§1.4 Derivation of Governing Eq. for Diffusion Phenomena.

Conservative Eq.

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} + w\frac{\partial \phi}{\partial z} = 0$$

Representing Material Transportation Due to Flows

If there is no flow $\mathbf{u} = (u, v, w) = 0$,

$$\frac{\partial \phi}{\partial t} + 0 \times \frac{\partial \phi}{\partial x} + 0 \times \frac{\partial \phi}{\partial y} + 0 \times \frac{\partial \phi}{\partial z} = 0$$

$$\therefore \frac{\partial \phi}{\partial t} = 0$$

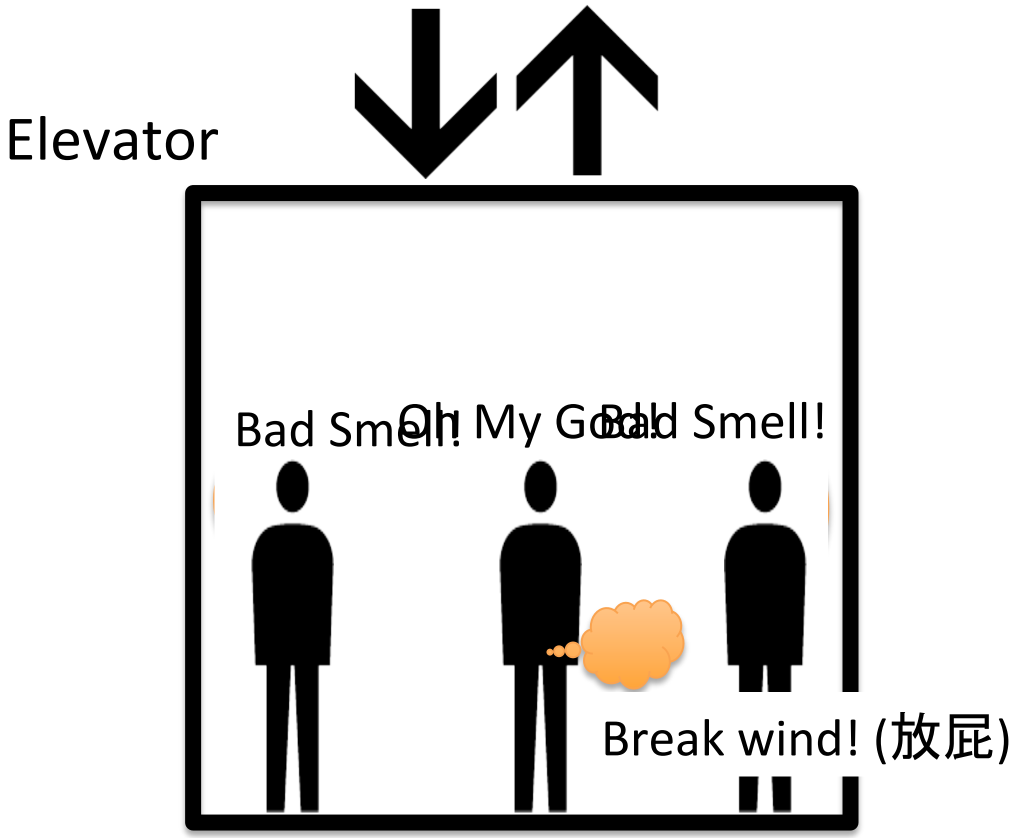
There should be no Transportation

and

Material Concentration not be changed.

But, we know,

Even if there is no flow in Closed Room, Smell Expand Gradually.



In the Actual Environments,

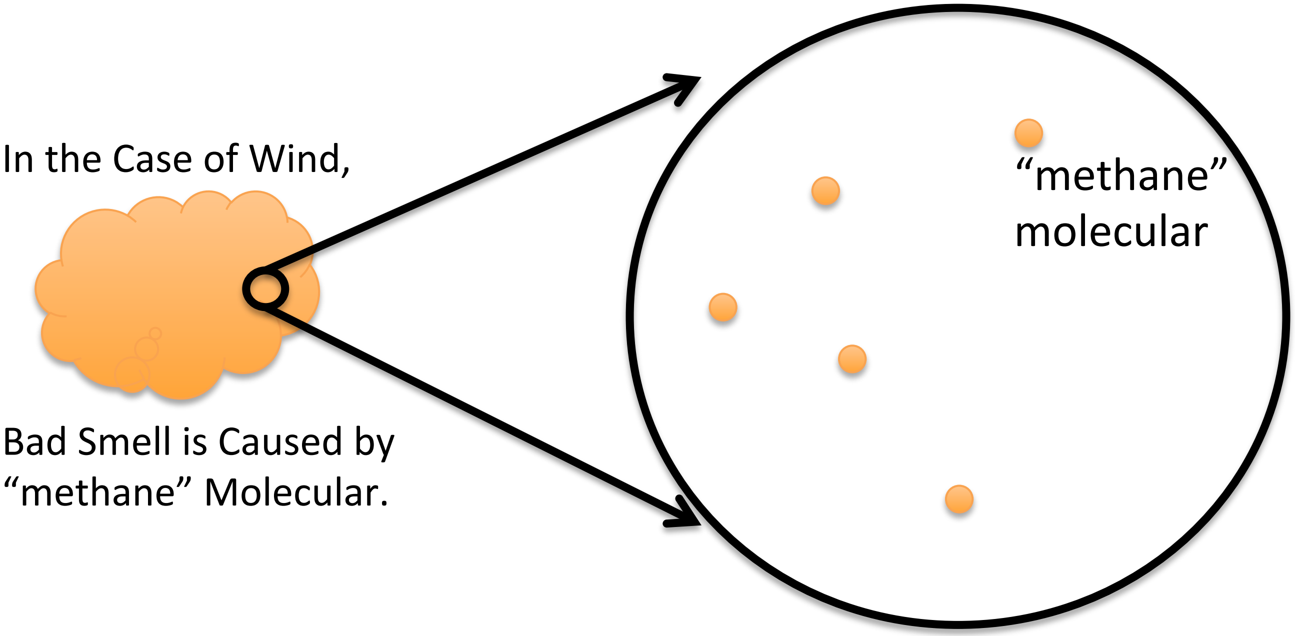
Another Transportation Mechanism exist.

Diffusion Phenomena

Mathematical Modeling of Diffusion Phenomena

All Substances Consist of Particles(Molecular)

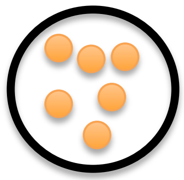
In the Case of Wind,



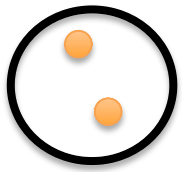
Bad Smell is Caused by
“methane” Molecular.

Concentration of Substances ϕ Means Number of Molecular.

High Concentration ⇔ Many Molecular Exist

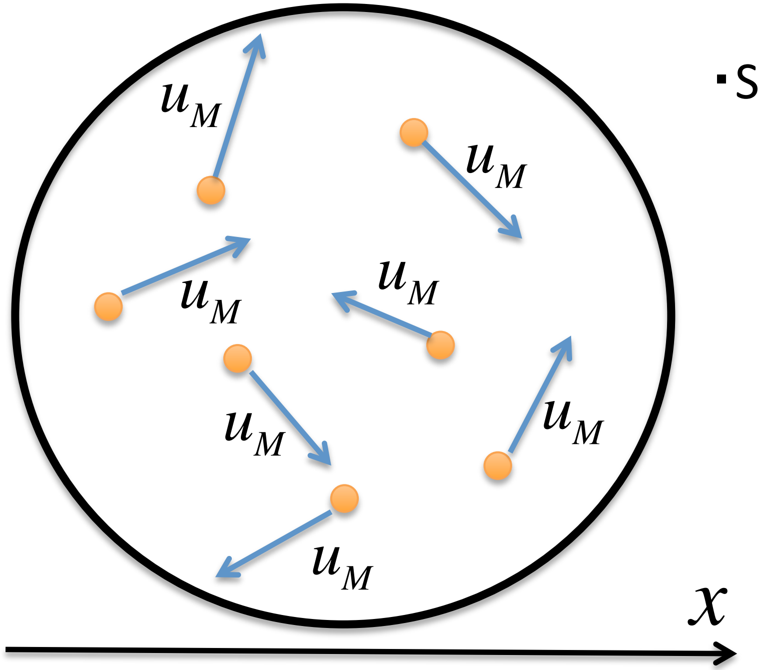


Low Concentration ⇔ Few Molecular Exist



The Molecular Motion

Even if There is no Flow, The Molecular does not Stop and Keep Moving!



・Speed of Molecular Motion u_M ;

Estimated from Temperature T [K].

$$\frac{1}{2} m_M u_M = \frac{3}{2} k_B T$$

m_M : Weight of Molecular

k_B : Boltzmann Constant

In the Ordinary Temp. (T =20[°C])

$$u_M \approx 2{,}160[km / hour]$$

・Direction of Molecular Motion; Entirely Random

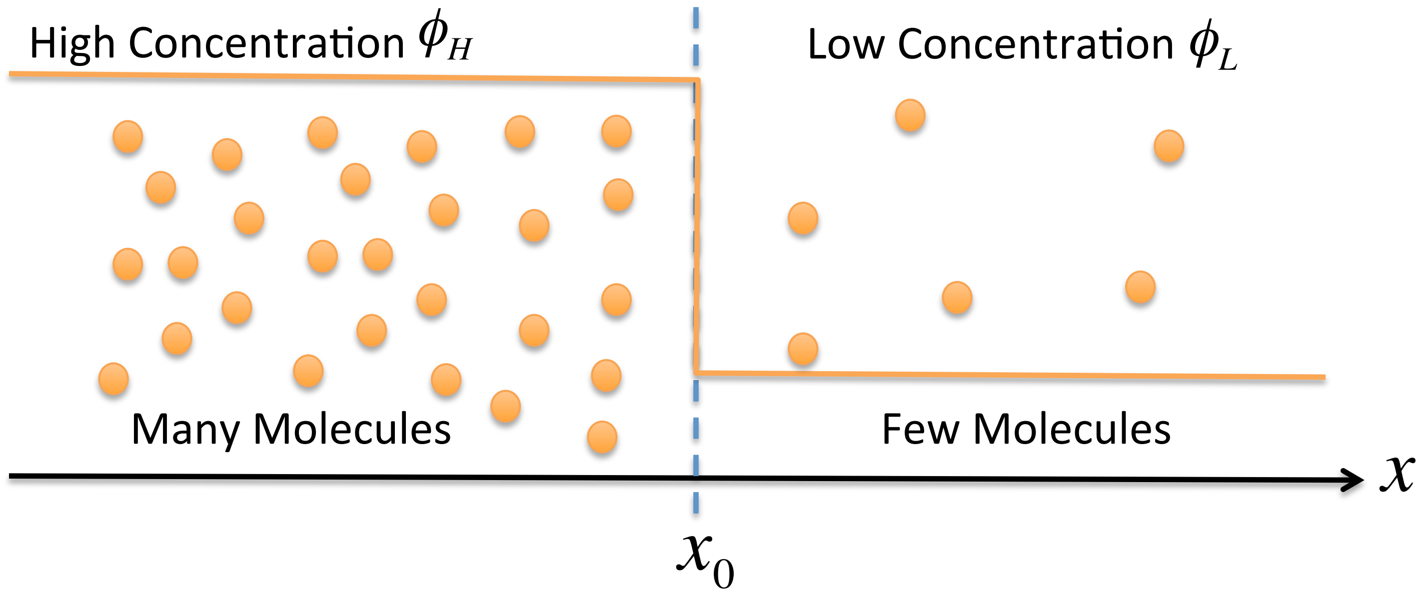
Namely,

Probability: "Move to $+x$ Direction" = "Move to $-x$ Direction" = 0.5

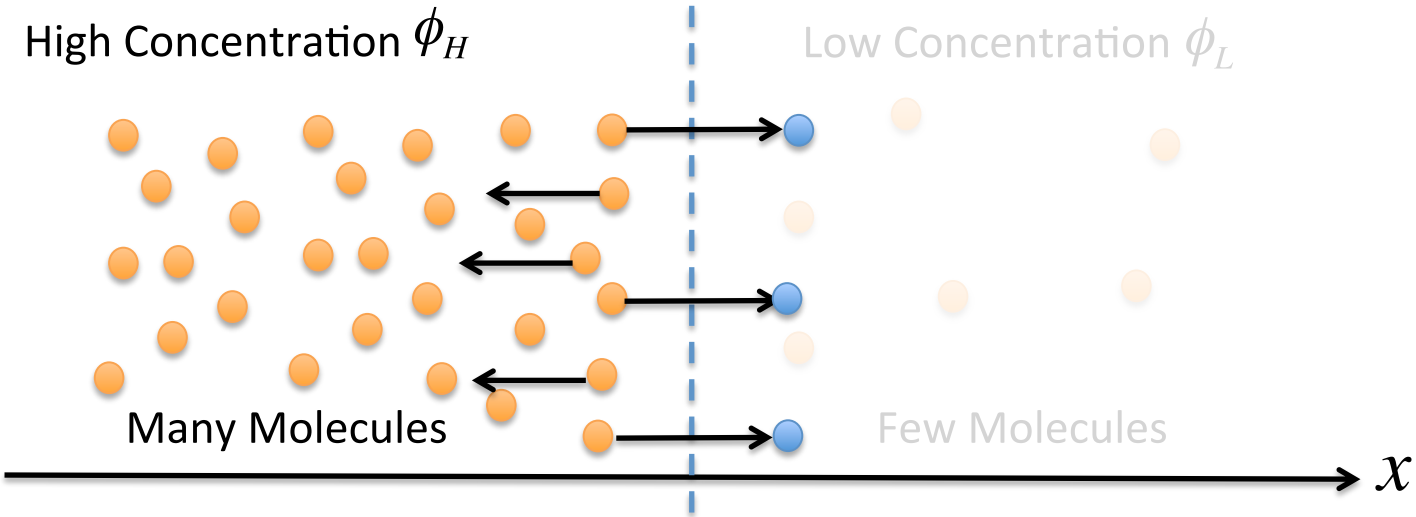
Deviation of Master Eq. for Diffusion Phenomena

- Thought Experiment
  - Assuming 1D Space (Molecular Moves only to x direction)
  - Concentration ϕ Changes Spatially at Initial Time

$$\phi = \begin{cases} \phi_H & \text{(High Concentration)} \quad for \quad x < x_0 \\ \phi_L & \text{(Low Concentration)} \quad for \quad x > x_0 \end{cases}$$



$$\phi \propto \text{"Number of Molecular"}$$



<u>Left Side (High Concentration Region)</u>

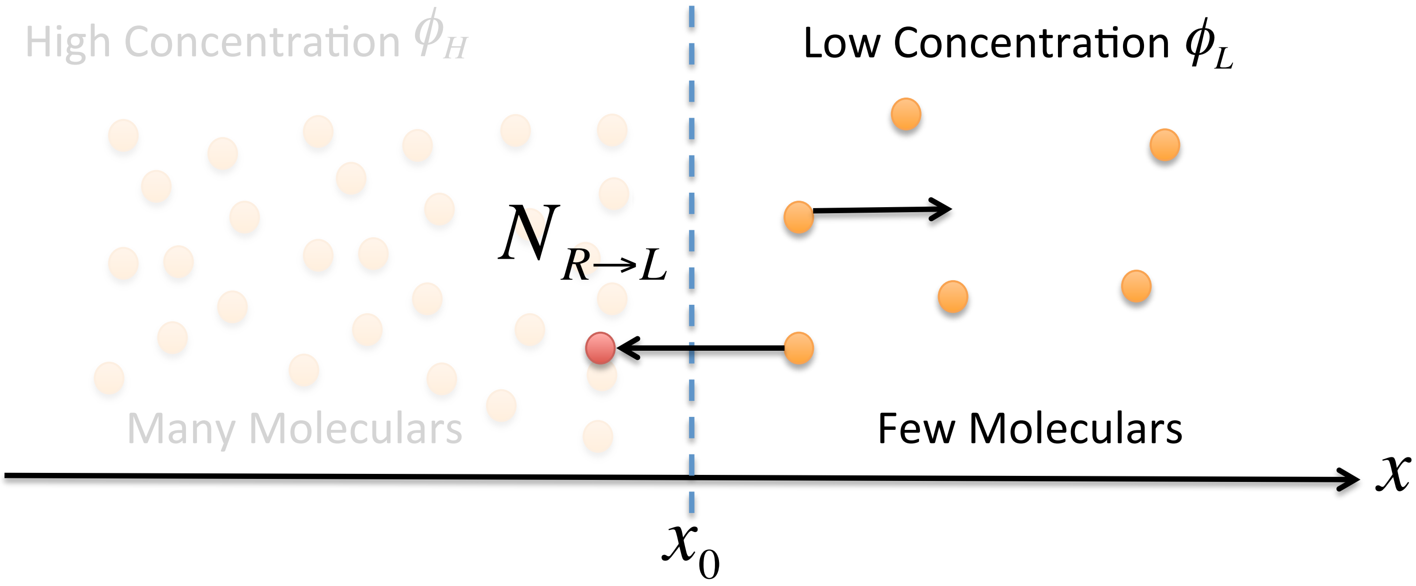
- Due to Random Motion, Near the Boundary, A Half of Molecules Move to the Right Across the x_0 .

- "Number of Molecules" ∝ ϕ_H

"Total Number of Molecules Moving to the Right Side" ; $N_{L\to R} \propto \frac{1}{2}\phi_H$

$$\therefore N_{L\to R} = \nu\phi_H$$

ν : Coefficient Representing Easiness of Molecules Movement.

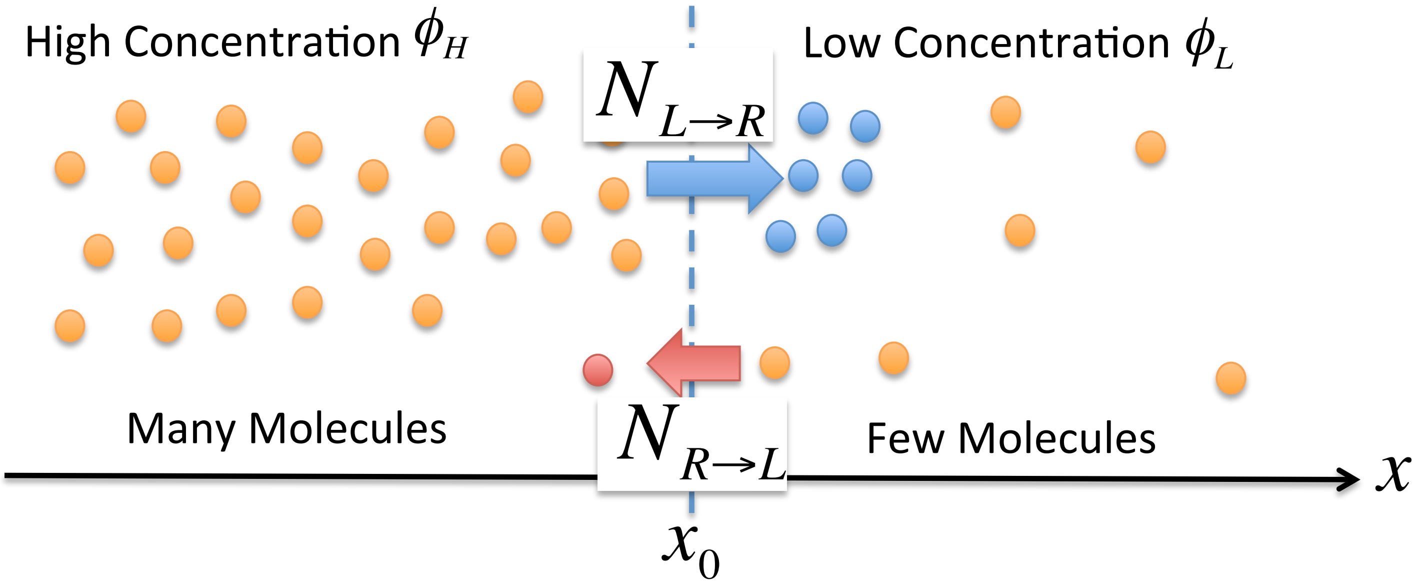


Total Number of Molecules Moving from Right to Left Side

$$\therefore N_{R \to L} = v\phi_L$$

Because Number of Molecules is Less than the Left Side,

$$N_{R \to L} < N_{L \to R}$$



Total Number of Molecules Moving Across x_0

From Left to Right Side $N_{L\to R} = \nu\phi_H$

From Right to Left Side $N_{R\to L} = \nu\phi_L$

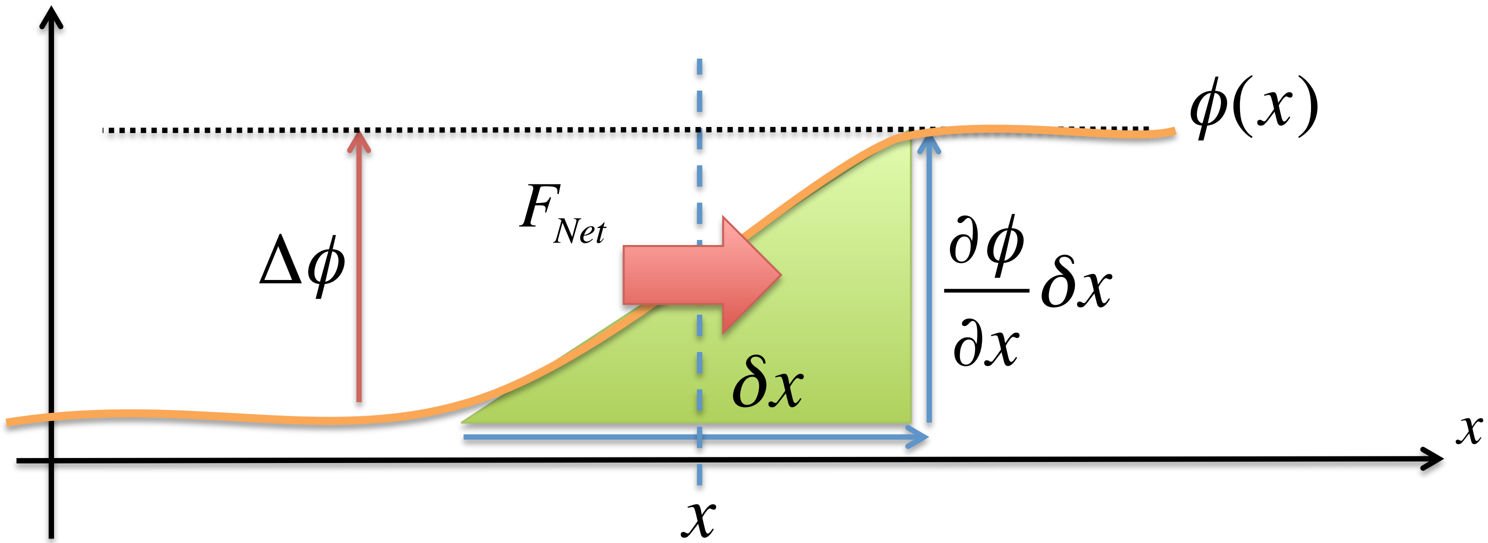
"Net Number of Molecules Moving to Right"

$$N_{Net} = N_{L\to R} - N_{R\to L} = \nu\phi_H - \nu\phi_L$$

$$\therefore N_{Net} = -\nu\left(\phi_L - \phi_H\right) = -\nu\Delta\phi$$

If there is spatial change of ϕ , Material is transported; Diffusion Phenomena

Speed of Transportation is Proportion to Spatial Change $\Delta\phi$



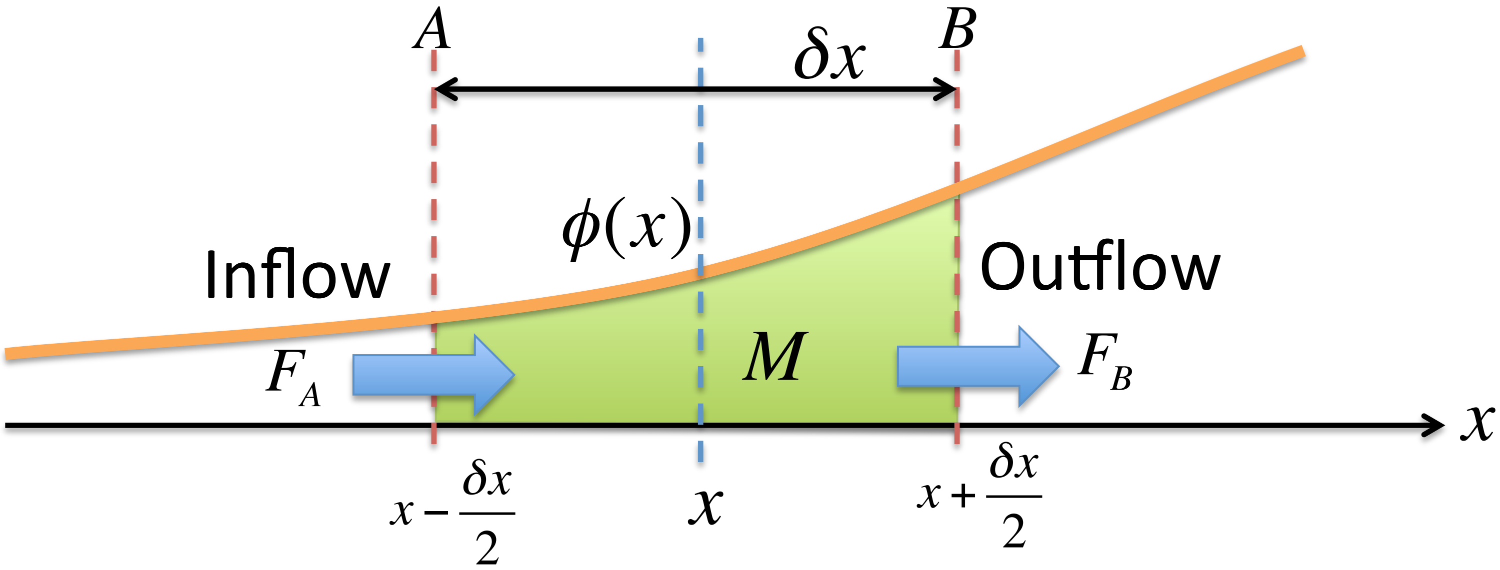
In General Case, $\phi(x)$ Changes Continuously.

Spatial Change $\Delta\phi$ around x is Represented by $\dfrac{\partial \phi}{\partial x}$

Transportation Due to Diffusion at x ; $F_{Net} = -\nu \dfrac{\partial \phi}{\partial x}$

Derivation of Mathematical Expression of Diffusion

Assuming Small Element [x-δx/2, x+δx/2] (δx Width)



- Total Amount of ϕ Substance included in Element; $M = \phi \times \delta x$

- Transported Amount across the $x-\frac{\delta x}{2}$; $F_A = -\nu \frac{\partial \phi(x-\delta x/2)}{\partial x}$

- Transported Amount across the $x+\frac{\delta x}{2}$; $F_B = -\nu \frac{\partial \phi(x+\delta x/2)}{\partial x}$

Change of M; $\frac{\partial M}{\partial t} = F_A - F_B$

Derivation of Mathematical Expression of Diffusion

$$\frac{\partial M}{\partial t} = F_A - F_B$$

$$\delta x \frac{\partial \phi}{\partial t} = -\nu \frac{\partial \phi(x - \delta x / 2)}{\partial x} + \nu \frac{\partial \phi(x + \delta x / 2)}{\partial x}$$

$$\frac{\partial \phi}{\partial t} = \frac{\nu \frac{\partial \phi(x + \delta x / 2)}{\partial x} - \nu \frac{\partial \phi(x - \delta x / 2)}{\partial x}}{\delta x}$$

Taking a limit $\delta x \rightarrow 0$

$$\frac{\partial \phi}{\partial t} = \lim_{\delta x \rightarrow 0} \frac{\nu \frac{\partial \phi(x + \delta x / 2)}{\partial x} - \nu \frac{\partial \phi(x - \delta x / 2)}{\partial x}}{\delta x} = \frac{\partial}{\partial x}\left(\nu \frac{\partial \phi}{\partial x}\right)$$

1D Expression of Diffusion Equation; $\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x}\left(\nu \frac{\partial \phi}{\partial x}\right)$

In 3D Case,

3D Diffusion Equation;

$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x}\left(\nu \frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\nu \frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\nu \frac{\partial \phi}{\partial z}\right)$$

Conservative Eq. is Rewritten so that Diffusion is introduced;

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} + w\frac{\partial \phi}{\partial z} = \frac{\partial}{\partial x}\left(\nu \frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\nu \frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(\nu \frac{\partial \phi}{\partial z}\right)$$

Transport Eq.