MATE 664 Lecture 09

Atomic Models for Diffusion (II): Gas & Liquid Phases

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Recap of Lecture 07

Key ideas from last lecture:

- Analytical solution to diffusion problems (infinite domain)
  - Semi-infinite (half-half) solution
  - Line / point source solution
  - Superimposition method
- Separation of variables method (finite / bounded domain)
- Laplace transform (will not be covered in exam)

Learning Outcomes

After this lecture, you will be able to:

- Recall the conditions behind the Einstein diffusion equation
- Understand why the Einstein relation is universal across states of matter
- Connect gas, liquid, and solid diffusion within a unified framework
- Derive Arrhenius-type diffusivity from a 1D potential well model
- Identify assumptions and missing physics in simple diffusion models

Recap: Linking Atomistic Motion to Diffusion

From last lecture:

- Diffusion emerges from random microscopic motion
- Mean squared displacement (MSD) is the key observable
- Einstein equation links MSD to macroscopic diffusivity

Einstein Diffusion Equation

Define MSD as the normalized second moment of concentration:

$$\langle R^2(t) \rangle = \frac{\int_0^\infty r^2 c(r,t)\, 4\pi r^2 dr}{\int_0^\infty c(r,t)\, 4\pi r^2 dr} \tag{1}$$

Using solution to point source diffusion, Einstein showed: - 3D: $\langle R^2 \rangle = 6Dt$ - 2D: $\langle R^2 \rangle = 4Dt$ - 1D: $\langle R^2 \rangle = 2Dt$