Stoichiometric Networks

Simple Pathways

$$\frac{dS_i}{dt} = \sum_j c_{ij} v_j \tag{2.7}$$

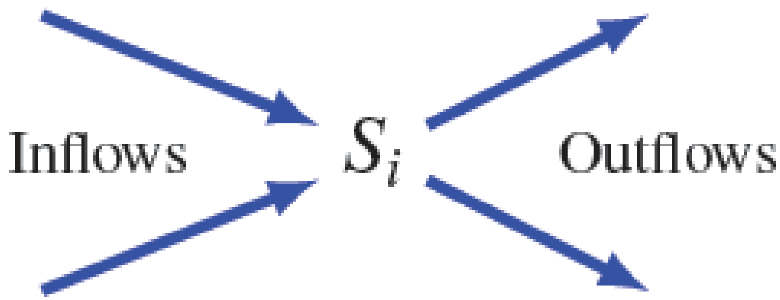
where c_{ij} is the stoichiometric coefficient for species i with respect to reaction, j.

For reactions that consume a species, the stoichiometric coefficient is often negative.

Simple Pathways

$$\xrightarrow{v_1} S \xrightarrow{v_2}$$

$$\frac{dS}{dt} = v_1 - v_2$$



$$dS_i/dt = \sum \text{Inflow} - \sum \text{Outflows}$$

Simple Pathways

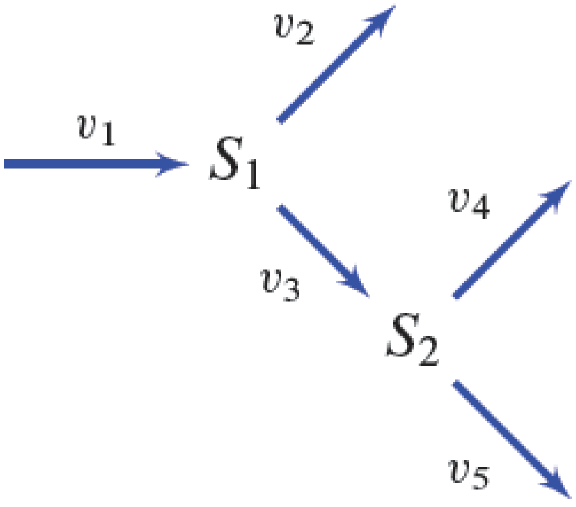
$$S_1 \xrightarrow{v_1} S_2 \xrightarrow{v_2} S_3 \xrightarrow{v_3} S_4 \xrightarrow{v_4} S_5$$

$$\frac{dS_1}{dt} = -v_1 \qquad \frac{dS_2}{dt} = v_1 - v_2$$

$$\frac{dS_3}{dt} = v_2 - v_3 \qquad \frac{dS_4}{dt} = v_3 - v_4$$

$$\frac{dS_5}{dt} = v_4$$

Branched Pathways



$$\frac{dS_1}{dt} = v_1 - v_2 - v_3$$

$$\frac{dS_2}{dt} = v_3 - v_4 - v_5$$

More Complex Pathways

Write out the mass-balance equations for the following networks:

$$
\begin{aligned}
A + X &\xrightarrow{v_1} 2X \\
X + Y &\xrightarrow{v_2} Z \\
Z &\xrightarrow{v_3} Y + B
\end{aligned}
$$

Stoichiometry Matrix

The stoichiometry matrix is a m row by n column matrix where m is the number of species and n the number of reactions:

$$\mathbf{N} = m \times n \text{ matrix}$$

$$\mathbf{N} = \begin{array}{cc} & v_j \\ S_i & \begin{bmatrix} c_{ij} & \cdots & \cdots \\ \vdots & & \\ \vdots & & \end{bmatrix} \end{array}$$

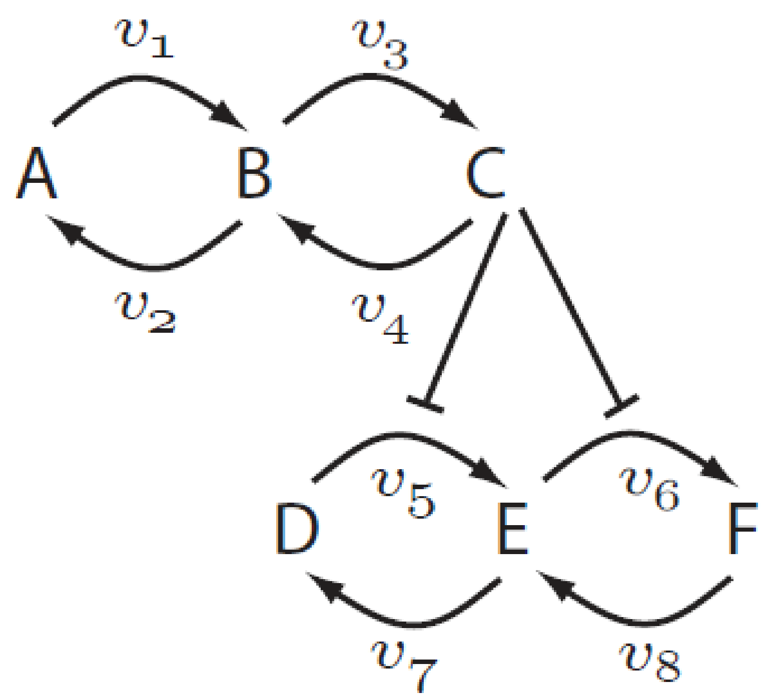
Stoichiometry Matrix

$$S_1 \xrightarrow{v_1} S_2 \xrightarrow{v_2} S_3 \xrightarrow{v_3} S_4 \xrightarrow{v_4} S_5$$

The stoichiometry matrix for this simple system is given by:

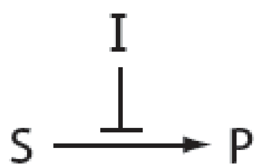
$$\mathbf{N} = \begin{array}{c} \begin{array}{cccc} v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{bmatrix} -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \begin{array}{c} \\ S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \end{array}$$

Stoichiometry Matrix

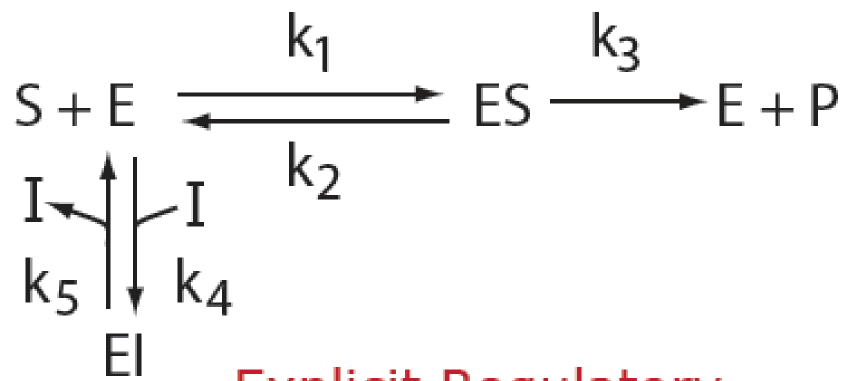


$$\mathbf{N} = \begin{array}{c} \\ A \\ B \\ C \\ D \\ E \\ F \end{array} \begin{array}{c} \begin{array}{cccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 \end{array} \\ \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \end{bmatrix} \end{array}$$

Explicit and Implicit Regulation



Implicit Regulatory Interaction

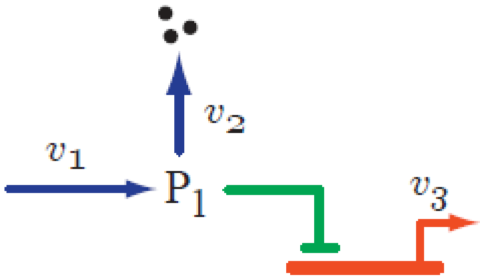


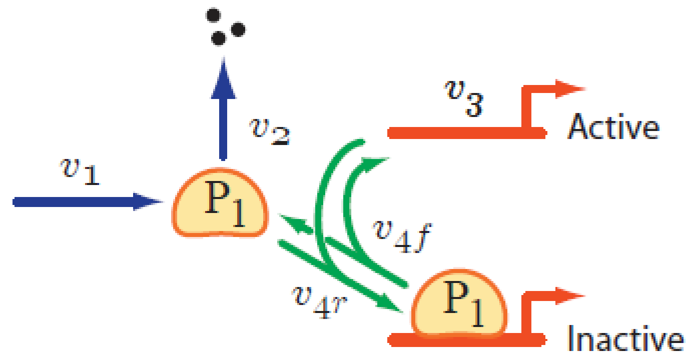
Explicit Regulatory Interaction

$$\mathbf{N} = \begin{array}{c} \\ S \\ P \\ I \end{array} \begin{array}{c} v_1 \\ \left[\begin{array}{r} -1 \\ 1 \\ 0 \end{array}\right] \end{array}$$

$$\mathbf{N} = \begin{array}{c} \\ S \\ P \\ I \\ ES \\ EI \end{array} \begin{array}{c} \begin{array}{ccccc} v_1 & v_2 & v_3 & v_4 & v_5 \end{array} \\ \left[\begin{array}{rrrrr} -1 & 1 & 0 & -1 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 1 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{array}\right] \end{array}$$

Explicit and Implicit Regulation





$$\mathbf{N} = \begin{array}{c} \\ P_1 \end{array} \begin{array}{cc} v_1 & v_2 \\ \left[\ 1 \right. & \left. -1\ \right] \end{array}$$

$$\mathbf{N} = \begin{array}{c} \\ P_1 \\ P_1(\text{Active}) \\ P_1(\text{InActive}) \end{array} \begin{array}{c} \begin{array}{cccc} v_1 & v_2 & v_{4r} & v_{4f} \end{array} \\ \left[\begin{array}{cccc} 1 & -1 & -1 & 1 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \end{array} \right] \end{array}$$

Stoichiometry Matrix

$$\frac{d\mathbf{s}}{dt} = \mathbf{N}\boldsymbol{v} \tag{2.12}$$

$$\frac{d\mathbf{s}}{dt} = \mathbf{N}\boldsymbol{v} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}$$

$$S_1 \xrightarrow{v_1} S_2 \xrightarrow{v_2} S_3 \xrightarrow{v_3} S_4 \xrightarrow{v_4} S_5$$

Stoichiometry Matrix

$$\frac{d\mathbf{s}}{dt} = \mathbf{N}\boldsymbol{v} \qquad (2.12)$$

Why bother?

1. Clean separation of structure from kinetics factors
2. Opens up a new field of structural analysis
3. Species conservation constraints (rows)
4. Flux constraints (columns)