

Algebra

- with n linear equations, and m < n unknowns, at most m values are needed to solve
  - [linear coefficients] x [unknowns] = [non-homogenous constants]
  - [n x m][m x 1] = [n x 1]

Calculus

- order of n order differential = order of n order system of 1st order differentials
  - n values required for n order differential to solve
  - n values required for n order system of 1st order differentials to solve

Mass Action

- general n order system of 1st order differentials

$$\frac{dx_i}{dt} = \sum_{j=1}^{a_i} b_{ij} \prod_{k=1}^{c_{ij}} x_{d_{ijk}}^{e_{ijk}} = \sum_{j=1}^{a_i} b_{ij} \prod_{k=1}^{g_{ij}} x_{d_{ijk}}^{f_{ijk}} = l_{ij}$$

$$x_{d_{ijk}} = \sum_{j=1}^{a_i} b_{ij} \prod_{k=1}^{g_{ij}} x_k^{f_{ijk}} = \sum_{j=1}^m b_{ij} \prod_{k=1}^n x_k^{f_{ijk}}$$

• parameters

- x is the species vector
- a is an amount of rates changing x
- b is a rate constant
- c is a number of different species involved
- d is a species involved
- e is a number of each species involved
- f is a number of species d involved
- g is a highest species involved
- l is a rate order
- m is the highest number of rates involved
- n is the number of species

• general rate equation

$$\sum_{i=1}^n r_{ij} = \sum_{l=0}^o \sum_{i=1}^n r_{lij} \leq o$$

$$\frac{dx_i}{dt} = \sum_{j=1}^m (p_{ij} - r_{ij}) c_j \prod_{k=1}^n x_k^{r_{kj}} = \sum_{l=0}^o \sum_{j=1}^m (p_{lij} - r_{lij}) c_{lj} \prod_{k=1}^n x_k^{r_{lkj}} = \sum_{l=0}^o \sum_{j=1}^m (p_{lij} - r_{lij}) c_{lj} \prod_{k=1}^n x_{h_{kj}}$$

$$\frac{dx}{dt} = \sum_{j=1}^m (P_j - R_j) c_j \prod_{k=1}^n x_k^{r_{kj}}$$

- x is the species vector
- m is the number of reactions
- p is a stoichiometric coefficient of the product
- r is a stoichiometric coefficient of the reactant
- c is a reaction rate constant
- n is the number of species
- h is a species involved
- P is the stoichiometric coefficient matrix for products
- R is the stoichiometric coefficient matrix for reactants

• simplifications

- simplified n order system of constant differential:

$$\frac{dx}{dt} = a$$

- x is a species vector
- a is a rate vector
- solution
- $x(t) = at + x(0)$
- calibration

$$a = (x(t) - x(0)) \frac{1}{t}$$

- simplified zero order rate equation

$$r_{ij} = 0$$

$$\frac{dx_i}{dt} = \sum_{j=1}^m p_{ij} c_j$$

$$\frac{dx}{dt} = Pc = a$$

- uses rate equation notation
- solution
- $x(t) = Pct + x(0)$
- calibration

$$c = P^{-1}(x(t) - x(0)) \frac{1}{t}$$

- simplified n order system of linear differential:

$$\frac{\partial}{\partial t} x = Ax + b$$

- x is a species vector
- A is a linear coefficient matrix
- b is a non-homogenous constant vector
- solution

$$x(t) = e^{At}(x(0) + A^{-1}b) - A^{-1}b$$

- steady state
- $x(\infty) = -A^{-1}b$

- stability
- $Ax = \lambda x$
- $\lambda < 0$

- optimization
- $\frac{dx(\infty)}{db} = -A^{-1} \neq 0$

$$\frac{dx(\infty)}{dA} = A^{-2}b = 0 = b$$

- calibration

$$A = -\ln((x(0)|^T - x(\infty)|^T)(X(t) - x(\infty)|^T)^{-1}) \frac{1}{t} = -\ln((X(0) - X(\infty))(X(t) - X(\infty))^{-1}) \frac{1}{t}$$

$$b = -AX(\infty) = \ln((x(0)|^T - x(\infty)|^T)(X(t) - x(\infty)|^T)^{-1}) \frac{x(\infty)}{t} = \ln((X(0) - X(\infty))(X(t) - X(\infty))^{-1}) \frac{x(\infty)}{t}$$

- X(t) is the matrix of measured data
- simplified 1st order rate equation

$$\sum_{i=1}^n r_{ij} = \sum_{l=0}^1 \sum_{i=1}^n r_{lij} \leq 1$$

$$\frac{dx_i}{dt} = \sum_{j=1}^m (p_{ij} - r_{ij}) c_j x_{h_j}^{r_{h_j i}} = \sum_{l=0}^1 \sum_{j=1}^m (p_{lij} - r_{lij}) c_l x_{h_j}^{r_{h_j i}} = \sum_{j=1}^m (p_{1ij} - r_{1ij}) c_1 x_{h_j} + \sum_{j=1}^m (p_{0ij} - r_{0ij}) c_0 = \sum_{l=0}^1 \sum_{j=1}^m (p_{lij} - r_{lij}) c_l \prod_{k=1}^l x_{h_k}$$

$$\frac{dx}{dt} = \sum_{j=1}^m (P_j - R_j) c_j x_{h_j}^{r_{h_j}}$$

• uses rate equation notation

• simplified n order system of quadratic differential:

$$\frac{dx_i}{dt} = x^T A_i x + b_i x + c_i$$

• x is the species vector

• A is a quadratic coefficient matrix

• b is a linear coefficient vector

• c is a non-homogenous constant

• simplified 2nd order rate equation

$$\sum_{i=1}^n r_{ij} = \sum_{l=0}^2 \sum_{i=1}^n r_{lij} \leq 2$$

$$\frac{dx_i}{dt} = \sum_{j=1}^m (p_{ij} - r_{ij}) c_j x_{h_j}^{r_{h_j i}} = \sum_{l=0}^2 \sum_{j=1}^m (p_{lij} - r_{lij}) c_l x_{h_{j1}}^{r_{h_{j1} i}} x_{h_{j2}}^{r_{h_{j2} i}} = \sum_{j=1}^m (p_{2ij} - r_{2ij}) c_2 x_{h_{j1}} x_{h_{j2}} + \sum_{j=1}^m (p_{1ij} - r_{1ij}) c_1 x_{h_{j1}} + \sum_{j=1}^m (p_{0ij} - r_{0ij}) c_0 = \sum_{l=0}^2 \sum_{j=1}^m (p_{lij} - r_{lij}) c_l \prod_{k=1}^l x_{h_k}$$

$$\frac{dx}{dt} = \sum_{j=1}^m (P_j - R_j) c_j x_{h_{j1}}^{r_{h_{j1}}} x_{h_{j2}}^{r_{h_{j2}}}$$

• uses rate equation notation