Mathematical Modelling

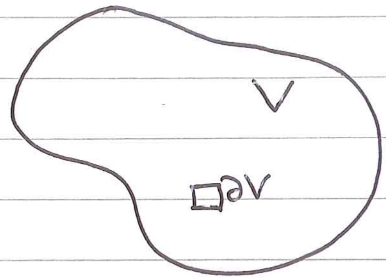
Case Study II:

Freezing and Melting Ice

Outline

1. Recap on Heat Equation and its solution
2. Introduction to
    a. Stefan problems
    b. Models for the growth and melting of ice

The Heat Equation



Let $c(\underline{x},t)$ be the amount of heat (or chemical) per unit vol. at position x & time t.

Mass conservation (assuming no internal sources or sinks of heat) $\Rightarrow$

$$\begin{pmatrix}\text{rate of change}\\ \text{of total heat}\end{pmatrix} = -\begin{pmatrix}\text{flow of heat}\\ \text{out of domain}\end{pmatrix}$$

ie $$\frac{d}{dt}\int_V c(x,t)\,dV = -\int_{\partial V} \underline{J}\cdot\underline{n}\,dS$$ $\underline{J}$ = heat flux

If V does not depend on time, & if we can apply the divergence theorem, then

$$\int_V \left(\frac{\partial c}{\partial t} + \nabla\cdot\underline{J}\right)dV = 0. \qquad (2.1)$$

$\boxed{\text{Exercise 2.1}}$: If Eqn (2.1) holds $\forall\, V$, then show that

$$\frac{\partial c}{\partial t} + \nabla\cdot\underline{J} = 0$$ (under certain continuity conditions)

To complete the equation, we must specify $\underline{J}$ in terms of c

Ficks Law / Fourier's Law of Cooling

$$\boxed{\underset{\sim}{J} = -D\nabla C}$$

where D = diffusion coefficient

heat assumed to move down spatial gradients

$$\Rightarrow \frac{\partial c}{\partial t} = D\nabla^2 C \qquad (2.2)$$

NB assumes D = constant.

Exercise 2.2

Suppose
$$\begin{cases} u_t = D u_{xx} & |x| < \infty,\ t > 0 \\ u(x,0) = g(x) & |x| < \infty \end{cases}$$

where $g(x) \geq 0$. Show that $u(x,t) \geq 0 \ \forall\ t$.

SOLUTION

Exercise 2.3

Suppose
$$\begin{cases} u_t = D u_{xx} & |x| < L \\ u_x = 0 & \text{at } x = \pm L \end{cases}$$
(ie Neumann or zero-flux BCs)

Show that the total amount of u in the domain is conserved.

SOLUTION

Similarity Solutions of the Heat Equation

Suppose $\quad u_t = D u_{xx} \quad |x| < \infty,\ t > 0.$

PDE is invariant under transformation

$$\left.\begin{aligned} t &\to a^2 t \\ x &\to a x \end{aligned}\right\} \quad a = \text{constant}$$

This suggests that solution should be a function of x^2/t or $x/\sqrt{t}$. Let's try $\boxed{u(x,t) = V(x/\sqrt{t})}$. Then,

$$\int_{-\infty}^{\infty} u(x,t)\,dx = \int_{-\infty}^{\infty} V(x/\sqrt{t})\,dx = \sqrt{t}\int_{-\infty}^{\infty} V(y)\,dy$$

$\to \infty$ as $t \to \infty$, contradicting heat/mass conservation.

$\Rightarrow$ Trial soln : $\boxed{u(x,t) = \frac{1}{\sqrt{t}}\, v(x/\sqrt{t})}$: similarity solⁿ.

Exercise 2.4

Show that $v(y) = C + A e^{-y^2/4D}$

where $y = x/\sqrt{t}$ & A, C are constants.

SOLUTION

$$u(x,t) = \frac{1}{\sqrt{t}} v(y) = \frac{C}{\sqrt{t}} + \frac{A}{\sqrt{t}} e^{-x^2/4Dt}$$

Exercise 2.6

Assume, WLOG, that $\int_{-\infty}^{\infty} u(x,t)\,dx = 1$.

Show that
$$\boxed{u(x,t) = \frac{1}{\sqrt{4\pi D t}} \cdot e^{-x^2/4Dt}}$$
fundamental solution of the heat eqn.

Sketch $u(x,t)$.

SOLUTION

Question how does fundamental soln generalise?

Solution: In $\mathbb{R}^n$,

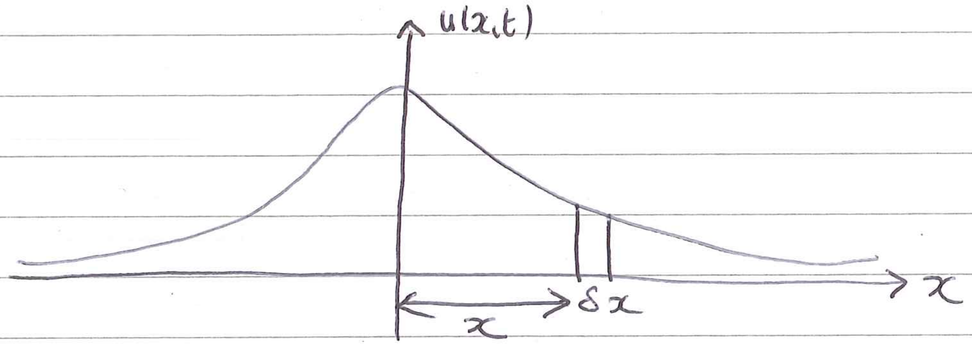
$$u(x,t) = \frac{1}{(4\pi D t)^{n/2}} \cdot e^{-|\underset{\sim}{x}|^2/4Dt}$$

Note: For $u(x,t) = \dfrac{1}{\sqrt{4\pi D t}} e^{-x^2/4Dt}$.

Fix spatial position x. Then

$$\begin{cases} \dfrac{du}{dt} = 0 & \text{at } t = x^2/2D \\ \dfrac{du}{dt} > 0 & \text{for } t < x^2/2D \\ \dfrac{du}{dt} < 0 & \text{for } t > x^2/2D. \end{cases}$$

Note: The mean displacement satisfies



$$\int_{-\infty}^{\infty} \frac{x\, e^{-x^2/4Dt}}{\sqrt{4\pi D t}}\, dx \equiv 0 \quad \text{(by symmetry)}$$

Exercise 2.7

Show that the mean-squared displacement (MSD)

$$\int_{-\infty}^{\infty} \frac{x^2 .\, e^{-x^2/4Dt}}{\sqrt{4\pi D t}}\, dx = 2Dt.$$

SOLUTION (integration by parts)

NOTE We can say that the diffusion lengthscale, L, satisfies

$$L^2 \sim DT$$

where T = diffusion timescale.

Exercise 2.8

Show that in 2D the MSD is 4DT.

SOLUTION

$$\left[c(x,y,t) = \frac{1}{4\pi Dt} \cdot e^{-(x^2+y^2)/4Dt} \right]$$

Example

For O_2 in blood, $D \sim 10^{-5}\ cm^2\ s^{-1}$

* $L = 1\,mm \Rightarrow T \sim L^2/D = \frac{10^{-2}}{10^{-5}} \sim 10^3\,s \sim \frac{1}{3}\,hr$

* $L = 10\,mm \Rightarrow T \sim \frac{100}{3}\,hr \sim 1$ day

* $L = 10\,cm \Rightarrow T \sim 100$ days !

These estimates limit the size of simple organisms (ie those without blood vessels).

Heat Equation

Let $Q(\underline{x},t)$ = heat energy / unit vol at $(\underline{x},t)$.

Then,

* $Q = c\rho T$ where T = temperature
  ρ = density
  c = specific heat capacity > 0

* $\underline{J} = -k\nabla T$ where k = thermal conductivity

Recall mass conservation:

$$\frac{\partial Q}{\partial t} = -\nabla\cdot\underline{J} \Rightarrow c\rho\frac{\partial T}{\partial t} = k\nabla^2 T$$ (assume c, ρ, k constant)

$$\Rightarrow \boxed{\frac{\partial T}{\partial t} = D\nabla^2 T} \quad \text{where } D = \frac{k}{c\rho}$$