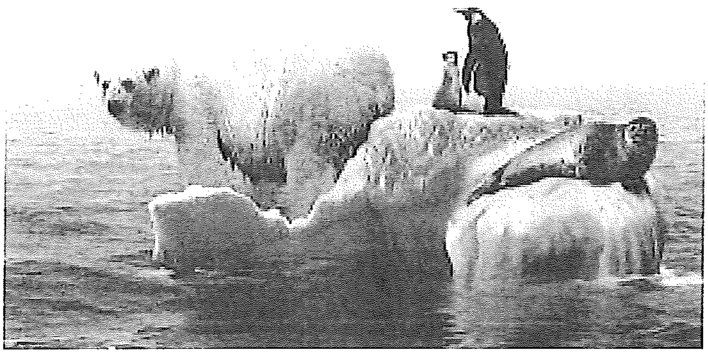
Mathematical Modelling

Case Study II:

Freezing and Melting Ice



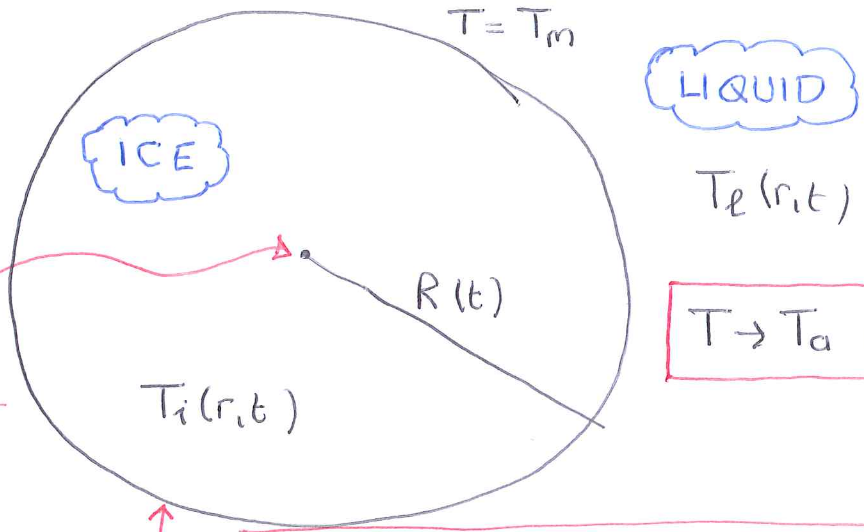
Outline

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

Spherical Ice Cube

Assumptions: infinite bath of water

same thermal properties & densities in each phase (no induced fluid motion due to phase change, as would happen with different densities).



$$\boxed{\frac{\partial T_i}{\partial r} = 0 \text{ at } r = 0}$$

$$\boxed{T \to T_a \text{ as } r \to \infty.}$$

$$\boxed{\rho L \frac{dR}{dt} = -k \left.\frac{\partial T_l}{\partial r}\right|_{R^+} + k \left.\frac{\partial T_i}{\partial r}\right|_{R^-}}$$

Governing Equations:

$r > R(t)$ (liquid): $$\rho c \frac{\partial T_l}{\partial t} = \frac{k}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_l}{\partial r}\right)$$

$r < R(t)$ (ice): $$\rho c \frac{\partial T_i}{\partial t} = \frac{k}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_i}{\partial r}\right)$$

with $T_i = T_{i0}$, $T_l = T_a$, $R = R_0$ at $t = 0$.

Nondimensionalise as follows:

$$\hat{R} = \frac{R}{R_0}, \quad \hat{r} = \frac{r}{R_0}, \quad \hat{T}_{\ell,i} = \frac{T_{\ell,i} - T_m}{T_a - T_m}$$

$$\hat{T}_{io} = \frac{T_{io} - T_m}{T_a - T_m}, \quad \hat{t} = \frac{\rho L R_0^2}{k(T_a - T_m)}$$

Then (omitting $\hat{}$s)

$$\begin{cases} \frac{1}{S}\frac{\partial T_\ell}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_\ell}{\partial r}\right) & r > R(t) \\ \frac{1}{S}\frac{\partial T_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_i}{\partial r}\right) & 0 < r < R(t). \end{cases}$$

with: $T_\ell \to 1$ as $r \to \infty$

$T_\ell = T_i = 1$ on $r = R(t)$

$$S = \frac{L}{c(T_a - T_m)}$$

$\frac{\partial T_i}{\partial r} = 0$ at $r = 0$

$T_\ell = 1, \quad T_i = T_{io}, \quad R = 1$ at $t = 0$

and $$\boxed{\frac{dR}{dt} = -\left.\frac{\partial T_\ell}{\partial r}\right|_{R^+} + \left.\frac{\partial T_i}{\partial r}\right|_{R^-}}$$

Assume $T_{io} = T_m$ at $t = 0$

Assume also that $\boxed{S \gg 1}$

With $\boxed{S \gg 1}$, in the liquid

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_\ell}{\partial r}\right) \approx 0 \qquad \text{for } r > R(t)$$

$$\Rightarrow \quad r^2 \frac{\partial T_\ell}{\partial r} = \hat{B}(t)$$

$$\Rightarrow \quad T_\ell = \frac{B(t)}{r} + A(t) \qquad \text{with } \begin{cases} T_\ell = 0 & \text{at } r = R \\ T_\ell \to 1 & \text{as } r \to \infty \end{cases}$$

$$\Rightarrow \quad \boxed{T_\ell(r,t) = 1 - \frac{R(t)}{r}}$$

In the ice $(0 < r < R(t))$:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_i}{\partial r}\right) \approx 0 \qquad \text{with } T_i = 0 \text{ on } r = R, \quad \frac{\partial T_i}{\partial r} = 0 \text{ at } r = 0$$

$$\Rightarrow \quad r^2 \frac{\partial T_i}{\partial r} = \hat{\beta}(t)$$

$$\Rightarrow \quad \frac{\partial T_i}{\partial r} = \frac{\hat{\beta}(t)}{r^2} = 0 \qquad \because \frac{\partial T_i}{\partial r} = 0 \text{ at } r = 0.$$

$$\Rightarrow \quad \boxed{T_i(r,t) = A(t) \equiv 0} \qquad \because T_i = 0 \text{ on } r = R(t).$$

Then, Stefan condition supplies

$$\frac{dR}{dt} = -\left.\frac{\partial T_\ell}{\partial r}\right|_{R^+} + \left.\frac{\partial T_i}{\partial r}\right|_{R^-}$$

$$= -R/R^2 + 0 \qquad \Rightarrow \frac{dR}{dt} = -1/R, \text{ with } R(0) = 1$$

$$\Rightarrow \boxed{R(t) = (1-2t)^{1/2}}$$

$R(t) = (1-2t)^{1/2} \Rightarrow R \to 0$ as $t \to 1/2$
(ice melts)

In dimensional terms, ice melts at time $\boxed{\frac{1}{2}\frac{\rho L R_0^2}{k(T_a - T_m)}}$

If R_0 large, then t large.

If $T_a \gg T_m$, then t small (liquid v. warm as $r \to \infty$)

If L large, then t large (energy/unit mass to melt solid is large)

If k large, then t small (heat conduction large)

BUT

$$T_\ell(r, t=0) = 1 - \frac{R(0)}{r} = 1 - 1/r \quad \text{for } r \geq 1.$$

But, we prescribe initial conditions with $T_\ell(r, t=0) \equiv 1$ ⋕

Recall,
$$\frac{1}{s}\frac{\partial T_\ell}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T_\ell}{\partial r}\right)$$

Initially (ie time, $t \ll 1$), $\frac{\partial T_\ell}{\partial t} = O(s)$. (ie rapid variation in T_ℓ wrt time, t)

ie quasi-steady approximation (QSSA) not valid at short times.
∃ short timescale on which temperature relaxes to satisfy the BCs (& to "forget" the ICs)

To analyse behaviour at early times, we set $\tau = st$ $(t = s/\tau)$

$$\begin{cases} \dfrac{\partial T_\ell}{\partial \tau} = \dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left(r^2 \dfrac{\partial T_\ell}{\partial r}\right) \\[2ex] s\dfrac{dR}{d\tau} = -\left.\dfrac{\partial T_\ell}{\partial r}\right|_{r=R^+} \end{cases}$$

Note: $\frac{dR}{d\tau} = O(s^{-1})$. We seek trial solution:

$$R(\tau) = 1 + \frac{R_1(\tau)}{s} + O(s^{-2})$$

s.t. as $\tau \to \infty$, $R(\tau)$ matches with outer solution derived above $\left(R(t) = (1-2t)^{1/2} = (1 - 2s/\tau)^{1/2}\right)$.

Exercise (matched asymptotics, separable solutions, ...)

Show that

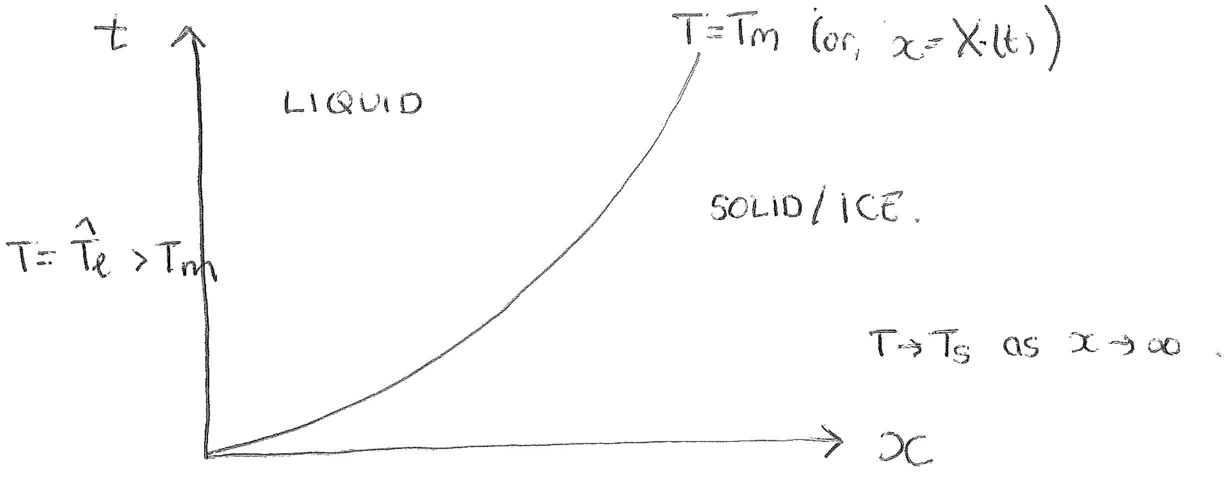
$$\frac{\partial}{\partial \tau}(r T_e) = \frac{\partial^2}{\partial r^2}(r T_e)$$

Use the above identity to construct sol^n's for $T_e(r,\tau)$ of the form:

$$T_e(r,\tau) = \left(1 - \frac{R(\tau)}{r}\right) + \sum_{\alpha} b_\alpha e^{-|\alpha|\tau} \cdot \frac{f_\alpha(r)}{r}$$

where $R(\tau) \approx 1$. Explain carefully how $f_\alpha(r)$ & the coefficients b_α are defined.

Two phase model (1D Cartesian geometry)



LIQUID : $\dfrac{\partial T_\ell}{\partial t} = \alpha_\ell \dfrac{\partial^2 T_\ell}{\partial x^2}$ $\qquad \alpha_\ell = k_\ell / \rho c_\ell$.

$(0 < x < X(t))$

SOLID : $\dfrac{\partial T_s}{\partial t} = \alpha_s \dfrac{\partial^2 T_s}{\partial x^2}$ $\qquad \alpha_s = k_s / \rho c_s$.

$(x > X(t))$

Stefan Condition : $$k_s \frac{\partial T_s}{\partial x} - k_\ell \frac{\partial T_\ell}{\partial x} = \rho L \frac{dX}{dt} \quad \text{on } x = X(t)$$

Initial conditions : $$\begin{cases} T(x,0) = T_s < T_m & \text{for } x > 0. \\ X(0) = 0 \end{cases}$$

Boundary conditions : $$\begin{cases} T(0,t) = \hat{T}_\ell > T_m \\ T(x,t) \to T_s < T_m & \text{as } x \to \infty. \end{cases}$$

In the liquid phase : $\begin{cases} T_\ell = f_\ell(\eta) \,, & \eta = \dfrac{x}{2\sqrt{\alpha_\ell t}} \\ X(t) = 2\lambda\sqrt{\alpha_\ell t} \,, & \lambda \text{ unknown}. \end{cases}$

As before, substitute into the heat equation to obtain

$$[f_\ell' \cdot e^{\eta^2}]' = 0$$

$$\Rightarrow \quad f_\ell' = K e^{-\eta^2} \qquad (K = \text{constant})$$

$$\Rightarrow \quad f_\ell(\eta) = K\int_0^\eta e^{-\tilde{\eta}^2}\, d\tilde{\eta} + \underbrace{K_1}_{\text{constant}}.$$

$$\Rightarrow \quad T_\ell(x,t) = K \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_\ell t}}\right) + K_1$$

Impose BCs :

$$T_\ell(0,t) = \hat{T}_\ell \quad \Rightarrow \quad K_1 = \hat{T}_\ell$$

$$T_\ell(X,t) = T_m \quad \Rightarrow \quad K \operatorname{erf}(\lambda) = T_m - \hat{T}_\ell$$

$$\Rightarrow \boxed{T_\ell(x,t) = \hat{T}_\ell - \frac{(\hat{T}_\ell - T_m)\operatorname{erf}\left(x/2\sqrt{\alpha_\ell t}\right)}{\operatorname{erf}(\lambda)}}.$$

In the solid phase (similarly),

$$T_s(x,t) = K_2 \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_s t}}\right) + K_3$$

Impose BCs :

$$T_s(\infty,t) = T_s \quad \Rightarrow \quad K_2 + K_3 = T_s .$$

$$T_s(X,t) = T_m \quad \Rightarrow \quad T_m = K_2 \operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_l}{\alpha_s}}\right) + K_3 .$$

$$\Rightarrow T_s(x,t) = \frac{(T_m - T_s)\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_s t}}\right) + T_s \operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_l}{\alpha_s}}\right) - T_m}{\operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_l}{\alpha_s}}\right) - 1}$$

Stefan condition :

$$\underbrace{\frac{\rho L \lambda . \sqrt{\alpha_l}}{\sqrt{t}}}_{\left(= \rho L \frac{dX}{dt}\right)} = k_s . \frac{\partial T_s}{\partial x}\bigg|_{x=X} - k_l \frac{\partial T_l}{\partial x}\bigg|_{x=X}$$

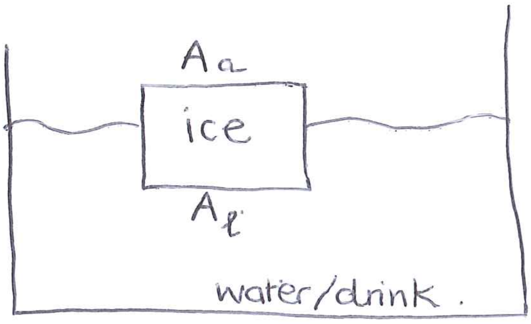
$\Rightarrow \dots \Rightarrow$ implicit expression for λ .

Exercise
* derive expression for λ .
* investigate limiting cases. (eg $L \gg 1$, $L \ll 1$)

Exercise : perform an experiment
measure rate of melting of block of ice

Lumped Model for Ice Cube & Drink.

Assumptions
- ignore spatial variation
- view T_i & T_ℓ as average values in each phase.



A_a, A_ℓ = SA of exchange with atmosphere & liquid.

Dependent variables

$T_i, V_i, T_\ell, V_\ell, A_a, A_\ell$.

Assumptions (ct'd):
- ice cube has volume $V_i(t)$
- liquid .. ... $V_\ell(t)$

- glass is perfectly insulating
- ignore heat exchange between liquid & air
- assume material properties of each phase are the same (eg densities are the same)

Governing Equations

* conservation of energy (in ice & liquid)

* conservation of mass (in "ice + liquid")

* ??

(3 additional eqns needed!)

Conservation of Energy

in ice :
$$\boxed{\frac{d}{dt}\left(\rho c V_i (T_i - T_m)\right) = -q_\ell A_\ell - q_a A_a .} \quad (*_1)$$

in liquid :
$$\boxed{\frac{d}{dt}\left(\rho c V_\ell (T_\ell - T_m)\right) = q_\ell A_\ell .} \quad (*_2)$$

where: (*) flow from liquid to ice, per unit SA $-q_\ell = \underbrace{h_\ell}_{\text{conductivity}} (T_\ell - T_m) > 0$.

(*) $\left(\begin{array}{c}\text{flow from air to ice} \\ \text{per unit SA}\end{array}\right)$, $-q_a = h_a (T_a - T_m)$

Conservation of total mass

$$\boxed{\rho V_i + \rho V_\ell = \underbrace{\rho (V_{i0} + V_{\ell 0})}_{\text{initial mass}} .} \quad (*_3)$$

$(*_1), (*_2), (*_3) \Rightarrow$ 3 equations for 6 unknowns !

Stefan Condition

$$(*_4) \quad \boxed{\rho L \frac{dV_i}{dt} = q_\ell A_\ell + q_a A_a - h_i(A)(T_i - T_m)}$$

$(*_1) - (*_4)$ define V_i, V_ℓ, T_i, T_ℓ .

what about A_a & A_ℓ ?

Exercise / project

By considering different shapes for V_i, propose functional relationships between A_e, A_a & V_i. Solve the resulting eqns (for V_i, V_e, T_i, T_e) & see how the dynamics depend on the functional forms you use.