Pores - reaction at walls

In - Out = Rxn

Homogeneous: -r = -1/V dNA/dt

Heterogeneous: -r = -1/S dNA/dt

-rA’’ = -1S dNA/dt = k’’CA

-r = kCA

k \* V = k’’ \* S

k \* πr2L = k’’ \* 2πrL

k = 2k’’/r

πr2(-D dC/dx)in - πr2(-D dC/dx)out = 2πrΔxk’’CA

Δx --> 0

d2CA/dx - 2k’’/Dr CA = 0

d2CA/dx - k/D CA = 0; m2 = k/D

d2CA/dx - m2CA = 0

CA = M1emx + M2e-mx

Boundary conditions:

X = 0: CA = CAg

X = L: dCA/dx = 0

M1 = CAse-mL/(emL+e-mL)

M2 = CAs emL/(emL+e-mL)

CA/CAs = (em(L-x)+ e-m(L-x))/(emL + e-mL)

CA/CAs = cosh(m(L-x))/cosh(mL)

Concentration when moving into the pore decreases

Profile depends on mL

MT = mL (Thiele modulus)

< 0.4, CA ~ CAs diffuses faster than reacts or short pore with slow reaction, not much diffusion resistance

Effectiveness factor: ξ = Actual Reaction Rate/Full Reaction Rate

MT < 0.4, ξ = 1

MT > 4, ξ = 1/MT

ξ = CA,average/CAs = ∫CAdx/L\*CAs = tanh(mL)/mL

Proper Measure of Particle Size: MT = L\*sqrt(k/D)

L = volume of particle/exterior surface available for reactant penetration)

Flat plate: L = AL/2A = L/2

Cylinder: L = πR2L/2πRL = R/2

Sphere: L = 4/3πR3/4πR2 = R/3

Reaction Rate effectiveness factor changes depending on geometry

Knowing MT, determine ξ (graph), then determine reaction rate ξkCA