3 p_7 p_{10} p_{11} p_{14} + p_7 p_{10} p_{11} p_{12} p_{16} + p_2 p_3 p_6 p_{10} p_{14}^2 + p_2 p_3 p_{10} p_{11} p_{14}^2 + p_2 p_3 p_5 p_6 p_{14}^2 p_{15} + p_1 p_2 p_6 p_{10} p_{13} p_{14} + p_3 p_5 p_6 p_7 p_{14} p_{15} + p_1 p_2 p_{10} p_{11} p_{13} p_{14} + p_2 p_{10} p_{11} p_{12} p_{14} p_{16})$$

$$ybar(2) = (q_1 (p_7 p_8 p_9 p_{12} p_{16} + p_7 p_9 p_{10} p_{12} p_{16} + p_4 p_7 p_8 p_{12} p_{13} p_{16} + p_2 p_9 p_{10} p_{12} p_{14} p_{16} + p_5 p_7 p_9 p_{12} p_{15} p_{16} + p_1 p_2 p_5 p_9 p_{13} p_{14} p_{15} + p_3 p_4 p_5 p_7 p_{13} p_{14} p_{15} + p_4 p_5 p_7 p_{12} p_{13} p_{15} p_{16} + p_2 p_5 p_9 p_{12} p_{14} p_{15} p_{16} + p_1 p_2 p_4 p_5 p_{13}^2 p_{14} p_{15} + p_2 p_3 p_4 p_5 p_{13} p_{14}^2 p_{15} + p_2 p_4 p_5 p_{12} p_{13} p_{14} p_{15} p_{16})) / (p_3 p_6 p_7 p_8 p_{14} + p_3 p_6 p_7 p_{10} p_{14} + p_3 p_7 p_8 p_{11} p_{14} + p_3 p_7 p_{10} p_{11} p_{14} + p_7 p_{10} p_{11} p_{12} p_{16} + p_2 p_3 p_6 p_{10} p_{14}^2 + p_2 p_3 p_{10} p_{11} p_{14}^2 + p_2 p_3 p_5 p_6 p_{14}^2 p_{15} + p_1 p_2 p_6 p_{10} p_{13} p_{14} + p_3 p_5 p_6 p_7 p_{14} p_{15} + p_1 p_2 p_{10} p_{11} p_{13} p_{14} + p_2 p_{10} p_{11} p_{12} p_{14} p_{16})$$

$$ybar(3) = (q_1 (p_1 p_6 p_8 p_9 p_{13} + p_1 p_6 p_9 p_{10} p_{13} + p_1 p_8 p_9 p_{11} p_{13} + p_1 p_9 p_{10} p_{11} p_{13} + p_8 p_9 p_{11} p_{12} p_{16} + p_1 p_4 p_6 p_8 p_{13}^2 + p_1 p_4 p_8 p_{11} p_{13}^2 + p_1 p_4 p_5 p_6 p_{13}^2 p_{15} + p_3 p_4 p_6 p_8 p_{13} p_{14} + p_1 p_5 p_6 p_9 p_{13} p_{15} + p_3 p_4 p_8 p_{11} p_{13} p_{14} + p_4 p_8 p_{11} p_{12} p_{13} p_{16})) / (p_3 p_6 p_7 p_8 p_{14} + p_3 p_6 p_7 p_{10} p_{14} + p_3 p_7 p_8 p_{11} p_{14} + p_3 p_7 p_{10} p_{11} p_{14} + p_7 p_{10} p_{11} p_{12} p_{16} + p_2 p_3 p_6 p_{10} p_{14}^2 + p_2 p_3 p_{10} p_{11} p_{14}^2 + p_2 p_3 p_5 p_6 p_{14}^2 p_{15} + p_1 p_2 p_6 p_{10} p_{13} p_{14} + p_3 p_5 p_6 p_7 p_{14} p_{15} + p_1 p_2 p_{10} p_{11} p_{13} p_{14} + p_2 p_{10} p_{11} p_{12} p_{14} p_{16})$$

$$4 + p7*p10*p11*p12*p16 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*p13*p14 + p2*p10*p11*p12*p14*p16)$$

$$\begin{aligned} \text{ybar}(4) = & (q1*(p7*p9*p11*p12*p16 + p1*p2*p4*p6*p13^2*p14 + p2*p3*p4*p6*p13*p14^2 + p1*p2*p6* \\ & p9*p13*p14 + p3*p4*p6*p7*p13*p14 + p1*p2*p9*p11*p13*p14 + p3*p4*p7* \\ & p11*p13*p14 + p4*p7*p11*p12*p13*p16 + p2*p9*p11*p12*p14*p16 + p2* \\ & p4*p11*p12*p13*p14*p16))/(p3*p6*p7*p8*p14 + p3*p6*p7*p10*p14 + p3* \\ & p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p16 + p2*p3*p6* \\ & p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*p15 + p1*p2*p6* \\ & p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*p13*p14 + p2*p1 \\ & 0*p11*p12*p14*p16) \end{aligned}$$

$$\text{ybar}(5) = q1$$

From ybar we construct the composite forward map psi_py :

$$k1 \quad | \rightarrow \quad p1$$

$$k2 \quad | \rightarrow \quad p2$$

$$k3 \quad | \rightarrow \quad p3$$

$$k4 \quad | \rightarrow \quad p4$$

$$k5 \quad | \rightarrow \quad p5$$

$$k6 \quad | \rightarrow \quad p6$$

$$k7 \quad | \rightarrow \quad p7$$

$$k8 \quad | \rightarrow \quad p8$$

$$k9 \quad | \rightarrow \quad p9$$

$$k10 \quad | \rightarrow \quad p10$$

$$k11 \quad | \rightarrow \quad p11$$

$$k12 \quad | \rightarrow \quad p12$$

$$\begin{aligned} x1 \quad | \rightarrow \quad & (q1*(p6*p7*p8*p9 + p6*p7*p9*p10 + p7*p8*p9*p11 + p7*p9*p10*p11 + \\ & p4*p6*p7*p8*p13 + p5*p6*p7*p9*p15 + p4*p7*p8*p11*p13 + p4*p5*p6*p \\ & 7*p13*p15) + p14*q1*(p2*p6*p9*p10 + p2*p9*p10*p11 + p2*p5*p6*p9*p \\ & 15 + p2*p4*p5*p6*p13*p15))/(p3*p6*p7*p8*p14 + p3*p6*p7*p10*p14 + \\ & p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p16 + p2*p3* \\ & p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*p15 + p1* \\ & p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*p13*p14 + \\ & p2*p10*p11*p12*p14*p16) \end{aligned}$$

$$\begin{aligned} x2 \quad | \rightarrow \quad & (q1*(p7*p8*p9*p12*p16 + p7*p9*p10*p12*p16 + p4*p7*p8*p12*p13*p16 \\ & + p2*p9*p10*p12*p14*p16 + p5*p7*p9*p12*p15*p16 + p1*p2*p5*p9*p13* \\ & p14*p15 + p3*p4*p5*p7*p13*p14*p15 + p4*p5*p7*p12*p13*p15*p16 + p2* \\ & p5*p9*p12*p14*p15*p16 + p1*p2*p4*p5*p13^2*p14*p15 + p2*p3*p4*p5* \\ & p13*p14^2*p15 + p2*p4*p5*p12*p13*p14*p15*p16))/(p3*p6*p7*p8*p14 + \\ & p3*p6*p7*p10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10* \\ & p11*p12*p16 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p \\ & 5*p6*p14^2*p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1* \\ & p2*p10*p11*p13*p14 + p2*p10*p11*p12*p14*p16) \end{aligned}$$

$$\begin{aligned} x3 \quad | \rightarrow \quad & (q1*(p1*p6*p8*p9*p13 + p1*p6*p9*p10*p13 + p1*p8*p9*p11*p13 + p1*p \\ & 9*p10*p11*p13 + p8*p9*p11*p12*p16 + p1*p4*p6*p8*p13^2 + p1*p4*p8* \\ & p11*p13^2 + p1*p4*p5*p6*p13^2*p15 + p3*p4*p6*p8*p13*p14 + p1*p5*p \\ & 6*p9*p13*p15 + p3*p4*p8*p11*p13*p14 + p4*p8*p11*p12*p13*p16))/(p3* \\ & p6*p7*p8*p14 + p3*p6*p7*p10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p \\ & 11*p14 + p7*p10*p11*p12*p16 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11* \end{aligned}$$

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p14^2 + p2*p3*p5*p6*p14^2*p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p
7*p14*p15 + p1*p2*p10*p11*p13*p14 + p2*p10*p11*p12*p14*p16)

x4  |--> (q1*(p7*p9*p11*p12*p16 + p1*p2*p4*p6*p13^2*p14 + p2*p3*p4*p6*p13*
p14^2 + p1*p2*p4*p11*p13^2*p14 + p2*p3*p4*p11*p13*p14^2 + p1*p2*p
6*p9*p13*p14 + p3*p4*p6*p7*p13*p14 + p1*p2*p9*p11*p13*p14 + p3*p4
*p7*p11*p13*p14 + p4*p7*p11*p12*p13*p16 + p2*p9*p11*p12*p14*p16 +
p2*p4*p11*p12*p13*p14*p16))/(p3*p6*p7*p8*p14 + p3*p6*p7*p10*p14
+ p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p16 + p2*
p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*p15 + p
1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*p13*p14
+ p2*p10*p11*p12*p14*p16)

x5  |--> q1
x6  |--> p13
x7  |--> p14
x8  |--> p15
x9  |--> p16

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

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vbar( 1) = (p1*p13*(q1*(p6*p7*p8*p9 + p6*p7*p9*p10 + p7*p8*p9*p11 + p7*p9*p1
0*p11 + p4*p6*p7*p8*p13 + p5*p6*p7*p9*p15 + p4*p7*p8*p11*p13 + p4
*p5*p6*p7*p13*p15) + p14*q1*(p2*p6*p9*p10 + p2*p9*p10*p11 + p2*p5
*p6*p9*p15 + p2*p4*p5*p6*p13*p15)))/(p3*p6*p7*p8*p14 + p3*p6*p7*p
10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p1
6 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*
p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*
p13*p14 + p2*p10*p11*p12*p14*p16)

vbar( 2) = (p2*p14*q1*(p1*p6*p8*p9*p13 + p1*p6*p9*p10*p13 + p1*p8*p9*p11*p13
+ p1*p9*p10*p11*p13 + p8*p9*p11*p12*p16 + p1*p4*p6*p8*p13^2 + p1
*p4*p8*p11*p13^2 + p1*p4*p5*p6*p13^2*p15 + p3*p4*p6*p8*p13*p14 +
p1*p5*p6*p9*p13*p15 + p3*p4*p8*p11*p13*p14 + p4*p8*p11*p12*p13*p1
6))/(p3*p6*p7*p8*p14 + p3*p6*p7*p10*p14 + p3*p7*p8*p11*p14 + p3*p
7*p10*p11*p14 + p7*p10*p11*p12*p16 + p2*p3*p6*p10*p14^2 + p2*p3*p
10*p11*p14^2 + p2*p3*p5*p6*p14^2*p15 + p1*p2*p6*p10*p13*p14 + p3*
p5*p6*p7*p14*p15 + p1*p2*p10*p11*p13*p14 + p2*p10*p11*p12*p14*p16
)

vbar( 3) = (p3*p14*(q1*(p6*p7*p8*p9 + p6*p7*p9*p10 + p7*p8*p9*p11 + p7*p9*p1
0*p11 + p4*p6*p7*p8*p13 + p5*p6*p7*p9*p15 + p4*p7*p8*p11*p13 + p4
*p5*p6*p7*p13*p15) + p14*q1*(p2*p6*p9*p10 + p2*p9*p10*p11 + p2*p5
*p6*p9*p15 + p2*p4*p5*p6*p13*p15)))/(p3*p6*p7*p8*p14 + p3*p6*p7*p
10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p1
6 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*
p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*
p13*p14 + p2*p10*p11*p12*p14*p16)

vbar( 4) = p4*p13*q1

vbar( 5) = (p5*p15*q1*(p7*p9*p11*p12*p16 + p1*p2*p4*p6*p13^2*p14 + p2*p3*p4*
p6*p13*p14^2 + p1*p2*p4*p11*p13^2*p14 + p2*p3*p4*p11*p13*p14^2 +
p1*p2*p6*p9*p13*p14 + p3*p4*p6*p7*p13*p14 + p1*p2*p9*p11*p13*p14
+ p3*p4*p7*p11*p13*p14 + p4*p7*p11*p12*p13*p16 + p2*p9*p11*p12*p1
4*p16 + p2*p4*p11*p12*p13*p14*p16))/(p3*p6*p7*p8*p14 + p3*p6*p7*p
10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p1
6 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*
p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*
p13*p14 + p2*p10*p11*p12*p14*p16)

vbar( 6) = (p6*q1*(p7*p8*p9*p12*p16 + p7*p9*p10*p12*p16 + p4*p7*p8*p12*p13*p
16 + p2*p9*p10*p12*p14*p16 + p5*p7*p9*p12*p15*p16 + p1*p2*p5*p9*p

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13*p14*p15 + p3*p4*p5*p7*p13*p14*p15 + p4*p5*p7*p12*p13*p15*p16 +
p2*p5*p9*p12*p14*p15*p16 + p1*p2*p4*p5*p13^2*p14*p15 + p2*p3*p4*
p5*p13*p14^2*p15 + p2*p4*p5*p12*p13*p14*p15*p16))/(p3*p6*p7*p8*p1
4 + p3*p6*p7*p10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*
p10*p11*p12*p16 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p
3*p5*p6*p14^2*p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 +
p1*p2*p10*p11*p13*p14 + p2*p10*p11*p12*p14*p16)

vbar( 7) = (p7*q1*(p1*p6*p8*p9*p13 + p1*p6*p9*p10*p13 + p1*p8*p9*p11*p13 + p
1*p9*p10*p11*p13 + p8*p9*p11*p12*p16 + p1*p4*p6*p8*p13^2 + p1*p4*
p8*p11*p13^2 + p1*p4*p5*p6*p13^2*p15 + p3*p4*p6*p8*p13*p14 + p1*p
5*p6*p9*p13*p15 + p3*p4*p8*p11*p13*p14 + p4*p8*p11*p12*p13*p16)))/
(p3*p6*p7*p8*p14 + p3*p6*p7*p10*p14 + p3*p7*p8*p11*p14 + p3*p7*p1
0*p11*p14 + p7*p10*p11*p12*p16 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p
11*p14^2 + p2*p3*p5*p6*p14^2*p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p
6*p7*p14*p15 + p1*p2*p10*p11*p13*p14 + p2*p10*p11*p12*p14*p16)

vbar( 8) = (p8*q1*(p7*p9*p11*p12*p16 + p1*p2*p4*p6*p13^2*p14 + p2*p3*p4*p6*p
13*p14^2 + p1*p2*p4*p11*p13^2*p14 + p2*p3*p4*p11*p13*p14^2 + p1*p
2*p6*p9*p13*p14 + p3*p4*p6*p7*p13*p14 + p1*p2*p9*p11*p13*p14 + p3
*p4*p7*p11*p13*p14 + p4*p7*p11*p12*p13*p16 + p2*p9*p11*p12*p14*p1
6 + p2*p4*p11*p12*p13*p14*p16)))/(p3*p6*p7*p8*p14 + p3*p6*p7*p10*p
14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p16 +
p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*p15
+ p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*p13*
p14 + p2*p10*p11*p12*p14*p16)

vbar( 9) = p9*q1

vbar(10) = (p10*q1*(p7*p9*p11*p12*p16 + p1*p2*p4*p6*p13^2*p14 + p2*p3*p4*p6*
p13*p14^2 + p1*p2*p4*p11*p13^2*p14 + p2*p3*p4*p11*p13*p14^2 + p1*p
2*p6*p9*p13*p14 + p3*p4*p6*p7*p13*p14 + p1*p2*p9*p11*p13*p14 + p
3*p4*p7*p11*p13*p14 + p4*p7*p11*p12*p13*p16 + p2*p9*p11*p12*p14*p1
6 + p2*p4*p11*p12*p13*p14*p16)))/(p3*p6*p7*p8*p14 + p3*p6*p7*p10*
p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p16 +
p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2*p15
+ p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11*p13
*p14 + p2*p10*p11*p12*p14*p16)

vbar(11) = (p11*q1*(p7*p8*p9*p12*p16 + p7*p9*p10*p12*p16 + p4*p7*p8*p12*p13*
p16 + p2*p9*p10*p12*p14*p16 + p5*p7*p9*p12*p15*p16 + p1*p2*p5*p9*
p13*p14*p15 + p3*p4*p5*p7*p13*p14*p15 + p4*p5*p7*p12*p13*p15*p16
+ p2*p5*p9*p12*p14*p15*p16 + p1*p2*p4*p5*p13^2*p14*p15 + p2*p3*p4
*p5*p13*p14^2*p15 + p2*p4*p5*p12*p13*p14*p15*p16))/(p3*p6*p7*p8*p
14 + p3*p6*p7*p10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7
*p10*p11*p12*p16 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*
p3*p5*p6*p14^2*p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 +
p1*p2*p10*p11*p13*p14 + p2*p10*p11*p12*p14*p16)

vbar(12) = (p12*p16*(q1*(p6*p7*p8*p9 + p6*p7*p9*p10 + p7*p8*p9*p11 + p7*p9*p
10*p11 + p4*p6*p7*p8*p13 + p5*p6*p7*p9*p15 + p4*p7*p8*p11*p13 + p
4*p5*p6*p7*p13*p15) + p14*q1*(p2*p6*p9*p10 + p2*p9*p10*p11 + p2*p
5*p6*p9*p15 + p2*p4*p5*p6*p13*p15)))/(p3*p6*p7*p8*p14 + p3*p6*p7*
p10*p14 + p3*p7*p8*p11*p14 + p3*p7*p10*p11*p14 + p7*p10*p11*p12*p
16 + p2*p3*p6*p10*p14^2 + p2*p3*p10*p11*p14^2 + p2*p3*p5*p6*p14^2
*p15 + p1*p2*p6*p10*p13*p14 + p3*p5*p6*p7*p14*p15 + p1*p2*p10*p11
*p13*p14 + p2*p10*p11*p12*p14*p16)

```

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

$q1 \mapsto y5$

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

$p1 \mapsto k1$
 $p2 \mapsto k2$
 $p3 \mapsto k3$


```

p4  |--> k4
p5  |--> k5
p6  |--> k6
p7  |--> k7
p8  |--> k8
p9  |--> k9
p10 |--> k10
p11 |--> k11
p12 |--> k12
p13 |--> x6
p14 |--> x7
p15 |--> x8
p16 |--> x9
q1  |--> x5

```

The complete steady state map ψ_{ss} is therefore

```

k1  |--> k1
k2  |--> k2
k3  |--> k3
k4  |--> k4
k5  |--> k5
k6  |--> k6
k7  |--> k7
k8  |--> k8
k9  |--> k9
k10 |--> k10
k11 |--> k11
k12 |--> k12

x1  |--> (x5*(k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k10*k11 +
k4*k6*k7*k8*x6 + k5*k6*k7*k9*x8 + k4*k7*k8*k11*x6 + k4*k5*k6*k7*x
6*x8) + x5*x7*(k2*k6*k9*k10 + k2*k9*k10*k11 + k2*k5*k6*k9*x8 + k2
*k4*k5*k6*x6*x8))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k1
1*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 +
k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 +
k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)

x2  |--> (x5*(k7*k8*k9*k12*x9 + k7*k9*k10*k12*x9 + k4*k7*k8*k12*x6*x9 + k2
*k9*k10*k12*x7*x9 + k5*k7*k9*k12*x8*x9 + k1*k2*k5*k9*x6*x7*x8 + k
3*k4*k5*k7*x6*x7*x8 + k4*k5*k7*k12*x6*x8*x9 + k2*k5*k9*k12*x7*x8*
x9 + k1*k2*k4*k5*x6^2*x7*x8 + k2*k3*k4*k5*x6*x7^2*x8 + k2*k4*k5*k
12*x6*x7*x8*x9))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11
*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 +
k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k
3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)

x3  |--> (x5*(k1*k6*k8*k9*x6 + k1*k6*k9*k10*x6 + k1*k8*k9*k11*x6 + k1*k9*k
10*k11*x6 + k8*k9*k11*k12*x9 + k1*k4*k6*k8*x6^2 + k1*k4*k8*k11*x6
^2 + k1*k4*k5*k6*x6^2*x8 + k3*k4*k6*k8*x6*x7 + k1*k5*k6*k9*x6*x8
+ k3*k4*k8*k11*x6*x7 + k4*k8*k11*k12*x6*x9))/(k3*k6*k7*k8*x7 + k3
*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k
12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2
*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x
7 + k2*k10*k11*k12*x7*x9)

x4  |--> (x5*(k7*k9*k11*k12*x9 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*x7^2

```

$$+ k1*k2*k4*k11*x6^2*x7 + k2*k3*k4*k11*x6*x7^2 + k1*k2*k6*k9*x6*x7 + k3*k4*k6*k7*x6*x7 + k1*k2*k9*k11*x6*x7 + k3*k4*k7*k11*x6*x7 + k4*k7*k11*k12*x6*x9 + k2*k9*k11*k12*x7*x9 + k2*k4*k11*k12*x6*x7*x9)/((k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)$$

x5 |--> x5

x6 |--> x6

x7 |--> x7

x8 |--> x8

x9 |--> x9

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

$$\mathbf{vbar}(1) = (k1*x6*(x5*(k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k10*k11 + k4*k6*k7*k8*x6 + k5*k6*k7*k9*x8 + k4*k7*k8*k11*x6 + k4*k5*k6*k7*x6*x8) + x5*x7*(k2*k6*k9*k10 + k2*k9*k10*k11 + k2*k5*k6*k9*x8 + k2*k4*k5*k6*x6*x8)))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)$$

$$\mathbf{vbar}(2) = (k2*x5*x7*(k1*k6*k8*k9*x6 + k1*k6*k9*k10*x6 + k1*k8*k9*k11*x6 + k1*k9*k10*k11*x6 + k8*k9*k11*k12*x9 + k1*k4*k6*k8*x6^2 + k1*k4*k8*k11*x6^2 + k1*k4*k5*k6*x6^2*x8 + k3*k4*k6*k8*x6*x7 + k1*k5*k6*k9*x6*x8 + k3*k4*k8*k11*x6*x7 + k4*k8*k11*k12*x6*x9))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)$$

$$\mathbf{vbar}(3) = (k3*x7*(x5*(k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k10*k11 + k4*k6*k7*k8*x6 + k5*k6*k7*k9*x8 + k4*k7*k8*k11*x6 + k4*k5*k6*k7*x6*x8) + x5*x7*(k2*k6*k9*k10 + k2*k9*k10*k11 + k2*k5*k6*k9*x8 + k2*k4*k5*k6*x6*x8)))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)$$

$\mathbf{vbar}(4) = k4*x5*x6$

$$\mathbf{vbar}(5) = (k5*x5*x8*(k7*k9*k11*k12*x9 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*x7^2 + k1*k2*k6*k9*x6*x7 + k3*k4*k6*k7*x6*x7 + k1*k2*k9*k11*x6*x7 + k3*k4*k7*k11*x6*x7 + k4*k7*k11*k12*x6*x9 + k2*k9*k11*k12*x7*x9 + k2*k4*k11*k12*x6*x7*x9))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)$$

$$\mathbf{vbar}(6) = (k6*x5*(k7*k8*k9*k12*x9 + k7*k9*k10*k12*x9 + k4*k7*k8*k12*x6*x9 + k2*k9*k10*k12*x7*x9 + k5*k7*k9*k12*x8*x9 + k1*k2*k5*k9*x6*x7*x8 + k3*k4*k5*k7*x6*x7*x8 + k4*k5*k7*k12*x6*x8*x9 + k2*k5*k9*k12*x7*x8*x9 + k1*k2*k4*k5*x6^2*x7*x8 + k2*k3*k4*k5*x6*x7^2*x8 + k2*k4*k5*k12*x6*x7*x8*x9))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)$$

```

vbar( 7) = (k7*x5*(k1*k6*k8*k9*x6 + k1*k6*k9*k10*x6 + k1*k8*k9*k11*x6 + k1*k
9*k10*k11*x6 + k8*k9*k11*k12*x9 + k1*k4*k6*k8*x6^2 + k1*k4*k8*k11
*x6^2 + k1*k4*k5*k6*x6^2*x8 + k3*k4*k6*k8*x6*x7 + k1*k5*k6*k9*x6*
x8 + k3*k4*k8*k11*x6*x7 + k4*k8*k11*k12*x6*x9))/(k3*k6*k7*k8*x7 +
k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k1
1*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x
7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x
6*x7 + k2*k10*k11*k12*x7*x9)

vbar( 8) = (k8*x5*(k7*k9*k11*k12*x9 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*x
7^2 + k1*k2*k4*k11*x6^2*x7 + k2*k3*k4*k11*x6*x7^2 + k1*k2*k6*k9*x
6*x7 + k3*k4*k6*k7*x6*x7 + k1*k2*k9*k11*x6*x7 + k3*k4*k7*k11*x6*x
7 + k4*k7*k11*k12*x6*x9 + k2*k9*k11*k12*x7*x9 + k2*k4*k11*k12*x6*
x7*x9))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*
k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10
*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k
7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)

vbar( 9) = k9*x5

vbar(10) = (k10*x5*(k7*k9*k11*k12*x9 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*
x7^2 + k1*k2*k4*k11*x6^2*x7 + k2*k3*k4*k11*x6*x7^2 + k1*k2*k6*k9*
x6*x7 + k3*k4*k6*k7*x6*x7 + k1*k2*k9*k11*x6*x7 + k3*k4*k7*k11*x6*
x7 + k4*k7*k11*k12*x6*x9 + k2*k9*k11*k12*x7*x9 + k2*k4*k11*k12*x6*
x7*x9))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*
k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k1
0*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*
k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9)

vbar(11) = (k11*x5*(k7*k8*k9*k12*x9 + k7*k9*k10*k12*x9 + k4*k7*k8*k12*x6*x9
+ k2*k9*k10*k12*x7*x9 + k5*k7*k9*k12*x8*x9 + k1*k2*k5*k9*x6*x7*x8
+ k3*k4*k5*k7*x6*x7*x8 + k4*k5*k7*k12*x6*x8*x9 + k2*k5*k9*k12*x7
*x8*x9 + k1*k2*k4*k5*x6^2*x7*x8 + k2*k3*k4*k5*x6*x7^2*x8 + k2*k4*
k5*k12*x6*x7*x8*x9))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8
*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^
2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7
+ k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9
)

vbar(12) = (k12*x9*(x5*(k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k1
0*k11 + k4*k6*k7*k8*x6 + k5*k6*k7*k9*x8 + k4*k7*k8*k11*x6 + k4*k5
*k6*k7*x6*x8) + x5*x7*(k2*k6*k9*k10 + k2*k9*k10*k11 + k2*k5*k6*k9
*x8 + k2*k4*k5*k6*x6*x8))/(k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*
k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k
10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10
*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12
*x7*x9)

```

The stoichiometric matrix S5 has a rank-deficiency of 1. In King-Altman, this free variable is x_tot. Unless specified, x_tot has an implicit value of 1:

```
>> simplify( sum(xbar_ka) ) =
```

1

In py-substitution, the free variable is x5. To equate the two solutions, we require that sum(x1...x5) = 1.

```
>> x5 = solve( sprintf('%s = 1',
char(sum(xbar_py))), 'x5' );
```

The resulting steady state expression for each enzyme i has the form

$N_{py}(i)/D_{py}$, where

$$N_{py}(1) = k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k10*k11 + k4*k6*k7*k8*x6 + k2*k6*k9*k10*x7 + k5*k6*k7*k9*x8 + k4*k7*k8*k11*x6 + k2*k9*k10*k11*x7 + k4*k5*k6*k7*x6*x8 + k2*k5*k6*k9*x7*x8 + k2*k4*k5*k6*x6*x7*x8$$

$$N_{py}(2) = k7*k8*k9*k12*x9 + k7*k9*k10*k12*x9 + k4*k7*k8*k12*x6*x9 + k2*k9*k10*k12*x7*x9 + k5*k7*k9*k12*x8*x9 + k1*k2*k5*k9*x6*x7*x8 + k3*k4*k5*k7*x6*x7*x8 + k4*k5*k7*k12*x6*x8*x9 + k2*k5*k9*k12*x7*x8*x9 + k1*k2*k4*k5*x6^2*x7*x8 + k2*k3*k4*k5*x6*x7^2*x8 + k2*k4*k5*k12*x6*x7*x8*x9$$

$$N_{py}(3) = k1*k6*k8*k9*x6 + k1*k6*k9*k10*x6 + k1*k8*k9*k11*x6 + k1*k9*k10*k11*x6 + k8*k9*k11*k12*x9 + k1*k4*k6*k8*x6^2 + k1*k4*k8*k11*x6^2 + k1*k4*k5*k6*x6^2*x8 + k3*k4*k6*k8*x6*x7 + k1*k5*k6*k9*x6*x8 + k3*k4*k8*k11*x6*x7 + k4*k8*k11*k12*x6*x9$$

$$N_{py}(4) = k7*k9*k11*k12*x9 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*x7^2 + k1*k2*k4*k11*x6^2*x7 + k2*k3*k4*k11*x6*x7^2 + k1*k2*k6*k9*x6*x7 + k3*k4*k6*k7*x6*x7 + k1*k2*k9*k11*x6*x7 + k3*k4*k7*k11*x6*x7 + k4*k7*k11*k12*x6*x9 + k2*k9*k11*k12*x7*x9 + k2*k4*k11*k12*x6*x7*x9$$

$$N_{py}(5) = k3*k6*k7*k8*x7 + k3*k6*k7*k10*x7 + k3*k7*k8*k11*x7 + k3*k7*k10*k11*x7 + k7*k10*k11*k12*x9 + k2*k3*k6*k10*x7^2 + k2*k3*k10*k11*x7^2 + k2*k3*k5*k6*x7^2*x8 + k1*k2*k6*k10*x6*x7 + k3*k5*k6*k7*x7*x8 + k1*k2*k10*k11*x6*x7 + k2*k10*k11*k12*x7*x9$$

and

$$D_{py} = k6*k7*k8*k9 + k6*k7*k9*k10 + k7*k8*k9*k11 + k7*k9*k10*k11 + k1*k6*k8*k9*x6 + k3*k6*k7*k8*x7 + k4*k6*k7*k8*x6 + k1*k6*k9*k10*x6 + k3*k6*k7*k10*x7 + k2*k6*k9*k10*x7 + k1*k8*k9*k11*x6 + k5*k6*k7*k9*x8 + k3*k7*k8*k11*x7 + k4*k7*k8*k11*x6 + k1*k9*k10*k11*x6 + k3*k7*k10*k11*x7 + k2*k9*k10*k11*x7 + k7*k8*k9*k12*x9 + k7*k9*k10*k12*x9 + k7*k9*k11*k12*x9 + k7*k10*k11*k12*x9 + k8*k9*k11*k12*x9 + k1*k4*k6*k8*x6^2 + k2*k3*k6*k10*x7^2 + k1*k4*k8*k11*x6^2 + k2*k3*k10*k11*x7^2 + k1*k2*k4*k6*x6^2*x7 + k2*k3*k4*k6*x6*x7^2 + k1*k4*k5*k6*x6^2*x8 + k1*k2*k4*k11*x6^2*x7 + k2*k3*k5*k6*x7^2*x8 + k2*k3*k4*k11*x6*x7^2 + k1*k2*k6*k9*x6*x7 + k1*k2*k6*k10*x6*x7 + k3*k4*k6*k7*x6*x7 + k3*k4*k6*k8*x6*x7 + k1*k5*k6*k9*x6*x8 + k1*k2*k9*k11*x6*x7 + k3*k5*k6*k7*x7*x8 + k4*k5*k6*k7*x6*x8 + k1*k2*k10*k11*x6*x7 + k2*k5*k6*k9*x7*x8 + k3*k4*k7*k11*x6*x7 + k3*k4*k8*k11*x6*x7 + k4*k7*k8*k12*x6*x9 + k2*k9*k10*k12*x7*x9 + k4*k8*k11*k12*x6*x9 + k5*k7*k9*k12*x8*x9 + k2*k10*k11*k12*x7*x9 + k1*k2*k5*k9*x6*x7*x8 + k2*k4*k5*k6*x6*x7*x8 + k3*k4*k5*k7*x6*x7*x8 + k2*k4*k11*k12*x6*x7*x9 + k4*k5*k7*k12*x6*x8*x9 + k2*k5*k9*k12*x7*x8*x9 + k1*k2*k4*k5*x6^2*x7*x8 + k2*k3*k4*k5*x6*x7^2*x8 + k2*k4*k5*k12*x6*x7*x8*x9$$

Verify the two solutions are equal.

```
>> delta_x = simplify(xbar_ka-xbar_py)
```

$$\begin{aligned} \text{delta_x}(1) &= 0 \\ \text{delta_x}(2) &= 0 \\ \text{delta_x}(3) &= 0 \\ \text{delta_x}(4) &= 0 \\ \text{delta_x}(5) &= 0 \end{aligned}$$