10.37 Chemical and Biological Reaction Engineering, Spring 2007
Prof. William H. Green
Lecture 1: Preliminaries & Remembrance of Things Past

This lecture covers: reaction stoichiometry, lumped stoichiometries in complex systems such as bioconversions and cell growth (yields), extent of reaction, independence of reactions, measures of concentrations, single reactions and reaction networks, and bioreaction pathways.

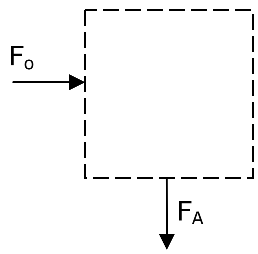

Figure 1. A schematic of a control volume with inflow of F_o and outflow of species A, F_A.

F = total molar flow rate (moles/sec)
F_o = total molar flow rate entering control volume
F_A = molar flow rate of species A
F_{Ao} = molar flow rate of species A entering control volume
N_A = Moles of species A

Mass balance: (change in "A" inside control volume)= (amount of "A" that entered)-(amount of "A" that exited) + (amount of "A" created inside the control volume) – (amount of "A" destroyed inside the control volume)

$$\frac{dN_A}{dt} = F_{Ao} - F_A + G_A$$

$$G_A [=] \frac{\text{moles}}{\text{sec}}$$

$$\text{If homogeneous, } G_A = r_A V$$

$$\text{else, } G_A = \int r_A dV$$

where V is volume and r_A is the rate of A created or destroyed (moles/sec/volume).

The mass balance can also be written as:

$$\frac{d\rho_A}{dt} = \overbrace{v\nabla\rho_A}^{\text{convection}} + \overbrace{D\nabla^2\rho_A}^{\text{diffusion}} + r_A$$

where v is velocity, D is the diffusion coefficient, and ρ_A is the molar density of A (moles/volume).

Example:

A+B→C+D

$$r_A = -k[A][B],\ \ r_C = +k[A][B],\ \ [A][=]\frac{\text{mole A}}{\text{liter}}$$

where k is a measurable rate constant that changes with respect to T and P but remains constant with respect to changing concentrations.

If $r_1 = k[A][B]$, then

$$r_A = \overbrace{\nu_{A,1}}^{=-1} r_1$$

where $\nu_{A,1}$ is the stoichiometric coefficient for species A in reaction 1. Likewise,

$$r_C = \overbrace{\nu_{C,1}}^{=+1} r_1$$

If there are n reactions involving species "A" then

$$r_A = \sum_{i=1}^{n} \nu_{A,i} r_i$$

$$G_A(t) = \iiint_{Vol.} \underbrace{r_A(x,y,z,t)}_{-k(T(x,y,z,t))[A(x,y,z,t)][B(x,y,z,t)]} dxdydz$$

$$\frac{d\overbrace{[A]}^{N_A/V}}{dt} = -k[A][B] \rightarrow \text{*only true if there are no flows!}$$

$$\frac{dN_A}{dt} = \int r_A dV \approx r_A V,\ \text{assume } r_A \text{ is true throughout volume}$$

If the system is homogeneous and there are no flows:

$$\frac{dN_A}{dt} = r_A V$$

Therefore:

$$\frac{d}{dt}\left(\frac{N_A}{V}\right) = r_A\ \ \text{iff homogeneous, no flow, constant V}$$

Extent of Reaction

$$\xi[=]\text{moles, extent of rxn.}$$

$$\dot{\xi}[=]\frac{\text{moles}}{\text{sec}}, \text{ rate of extent of rxn.}$$

$$A + B \rightarrow C + D$$

$N_A = N_{A,\text{initially}} - \xi$, if there is one reaction involving A

$N_A = N_{A,\text{initially}} - \sum_n \nu_{A,n}\xi_n$, if there are several reactions

$\dot{\xi}_n = \int r_n dV$, n is the reaction number

$G_A = \int r_A dV$, A is the species

Conversion

$A + B \rightarrow C + D$

$X_A = \frac{N_{A,\text{initial}} - N_A}{N_{A,\text{initial}}}$ (dimensionless)

$X_C = \frac{N_C}{N_{A,\text{initial}}}$ (≈ 1 since rxn is 1:1)

$\begin{pmatrix} A + B \rightarrow C + D \\ A \rightarrow U \end{pmatrix}$ Selectivity is good if $A \rightarrow C$, bad if $A \rightarrow U$.

*May worsen as rxn. goes on ($A \rightarrow C$ slows, $A \rightarrow U$ keeps going)