**Heterogeneous Catalytic Reactions**

Examples: digesting food, burning carbon/coal, cellular respiration

Burning coal: reaction occurs on surface, solid phase, heterogeneous system

Digesting food: in stomach, enzymes

C + O2 --> CO2

Solid + Gas --> Gas

Concentration gradient (diffusion; Fick’s Law)

Bulk/Convection Flow

Involves two phases (solid/gas)

Modeling reaction kinetics, must think about mass transport between two phases

In reality, in biological systems, reactions happen in multiple phases

Must model heterogeneous reactions

Reactions only happen when reactants are in contact with catalysts

Reactions only occur at surface

What governs the rate of reaction in heterogeneous systems?

* Surface area
* Diffusion of the reactants
* Phases
* Flow behavior
* Reaction mechanism kinetics

Need to determine how much is moving toward the surface via diffusion/bulk flow.

Mass flow/Time\*area = flux

1. Bulk flow: q\*C/A = volumetric flow rate \* concentration / area = u\*C
2. Diffusion: Fick’s Law: -D dC/dx

In biological systems, most reactions do not occur in bulk solutions (homogeneous reactions)

We must model mass transport and reactions

Derivation of transport equations

1. Conservation principles (first law)
   * In - out = accumulation
   * In = Out + accumulation + reaction
   * In - Out = Reaction + Accumulation
     + Assume no reactions
   * In - Out = Accumulation
     + In a general case: accumulation = Volume\*dC/dt
     + Combine with flux
   * (Flux)Area|in - (Flux)Area|out = V\*dC/dt
   * (V\*C - DdC/dz)\*A|z - (V\*C - DdC/dz)\*A|z+∆z = A\*∆z\*dC/dt
   * [(DdC/dz)|z+∆z - (DdC/dz)|z]/∆z - [(V\*C)|z+∆z - (V\*C)|z]/∆z= dC/dt
     + ∆z-->0
   * Dd2C/dz2 - d(V\*C)/dz = dC/dt
     + Mass density (ρ)
     + C = mol/L3, ρ = mass/L3
   * Dd2ρ/dz2 - d(V\*ρ)/dz = dρ/dt
     + D = 0
   * - d(V\*C)/dz = dC/dt or d(V\*ρ)/dz + dρ/dt = 0
     + Continuity equation
     + v = 0
   * Dd2C/dz2 = dC/dt
     + Fick’s second law
   * What if there is a reaction?
     + Assume accumulation = 0
     + (Flux)Area|in - (Flux)Area|out = -rV\*f(C)
       - (V\*C - DdC/dz)\*A|z - (V\*C - DdC/dz)\*A|z+∆z = A\*∆z\*f(C)
       - [(DdC/dz)|z+∆z - (DdC/dz)|z]/∆z - [(V\*C)|z+∆z - (V\*C)|z]/∆z= f(C)
       - Dd2C/dz2 - d(V\*C)/dz = f(C)
2. Transport principles for mass, energy system

Bulk flow (mass) q/A \* C = v\*C

Starting from first principles, derive differential equation