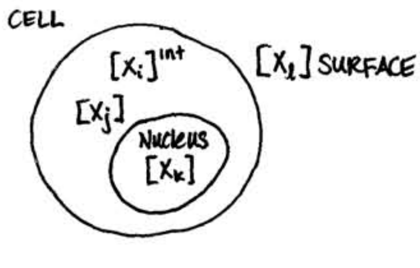
6.581/20.482

LECTURE 14: FORMULATING MODELS

TUESDAY 4 APRIL 2006

DIFFERENTIAL EQUATION MODEL



VERY GENERAL SETTING

$$\begin{bmatrix}[x_1]\\ \vdots \\ [x_N]\end{bmatrix} = \overset{\text{unknown}}{\vec{X}} \qquad \vec{u} = \begin{bmatrix}[u_1]\\ \vdots \\ [u_K]\end{bmatrix}$$

time-variation of concentrations

$$\frac{d}{dt}[x_i] = \underbrace{V^+(\vec{X},\vec{u})}_{\text{rate of production}} - \underbrace{V^-(\vec{X},\vec{u})}_{\text{rate of consumption}}$$

Ex: $A+B \underset{K_2}{\overset{K_1}{\rightleftharpoons}} C$

$$\frac{d}{dt}[C] = K_1[A][B] - K_2[C]$$
$$\frac{d}{dt}[A] = K_2[C] - K_1[A][B]$$
$$\frac{d}{dt}[B] = K_2[C] - K_1[A][B]$$

+ Initial conditions $A(0), B(0), C(0)$

Ex: Dimerization

$A \underset{K_2}{\overset{K_1}{\rightleftharpoons}} A_2$

$$\frac{d}{dt}[A_2] = K_1[A][A] - K_2[A_2]$$
$$\frac{d}{dt}[A] = 2K_2[A_2] - 2K_1[A][A]$$

STEADY-STATE (Equilibrium)

Reactions are in balance

$$\frac{d}{dt}[x_i] = 0$$

continuum approximation b/c molecules are reacting, but overall the net rate is balanced

$\Downarrow$

Lots of copies of x

Dimerization case:

$$K_1[A][A] = K_2[A_2]$$
$$[A]^2 = \frac{K_2}{K_1}[A_2]$$
$$[A] = \sqrt{\frac{K_2}{K_1}}[A_2]^{1/2}$$

Also given:

$A(0)=A_0 \quad A_2(0)=0$

$\rightarrow$ intial conditions

Steady-state:

$$[A] + 2[A_2] = A_0$$

CHEMICAL KINETICS FORM

$$\frac{d}{dt}[x_i] = \sum_{j=1}^{N} \gamma_j^i [x_j]$$

destination, source

(Typical Case $\gamma_i^i < 0$ degradation process)

$$\frac{d}{dt}[x_i] = \sum_{j=1}^{N} \gamma_j^i [x_j] + \sum_{j=1}^{N}\sum_{k=1}^{N} \gamma_{j,k}^i [x_j][x_k]$$

(Typical Consumption Process $\gamma_{i,k}^i < 0$
Typical Production Process $\gamma_{j,k}^i > 0$)

$$\frac{d}{dt}[x_i] = \sum_{j=1}^{N} \gamma_j^i [x_j] + \sum_{j=1}^{N}\sum_{k=1}^{N} \gamma_{j,k}^i [x_j][x_k] + \sum_{j=1}^{M} \alpha_j^i [u_j] + \sum_{j=1}^{M}\sum_{k=1}^{N} \alpha_{j,k}^i [u_j][x_k]$$
$$\underbrace{+ \sum_{j=1}^{M}\sum_{k=1}^{M} \beta_{j,k}^i [u_j][u_k]}_{\text{MULTIPLE INPUTS}}$$

$\gamma_i^i < 0 \Rightarrow$ models degradation

$\gamma_j^i \neq 0 \Rightarrow$ models conversion $\quad x_i \underset{\gamma_j^i}{\overset{\gamma_i^j}{\rightleftharpoons}} x_j$

$\gamma_{j,k}^i \quad x_j + x_k \underset{\gamma_i^j \ \gamma_i^k}{\overset{\gamma_{j,k}^i}{\rightleftharpoons}} x_i$

unnecessary for following proof

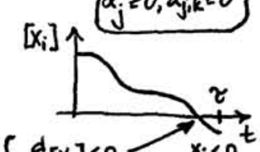
If $[x_i]$ is involved only in reactions that consume $[x_i] \Rightarrow \gamma_i^i \le 0, \gamma_{i,k}^i \le 0, \alpha_{j,i}^i \le 0$

and reactions that consume $[x_i]$ Must include $[x_i] \Rightarrow$ $\boxed{j,k \neq i \quad \gamma_j^i \ge 0, \gamma_{j,k}^i \ge 0 \quad \alpha_j^i \ge 0, \alpha_{j,k}^i \ge 0}$

$[x_i] \ge 0$ at $t=0$

Then All $[x_i]$'s ≥ 0 for all t

PROOF: Suppose $[x_i] < 0$ for some i at some t



CONTRADICTION $\left\{ \frac{d}{dt}[x_i] < 0 \text{ when } [x_i] = 0 \right.$

$$\frac{d}{dt}\vec{X} = \underbrace{A^{(1)}\vec{X}}_{\text{terms}} + A^{(2)} \begin{bmatrix} [X_1][X_1] \\ [X_1][X_2] \\ \vdots \\ [X_1][X_N] \\ [X_2][X_1] \\ [X_2][X_2] \\ \vdots \\ [X_2][X_N] \\ [X_3][X_1] \\ \vdots \\ [X_N][X_N] \end{bmatrix}$$

terms appear twice ... not a big deal

N^2 terms

$$\vec{X} = \begin{bmatrix} [X_1] \\ \vdots \\ [X_N] \end{bmatrix}$$

terms

$$\sum \gamma^i_j [X_j]$$

$$\Rightarrow A^{(1)}_{ij} = \gamma^i_j$$

$$A^{(2)} \quad N \times N^2$$

$$\Rightarrow A^{(2)}_{ij} = \underbrace{\boxed{\;\;}}_{[(j-1)n+k+1]} \gamma^i_{j,k}$$

KROENEKER PRODUCT:

$$\vec{X} \otimes \vec{X} = \begin{bmatrix} x_1\vec{X} \\ x_2\vec{X} \\ x_3\vec{X} \\ \vdots \\ x_N\vec{X} \end{bmatrix}$$

$$\frac{d}{dt}\vec{X} = A^{(1)}\vec{X} + A^{(2)}\vec{X}\otimes\vec{X} + B\vec{u} + C\underbrace{\vec{u}\otimes\vec{X}} + D\,\vec{u}\otimes\vec{u}$$

$$\Downarrow$$

$$\begin{bmatrix} u_1\vec{X} \\ u_2\vec{X} \\ \vdots \\ u_M\vec{X} \end{bmatrix} = \begin{bmatrix} [u_1][X_1] \\ [u_1][X_2] \\ \vdots \\ [u_1][X_N] \\ [u_2][X_1] \\ \vdots \\ [u_M][X_M] \end{bmatrix}$$