THE FREEZING TIME FOR PSEUDO-ELLIPSOIDS

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1 Introduction

When a homogeneous isotropic conducting region G, initially at a constant temperture T_0 is immersed in a cooler environment at a temperture T_1, it takes forever to reach thermal equilibrium. In some practical sense though, similarity arguments convince us that it takes four times as long to cool a region twice the size of G when subject to Dirichlet boundary conditions. But, is there a natural finite time to associate with the thermal transition between steady states that leads to a more specific dependence of the process on geometric factors of size and shape?

The Greens function formulation of the solution for linear conduction problems leads us to consider a function $\theta(x)$ we call the mean action time for this role by associating $\theta(x)$ with the mean residence time in G of a unit pulse of diffusing particles released at x. This mean residence time can also be identified with a time lag function describing the asymptotic behaviour of associated particle fluxes out of G generated by switching on constant sources. The mean action time concept is established and shown to satisfy a Poisson problem in section two. The next section explores the time lag connection and associates $\theta(x)$ with the time lag constant and asymptotic properties of the flux of heat into G generated by small disturbances of the solution produced by maintaining the initial temperature T_0 on very small spheres centred at x. In section five the concepts are generalised to conduction problems with phase changes. The generalised mean action time θ also satisfies a Poisson equation and there are associated boundary conditions when the conductivity is constant or Dirichlet boundary conditions apply.

An inverse approach demonstrates the existence of unique ellipsoid - like regions for which there are quadratic solutions of Poissons equation satisfying mixed linear boundary conditions. These solutions lead to simple formulae for cooling and freezing times of near ellipsoidal regions and provide a convenient rule-of-thumb expression for the cooling and freezing times of such convex shapes. Graphs of these pseudo-ellipses are given, comparing their shapes for a wide range of values of the heat transfer coefficient.

2 Mean Action Time

The thermal transition time problem is in some ways similar to that of comparing rates of decay of radioactive elements. If m is the mass of undecayed matter of some element at time t, there is a decay constant k, characteristic of each element such that

$$\frac{dm}{dt} = -km. \tag{2.1}$$

It takes forever for m to vanish exponentially, but for each k there is a finite mean life time t for undecayed atoms given by the expression

$$\tilde{t} = -\int_0^\infty t\frac{dm}{dt}dt \Big/ \int_0^\infty -\frac{dm}{dt}dt = \int_0^\infty mdt \Big/ \int_0^\infty kmdt = \frac{1}{k}. \tag{2.2}$$

For linear heat conduction problems there is an analogous finite comparitive time $\theta(x)$, the mean action time defined at each point x by

$$\theta(x) = \int_0^\infty t\frac{\partial T}{\partial t}dt \Big/ \int_0^\infty \frac{\partial T}{\partial t}dt \tag{2.3}$$

which associates a mean local energy decay time with the transition process. The analogy is clearer and more compelling if we compare the radioactive decay problem with the problem for linear diffusion of a chemical from a region G.

Suppose $C(x,t)$ is a suitable measure of concentration or diffusion potential of a chemical per unit volume at x in a region G at time t, and that $C = C_0$ in G at

$t = 0$ and satisfies the linear diffusion equation

$$\frac{\partial C}{\partial t} = D\nabla^2 C \text{ in } G, \quad t > 0, \tag{2.4}$$

and boundary conditions

$$C + \beta\frac{\partial C}{\partial n} = 0 \text{ on } \partial G \text{ the boundary of } G, \quad t > 0. \tag{2.5}$$

The diffusivity coefficient D is the ratio $\bar{D}/a$ of the diffusion constant $\bar{D}$ and a storage capacity coefficient a.

If G has a sufficiently smooth boundary, the solution of this problem is given in terms of an associated Green's function $g(x, x^*; t - t^*)$ by the expression

$$C(x,t) = C_0 - C_0 \int_0^t \int_{\partial G} D\frac{\partial G}{\partial n^*}(x, x^*; t - t^*) ds^* dt^*, \tag{2.6}$$

so that

$$\frac{\partial C}{\partial t}(x,t) = q_G(x,t) = -C_0 \int_{\partial G} D\frac{\partial G}{\partial n^*}(x, x^*; t) ds^* \tag{2.7}$$

where q_G is the flux of chemical out of G when it is initially free of matter and a unit pulse of chemical is released at x at time zero. For such a pulse the molecules have a mean residence time θ in G given by

$$\theta(x) = \int_0^\infty t q_G dt \Big/ \int_0^\infty q_G dt$$

and if $Q_G(x,t)$ is the amount of chemical which has passed out of G at time t so that

$$Q_G(x,t) = \int_0^t q_G(x,\tau) d\tau,$$

then from equation (2.6) and (2.7),

$$C(x,t) = C_0 - Q_G(x,t)$$

and $\theta(x) = \int_0^\infty [Q_G(x,\infty) - Q_G(x,\tau)]\, d\tau / Q_G(x,\infty) = \int_0^\infty C(x,\tau) d\tau / C_0$.

Note that θ satisfies the Poisson problem

$$\begin{aligned} D\nabla^2\theta &= \int_0^\infty \frac{\partial C}{\partial t} dt / C_0 = -1 \text{ in } G \\ \theta + \beta\frac{\partial \theta}{\partial n} &= 0 \text{ on } \partial G. \end{aligned} \tag{2.8}$$

For our original problem (2.4), (2.5), the molecules also have a mean residence time $\mathbf{t}$ in G given by

$$\begin{aligned} \mathbf{t} &= -\int_0^\infty t \int_{\partial G} D\frac{\partial C}{\partial n} ds dt / -\int_0^\infty \int_{\partial G} D\frac{\partial C}{\partial n} ds dt \\ &= -\int_0^\infty t \int_G \frac{\partial C}{\partial t} dv dt / -\int_0^\infty \int_G \frac{\partial C}{\partial t} dv dt \\ &= \int_G \theta(x) dv / \int_G dv. \end{aligned} \tag{2.9}$$

(In the case of zero β, and G a cylinder, $\mathbf{t}$ is the torsional rigidity of the cylinder.)

If $q(t)$ is the flux of chemical through ∂G at time t for our problem (2.4), (2.5) and $Q(t)$ is the accumulated mass lost from G in time t, then

$$\begin{aligned} \mathbf{t} &= \int_0^\infty t q(t) dt / \int_0^\infty q(t) dt \\ &= \int_0^\infty [Q(\infty) - Q(t)]\, dt / Q(\infty) \end{aligned} \tag{2.10}$$

The mass loss function $Q(t)$ is readily measured experimentally and leads to an estimate for $\mathbf{t}$. On the other hand, $\mathbf{t}$ can be calculated from the Poisson problem (2.8), (2.9), and so formula (2.10) can be used to estimate the diffusivity D of the medium. Since Q_∞ is VaC_0 where V is the volume of G and aC_0 is the total storage capacity for the chemical of unit volume of the medium when the initial concentration is C_0, the diffusion constant $\bar{D}$ is obtained from $\bar{D} = Da$.

3 The Time Lag Function

We can view expression (2.6) from another point of view. The function

$$H(x, x^*, t) = \int_0^t G(x, x^*, t - t^*) dt^*$$

represents a source of unit strength switched on at the point x in G at time $t = 0$. The function $Q_G(x, t)$ is then the flux through ∂G at time t due to such a constant source of strength C_0 and tends to a limiting constant value $Q_G(x, \infty) = C_0$ at

large times. If $P_G(x,t)$ is the total mass of chemical out of ∂G at time t so that

$$P_G(x,t) = \int_0^t Q_G(x,\tau)d\tau,$$

then as t tends to infinity, P_G approaches a linear asymptote. Since $Q_G(x,\infty) = C_0$ it can be seen that

$$\begin{aligned} P_G(x,t) &\sim C_0 t - \int_0^\infty [Q_G(x,\infty) - Q_G(x,\tau)]\, d\tau \\ &= C_0 [t - \theta(x)]. \end{aligned}$$

and hence $\theta(x)$ is the time lag for this unit source switched on at x at time zero.

This is a general property of linear systems. If θ is the mean passage time for particles leaving a linear system through a gate and these same particles originate from a pulse released at $t = 0$ at a certain point in the system, then θ is also the time lag constant for the flux through the gate produced by a uniform source switched on at $t = 0$ at the same point [1].

Ussing's flux ration theorem [5] leads to another physical interpretation for $\theta(x)$ for linear diffusion problems which is of special interest since it remains viable for an important class of non linear diffusion problems.

Consider an infinitisimal constant source $\epsilon H(x,x^*,t)$ switched on at x in G at $t = 0$. In a time of order ϵ^2, C is almost 1 on a small sphere $S(x,\epsilon^*)$ of radius $\epsilon^* = \epsilon/4\pi D$ centred at x and ϵH is a very good approximation to the solution C_ϵ of the following problem: C_ϵ satisfies equation (2.4) in G less the sphere $S(x,\epsilon^*)$, and the initial condition, $C_\epsilon = 0$; $C_\epsilon = 1$ on $S(x,\epsilon^*)$ for $t > 0$.

The flux of chemical over ∂G has a time lag constant $\theta(x)$ in the limit as ϵ goes to zero. Now Ussings flux ratio theorem considers a complimentary solution C_ϵ^* of (2.4) satisfying boundary conditions; $C_\epsilon^* = 0$ in $G - S(x,\epsilon^*)$ at $t = 0$, $C_\epsilon^* = 0$ on $S(x,\epsilon^*)$ for $t > 0$, $C_\epsilon^* + \beta\frac{\partial C_\epsilon^*}{\partial n} = 1$ on ∂G for $t > 0$, and equates the flux $q_{\partial G}(x,t)$ out of the region through ∂G for the first problem in $G - S(x,\epsilon^*)$ to the complimentary flux $q_s^*(x,t)$ through $S(x,\epsilon^*)$ associated with the complimentary solution C_ϵ^*. The

flux $q_s^*(x,t)$ must therefore have the same asymptotic properties and hence the same limiting time lag constant $\theta(x)$ as ϵ tends to zero, as $q_{\partial G}(x,t)$. In the limit as ϵ tends to zero C_ϵ^* tends to the solution $1-C$ where C satisfies the problem (2.4),(2.5) except at the point x, the centre of $S(x,\epsilon^*)$.

This gives an important physical interpretation for mean action time for conduction problems. Suppose our medium G is initially at a constant temperature T_i and at $t=0$ is immersed in an environment at an ambient temperature T_a. If the temperature on a small sphere $S(x,\epsilon)$ is maintained at T_i, then the flux of the heat through $S(x,\epsilon)$ has a time lag constant $\theta_\epsilon(x)$ which tends to the function $\theta(x)$, the mean action time at x as ϵ tends to zero, which for some constant A, satisfies a Poisson problem $\nabla^2\theta = -A$ in G, $\theta + \beta\frac{\partial\theta}{\partial n} = 0$ on ∂G.

4 Freezing and Thawing Problems

A more general setting for our thermal transition problem involving a homogeneous isotropic region G of material with heat conductivity $k(T)$ and internal energy $E(T)$ per unit volume which can handle discontinuities in E at temperatures where phase changes occur is as follows.

Physical considerations require a positive conductivity $k(T)$ and an internal energy E which is a monotone increasing function of the temperature T. Since energy is conserved in any arbitrary volume V in G (if you like, all spheres in G), and if V has a smooth enough boundary ∂V, we must have

$$\frac{\partial}{\partial t}\int_v E dV = \int_{\partial V} k(T)\frac{\partial T}{\partial n} ds \tag{4.1}$$

where $\frac{\partial T}{\partial n}$ is the temperature gradient along outwardly directed normals to ∂V. If, on the boundary ∂G of G the energy flux (per unit surface area) out of G is $\alpha(T-T_a)$, where T is the temperature on ∂G and T_a is the ambient temperature

ultimately assumed by G, then

$$k(T)\frac{\partial T}{\partial n} + \alpha(T - T_a) = 0, \text{ on } \partial G \tag{4.2}$$

If $T = T_i$ in G at $t = 0$, and T satisfies the conservation equation (3.1) and boundary condition (3.2) there is a generalisation of the mean action time (2.3) for linear problems, defined by the density function $J(x,t)$ given by,

$$J(x,t) = \frac{\partial}{\partial t}\int_{T_a}^{T} k(s)ds / \int_{T_a}^{T_i} k(s)ds. \tag{4.3}$$

Consider the expression

$$\phi(x) = \int_0^\infty tJ(x,t)dt = \int_0^\infty \int_{T_a}^{T} k(s)ds / \int_{T_a}^{T_i} k(s)ds. \tag{4.4}$$

We see from (4.1) that for any volume V with a suitably smooth surface ∂V in G,

$$\begin{aligned}
\int_{\partial V} \frac{\partial \phi}{\partial n} ds &= \int_0^\infty \int_{\partial V} k(T)\frac{\partial T}{\partial n} ds dt / \int_{T_a}^{T_i} k(s)ds \\
&= \int_0^\infty \frac{\partial}{\partial t}\int_V E dv dt / \int_{T_a}^{T_i} k(s)ds \\
&= -\int_V [E(T_i) - E(T_a)] / \int_{T_a}^{T_i} k(s)ds
\end{aligned}$$

If gradϕ is continuously differentiable in G, the divergence theorem and arbitrariness of V leads to a Poisson equation

$$\nabla^2\phi = -[E(T_i) - E(T_a)] / \int_{T_a}^{T_i} k(s)ds = -A \tag{4.5}$$

for ϕ in G. If ϕ is normalised by defining $\Psi \equiv \phi/A$, we see that

$$\nabla^2\Psi = -1 \text{ in } G. \tag{4.6}$$

The function Ψ can be found via equation (4.6) when known boundary conditions exist for it on ∂G. This is immediately true in two useful special cases. The first case is concerned with Dirichlet boundary conditions for T in the case $\beta = 0$.

From (4.4) we see that when $T = T_a$ on ∂G, $\phi(x) = 0$ on ∂G. The second case is associated with constant conductivity k. In this case; $k(T)$ constant and equal to K say, we see that from equation (4.2) that

$$\phi(x) = \int_0^\infty \frac{(T - T_a)}{(T_i - T_a)} dt = -\frac{K}{\alpha} \int_0^\infty \frac{\partial}{\partial n} \frac{(T - T_a)}{(T_i - T_a)} dt \tag{4.7}$$

$$= -\frac{K}{\alpha} \frac{\partial \phi}{\partial n} \text{ on } \partial G. \tag{4.8}$$

and hence

$$\beta \frac{\partial \Psi}{\partial n} + \Psi = 0 \text{ on } \partial G, \text{ where } \beta = K/\alpha. \tag{4.9}$$

In these two cases Ψ is a geometric factor in the mean action time expression $\theta = A\Psi$, dependent on size, shape, and the boundary constant β in the second case. Once again it can be shown [1] that $\phi(x)$ is the limiting value for the time lag of fluxes down a spherical hole $S(x, \epsilon)$ in G as ϵ goes to zero when T is maintained at T_i on the sphere.

For freezing problems, t^* the greatest value of ϕ in G is a useful comparative time for the transition from T_i to T_a when T_m the melting point lies between T_i and T_a and is associated with most of the energy change ΔE. Consider the case $T_i = T_m > T_a$ and the material is initially unfrozen at its freezing point. Let t_{fr} be the time the last point in G freezes and suppose this happens at x^*. Then at x^*, $T = T_i = T_m$ for $0 \leq t \leq t_{fr}$ so that from (4.4)

$$t^* = \phi(x^*) = \int_0^{t_{fr}} \frac{(T_i - T_a)}{(T_i - T_a)} dt + \int_{t_{fr}}^\infty \frac{(T - T_a)}{(T_i - T_a)} dt$$

$$\geq t_{fr}$$

In the extreme case where E is a step function and $E = E(T_a) \equiv E_a$ for $T_m < T \leq T_a$, $E = E(T_i) = E_i$ for $T = T_i = T_m^+$ we see that $t^* = t_{fr}$.

In this case the time and position for the last point to freeze in G can be found from $\Psi(x)$ the solution of a Poisson problem.

5 Simple Solutions and Pseudo-Ellipsoids

Simple exact solution of the Poisson problem (4.6), (4.8) can be found for spheres, box shapes, finite cylinders and even equilateral triangles in two dimensions. [2]. When $\beta = 0$ and G is an ellipsoid with semi-axis a, b and c, the Poisson problem has the solution

$$w = \left(1 - \frac{x^2}{a^2} - \frac{y^2}{b^2} - \frac{z^2}{c^2}\right) / 2 \left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right) \tag{5.1}$$

In this cas

$$t^* = (E_i - E_a)/2K(T_i - T_a) \left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right) \tag{5.2}$$

gives a useful comparative formula for freezing or chilling of regions G which are roughly ellipsoidal in shape with axial diameters 2a, 2b and 2c. Even for non-symmetric lens shapes, formulae like (5.2) using inner and outer radii do very well for the $\beta = 0$ case. [3]

For the more realistic $\beta > 0$, there is no known corresponding exact solution for G an ellipsoid. However, the global solution (5.1) of (4.6) can be used in conjunction with (4.8) to derive a first order partial differential equation for surfaces ∂G. It is shown in [4] that there are many simply connected closed surfaces ∂G which contain the origin and define a region G in which (5.1) is an exact solution of (4.6), (4.8), but only one of these surfaces has a continuously varying and well-defined normal at all its points. We call this surface a pseudo-ellipsoid for the following reasons. When β is less than one, the surface is very close to an ellipsoid with semi axes x_1, y_1, z_1, given by the positive roots of

$$a^2 = x_1^2 + 2\beta x_1, \quad b^2 = y_1^2 + 2\beta y_1, \quad c^2 = z_1^2 + 2\beta z_1, \tag{5.3}$$

As β increases, the shape change from ellipsoidal to a limiting convex surface S^*. In the case $a = b = c$, the pseudo-ellipsoids and S^* are spheres, but otherwise S^* is more box-like, expecially for $c \gg a$. For all β, the pseudo-ellipsoid lies inside

and touches all sides of the box $|x| = x_1$, $|y| = y_1$, $|z| = z_1$, and lies outside the surface S_0 on which

$$w = \beta|\text{grad } w| = \beta(w_x^2 + w_y^2 + w_z^2)^{\frac{1}{2}} \tag{5.4}$$

Graphs of axial cross sections of pseudo-ellipsoids $S(x_1, y_1, z_1, \beta)$ for various values of β and axial dimensions are shown in Figure 1. These surfaces have simple quadratic exact solutions for problem (4.6), (4.8) and t^* is given by the expression;

$$t^* = (E_i - E_a)/\left\{2K(T_i - T_a)\left[(x_1^2 + 2\beta x_1)^{-1} + (y_1^2 + 2\beta y_1)^{-1} + (z_1^2 + 2\beta z_1)^{-1}\right]\right\} \tag{5.5}$$

This formula provides a simple rule-of-thumb for the comparative assessment of freezing and chilling times for ellipsoid-like shapes with semi-axes x_1, y_1 and z_1.

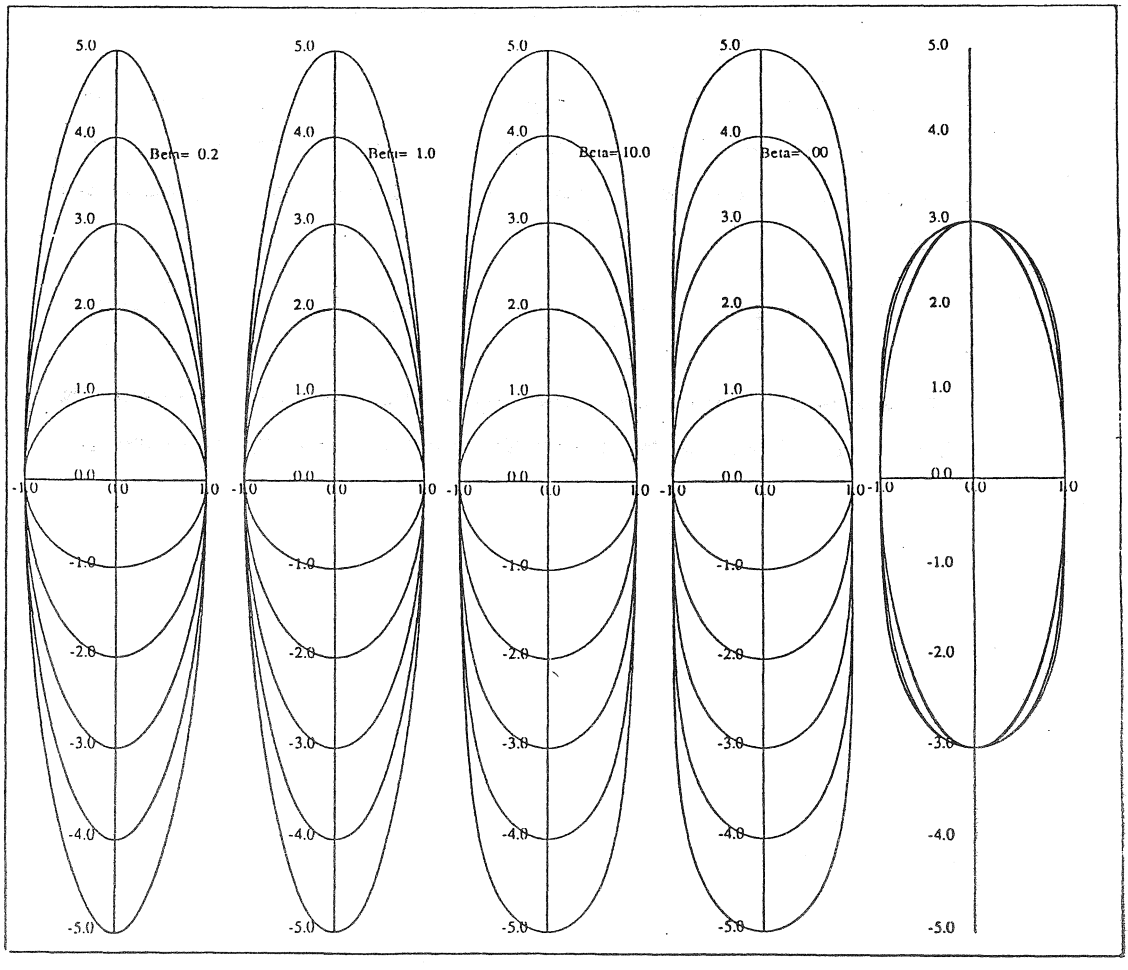

Figure 1. Pseudo-ellipses for $y_1 = 1$; $z_1 = 1, 2, 3, 4, 5$; $\beta = 0.2, 1.0, 10, \infty$; and a superposition of the curves in the case $z_1 = 3$. The $\beta = 0$ and $\beta = 0.2$ curves are indistinguishable. These diagrams are in the $y - z$ plane with y horizontal and z vertical.

References.

1. McNabb, A., and Wake, G.C. Heat Conduction and finite transition times between steady-states. I.M.A. Journal of Applied Mathematics (1991, to appear).

2. McNabb, A., and Wake, G.C. Massey University, Palmerston North, New Zealand, Department of Mathematics and Statistics Research report No. 17, February 1989.

3. McNabb, A., and Keady, G. Some explicit solutions of $-\Delta w = 1$ with zero boundary data. University of Western Australia, Department of Mathematics, Research Report 42, December 1988.

4. McNabb, A., Wake, G.C., Lambourne, R.D. and Anderssen, R.S. Theoretical derivation of rules-of-thumb for freezing times. The Australian National University, Centre for Mathematical Analysis, Research Report CMA - R40 - 90 (1990).

5. Ussing, H.H. Interpretation of tracer fluxes. Membrane Transport in Biology. G. Giebisch, D.C. Tosteson and H.H. Ussing, Eds Vol. 1, 115-140, New York, Springer (1978).

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