Similarity of mass, momentum, and heat transport laws

(Empirical laws)

Fick's first law : diffusion of mass

$$J_{ix} = -D \frac{\partial C_i}{\partial x} \qquad J: [ML^{-2}\ T^{-1}] \qquad D : [L^2T^{-1}]$$

Newton's law : dissipation of momentum (force) through fluid viscosity

$$\tau_{yx} = -\mu \frac{\partial \ _x}{\partial y} \qquad \tau_{yx} : [ML^{-1}\ T^{-2}]$$

fluid shear

$$= -\frac{\mu}{\varrho}\frac{\partial\ \varrho u_x)}{\partial y} \qquad \upsilon = \frac{\mu}{\varrho}[L^2T^{-1}]$$

kinematic viscosity

Fourier's law : heat conduction

$$q_x = -\kappa \frac{\partial T}{\partial x} \qquad q : [\mathrm{cal}\ M^{-1}T^{-1}]$$

$$= \frac{-\kappa}{C_P\varrho}\frac{\partial\ TC_P\varrho)}{\partial x} \qquad \alpha \quad \frac{\kappa}{C_P\varrho}[L^2T^{-1}]$$

thermal diffusivity

Table 4.1

Diffusion coeff	order of magnitude Air	 Water	
υ_j	0.2	0.01	(momentum)
α	0.2	1.5×10^{-3}	(heat)
D_{ij}	0.2	10^{-5}	(diffusion)

why equal? why different?

$$Sc = \frac{\text{momentum diffusivity}}{\text{chemical diffusivity}} = \frac{\upsilon}{D} \qquad \text{Schmidt number}$$

$$Pr = \frac{\text{momentum diffusivity}}{\text{thermal diffusivity}} = \frac{\upsilon}{\alpha} \qquad \text{Prandtl number}$$

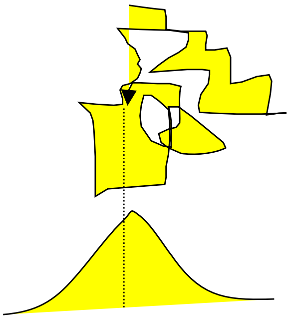
for air (or low pressure gaseous systems) $Pr \approx \ \approx$

Principle of Diffusion : random molecular motion

→ complete mixing in a confined space

thermally induced fluctuation

translational kinetic energy = 3/2 κ ˋ = 1/2 mU



probability of a displacement
between x and x dx after n random
steps of length is given by
the Gaussian distribution

$$P(x\ \,)\qquad \pi \qquad e^{-x/2nl}\,dx$$

n=kt

$$C = Co\ \ P(x\ \ t)$$

This is the solution of one-dimensional diffusion eqn

$$\frac{\partial}{\partial} = D\,\frac{\partial^2 c}{\partial x^2}$$

$$C = Co\,\frac{1}{2\ \ \pi\ \ t}\,e^{-x\ \ Dt}$$

in gases diffusion progress about 10 cm min
liquid 0.05 cm min
solid 0.00001 cm min

Diffusion : random molecular motion (Brownian motion)

→ complete mixing

slowest step in the sequence

compared to convective flow, reaction, mixing(stirring)

wind 100 m/min

but determine the efficiency of a unit operation

mixing ~ hydrodynamic movement
diffusion ~ molecular movement

$$\text{flux} = \frac{\text{amount transported}}{\text{(time) (area)}}$$

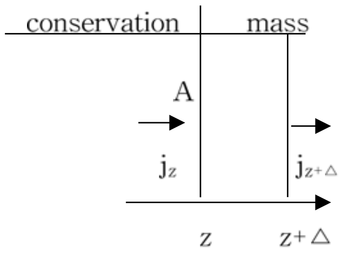
Fick's second law (conservation of mass)

Fick's first law

total flux $J = Aj = AD\frac{\partial}{\partial}$

one-dimensional diffusion equation (empirical equation)

why $\frac{\partial}{\partial} > 0,\ j_1 < 0$



$$\frac{\partial}{\partial} \underbrace{A \cdot \triangle}_{\text{volume}} = (j_z - j_{z+\triangle})\, A$$

$$\frac{\partial}{\partial} = -\frac{j_{z+\triangle} - j_z}{\triangle}$$

$$= -\frac{\partial}{\partial}$$

$$\frac{\partial}{\partial} = +D\frac{\partial^2 c}{\partial^{\ 2}}$$

: one-dimensional Fick's second law

3-dimensional or vector form of Fick's law

$$j = -D\nabla \qquad j = -D\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial} + \frac{\partial}{\partial}\right)$$

$$\frac{\partial}{\partial} = +D\nabla^2 C \qquad \frac{\partial}{\partial} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial^{\ 2}} + \frac{\partial^2 c}{\partial^{\ 2}}\right)$$

case 1. A is not constant $\quad \frac{\partial}{\partial} = D\left(\frac{\partial^2 c}{\partial^{\ 2}} + \frac{1}{A}\frac{2A}{\partial}\frac{\partial^2 c}{\partial}\right)$

case 2. D is directional $\quad \frac{\partial}{\partial} = D_x\frac{\partial^2 c}{\partial x^2} + D_y\frac{\partial^2 c}{\partial^{\ 2}} + D_z\frac{\partial^2 c}{\partial^{\ 2}}$

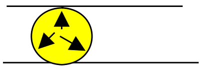
general (constitutive) transport equation $\qquad$ for constant D

$$\frac{\partial}{\partial} = -(u \cdot \nabla \quad - \nabla \cdot (-D\nabla \quad + Rc \Rightarrow \frac{\partial}{\partial} + u \cdot \nabla \quad - D\nabla^2 c - Rc = 0$$

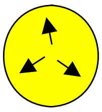
coordinates of Fick's law

$$j_1 = -D\frac{d}{d}$$ one-dimensional cartesian coordinate

$$j_1 = -D\frac{d_{\;1}}{d}$$ radial direction in cylindrical coordinate



$$j_1 = -D\frac{d_{\;1}}{d}$$ radial direction in spherical coordinate

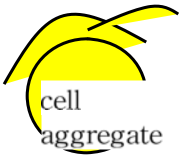


2nd law is different for each coordinate

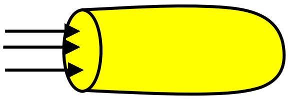
$$\frac{\partial}{\partial} = D\frac{1}{r}\frac{\partial}{\partial}\left(r\frac{\partial}{\partial}\right)$$ cylindrical

$$\frac{\partial}{\partial} = D\frac{1}{r}\frac{\partial}{\partial}\left(r\frac{\partial}{\partial}\right)$$ spherical

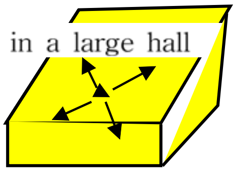
*** coordinate is not determined by the geometry itself.**



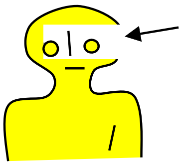
analysis of thin layer → can be simplified to one-dimensional cartesian coordinate



transport in a capillary tube → 〃 〃



diffusion from a point source in a large room → cartesian or spherical coordinate

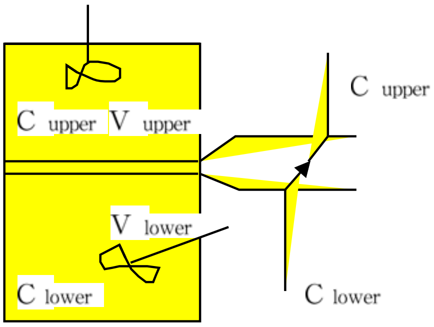


acid rain very slow diffusion → one dimensional cartesian

Diffusion Coefficient

Air-CO_2	0.142 ㎠ sec	at 276.2 K
Air-benzene	0.096 ㎠ sec	at 298 K
O_2 in water	2.10×10^{-5} ㎠ sec	at 298 K
Cl_2 in water	1.25×10^{-5} ㎠ sec	ar 298 K

Experimental Determination of Diffusion Coefficient

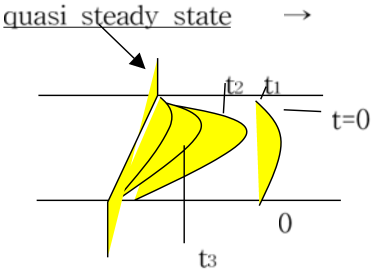


$$j = \frac{DH}{\ell}(C_{lower} - C_{upper})$$

rate of decease in the lower compartment $V_{lower}\frac{dC_{lower}}{d} = -Aj$, $\frac{dC_{lower}}{d} = -\frac{A}{V_{lower}} j$ ①

rate of increase in the upper compartment $V_{upper}\frac{dC_{upper}}{d} = Aj$, $\frac{dC_{upper}}{d} = \frac{A}{V_{upper}} j$ ②

Assume quasi steady state → $j = \frac{DH}{\ell}(C_{lower} - C_{upper})$



for a thin layer

① ②

$$\frac{d}{d}(C_{lower} - C_{upper}) = -\left(\frac{A}{V_{lower}} + \frac{A}{V_{upper}}\right)\frac{DH}{\ell}(C_{lower} - C_{upper})$$

$y \equiv C_{lower} - C_{upper}$ $\beta \left(\frac{A}{V_{lower}} + \frac{A}{V_{upper}}\right)\frac{DH}{\ell}$

initial concentration

$\frac{d}{d} = -\beta$ at t=0 $y = C_{\circ\ lower} - C_{\circ\ upper} = y^{\circ}$

$$y = y^{\circ}e^{-\beta}$$

$$\frac{C_{lower} - C_{upper}}{C_{\circ\ lower} - C_{\circ\ upper}} = e^{-\beta}$$

experimental data (unsteady state)
→ data regression
→ β → D

H : distribution coefficient
H ~ 1 preferred (chemically inert membrane-separator)

General transport equations for various coordinates

Table 3.4-2. *Mass balance for species 1 combined with Fick's law*

Rectangular coordinates

$$\frac{\partial c_1}{\partial t} + v_x^0 \frac{\partial c_1}{\partial x} + v_y^0 \frac{\partial c_1}{\partial y} + v_z^0 \frac{\partial c_1}{\partial z} = D \left(\frac{\partial^2 c_1}{\partial x^2} + \frac{\partial^2 c_1}{\partial y^2} + \frac{\partial^2 c_1}{\partial z^2} \right) + r_1 \tag{A}$$

Cylindrical coordinates

$$\frac{\partial c_1}{\partial t} + v_r^0 \frac{\partial c_1}{\partial r} + \frac{v_\theta^0}{r} \frac{\partial c_1}{\partial \theta} + v_z^0 \frac{\partial c_1}{\partial z} = D \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c_1}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 c_1}{\partial \theta^2} + \frac{\partial^2 c_1}{\partial z^2} \right] + r_1 \tag{B}$$

Spherical coordinates

$$\frac{\partial c_1}{\partial t} + v_r^0 \frac{\partial c_1}{\partial r} + v_\theta^0 \frac{\partial c_1}{\partial \theta} + \frac{v_\theta^0}{r \sin\theta} \frac{\partial c_1}{\partial \phi}$$

$$= D \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_1}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial c_1}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 c_1}{\partial \phi^2} \right] + r_1 \tag{C}$$

Note: The diffusion coefficient D and the density ρ are assumed constant. In this case, the mass average and volume average velocities are equal. Again, r_1 is the rate of production of species 1 per volume.

Table 3.4-3. *Total mass balance in several coordinate systems*

Rectangular coordinates

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}(\rho v_x) - \frac{\partial}{\partial y}(\rho v_y) - \frac{\partial}{\partial z}(\rho v_z) \tag{A}$$

Cylindrical coordinates

$$\frac{\partial \rho}{\partial t} = -\frac{1}{r} \frac{\partial}{\partial r}(\rho r v_r) - \frac{1}{r} \frac{\partial}{\partial \theta}(\rho v_\theta) - \frac{\partial}{\partial z}(\rho v_z) \tag{B}$$

Spherical coordinates

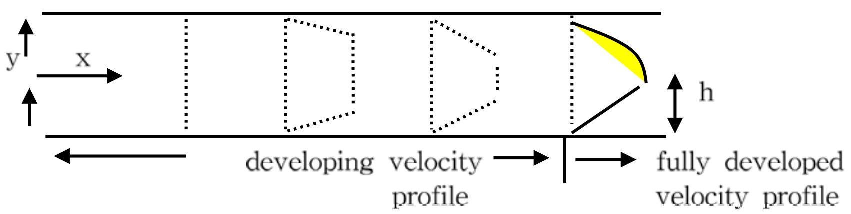
$$\frac{\partial \rho}{\partial t} = -\frac{1}{r^2} \frac{\partial}{\partial r}(\rho r^2 v_r) - \frac{1}{r \sin\theta} \frac{\partial}{\partial \theta}(\rho v_\theta \sin\theta) - \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi}(\rho v_\phi) \tag{C}$$

Note: The velocity here is the mass average and not the volume average commonly used with Fick's law.

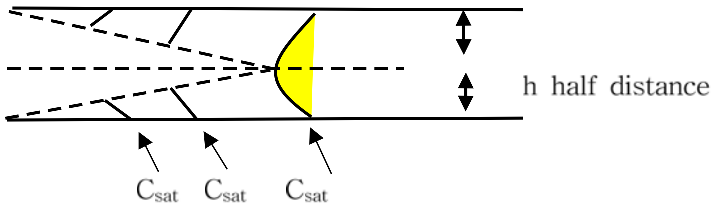
General Transport Equations and Their Applications

Two Case Studies on Analytical Solutions of Partial Differential Equations in Mass Transfer using Similarity Variables

Case 1 Mass transfer in a channel flow
flow development in a channel



development of concentration profile in a channel with slightly soluble walls (no change in gap)



" Concentration profile in a fully developed flow"
velocity profile for a fully developed flow

Navier Stokes eqn

$$\rho \frac{Du}{Dt} = \mu \nabla^2 u - \nabla \quad + \rho g \qquad (4\text{-}17)$$

steady state Du/Dt = 0
No gravity $\rho g = 0$
△ is the only driving force

$$\nabla^2 u = \triangle \ /\mu \qquad (1)$$

$$d^2u/dy^2 = \triangle \ /\mu \qquad \text{BC I} \quad y=0 \quad du/dy=0 \qquad (2)$$
$$\text{II} \quad y=h \quad u=0$$

$$\frac{du}{dy} = \frac{\triangle}{\mu} y + C_1 \qquad \text{BC I. } 0=C_1 \qquad (3)$$

$$u = \frac{\triangle}{2\mu} y^2 + \cancel{C_1 y} + C_2 \qquad \text{BC II} \qquad 0 = \frac{\triangle}{2\mu} h^2 + C_2 \qquad (4)$$

$$u = -\frac{\triangle}{2\mu}(h^2 - y^2 \qquad C_2 = \frac{\triangle}{2\mu} h^2 \tag{5}$$

$$u = -\frac{\triangle}{2\mu}\left[1-\left(\frac{y}{\ }\right)^2\right] \qquad r=0 \quad u_{max} = \frac{\triangle}{\mu} \tag{6}$$

near the wall

$$1-(y/h)^2 \qquad 1-[\cancel{(}y^2-2yh+h^2)/h^2] \simeq 2y/h \qquad y^2 \ll {}^2 \tag{7}$$

$$u=u_{max}(2y/h) \tag{8}$$

(how to derive from force balance ?)

Constitutive transport equation

$$(\partial \ _1/\partial \ + u\cdot \ \nabla \ _1 = D\nabla^2 C_1 + R_1 \tag{4-28}$$

steady state $\partial \ _1/\partial \ = 0$

no reaction $R_1 = 0$

$$u.\cdot\nabla \ = D\nabla^2 C \tag{9}$$

for cartesian coordinate

$$u_x \frac{\partial}{\partial x} + \underbrace{u_y \frac{\partial}{\partial \ }}_{0} + \underbrace{u_z \frac{\partial}{\partial \ }}_{0} = \underbrace{D\frac{\partial^2 C}{\partial x^2}}_{0} + D\frac{\partial^2 C}{\partial \ ^2} + \underbrace{D\frac{\partial^2 C}{\partial \ ^2}}_{0}$$

$$\frac{2y}{h} u_{max} \frac{\partial}{\partial x} = D\frac{\ }{\partial \ ^2} \qquad \text{two independent var. } x \ y \quad \text{one dependent var, } c \tag{10}$$

$$C = C_{sat} \quad \text{at } y = 0 \tag{11}$$

$$C = 0 \quad \text{as } y \to \infty \qquad ** \quad \partial \ '\partial \ = 0 \quad \text{at } y=h$$

$$\frac{C}{C_{sat}} = C* \quad f'n\left(x \quad y, \frac{u_{max}}{Dh}\right)$$

Similarity : non-dimensional combination

similarity variable

$$\eta = y\left(\frac{2u_{max}}{hDx}\right)^{1/3} \tag{12}$$

chain rule $C^{*} = f'n\ (\eta$

$$\frac{\partial \quad {}^{*}}{\partial x} = \frac{dC^{*}}{d\eta}\,\frac{\partial \eta}{\partial x}\bigg|_{y\ \mathrm{const}} = y\left(\frac{2u_{max}}{hD}\right)^{1/3}\left(-\frac{1}{3}\right)x^{-4/3}\,\frac{dC^{*}}{d\eta} = \frac{\eta}{3x}\,\frac{dC^{*}}{d\eta} \qquad (13)$$

$$\frac{\partial \quad {}^{*}}{\partial} = \frac{dC^{*}}{d\eta}\,\frac{\partial \eta}{\partial}\bigg|_{x\ \mathrm{const}} = \left(\frac{2u_{max}}{hDx}\right)^{1/3}\frac{dC^{*}}{d\eta} \qquad (14)$$

$$\frac{\partial^{2}C^{*}}{\partial \quad {}^{2}} = \left(\frac{2u_{max}}{hDx}\right)^{1/3}\frac{dC^{*}}{d\eta}\,\frac{\partial \eta}{\partial} = \left(\frac{2u_{max}}{hDx}\right)^{2/3}\left(\frac{d^{2}C^{*}}{d\eta^{2}}\right) \qquad (15)$$

$$\cancel{2}\,\frac{y}{h}\,u_{max}\left(-\frac{\eta}{3x}\right)\frac{dC^{*}}{d\eta} = D\left(\frac{2u_{max}}{hDx}\right)^{2/3}\frac{dC^{*}}{d\eta} \qquad (16)$$

$$\frac{dC^{*}}{d\eta} + \frac{\eta}{3}\,\frac{dC^{*}}{d\eta} = 0 \qquad (17)$$

$$\begin{aligned} \mathrm{BC}\quad C^{*} \quad 1\ \mathrm{at}\quad \eta &= 0 \leftarrow y = 0 \\ C^{*} \quad 0 \qquad \eta &= \infty \leftarrow y \rightarrow \infty \end{aligned} \qquad (18)$$

$$\frac{d}{d\eta}\ln\left(\frac{dC^{*}}{d\eta}\right) = -\frac{\eta}{3} \qquad (19)$$

$$C^{*} = A\int_{0}^{\eta} e^{-\eta^{2}/9}\,d\eta + B \qquad (20)$$

$$C^{*} \quad 1 - \frac{\int_{0}^{\eta} e^{-\eta^{2}/9}\,d\eta}{\int_{0}^{\infty} e^{-\eta^{2}/9}\,d\eta} \qquad (21)$$

$$\text{Gamma function}\ \Gamma\ n) = \int_{0}^{\infty} Z^{n-1}\,e^{-z} \quad (n>0) \qquad (22)$$

$$\Gamma\ \imath+1) = \int_0^{\infty} Z\ e^{-z^2}\ d \qquad \Gamma\ \imath+1) = n\Gamma\ \imath)$$

$$\frac{C}{C_{sat}} = 1 - 0.538 \int_{0w}^{\eta} e^{-\eta^2/9}\, d\eta \qquad (23)$$

Flux at wall

$$j^* = -D\left(\frac{\partial}{\partial}\right)_w = -\ C_{sat}\, D\left(\frac{2u_{max}}{hDx}\right)^{1/3}\left(\frac{dC^*}{d\eta}\right)_w \ (y=h) \qquad (24)$$

$$= 0.678\ C_{sat}\, D\left(\frac{u_{max}}{hDx}\right)^{1/3} \qquad (25)$$

Equation (25) is useful, since the solubility (or total flux) is expressed as a function of distance. Also it is coincident with the empirical relations for mass transfer.

Case 2 Unsteady state diffusion in a semi-infinite slab starting from mass balance (free diffusion)

slab
semi-infinite slab   physically semi-infinite
or D≪ℓ   n a slab

$$\left(\begin{matrix}\text{solute accumulation}\\ \text{in volume A}\triangle\end{matrix}\right) = \left(\begin{matrix}\text{rate of diffusion}\\ \text{into the layer}\\ \text{at Z}\end{matrix}\right) - \left(\begin{matrix}\text{rate of diffusion}\\ \text{out of the layer}\\ \text{at Z+}\triangle\end{matrix}\right)$$

$$\frac{\partial}{\partial}(A\triangle\ C_1) = A\left(j_1\Big|_{Z} - j_1\Big|_{Z+\triangle} \right)$$

$$\frac{\partial\ \ _1}{\partial} = -\frac{j_1\Big|_{Z+\triangle} - j_1\Big|_{Z}}{(Z+\triangle\ ) - Z}$$

t=0   all z $C_1 = C_{1\,\infty}$
t→   z=0 $C_1 = C_{1\,0}$
z=∞ $C_1 = C_{1\,\infty}$

$$\frac{\partial\ \ _1}{\partial} = -\frac{\partial j_1}{\partial} \qquad j_1 = -D\frac{\partial}{\partial}$$

$$\frac{\partial\ \ _1}{\partial} = D\frac{\partial^2 C_1}{\partial\ \ ^2}$$

Fick's 2nd law (1)
Diffusion equation

← Boundary condition

$$\zeta \equiv \frac{z}{\sqrt{\ \ Dt}}$$

combination of variables (2)

$$\frac{dC_1}{d\zeta}\left(\frac{\partial\zeta}{\partial}\right) = D\frac{d^2C_1}{d\zeta^2}\left(\frac{\partial\zeta}{\partial}\right) \tag{3}$$

$$\text{LHS}: \frac{d\zeta}{dt} = \frac{d}{d}\left(Z\ (4Dt)^{1/2}\right) = Z\ (-1/2)\ (4Dt) \qquad 4D \tag{4}$$

$$\text{RHS}: \left(\frac{d\zeta}{d}\right)^2 = \left(\frac{}{\sqrt{\ \ Dt}}\right) = \frac{1}{4Dt} \tag{5}$$

$$\frac{dC_1}{d\zeta}\left(-\frac{2\ z}{4t\sqrt{\ \ Dt}}\right) = D\frac{d^2C_1}{d\zeta^2}\frac{1}{4Dt} \qquad (6)$$

$$\frac{d^2C_1}{d\zeta^2} + \frac{2\ z}{\sqrt{\ \ Dt}}\frac{dC_1}{d\zeta} = 0 \qquad (7)$$

$$\frac{d^2C_1}{d\zeta^2} + 2\zeta\frac{dC_1}{d\zeta} = 0 \qquad (8)$$

$$\begin{array}{llll} z=0 & C_1 = C_{1\,0} & \Rightarrow & \zeta\quad 0 \quad C_1 = C_{1\,0} \qquad (9) \\ t=0\ \big) & & & \\ z=\infty & C_1 = C_{1\,\infty} & \Rightarrow & \zeta\quad \infty \quad C_1 = C_{1\,\infty} \end{array}$$

integrate

$$\frac{dC_1}{d\zeta} = a\ e^{-\zeta}$$

confirm

$$\frac{d\ \ C_1}{d\zeta} = a\ e^{-\zeta}\ (-2\zeta$$

$$= \cancel{a}\frac{1}{\cancel{\ }}\ \frac{dC_1}{d\zeta}\ (-2\zeta$$

$$\frac{d\ \ C_1}{d\zeta} + 2\zeta\frac{dC_1}{d\zeta} = 0 \qquad (10)$$

integrate $\int dC_1 = \int a\ e^{-\zeta}\ d\zeta$

$$C_1 - C_{1\,0} = a\int_o^x e^{-y}\ d$$

independent
variable?

$$\boxed{\mathrm{erf}x \equiv \frac{2}{\sqrt{\pi}}\int_o^x e^{-y}\ d}$$

$$C_1 - C_{1\,0} = a\frac{\sqrt{\pi}}{2}\mathrm{erf}\zeta \qquad (11)$$

a=?

at $\zeta\quad\infty \quad C_1 = C_{1\,\infty}$

$$C_{1\infty} - C_{1\,0} = a\frac{\sqrt{\pi}}{2}\mathrm{erf}\infty \qquad \mathrm{erf}\infty = 1$$

$$= \frac{a\sqrt{\pi}}{2}$$

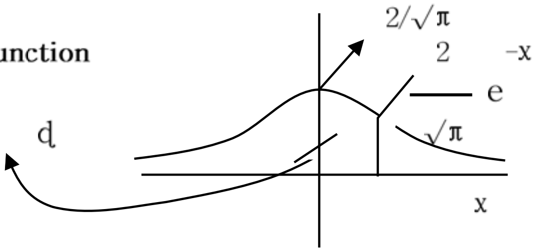
$$a = (C_{1\infty} - C_{1\,0})\frac{2}{\sqrt{\pi}}$$

$$C_1 - C_{1\,0} = (C_{1\infty} - C_{1\,0})\,\frac{\sqrt{\pi}}{2}\,\frac{2}{\sqrt{\pi}}\,\mathrm{erf}\zeta$$

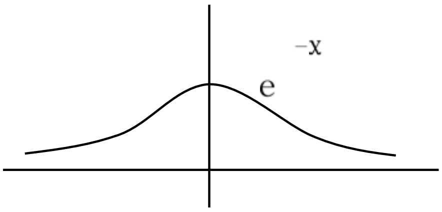
$$\frac{C_1 - C_{1\,0}}{C_{1\infty} - C_{1\,0}} = \mathrm{erf}\zeta \qquad (12)$$

Properties of error function

$$\mathrm{erf}\ x \quad \frac{2}{\sqrt{\pi}}\int_o^x e^{-y}\quad d$$



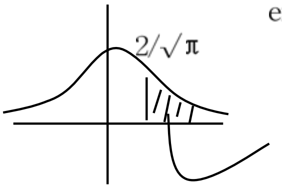
$$\begin{cases} \mathrm{erf}(\infty = 1 \\ \mathrm{erf}\ 0 = 0 \end{cases}$$



$$\frac{d}{dx}\,\mathrm{erf}x = \frac{2}{\sqrt{\pi}}\,e^{-x}$$

$$\int_o^{\infty} e^{-x} = \frac{\sqrt{\pi}}{2}$$

$$\mathrm{erfc}\ x = 1-\mathrm{erf}x$$



$$\mathrm{erfc}(x = \frac{2}{\sqrt{\pi}}\int_x^{\infty} e^{-y}\quad d$$

$$\begin{cases} \mathrm{erfc}\ 0 = 1 \\ \mathrm{erfc}\ \infty = 0 \end{cases}$$

Flux

$$j_1 = -D\frac{\partial\ \ 1}{\partial} = -D(C_{1\infty} - C_{1\,0})\,\frac{2}{\sqrt{\pi}}\,e^{-\zeta}\quad\frac{d\zeta}{d} \qquad (13)$$

$$= -D(C_{1\infty} - C_{1\,0})\,\frac{2}{\sqrt{\pi}}\,e^{-Z\ /4Dt}\quad\frac{1}{\sqrt{\ Dt}}$$

$$= (C_{10} - C_{1\infty})\,\frac{\sqrt{\ }}{\sqrt{\pi}}\,e^{-Z\ /4Dt} \qquad (14)$$

flux at z=0

$$j_1\Big|_{z=0} = (C_{1\infty} - C_{1\,0})\sqrt{\frac{D}{\pi}} \qquad (15)$$

Superposition method

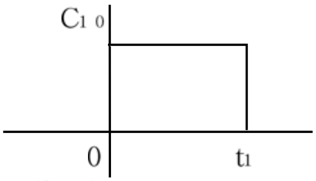
$$\frac{C_1 - C_{1\,0}}{C_{1\infty} - C_{1\,0}} = \mathrm{erf}\zeta$$

$C_{1\infty} = 0$ (or initial condition)

$$1 - C_1/C_{1\,0} = \mathrm{erf}\zeta$$

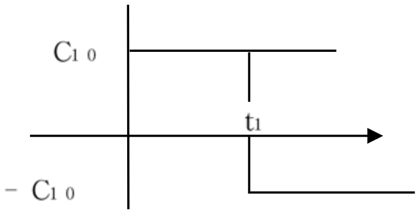
$$C_1/C_{1\,0} = 1 - \mathrm{erf}\zeta = \mathrm{erfc}\zeta$$

$$\begin{cases} 0 < t < t_1 & C = C_{1\,0} \\ t_1 \leq & C = 0 \end{cases}$$



Du Hamel's theorem

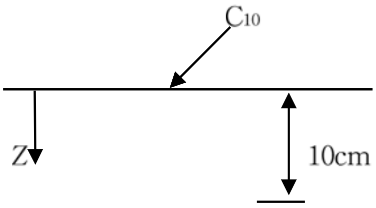
$$C_1 = C_{1\,0}\,\mathrm{erfc}\zeta \quad 0 < t < t_1)$$
$$C_1 = C_{1\,0}\,\mathrm{erfc}\zeta - C_{1\,0}\,\mathrm{erfc}\zeta_1$$



$$\zeta \quad \frac{z}{\sqrt{Dt}} \qquad \zeta_1 = \frac{z}{\sqrt{D(t-t_1)}}$$

$$C_1 = C_{1\,0}(1 - \mathrm{erf}\zeta \quad 1 + \mathrm{erf}\zeta_1) = C_{1\,0}(\mathrm{erf}\zeta_1 - \mathrm{erf}\zeta$$

Example (soil contamination)



semi infinite

at what time
C at 10cm = 0.02 kg/kg soil

$$\frac{\partial \quad {}_A}{\partial} = D\frac{\partial^2 C_A}{\partial \quad ^2}$$

$C_{sat} = 0.05$ kg/kg soil
$D_{eff} = 5\times10^{-4}$ m²/sec

IC t=0 for all Z $C_A = C_{A\infty}$
t>0 Z=0 $C_A = C_{A0} = 0.05$ kg/kg
Z=∞ $C_A = C_{A\infty} = 0$

$$\frac{C_A - C_{A0}}{0 - C_{A0}} = \mathrm{erf}\zeta \qquad \zeta \quad \frac{Z}{\sqrt{Dt}}$$

$$-(C_A/C_{A0}) + 1 = \mathrm{erf}\zeta$$

$$C_A/C_{A0} = 1 - \mathrm{erf}\zeta$$

$$\mathrm{erf}\zeta \qquad 1-(0.02/0.05)=0.6 \quad \rightarrow \zeta \quad 0.6$$

$$\zeta = 0.55 + 0.05\left(\frac{0.6 - 0.563}{0.604 - 0.563}\right) = 0.595$$

$$0.595 = \frac{10\text{cm}}{\sqrt{\times 5\times10^{-4} \qquad \text{sec}\ t}}$$

$$(0.595) = \frac{100}{20\times10^{-4} \qquad t}$$

$$t = \frac{100}{(20\times10^{-4})\ (0.595)} = 14100\ \text{sec}$$

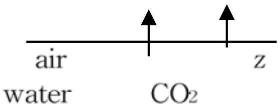
or 39 hr

= 1.6 day

More problems to be analyzed by error functions

Carbon dioxide enrichment of a stagnant air mass

A region of air enriched with CO_2 grows upward from the interface as the air mass remains in contact with the water body. Consider the CO_2 distribution in the stagnant air T= 20℃ P=1atm



$$\frac{y_1 - y_{10}}{y_{1\infty} - y_{10}} = \text{erf}\zeta \qquad \zeta \quad \frac{z}{\sqrt{\ \ Dt}}$$

D = 0.153 ㎠ s $\qquad y_{1\infty} = 0.03 \quad y_{10} = 0.0658$

time	Penetration Distance z (cm)		
	0.1	1	10
10 sec	0.0642	0.0503	0.03
1 min	0.0651	0.0592	0.0307
1 hr	0.0657	0.0649	0.0574

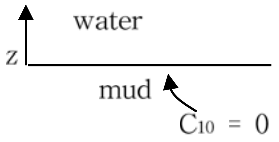
Homework Problem

consider a stagnant layer of O_2-rich water suddenly placed above an anaerobic mud layer capable of consuming O_2 and depleting the water of its O_2 content

Initially water was saturated at 9.17 mg/L

The Diffusivity of O_2 in water is 1.80×10 ㎠ s

Calculate the concentration of O_2 at given time and distance



time	distance		
	0.001 cm	0.1 cm	10 cm
5 min			
1 hr			
1 day			

Exercises

1. Reverse osmosis takes place in a plate and frame module (between two flat membranes), i.e., the salt is rejected by the membranes and concentrated while water permeate through the membrane. Derive the transport equation that describes the salt concentration, starting from a mass balance on the differential control volume. Assume steady state and no movement in y-direction.

2. A chemical is injected into a fully-developed pipe flow and degraded by a first-order reaction. Starting from mass balance in a differential control volume, derive a differential equation for one-dimensional non-steady transport of the chemical in the pipe in terms of diffusion and bulk velocity. (Boundary conditions not needed)

3. We consider a case where a vessel containing a selective membrane is initially filled to a volume V_0 with solution at a concentration of chemical able to pass through the membrane, c_{r0}. At t = 0 fluid begins leaving the vessel at a constant rate Q. The concentration in the effluent (or membrane permeate), c_p, is always less than the concentration in the vessel, c_r, by the constant ratio $pc = c_p/c_r$ ($p_c < 1$). The effluent is received in another vessel which is well mixed. Derive an expression for the concentration of the chemical in the receiving vessel as a function of time. The receiving vessel is initially empty. If possible, keep the symbols used in Example 1.6, p17, Logan.

4. A stagnant water is saturated with oxygen in air at 25 ^{o}C. Suddenly (at time zero) the air is replaced by pure oxygen, and the interface is saturated with the pure oxygen immediately and oxygen diffuses into the water. Calculate the oxygen concentration at 0.5 cm under the interface and the oxygen flux at the interface at 1 hr.

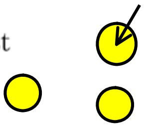
mass transfer

diffusion : diffusion coeff (D)
(internal mass transfer) intraphase, continuous phase
(internal diffusion) Fick's law

mass transfer: mass transfer coeff(κ
(external mass transfer) interphase phenomena
(external diffusion) discontinuous

Exercise **Diffusion problems vs. mass transfer problem (D or κ**

(1) catalyst



intraparticle phenomena
D

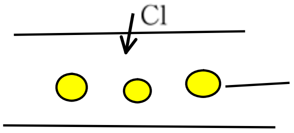
(2) penetration of acid rain into a mable stature
D

(3) O_2 transfer in a activated sludge process
aeration. bubble → bulk O_2 transfer κ

(4) In an activated sludge
nutrient transport into a floc
(substrate) D

(5) SO_2 scrubbing $SO_2 + CaO \rightarrow$ ƆaSO$_3$
"κ scale up

(6) Cl_2 penetration into bridge

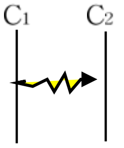


steel frame corrosion
→ ridge collapsed
D

(7) odor control by plastic film
leak or diffusion

mass
transfer

flux = κ (concentration difference)



κ △)

flux variation with position ignored

$$\text{flux} = D\left(\frac{\text{conc difference}}{\text{length}}\right)$$

$$-D\frac{\partial}{\partial}$$

variation with position predicted

$$= \frac{D}{\ell}\,(\text{conc difference})$$

"lumped-parameter" vs "distributed parameter"