MATE 664 Lecture 07

Solution to Diffusion Equations (II)

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2026-01-26

Recap of Lecture 06

Key ideas from last lecture:

- Governing equation for diffusion problems
- Steady state solutions to diffusion problems (without convection)
- Introduction to nonsteady state diffusion solutions

Recap: Steady-State Solutions to Diffusion Equations

Just to solve Laplace equation $\nabla^2 c = 0$. But ∇^2 terms depend on the coordinate system!

- Cartesian: $c(x) = k_1 x + k_2$
- Cylindrical: $c(r) = k_1 \ln r + k_2$
- Spherical: $c(r) = k_1 / r + k_2$

k_1, k_2 are determined by the boundary conditions.

- *Can we determine D using steady state profile?*

Influence of Geometry on S.S. Solutions

Learning Outcomes

After today's lecture, you will be able to:

- **Recall** analytical solutions to diffusion problems
- **Analyze** superposition of the source method in diffusion problems
- **Analyze** the diffusion length scale in $\sqrt{4Dt}$ and its implications

- **Describe** the key process in separation of variables method
- **Apply** Laplace transform in initial value problems

Part II: Non-steady State Diffusion

Different strategies (review)

- Superposition with known "source" solutions
- Separation of variables (finite domains)
- Laplace transform (initial condition handling)
- Numerical methods (general geometry / $D(c)$)

Dimensionless Transform of Diffusion

- Analysis of many diffusion problems will benefit by transforming into dimensionless forms
- Diffusion length scale $\sqrt{Dt}$ (or $\sqrt{4Dt}$)
- Dimensionless variable $\eta = \frac{x}{\sqrt{Dt}}$
- Transform from ODE to PDE

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{1}$$

$$\frac{\partial c}{\partial \eta} = -\frac{\eta}{2}\frac{\partial^2 c}{\partial \eta^2} \tag{2}$$

Solution to Dimensionless Diffusion Problem

- Step 1: Let $u = \frac{\partial c}{\partial \eta}$

$$u = C_1 \exp(-\frac{1}{4}\eta^2)$$

- Step 2: integrate $u = \frac{\partial c}{\partial \eta}$

$$c(\eta) = K_1 + K_2 \,\mathrm{erf}(\frac{\eta}{2})$$

where $\mathrm{erf}(\xi) = \frac{2}{\sqrt{\pi}}\int_0^{\xi} e^{-x^2}dx$ is the **error function**

- Step 3: fit initial condition and boundary conditions (**the hardest part**!)
- How do the solution look like?

Inifinite Space: Half-Half Situation

Geometry: $x \geq 0$

I.C.

- $c(x < 0, t = 0) = c_L$
- $c(x > 0, t = 0) = c_R$

Solution form

$$c(x,t) = \frac{c_L + c_R}{2} + \frac{c_L - c_R}{2} \ \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right)$$

How do we get here?

Limits and Checks

- $t \to 0^+$: $\mathrm{erfc}(x/(\sqrt{4Dt})) \to 0$ for $x > 0 \quad c \to c_R$
- $t \to 0^+$: $\mathrm{erfc}(x/(\sqrt{4Dt})) \to 0$ for $x > 0 \quad c \to c_L$
- $x \to \infty$: $\mathrm{erfc}(\infty) = 0 \quad c \to \frac{c_L + c_R}{2}$
- Takes **infinite** amount of time to reach steady-state, but we can often take intermediate snapshots

Inifinite Space: Half-Half Situation Time Scale

Line Source as Superposition

Notes: “line source” can be built from two semi-infinite problems. For a line source with concentration c_0 and thickness δ, solution $c(x,t)$ follows

$$c(x,t) = c_1(x,t) + c_2(x,t)$$

Idea:

- c_1 and c_2 are solutions for 2 semi-infinite geometries
- decompose initial profile into steps
- add corresponding erfc solutions

Superposition Solution For Slab Geometry

- Step 1: write 2 half-space solutions

$$c_1(x,t) = \frac{c_0}{2} + \frac{c_0}{2}\,\mathrm{erf}\Big(\frac{x}{\sqrt{4Dt}}\Big) \tag{3}$$

$$c_2(x,t) = -\frac{c_0}{2} - \frac{c_0}{2}\,\mathrm{erf}\Big(\frac{x-\delta}{\sqrt{4Dt}}\Big) \tag{4}$$

- Step 2: combine them!

$$c(x,t) = \frac{c_0}{2}\left[\mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right) - \mathrm{erf}\left(\frac{x-\delta}{\sqrt{4Dt}}\right)\right] \tag{5}$$

is obtained by superposition and is valid under the following conditions:

Infinite Domain: Point Source (1D)

Initial conditions

$$c(x,0) = N\,\delta(x)$$

Solution (thin-film limit)

$$c(x,t) = \frac{N}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right)$$

Gaussian Interpretation

- point source spreads as a Gaussian
- variance grows linearly with time

$$\sigma^2 = 2Dt$$

So width $\sigma \sim \sqrt{2Dt}$.

Error Function and Gaussian Integral

Define

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-s^2}\, ds$$

and

$$\mathrm{erfc}(z) = 1 - \mathrm{erf}(z)$$

These appear in semi-infinite diffusion solutions.

Step Source

Finite step (width Δx) can be treated as

- difference of two semi-infinite step solutions
- in the limit $\Delta x \to 0$ recovers point source Gaussian

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3D Point Source

c is separabile across axes!

For 3D infinite space

$$c(x, y, z, t) = \frac{N}{(4\pi Dt)^{3/2}} \exp\left(-\frac{x^2 + y^2 + z^2}{4Dt}\right)$$

General Principle: Linear PDE → Build Solutions

Because diffusion equation is linear (for constant D)

- complex IC can be decomposed into simpler components
- solutions are sums (or integrals) of known kernels

Hard part

- enforcing boundary conditions in finite domains

Method 2: Separation of Variables

Used often for finite domains

Assume product form

$$c(x, t) = X(x)\, T(t)$$

Substitute into

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

gives

$$\frac{1}{DT}\frac{dT}{dt} = \frac{1}{X}\frac{d^2 X}{dx^2} = -\lambda^2$$

Time Part and Spatial Eigenfunctions

Time ODE

$$\frac{dT}{dt} = -\lambda^2 D T \Rightarrow T(t) = \exp(-\lambda^2 D t)$$

Space ODE

$$\frac{d^2 X}{dx^2} + \lambda^2 X = 0$$

Solutions depend on BCs (sine/cosine, etc.).

Eigenvalues from Boundary Conditions

- Dirichlet BC $\lambda_n = n\pi/L$
- Neumann BC $\lambda_n = n\pi/L$ with different eigenfunctions
- Mixed BC   different transcendental conditions

Physical meaning in notes

- λ sets spatial wavelength $\sim 1/\lambda$
- higher n modes decay faster (via $e^{-\lambda^2 D t}$)

General Series Solution Form

Superposition over modes

$$c(x,t) = \sum_{n=0}^{\infty} A_n X_n(x)\, e^{-\lambda_n^2 D t}$$

Coefficients A_n from initial condition projection.

Modal Picture: What Decays First?

- high spatial-frequency components (large λ_n) vanish quickly
- long-wavelength components persist longer
- diffusion acts as a low-pass filter on concentration profiles

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Method 3: Laplace Transform (Time Domain)

Notes: convert time-dependence into algebraic parameter p

Define

$$\hat{c}(x,p) = \mathcal{L}\{c(x,t)\} = \int_0^\infty e^{-pt} c(x,t)\,dt$$

Laplace transform replaces time derivative with initial-value term.

Key Property: Transform of $\partial c/\partial t$

Using integration by parts (as in notes)

$$\mathcal{L}\left\{\frac{\partial c}{\partial t}\right\} = p\hat{c}(x,p) - c(x,0)$$

Spatial derivatives remain derivatives in x:

$$\mathcal{L}\left\{\frac{\partial^2 c}{\partial x^2}\right\} = \frac{\partial^2 \hat{c}}{\partial x^2}$$

Fick's 2nd Law in Laplace Space

Transform

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

becomes

$$p\hat{c}(x,p) - c(x,0) = D\frac{\partial^2 \hat{c}}{\partial x^2}$$

Now an ODE in x (parameter p).

Example Setup: Semi-infinite with Fixed Surface

From notes example

- $c(x,0) = 0$ for $x > 0$
- $c(0,t) = c_0$
- $c(\infty,t) = 0$

Boundary conditions in Laplace domain

$$\hat{c}(0,p) = \frac{c_0}{p}, \qquad \hat{c}(\infty,p) = 0$$

Solve ODE in x

With $c(x,0) = 0$, equation reduces to

$$D\frac{\partial^2 \hat{c}}{\partial x^2} - p\hat{c} = 0$$

General solution

$$\hat{c}(x,p) = Ae^{+\sqrt{p/D}\,x} + Be^{-\sqrt{p/D}\,x}$$

Semi-infinite boundedness $\quad A = 0$.

Apply BC at $x = 0$

At $x = 0$

$$\hat{c}(0, p) = B = \frac{c_0}{p}$$

So

$$\hat{c}(x, p) = \frac{c_0}{p} \exp\left(-\sqrt{\frac{p}{D}}\, x\right)$$

Back-transform: Error Function Result

Inverse Laplace yields the erfc solution (notes)

$$c(x, t) = c_0 \ \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Interpretation

- Laplace method packaged IC automatically into transformed equation
- remaining work: solve ODE in x + apply BCs

General Laplace Workflow (Notes Summary)

1) Write PDE and IC/BC

2) Laplace in time: $c \to \hat{c}(x, p)$

3) Solve ODE in x (parameter p)

4) Fit BCs (Dirichlet / Neumann) to get coefficients

5) Invert transform (analytic or numeric)

Meaning of the p-space Parameter

From your sketch (page 17)

- $\hat{c}(x, p)$ is a weighted time integral of $c(x, t)$
- large p emphasizes early-time behavior
- small p emphasizes long-time behavior

Conceptual plots

- $c(x, t)$ evolves in t
- $\hat{c}(x, p)$ "compresses" time into the p axis

When to Use Which Method?

- Known source solutions + superposition
  - infinite / semi-infinite, simple BCs
- Separation of variables
  - finite domains, classical BCs, eigenfunction expansions
- Laplace transform
  - strong control over initial conditions, semi-infinite problems
- Numerical
  - complex geometry, nonlinear $D(c)$, complicated BCs

Summary

- Steady state   Laplace equation $\nabla^2 c = 0$ (solve by geometry)
- Non-steady constant-D diffusion is linear
- Key kernels: Gaussian (point source) and erfc (semi-infinite boundary)
- Separation of variables: eigenmodes decay as $e^{-\lambda_n^2 D t}$
- Laplace transform: time derivative becomes $p\hat{c} - c(x, 0)$, ODE in x

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Next Steps

- Numerical solutions to diffusion problems
- Estimation of diffusivity from solutions
- Introduction to atomic model of diffusion