GPHS/MATH 323 Mathematics for Earth Science IV

The Diffusion Equation

Fourier's law of heat conduction

This can be stated as: "Heat flows by conduction from high temperatures to low at a rate, dq/dt, depending on the temperature gradient." The constant of proportionality is called the thermal conductivity, k, and depends on the material.

This can be written:

$$d\mathbf{q}/dt = -k \nabla T$$

where T is temperature and d**q** / dt is the rate of heat flow at a point. It is a vector quantity because it may flow in different directions. The negative sign is because of the flow from high T to low T.

In tensor notation:

$$dq_j/dt = -k \, \partial T / \partial x_j$$

Darcy's Law

Darcy's law describes the flow of fluids in a permeable material, and may be stated as: "Fluid flows from high pressure to low at a rate dq / dt depending on the pressure gradient".

This is consistent with the special case of the Navier-Stokes equations for low viscosity fluids (like water).

The constant of proportionality increases with permeability, k, and decreases with increasing fluid viscosity, μ, so may be written k/μ. This can be written

$$d\mathbf{q}/dt = -k/\mu \, \nabla P$$

where P is pressure and d**q** / dt is the rate of fluid flow at a point. It is a vector quantity because it may be different in different directions.

$$dq_j/dt = -k/\mu \, \partial P / \partial x_j$$

The similarity between the two laws is obvious. Both the processes are examples of *diffusion* of something through a medium offering resistance to the flow. The PDE we will develop can be applied to all such processes.

Returning to heat: dq_j /dt points in the direction of maximum decrease of T. If we want the flow in a direction n_j, we calculate this by $n_j \, dq_j$ /dt (scalar product).

We calculate the amount of heat flowing into a volume V bounded by a surface S. At the right moment we shall use Gauss's divergence theorem.

First we need the relationship between change in heat content and change of temperature of a material. The two are related by the *specific heat c*, which depends on the particular material.

Specific heat *c* is defined to be the amount of heat dQ required to raise the temperature of a unit mass by 1 K (we shall use both the Celsius and the Kelvin temperature scale: degrees K = degrees Celsius + 273.15)

Symbolically: *c* = dQ/dT per unit mass.

(NB a distinction is made between Q and q for clarity: but BOTH represent a *quantity of heat*)

Note that for gases c may be defined per unit volume as an alternative to per unit mass.

The heat increase dQ inside V in time dt is

$$dQ = \{ - \iint_S n_j (dq_j /dt) dS + \iiint_V g \, dV \} \, dt$$

where we allow the possibility that heat is being generated inside V by $g(x_j)$ per unit volume per unit time.

Apply Gauss's theorem to the first term:

$$dQ = \{ - \iiint_V \partial (dq_j /dt) / \partial x_j \, dV + \iiint_V g \, dV \} \, dt$$

This results in an increase of temperature $= (\partial T / \partial t) \, dt$. So we have

$$dQ = \iiint \partial T / \partial t \; dt \; c \, \rho \, dV = \{ \iiint c \, \rho \, \partial T / \partial t \; dV \} \, dt$$

Equate the two expressions for dQ and collect under one integral sign:

$$\{ \iiint_V [- \partial (dq_j /dt) / \partial x_j + g - c \, \rho \, \partial T / \partial t] \, dV \} \, dt = 0$$

Now we apply a familiar argument. For this to be true for any volume V, we require that the integrand inside [ ] be zero everywhere. So:

$$- \partial (dq_j /dt) / \partial x_j + g - c \, \rho \, \partial T / \partial t = 0$$

Now substitute for (dq_j /dt) using Fourier's law:

$$- \partial (- k \, \partial T / \partial x_j) / \partial x_j + g - c \, \rho \, \partial T / \partial t = 0$$

or

$$c \, \rho \, \partial T / \partial t = \partial (k \, \partial T / \partial x_j) / \partial x_j + g$$

If the thermal conductivity k is constant, we can take this outside the gradient operator and write

$$\partial T / \partial t = (k / c \, \rho) \, \partial^2 T / \partial x_j \partial x_j + g / c \, \rho \qquad\qquad (1)$$

This is the Heat Diffusion equation (with constant conductivity) with sources g. The constant

$k / c \, \rho$ is called the *thermal diffusivity* K. We recognise $\partial^2 T / \partial x_j \partial x_j$ as $\nabla^2 T$.

So :

$$\partial T / \partial t = K \nabla^2 T + (g / c \, \rho) \qquad\qquad (1a)$$

This completes our trio of famous and important PDEs for the physical world.

Units of constants (courtesy Wikipedia)

J = Joule – units of heat – work done by a force of 1 Newton over 1 metre.
k thermal conductivity (SI units : $W\ m^{-1}\ K^{-1}$) (W = Watt = $J\ s^{-1}$)
ρ density (SI units : $kg\ m^{-3}$)
c specific heat capacity (SI units : $J\ kg^{-1}\ K^{-1}$) (J Joule)
c ρ volumetric heat capacity (SI units : $J\ m^{-3}\ K^{-1}$))

K = k / *c* ρ thermal diffusivity (SI units : $m^2\ s^{-1}$)

Material	Thermal conductivity $W\ m^{-1}\ K^{1}$	Specific heat $10^3\ J\ kg^{-1}\ K^{-1}$	Diffusivity $10^{-6}\ m^2\ s^{-1}$
Diamond	900-2320	0.51	1100
Silver	429	0.233	200
Stainless steel	12-45		1
Rock	1.7-2.4	0.8-0.9	1
Concrete	1.7	0.88	1
Glass	1.1	0.5-0.9	1
Ice	2	2.05	1
Air	0.025	1.0	24

Functional forms of solutions to the (heat) diffusion equation

At this stage we will omit the possibility of sources, and consider the heat diffusion equation without internal sources:

$$\partial T / \partial t = K \nabla^2 T$$

Separated solution

We start with our first trial method of separated solutions.

Write $T(x_j, t) = X(x_1)\ Y(x_2)\ Z(x_3)\ C(t)$. Then

$$\partial T / \partial t - K \nabla^2 T = 0$$

is satisfied if

$$XYZ\ dC/dt - K\{ YZC\ d^2X/dx_1^2 + XZC\ d^2Y/dx_2^2 + XYC\ d^2Z/dx_3^2 \} = 0$$

Divide through by XYZC:

$$(1/C)\ dC/dt - K\{ (1/X)\ d^2X/dx_1^2 + (1/Y)\ d^2Y/dx_2^2 + (1/Z)\ d^2Z/dx_3^2 \} = 0$$

which is quite like the result for the wave equation except that it is the *first* derivative of C(t) that appears, not the second.

As before, each term only depends on one variable, so set

$$(1/X)\ d^2X/dx_1^2 = \nu_1^2 ,$$

$$(1/Y)\ d^2Y/dx_2^2 = \nu_2^2 ,$$

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$$(1/Z)\, d^2Z/\, dx_3^{\,2} = \nu_3^{\,2}\ ,$$

Then the constant for the C term is specified by the ν_j:

$$(1/C)\, dC/dt = K\{\ \nu_1^{\,2}\ +\ \nu_2^{\,2}\ +\ \nu_3^{\,2}\ \}$$

Physical problems could involve situations where dC/dt is negative (heat loss with time) or positive (heat accumulating in a furnace or reactor). Since K is positive, the RHS is positive unless (some of) the ν_j are complex.

Write $K\{\ \nu_1^{\,2}\ +\ \nu_2^{\,2}\ +\ \nu_3^{\,2}\ \} = \lambda$. Then the solution for C is

$$C(t) = C_0\, \exp(\ \lambda\ t).$$

λ could also be complex. The appropriate choice for these constants will depend, as usual, on the boundary conditions.

So the full solution is of the form:

$$T(x_j,\ t\ ) = C_0\, \exp(\ \lambda\ t)\, \exp(\pm\nu_1\ x_1)\, \exp(\pm\nu_2\ x_2)\, \exp(\pm\nu_3\ x_3)$$

We will find an application for this solution later.

A change of variable

The second spatial derivative and only one time derivative mean that there is a class of solutions to the diffusion equation that depend on $\xi = a\,(\ x_1^{\,2} + x_2^{\,2} + x_3^{\,2}\ )/\,t$ for a suitable constant *a*.

Without too much loss of generality, we will drop to one spatial dimension. It will be easy to see the generalisation of 3-D later.

So, with one eye on the solution to the diffusion equation above, and also the wave equation and Laplace's equation, try a solution

$$T(x,\ t) =\ t^{\,-1/2}\, \exp(\ -\ a\, x^2/\,t\ )$$

The appearance in the 'trial' solution of the $t^{\,-1/2}$ term is distinctive.

Now:
$$\partial T/\, \partial t =\ -1/2\ t^{\,-3/2}\, \exp(\ -\ a\, x^2/\,t\ ) + a\, x^2\, t^{\,-5/2}\, \exp(\ -\ a\, x^2/\,t\ )$$

$$\partial T/\, \partial x =\ -2\, a\, x\, t^{\,-3/2}\, \exp(\ -\ a\, x^2/\,t\ )$$

$$\partial T^2/\, \partial x^2 =\ -2\, a\, t^{\,-3/2}\, \exp(\ -\ a\, x^2/\,t\ )\ +\ 4\, a^2\, x^2\, t^{\,-5/2}\, \exp(\ -\ a\, x^2/\,t\ )$$

So to satisfy:

$$\partial T\, /\partial t\ -\ K\, \nabla^2 T = 0$$

we need $(-1/2) = K\,(-2a)$ and $a = K\,(4\,a^2)$

which fortunately (!) are both satisfied if $a = 1/\,(4K)$

So
$$T(x,\ t) =\ t^{\,-1/2}\, \exp[\ -\ x^2/(4K\,t\ )\ ]$$

is a particular solution to the heat diffusion equation.

Interpretation

For any $x \neq 0$,

$$\lim_{t \to 0} \{ \exp[- x^2/(4K t)] / t^{1/2} \}$$

$$= \lim \zeta = 1/t \to \infty \quad \zeta^{1/2} \exp[- x^2 \zeta /(4K)]$$

$= 0$, because $\exp(- \zeta)$ goes to zero faster than $\zeta^{1/2}$ increases.

Proof: L'Hôpital's rule. Put $\zeta^{1/2} \exp[- x^2 \zeta /(4K) = \zeta^{1/2} / \exp[+ x^2 \zeta /(4K)]$.

However, at $x = 0$,

$$\lim_{t \to 0} \{ \exp[- x^2/(4K t)] / t^{1/2} \} = \lim_{t \to 0} \{ \exp[0] / t^{1/2} \} = \infty$$

So there is some sort of singularity at $t = 0$.

From before, heat and temperature are linked by:

$$dQ = c \rho \, dT$$

where dQ is the amount of heat required to raise the temperature by dT in a unit volume. If c is independent of T, we can write

$$Q = c \rho (T - T_0)$$

So in a volume of area 1 unit in the plane $x = 0$ and thickness dx, the heat required for an *increase* of T from $T_0 = 0$ is

$$Q = c \rho \, T \, dx$$

Add this up per unit (zy) area for all x:

$$Q(\text{total}) = \int_{-\infty}^{\infty} c \rho \, T \, dx$$

$$= c \rho \int_{-\infty}^{\infty} t^{-1/2} \exp[- x^2/(4K t) \, dx$$

for any $t > 0$.

We evaluate this by making use of a result from statistics. The Gaussian probability density function is

$$f(x) = 1/ \sqrt{(2\pi \sigma^2)} \exp[- x^2/(2 \sigma^2)]$$

where the constant at the front has been chosen so that (as required for pdfs)

$$\int_{-\infty}^{\infty} 1/ \sqrt{(2\pi\sigma^2)} \exp[- x^2/(2 \sigma^2)] \, dx = 1$$

So put $\sigma^2 = 2K t$, and then

$$\int_{-\infty}^{\infty} t^{-1/2} \exp[- x^2/(4K t)] \, dx = 2 \sqrt{(\pi K)}$$

So

$$Q(total) = c\,\rho\,2\,\sqrt{(\pi K)}$$

So we have the interpretation: this amount of heat *per unit area* was released (in a spike) at t = 0 at x = 0 uniformly over the yz plane and then diffused throughout all space.

This may have application in some circumstances e.g. the sudden production of heat in an explosion, etc.

Derivatives and integrals of a solution

If w(x, t) is a solution of the diffusion equation, then so is

$$W(x, t) = \int_0^x w(t, \xi)\, d\xi$$

Proof: $\partial W/\partial x = w$, and w satisfies the diffusion equation

$$\partial T/\partial t - K\,\nabla^2 T = 0$$

So

$$\partial w/\partial t - K\,\nabla^2 w = 0$$

Substitute for w:

$$\partial\,(\partial W/\partial x)/\partial t - K\,\nabla^2(\partial W/\partial x) = 0$$

and switch the order of the differentiation

$$\partial\,(\partial W/\partial t)/\partial x - K\,(\partial/\partial x)\,\nabla^2 W = 0$$

or

$$\partial/\partial x\,(\partial W/\partial t - K\,\nabla^2 W) = 0$$

so

$$\partial W/\partial t - K\,\nabla^2 W = constant$$

so we choose the constant to be 0! Or we could recognise that we have solved the problem:

$$\partial W/\partial t = K\,\nabla^2 W + (g/c\,\rho) \qquad\qquad (1a)$$

for a constant distribution of heat sources in the material e.g. from radioactive minerals in rock.

Application to $T(x, t) = t^{-1/2}\exp(-a\,x^2/t)$

From the above,

$$T(x, t) = \int_0^x t^{-1/2}\exp[-\xi^2/(4K t)]\, d\xi$$

is a particular solution for the diffusion equation.

Substitute $\zeta^2 = \xi^2/(4K t)$.   Then

$$2\zeta\, d\zeta = 2\,\xi/(4K t)\, d\xi$$

or

$$d\xi = [\xi/\sqrt{(4K t)}\,]/\,\xi/(4K t)\, d\zeta = 2\,\sqrt{(K t)}\, d\zeta$$

So

$$T(x, t) = \int_0^{x(4Kt)^{-1/2}} t^{-1/2} \exp(-\zeta^2) \, 2\sqrt{(Kt)} \, d\zeta$$

$$= 2\sqrt{K} \int_0^{x(4Kt)^{-1/2}} \exp(-\zeta^2) \, d\zeta$$

Now from the discussion about the Gaussian pdf above:

$$\int_{-\infty}^{\infty} 1/\sqrt{(2\pi)} \exp[-x^2/2] \, dx = 1$$

(put $\sigma = 1$) and because of symmetry

$$\sqrt{(2/\pi)} \int_0^{\infty} \exp[-x^2/2] \, dx = 1$$

The linkages between these has led to the naming of the integral:

$$\mathrm{erf}(y) = \sqrt{(2/\pi)} \int_0^{\sqrt{2}y} \sqrt{2} \exp(-\zeta^2/2) \, d\zeta /\sqrt{2} = 2/\sqrt{\pi} \int_0^{y} \exp(-\xi^2) \, d\xi$$

as the *Error Function*, with the property that

$$\mathrm{erf}(\infty) = 1.$$

We also define the complementary error function

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

And we have shown that $A \, \mathrm{erf}(x(4Kt)^{-1/2})$ is a solution of the diffusion equation

Properties of the erf() solution

We already have most of this function's limits.

For any $x \neq 0$,

$$\lim \, t \to 0 = A \, \mathrm{erf}(\infty) = A.$$

At $x = 0$, $A \, \mathrm{erf}(x(4Kt)^{-1/2}) = A \, \mathrm{erf}(0(4Kt)^{-1/2}) = 0$ for all time $t \neq 0$.

So at x=0,

$$\lim \, t \to 0 \quad A \, \mathrm{erf}(0(4Kt)^{-1/2}) = 0$$

So we have the solution to the problem in the half-space $x \geq 0$ with these boundary conditions:

$T = 0$ on $x = 0$ for all t; $T = A$ at $t = 0$ for all $x \neq 0$.

So this can be thought of as the problem of suddenly (at $t = 0$) reducing the temperature on the surface of a half space (bounded by $x = 0$) from A to 0.

It happens that this is an important problem in several branches of science!

Problem 1: The cooling Earth

Specifically, we are interested in understanding the cooling of the crust under the oceans.

There are a number of reasons for this. For example, it is the cooling of the ocean *lithosphere* (crust plus uppermost mantle) that is the principal driver of plate tectonics.

A pragmatic reason is that the bottom of the ocean is at a near constant temperature of 0 C. This makes the modelling simple!

So we have this problem: A volume of rock at melting point (temperature A) wells up from the mantle at a mid-ocean ridge and (at t = 0) freezes in contact with the water at the bottom of the ocean (the pressure is too great for the water to boil). It moves away from the ridge at some steady speed (order 10-50 mm/yr). Its upper surface is maintained at 0 C. *What is the temperature distribution inside the rock after time t?*

We have a half space problem. The movement of the plate can be dealt with by using Lagrangian coordinates! We will ride with the plate and 'observe' its subterranean cooling.
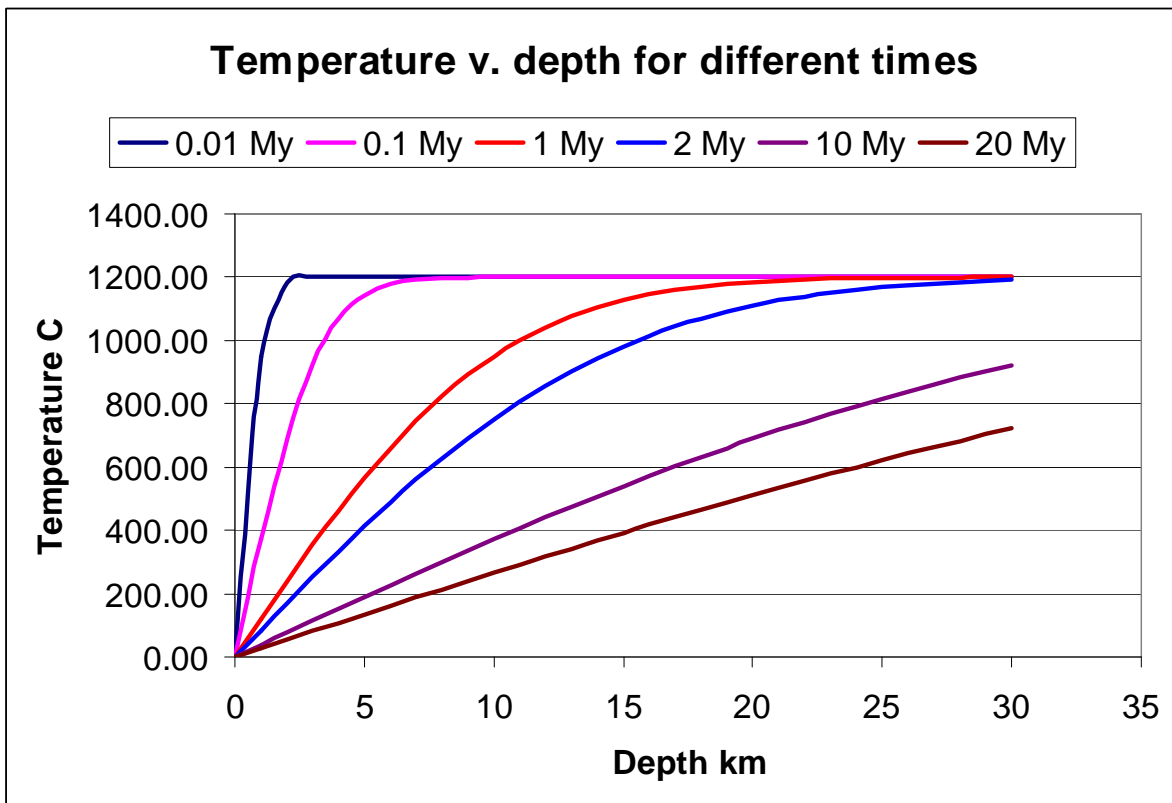
Problem geometry

T = 0 at all time

y axis

Sea bottom

T = *A* ~ 1200 C

at time t = 0.

x axis

(depth)
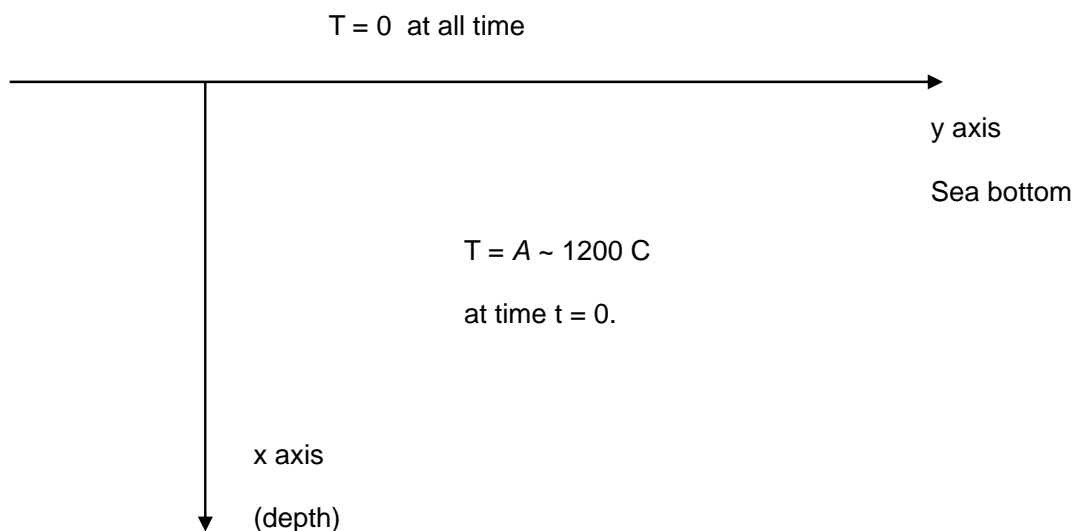
We just write down the answer:

$$T(x, t) = A \, \text{erf}(x \, (4Kt)^{-1/2})$$

$$= \frac{2A}{\sqrt{\pi}} \int_0^{x \, (4Kt)^{-1/2}} \exp(-\xi^2) \, d\xi$$

We can take $A = 1200$ C and $K = 10^{-6}$ m^2 s^{-1}

We get a picture that looks like this:

Temperature v. depth for different times

Testing the model – consequences of cooling

As the rock cools from its initial temperature, it will contract. The contraction is described by the *coefficient of thermal contraction* (volumetric or linear) which may itself depend on temperature.

α = 1/V dV/dT

For sea-floor rocks this is about 3-5 x 10^{-5} K^{-1}.

We can calculate the contraction of a column of sea-floor rock or unit area at any time t using

$$T(x, t) = 2400/\sqrt{\pi} \int_0^{x (4Kt)^{-1/2}} \exp(-\xi^2) \, d\xi$$

At time t, the rock at depth x is at T(x, t), so a column of unit area and length dx has contracted by α (1200-T) dx.

So the total contraction C(t) is

$$C(t) = \int_0^\infty \alpha (1200-T(x, t)) \, dx. = 1200 \alpha \int_0^\infty [1 - 2/\sqrt{\pi} \int_0^{x (4Kt)^{-1/2}} \exp(-\xi^2) \, d\xi] \, dx$$

$$= 1200 \alpha \int_0^\infty \operatorname{erfc}(x (4Kt)^{-1/2}) \, dx$$

Differentiate this with respect to time t:

$$dC(t)/dt = 1200\,\alpha \int_0^\infty \partial/\partial t\,[\,1 - 2/\sqrt\pi \int_0^{x\,(4Kt)^{-1/2}} \exp(-\xi^2)\,d\xi\,]\,dx$$

$$= 1200\,\alpha \int_0^\infty [\,-2/\sqrt\pi\;\partial/\partial t \int_0^{x\,(4Kt)^{-1/2}} \exp(-\xi^2)\,d\xi\,]\,dx$$

$$= 1200\,\alpha \int_0^\infty -2/\sqrt\pi\,[\,\exp(-x^2/(4Kt))\,(-1/2\;x\;4K^{-1/2}\;t^{-3/2})\,]\,dx$$

$$= 1200\,\alpha/\sqrt\pi \int_0^\infty x\,(4Kt)^{-1/2}\;t^{-1}\,[\,\exp(-x^2/(4Kt))\,]\,dx$$

Substitute again: $\xi = x^2\,(4Kt)^{-1}$

So $d\xi = 2\,x\,(4Kt)^{-1}\,dx$ and

$$dC(t)/dt = 1200\,\alpha/\sqrt\pi\;t^{-1} \int_0^\infty (4Kt)^{-1/2}\,[\,\exp(-\xi)\,]\,d\xi\,(2Kt)$$

$$= 1200\,\alpha/\sqrt\pi\;2K\,(4Kt)^{-1/2} \int_0^\infty \exp(-\xi)\,d\xi$$

The integral = 1. So

$$dC(t)/dt = 1200\,\alpha/\sqrt\pi\;K^{1/2}\,t^{-1/2}$$

Now we can integrate this:

$$C(t) = 2400\,\alpha/\sqrt\pi\;K^{1/2}\,t^{1/2} + \text{const.}$$

At t = 0 there is no contraction; so the constant is 0 and

$$C(t) = 2400/\sqrt\pi\;\alpha\,K^{1/2}\,t^{1/2}$$

For $\alpha = 4 \times 10^{-5}\;C^{-1}$ and $K = 10^{-6}\;m^2\,s^{-1}$, and substituting for t in M years, (1 year = $3.156\;10^7$ s)

$$C(t) = 230\,t^{1/2}\;\text{m, with t in Myear}$$

This gives the amount the rocks 'shrink' over time. It predicts that the ocean sea floor will deepen as $t^{1/2}$ as one moves away from a mid-ocean ridge.

However, this is only part of the story. The extra weight of water from the shrinkage is a load on the Earth's surface, under which it will sink some more. The total subsidence is found using the Principle of Isostasy, and is given by:

C(t) (density of the asthenosphere)/(density of the asthenosphere – density of water) ~ 1.45 C(t)

for an asthenosphere density of 3.35 Mg/m^3 and a density of sea water of about 1.04 Mg/m^3.

We can now compare this with the observed water depth.

Our formula predicts an increased water depth of 3300 m at 100 My.

The model has not allowed for a steady input of heat into the lithosphere from the fluid asthenosphere below it, or from radioactive minerals in the lithosphere, or from variation of thermal diffusivity with temperature. These inhibit cooling, so the curves start to diverge at ~ 70 Ma.
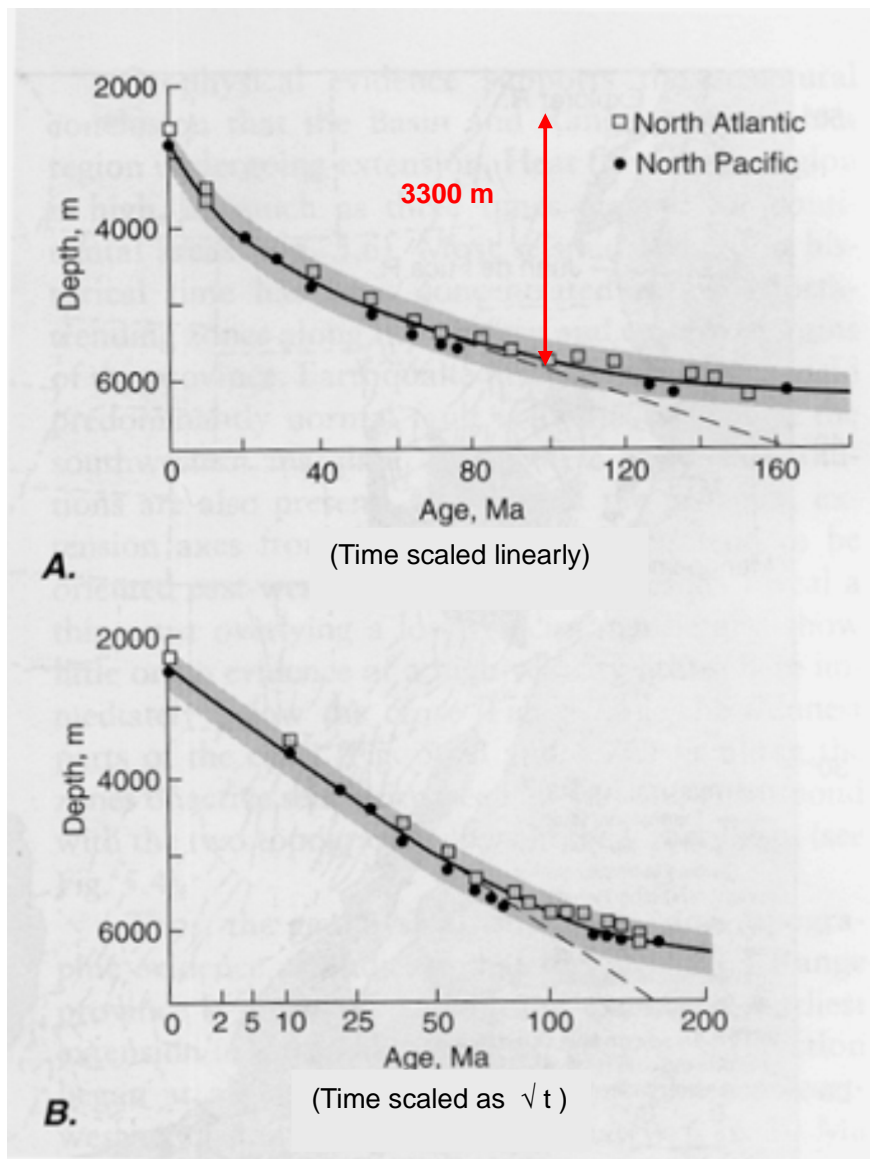
Water depth v. age of ocean floor for the north Pacific and north Atlantic