CME 550 Fall 2005

Review for Exam 1

Reading: Levenspiel Chapters 1-3. You may use one 8.5" x 11" sheet of notes + calculator.

Definitions

Homogeneous / heterogeneous reaction

Catalyzed or uncatalyzed reaction

r, r', r'', r''', r'''' (moles of species formed per time per some reactor quantity)

Chemical Kinetics

One of main influences on rate is species concentration

If rate is power law, power is order with respect to species or overall $-r_A = kC_A^{\alpha}C_B^{\beta}$

Stoichiometry used to relate moles produced / consumed

Elementary reactions: order = stiochiometry

Units of rate coefficient for any order (should be able to relate the two)

Other main influence: temperature through Arrhenius law

$k = k_0e^{-E/(RT)}$ (What is the linearized form of this equation used to get E?)

Thermodynamics

Definition of ΔH_{Rxn}

Definition and use of equilibrium coefficient (K_C) and ΔG_{Rxn}

Thermodynamically, what does "irreversible" mean?

Reaction mechanisms

Pseudo-steady state approximation for reactive intermediates

Quasi-equilibrium assumption for fast reversible reactions

Reactions with changing order, such as Michaelis-Menten kinetics

Batch Reactors and Treatment of Batch Reactor Data (All isothermal for now!)

Constant volume batch reactor: $r_A = dC_A/dt$

Conversion of species A: $X_A = (N_{A0}-N_A)/N_{A0}$

Using stoichiometry to express all concentrations in terms of X_A

Dependence of P on X_A for reaction with changing number of moles

Differential method of analysis

For power law plot $\ln(-r_A)$ vs. $\ln(C_A)$ (slope = order, intercept = $\ln(k)$)

Other rate expressions require other linearized forms (e.g. $1/r_A$ vs. $1/C_A$)

Method of initial rates

Getting order with respect to one species: use large concentration of other

If $C_B >> C_A$, $-r_A = kC_A{}^{\alpha} C_B{}^{\beta} \cong k' C_A{}^{\alpha}$

Integral method of analysis

$$-r_A = -\frac{dC_A}{dt} = f(C_A) \Rightarrow \int_{C_{A0}}^{C_A} \frac{dC_A}{f(C_A)} = -\int_0^t dt \text{ (Or equivalent in terms of } X_A\text{)}$$

First order C_A decays exponentially, 2^{nd} order $1/C_A$ is proportional to *t*, others…

Half lives

Half life constant for 1^{st} order, otherwise, $t_{1/2} = \frac{(1/2)^{(1-n)} - 1}{k(n-1)} C_{A0}{}^{(1-n)}$

If order known, can get rate coefficient from half life

Multiple reactions

Parallel reactions (just add together rate constants if orders are same)

Homogeneous catalyzed reaction (parallel rxns. w/ constant [C])

Autocatalytic

Series reactions (intermediate goes through maximum)

Reversible first order (exponential but final state is equilibrium)

Variable volume

$\varepsilon_A = [V(X_A{=}1) - V(X_A{=}0)]/ V(X_A{=}0)$

$V = V_0(1+ \varepsilon_A X_A)$ and $C_A = C_{A0}(1-X_A)/(1+ \varepsilon_A X_A)$

Go back to definition of rate!! $(1/V)dN_A/dt$

Differential method based on volume evolution

Integral equations in terms of conversion or volume