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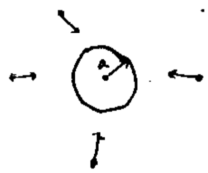
Course 565/665 Lecture Number ______ Date 4/24/03

Lecturer Dr. Silvia Covagnero Note Taker Eric Fulmer

Diffusion - Controlled Reactions



$$\left(\frac{\partial c}{\partial t}\right)_{x,y,z} = D\,\nabla^2 c = 0$$

Steady State Conditions.

Let the sphere with radius a be called the "absorbing sphere."

$$0 = \frac{1}{r}\frac{d^2(rc)}{dr^2} \qquad \text{(spherical coordinates).}$$

$$0 = \frac{d\,rc}{dr} + A_1$$

$$= rc + A_1' r + A_2'$$

$$c = A_1 + \frac{A_2}{r} \qquad \text{where } \begin{array}{l} A_1 = -A_1' \\ A_2 = -A_2' \end{array}$$

Boundary Conditions

$r = \infty$, $c = c_\infty$

$r = a$, $c = 0$

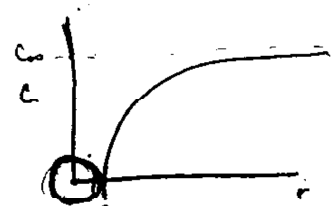
bulk concentration $= c_\infty$

$$c_\infty = A_1 + \frac{A_2}{\infty} = A_1$$

$$0 = c_\infty + \frac{A_2}{a}$$

$$A_2 = -c_\infty a$$

$$\boxed{c(r,t) = c_\infty\left(1 - \frac{a}{r}\right)}$$



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I_a = number of collisions of the small molecules with the sphere per second.

$I_a = J_a \, 4\pi a^2 = -4\pi D c_\infty a$ # collisions/second.

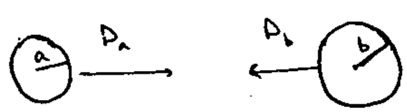
This ~~diffusion controlled~~ collision rate corresponds to the fastest possible reaction.

$I_a = -k_a c_\infty$ $k_a = 4\pi D a$

$$\boxed{k_a = 4\pi D a}$$

<u>In General</u>.

2 molecules of radius r_A and r_b colliding and reacting as soon as they collide:



$I_a = -4\pi (D_A + D_b) \, c_\infty \, (r_A + r_B) \, N_A$ # molecules colliding.

$k_a = 4\pi (D_a + D_b)(r_a + r_b) N_A$ The N_A is strange.

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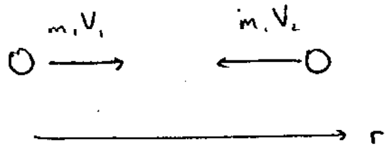
<u>Many Colliding Particles</u>



More complex forces (other than the purely diffusive forces) are present in solution, f_c.

$f_c = 6\pi\eta a$ for spherical particles of radius a.

$$D = \frac{kT}{6\pi\eta a}$$ Stokes-Einstein Equation

Diffusion by Brownian Motion (Random Diffusion)

$\langle x^2 \rangle = 2Dt$ <u>1D</u>

$\langle r^2 \rangle = 4Dt$ <u>2D</u>

$\langle r^2 \rangle = 6Dt$ <u>3D</u>