Diffusion Equation

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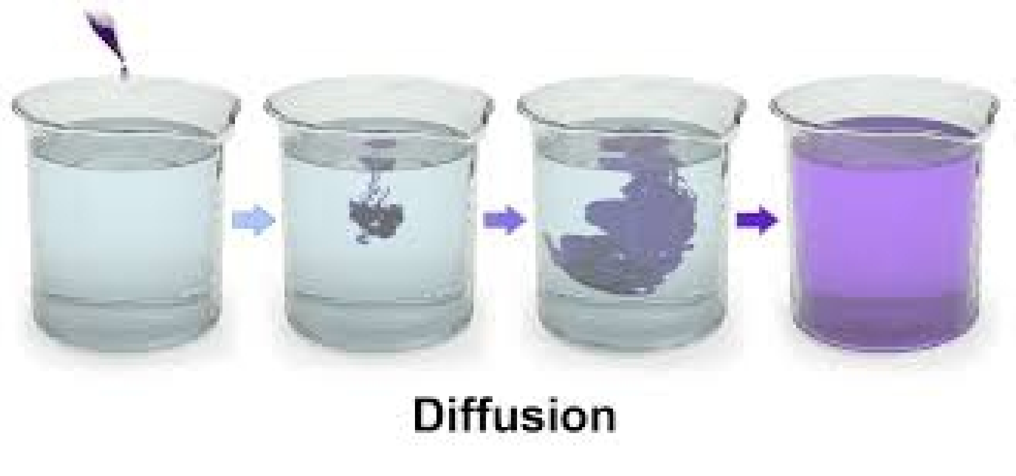
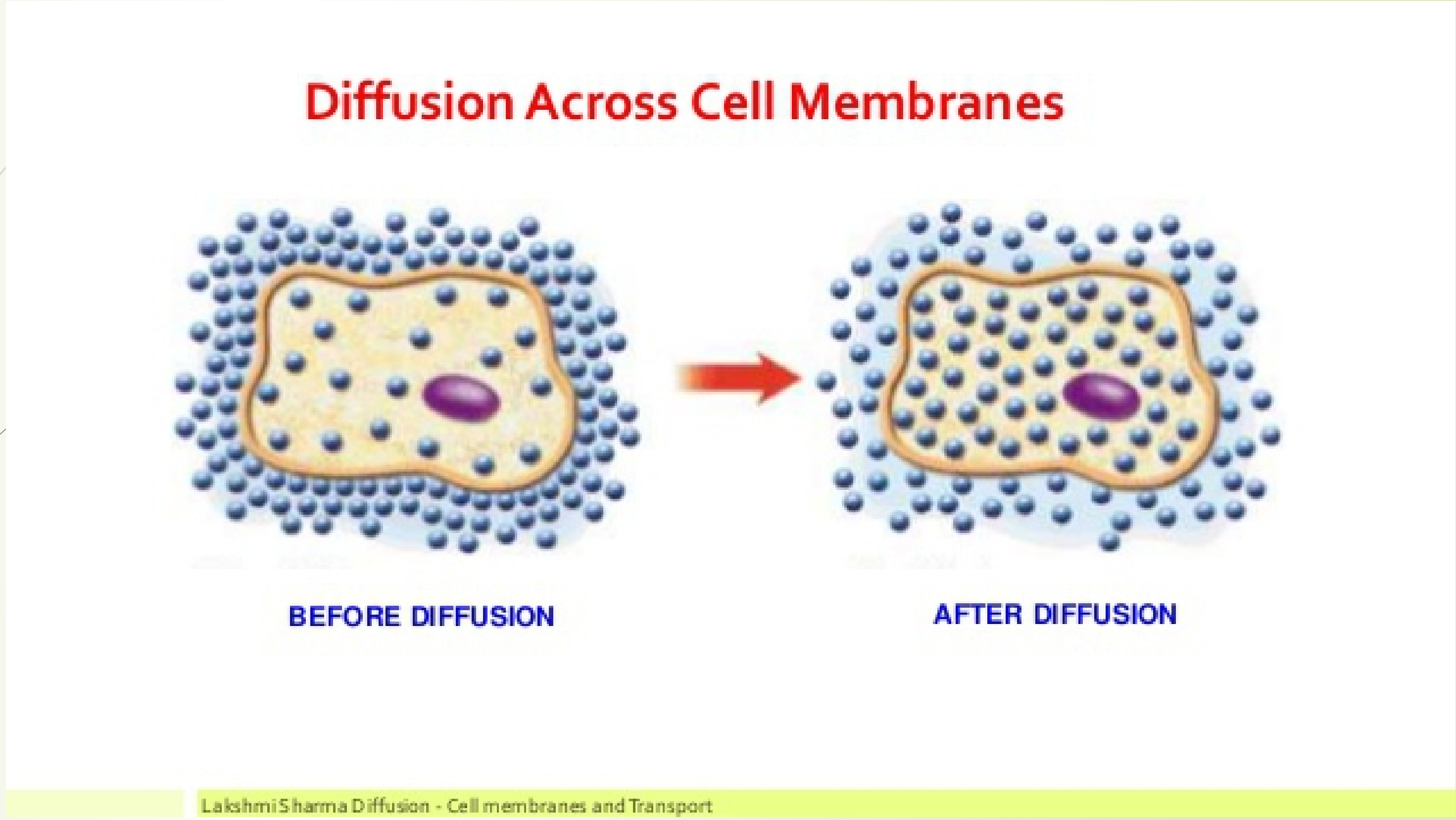
What is diffusion?

Diffusion is the movement of a dispersed material from an area of higher concentration to an area of lower concentration within a matrix



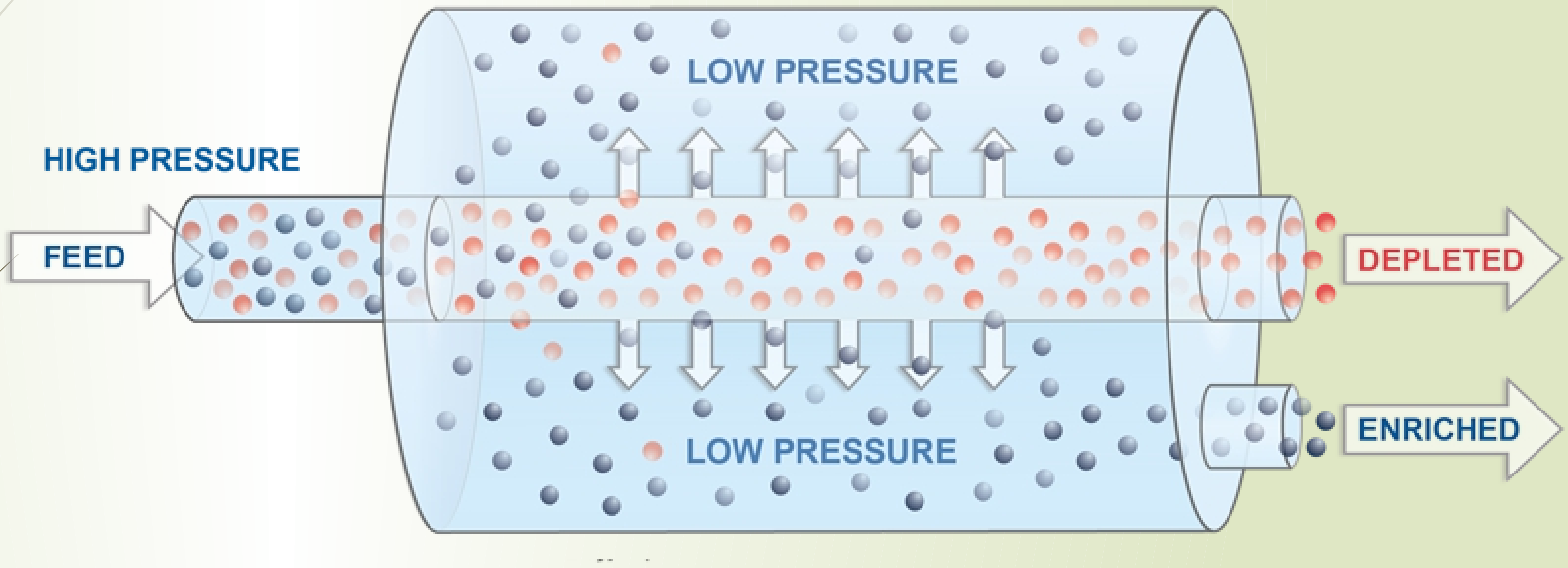
https://commons.wikimedia.org/wiki/File:Blausen_0315_Diffusion.png



https://commons.wikimedia.org/wiki/File:Blausen_0315_Diffusion.png

Gaseous diffusion

= U235
= U238



http://www.centrusenergy.com/learn-more/uranium-enrichment/gaseous-diffusion/

The equation

$$\frac{\partial \phi(\mathbf{r},t)}{\partial t} = \nabla \cdot \left[D(\phi,\mathbf{r})\ \nabla \phi(\mathbf{r},t) \right]$$

https://en.wikipedia.org/wiki/Diffusion_equation

The terms

- $\varphi(r, t)$ = density/concentration as a function of position (r) and time (t)
- $D(\varphi, r)$ = diffusion coefficient as a function of density/concentration and position
- ∇ = divergence of vector field when in dot product, gradient of function (d/dx, d/dy, d/dz) when used as function operator

History

- 1822 : Fourier proposes heat eqution
- 1827 : Brownian motion discovered
- 1855 : Fick uses heat equation to solve diffusion problem
- 1905 : Brownian motion recognized as a diffusion problem

Derivation

- The trivial diffusion equation can be derived from the continuity equation, which is based on the conservation of mass, combined with Fick's first Law

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{j} = 0$$

, where j is flux (continuity)

$$\mathbf{j} = -D(\phi, \mathbf{r})\, \nabla \phi(\mathbf{r}, t).$$

(Fick's 1st law)

- Generalization comes from the Smoluchowski equation is drift must be accounted for

https://en.wikipedia.org/wiki/Diffusion_equation

Fun facts

- If the diffusion coefficient (material dependent) is a constant (D = constant), then the diffusion equation simplifies to the heat equation in 3 dimensions

$$\frac{\partial \phi(\mathbf{r},t)}{\partial t} = D\nabla^2 \phi(\mathbf{r},t)$$

https://en.wikipedia.org/wiki/Diffusion_equation

- Einstein proposed Brownian motion as diffusion problem
- Gauss Divergence theorem proves diffusion equation holds for all states of matter, assuming there are no sources or sinks in the system

Diffusion in chemical engineering

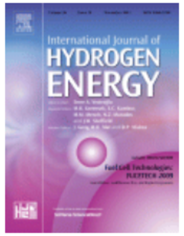
- Local concentrations
- Boundary/interfacial zones in processes
- Membranes
- Separations

Example

ELSEVIER

International Journal of Hydrogen Energy

Volume 36, Issue 22, November 2011, Pages 14779-14786



Dynamic modeling and simulation of a proton exchange membrane electrolyzer for hydrogen production

A. Awasthi [a], Keith Scott [b], S. Basu [a]

- Proton exchange across membrane for hydrogen production
- Gas diffusion out of the cell

https://www.sciencedirect.com/science/article/pii/S0360319911006343

Diffusion in environmental engineering

- Contaminant fate and transport
- Groundwater contamination

Example

Journal of Contaminant Hydrology

Volume 53, Issues 1–2, 1 December 2001, Pages 85-100

Tracer diffusion coefficients in sedimentary rocks: correlation to porosity and hydraulic conductivity

Thomas B Boving [a], Peter Grathwohl [b, 1]

- Diffusion in porous media
- Solid-liquid interface

https://www.sciencedirect.com/science/article/pii/S0169772201001383

Additional fields in which diffusion matters

- Physics
- Cell biology / biochemistry/ biomedical engineering
- Materials science
- Rheology
- Many more: basically whenever there is contact between 2 different materials

End

Thank you!

Questions?

Sources

- https://en.wikipedia.org/wiki/Diffusion_equation
- https://commons.wikimedia.org/wiki/File:Blausen_0315_Diffusion.png
- http://www.centrusenergy.com/learn-more/uranium-enrichment/gaseous-diffusion/
- https://www.sciencedirect.com/science/article/pii/S0360319911006343
- https://www.sciencedirect.com/science/article/pii/S0169772201001383