Note that for the step change problem $T(0, t) = 0.5 \ T_0$, for $t > 0$. The step smears over time and, unlike the diffusion problem, the concentration at the origin changes. It is not a boundary condition.

**Transform Solutions to Heat Diffusion** (see Crank, §2.2)

It can be shown by dimensional analysis that solutions to (30) are often of the form

$$ T(x, t) = \frac{A}{t^{1/2}} \Phi \left[ -\frac{x^2}{4Dt} \right] $$

(68)

where $\Phi$ is a function to be determined\(^\text{19}\). In particular, we’ve already found Gaussian and error function solutions. Notice that the function is *self-similar*. That is, the function is stretched one way or another, but the shape remains unchanged over time-space. You’ve seen such similarity solutions before, in the Theis Well function, which has similarity variable $u = r^2 S / 4 T t$, where the parameters take on the normal well-hydraulics definitions, and hydraulic diffusivity is $D = T / S$.

It is not unusual to assume a solution of the form of (68) and then to seek the coefficient $A$, that matches the boundary and initial conditions. As a demonstration, let’s take a look at one such application of similarity to find another path to a familiar solution.

**Boltzmann Transformation** (Crank, 1975, p. 105; this page is not included in the supplemental reading.) Reconsider the diffusion equation given by

$$ \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( D(T) \frac{\partial T}{\partial x} \right) $$

(69)

with initial and boundary conditions for a semi-infinite domain ($0 \leq x \leq \infty$) described by

- **IC**: $T(x, 0) = T_i$, a constant
- **BC1**: $T(0, t) = T_0$, a constant
- **BC2**: $T(\infty, t) = T_i$, a constant

(79a,b,c)

From our previous work we might expect that the solution involves an error function. Instead, let’s assume only that it is a similarity solution of the type shown in (68). Define a similarity variable

$$ \eta = \frac{x}{\sqrt{4Dt}} $$

(71)

Then apply this change in variables and some chain rules to convert (69) into an ODE. Converting a PDE to an ODE is the goal of many methods that solve parabolic PDEs.

In this case the chain rules are

---

\(^{19}\) Typically its some combination of exponential or error functions.
\[
\frac{\partial (\eta)}{\partial t} = \frac{\partial \eta}{\partial t} \frac{d(\eta)}{d \eta} = \frac{x}{2} D^{1/2} x^{3/2} \frac{d(\eta)}{d \eta} \frac{d(\eta)}{d \eta} \frac{d(\eta)}{d \eta} = \frac{-x}{4 D^{1/2} x^{3/2}} \frac{d(\eta)}{d \eta} \\
\frac{\partial (\eta)}{\partial x} = \frac{\partial \eta}{\partial x} \frac{d(\eta)}{d \eta} = \frac{1}{\sqrt{4Dt}} \frac{d(\eta)}{d \eta} \\
\frac{\partial^2 (\eta)}{\partial x^2} = \frac{\partial}{\partial x} \left[ \frac{\partial \eta}{\partial x} \frac{d(\eta)}{d \eta} \right] = \frac{1}{\sqrt{4Dt}} \frac{d}{d \eta} \left[ \frac{\partial \eta}{\partial x} \frac{d(\eta)}{d \eta} \right] = \frac{1}{\sqrt{4Dt}} \frac{d}{d \eta} \left[ \frac{1}{\sqrt{4Dt}} \frac{d(\eta)}{d \eta} \right] = \frac{1}{4Dt} \frac{d^2(\eta)}{d \eta^2} 
\]

Notice the ordinary derivatives with respect to the similarity variable, \( \eta \). We can substitute into the diffusion equation,

\[
\frac{\partial T}{\partial t} = \frac{-x}{4 D^{1/2} x^{3/2}} \frac{dT}{d \eta} = D \frac{\partial^2 T}{\partial x^2} \frac{d(\eta)}{d \eta} \frac{d(\eta)}{d \eta} \frac{d(\eta)}{d \eta} = \frac{D}{4Dt} \frac{d^2T}{d \eta^2}, \text{ or} \\
\frac{-x}{4 D^{1/2} x^{3/2}} \frac{dT}{d \eta} = \frac{1}{4t} \frac{d^2T}{d \eta^2} 
\]

This simplifies to

\[
\frac{d^2T}{d \eta^2} + \frac{2x}{\sqrt{4Dt}} \frac{dT}{d \eta} = 0 \quad \text{or} \quad \frac{d^2T}{d \eta^2} + 2 \eta \frac{dT}{d \eta} = 0 \quad (73) 
\]

which is a second order ODE. We can solve by reduction in order, say be defining

\[
v = \frac{dT}{d \eta} \quad (75) 
\]

where the symbol \( v \) was chosen arbitrarily. The ODE becomes 1st order,

\[
\frac{dv}{d \eta} + 2 \eta v = 0 \quad (76) 
\]

Its solution, by separation of variables (SOV) and integration, is

\[
\frac{1}{v} \frac{dv}{d \eta} = 2 \eta \frac{d \eta}{d \eta} \rightarrow \ln v = \eta^2 + c_1 \rightarrow v = a_1 \exp \eta^2 \\
\frac{dT}{d \eta} = a_1 \exp \eta^2 \quad (77) 
\]

where \( c_1 \) and \( a_1 \) are constants, and we have derived a new 1st order ODE to solve. We can apply SOV again to get
\[ dT = a_i \exp \eta^2 d\eta \]  

(78)

Obviously, we should integrate this expression.

However, to progress further we need to apply initial and boundary conditions. Recall that it is these conditions that determine the form of the solution to the PDE. In fact, with the Boltzmann approach, it is “only when the initial and boundary conditions are expressible in terms of \( \eta \) alone, and \( x \) and \( t \) are not involved separately, that …” the Boltzmann transformation can be used (Crank, 1975, p. 106). For example, in our case, when \( t=0 \), no matter the value of \( x \), then \( \eta=\infty \). Similarly, when \( x=0 \), then \( \eta=0 \). What about when \( x=\infty \)? We have \( \eta=\infty \), again. Thus our conditions become

\[
\begin{align*}
\text{IC & BC2} & \quad T(\eta=\infty) = T_i, \text{ a constant} \\
\text{BC1} & \quad T(\eta=0) = T_0, \text{ a constant}
\end{align*}
\]

(79a,b)

Let’s use the second condition and integrate from \( \eta=0 \) to \( \eta=x/\sqrt{4Dt} \),

\[
\int_{T_0}^{T} dT = a_i \int_{0}^{\sqrt{4Dt}} \exp \eta^2 d\eta \\
T - T_0 = a_i \frac{\pi}{4} \sqrt{4Dt} \frac{x}{\sqrt{4Dt}}
\]

(80)

where we can recognize the integral as appearing in the error function. That leaves one constant to determine, from the other condition, \( T(\eta=\infty) = T_i \), where \( \text{erf}(\eta) = \text{erf}(\infty) =1 \), or

\[
T_i - T_0 = a_i \frac{\pi}{4} \text{erf}(\infty) \quad \rightarrow \quad a_i = \frac{2}{\pi^{1/2}}(T_i - T_0)
\]

(81)

Substituting back into (80) gives the final solution of the PDE,

\[
\frac{T - T_0}{T_i - T_0} = \text{erf} \frac{x}{\sqrt{4Dt}}
\]

(82a)

Flux calculation at \( x=0 \): One application of this solution is to the calculation of the time varying flux of heat into the domain from the boundary, or to the calculation of the total heat added. The first of these involves Fourier’s law and taking the derivative of (82) wrt \( x \), while the second involves the integral of that derivative over time, or of (82) over space. The flux is given by

\[
T(x,t) = T_0 + (T_i - T_0) \text{erf} \frac{x}{\sqrt{4Dt}}
\]

(82b)

\[
\text{Diffusive flux} = -K \frac{dT}{dx} = -K(T_i - T_0) \frac{d}{dx} \left[ \text{erf} \frac{x}{\sqrt{4Dt}} \right]
\]

(83)

where \( K \) is the heat conductivity, and \( D=K/\rho c_p \). The derivative on the right evaluates using the chain rule (p. 24 of these notes) and by applying the derivative of an integral with a variable upper limit (i.e., the derivative of an error function; p. 44 of these notes).
\[
\frac{dT}{dx} = (T_i - T_o) \frac{d}{dx} \left[ \text{erf}(\eta) \right] = (T_i - T_o) \frac{d\eta}{dx} \frac{d}{d\eta} \left[ \text{erf}(\eta) \right] = \\
= (T_i - T_o) \frac{d}{dx} \left[ \frac{x}{\sqrt{4Dt}} \right] \cdot \frac{2}{\sqrt{\pi}} \exp(-\eta^2) \\
= \frac{(T_i - T_o)}{\sqrt{\pi Dt}} \exp(\frac{-x^2}{4Dt})
\]

(84)

Thus, the diffusive flux any \( x,t \) is

\[
\text{Flux} = -K \frac{dT}{dx} = -K \left( \frac{T_i - T_o}{\sqrt{\pi Dt}} \right) \exp(\frac{-x^2}{4Dt})
\]

(85)

At the boundary, the flux into (or out of) the domain is given by applying this model at \( x=0 \), or

\[
\text{Boundary diffusive flux at } x=0 = -K \left. \frac{dT}{dx} \right|_{x=0} = -K \left( \frac{T_i - T_o}{\sqrt{\pi Dt}} \right) = \sqrt{K \rho c} \left( \frac{T_0 - T_i}{\sqrt{\pi t}} \right)
\]

(86)

The boundary flux is greater for higher thermal conductivity and heat capacity \( (c) \), larger temperature differences \( (T_0 - T_i) \), and smaller time. It decreases with the square root of time.

We integrate this over time to get the quantity of heat added as a function of time, \( H(t) \), or

\[
H = \sqrt{K \rho c} \left( \frac{T_0 - T_i}{\sqrt{\pi}} \right) \int_0^t dt = \sqrt{K \rho c} \left( \frac{T_0 - T_i}{\sqrt{\pi}} \right) \frac{1}{1/2} = \sqrt{K \rho c (T_0 - T_i)} \sqrt{\frac{4t}{\pi}}
\]

(87)

The amount of heat added increases with the square root of time. The amount \( H \) should also equal the spatial integral of heat added, or

\[
H = \int_0^\infty \rho c [T(x,t) - T_i] dx = \rho c (T_0 - T_i) \int_0^\infty \left[ 1 - \text{erf} \left( \frac{x}{\sqrt{4Dt}} \right) \right] dx
\]

\[
= \rho c (T_0 - T_i) \int_0^\infty \text{erfc} \left( \frac{x}{\sqrt{4Dt}} \right) dx = \rho c (T_0 - T_i) \sqrt{4Dt} \int_0^\infty \text{erfc}(\eta) d\eta
\]

(88)

which agrees with (87). I had to look up the integral at http://mathworld.wolfram.com/Erfc.html, the mathematica web site, to find that

\[
\int_0^\infty \text{erfc}(\eta) d\eta = \frac{1}{\sqrt{\pi}}
\]

(89)

In application, if I had not been able to find this integral, I would have relied on (87). It’s nice to have more than one way to solve a problem.
Other applications We can apply this model elsewhere in hydrology. One common application is bank storage due to a passing flood wave. If \( h_i \) is the initial head in the aquifer, \( h_0 \) is the height of the flood wave (using the same datum), \( D \) is hydraulic diffusivity (\( = T/S_y \)), then by homology to (82), (86) and (87) the aquifer head, the boundary flux into the aquifer, and the volume of water stored are given by

\[
h(x, t) = h_0 + (h_i - h_0) \text{erf} \frac{x}{\sqrt{4Dt}}
\]

\[
-T \frac{dh}{dx} \bigg|_{x=0} = -T \frac{h_i - h_0}{\sqrt{\pi Dt}} = \sqrt{TS_y} \frac{h_0 - h_i}{\sqrt{\pi t}}
\]

\[
V = \sqrt{TS_y} (h_0 - h_i) \frac{4t}{\pi}
\]

This tells us that the rate of bank infiltration and the amount of bank storage is greater for higher transmissivity and storage coefficient, and larger head differences \((h_0 - h_i)\). The rate decreases with the square root of time, while the storage volume increases with the square root of time.

Another common application is moisture “absorption” into a drier (or “desorption from a wetter) porous material due to capillarity (and ignoring gravity), provided we assume that “capillary diffusion” is a linear process. If \( \theta_i \) is the initial moisture content in the soil (volume of water per volume of soil), \( \theta_0 \) is boundary moisture content, \( D \) is capillary (soil moisture) diffusivity (\( = K \psi/d\theta \), where \( \psi \) is soil moisture tension and \( K \) is hydraulic conductivity), then by homology to (82), (86) and (87), the moisture content, boundary flux into the soil, and the total amount of absorption are given by

\[
\theta(x, t) = \theta_0 + (\theta_i - \theta_0) \text{erf} \frac{x}{\sqrt{4Dt}}
\]

\[
-D \frac{d\theta}{dx} \bigg|_{x=0} = -D \frac{\theta_i - \theta_0}{\sqrt{\pi Dt}} = \sqrt{D} \frac{(\theta_0 - \theta_i)}{\sqrt{\pi t}}
\]

\[
V = \sqrt{D} (\theta_0 - \theta_i) \frac{4t}{\pi}
\]

The rate and amount of moisture absorption is greater for higher soil moisture diffusivity and larger moisture differences \((\theta_0 - \theta_i)\). The rate decreases and the amount increases with the square root of time. If we add gravity\(^{20}\) to this moisture problem we can study infiltration, but continuing to assume that \( K \) and \( D \) are constants (and the problem linear). In this case only the flux changes, or

\[
(-D \frac{d\theta}{dx} + K) \bigg|_{x=0} = \sqrt{D} \frac{(\theta_0 - \theta_i)}{\sqrt{\pi t}} + K
\]

Thus the presence of gravity increases the infiltration rate, but the rate is suppressed by higher initial moisture, \( \theta_i \). The actual problem is more complicated than this. Both \( D \) and \( K \) depend on

\(^{20}\) Assuming that \( x \) is positive downward.
moisture content. The problem is actually non-linear. Let’s return to the heat diffusion problem to explore this issue.

Non-linear diffusion  Reconsider the diffusion equation but for the case of a diffusion coefficient that depends on the state. For heat diffusion this would be given by

$$\frac{\partial T}{\partial t} = \frac{1}{\partial x} \left( D(T) \frac{\partial T}{\partial x} \right)$$

(93)

Other applications of state dependent diffusion coefficient include solute diffusion, groundwater hydraulic diffusion (where in a phreatic aquifer the transmissivity depends on the saturated thickness and thus on the water table elevation), and moisture absorption and infiltration. How can we solve (68) for any general function $D(T)$, without specifying that function explicitly? We’ll see that what we can do is to develop a solution approach, implement it and carry out the symbolic calculations to a certain point, but then we’ll have to apply a particular function $D(T)$ and complete the remainder of the calculation numerically. Below we assume that $D$ depends on temperature through a dependence of thermal conductivity $K(T)$ on temperature. Heat capacity is assumed constant.

While there are some very good non-linear solution approaches for (68), also capable of handling advection, we’ll focus on the simplest. It is to illustrate only; you won’t be applying this method yourself.

Basically, the idea is to use the Boltzmann transformation again. We assume that the solution will be something like that in the similarity solution of (68), apply the change of variables in (71) but in terms of a fixed $D_0=D(T_0)$ taken at the boundary,

$$\eta = \frac{x}{\sqrt{4D_0 t}}$$

(94)

and derive a non-linear ODE similar to (73), or

$$\frac{d}{d\eta} \left[ \frac{D(T)(dT)}{D_0 (d\eta)} \right] + 2\eta \frac{dT}{d\eta} = 0$$

(95)

This is presented in some detail in Crank (1975, Chap. 7), and reviewed in the context of soil moisture absorption and infiltration in Eagleson (Dynamic Hydrology, Prentice Hall, 1970, pp. 291-299). For example, the boundary diffusive flux at $x=0$ becomes,

$$-K \frac{dT}{dx} \bigg|_{x=0} = \frac{1}{2} \sqrt{\frac{K\rho c}{t}} \frac{dT}{d\eta} \bigg|_{\eta=0}$$

(86)

21 John Phillip (CSIRO) and Yves Parlange (Cornell) are well known in hydrology, soil physics, and mathematical physics for their contributions along these lines. For example, both worked on something called the “flux concentration approach”.

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which, by comparison to the linear case, we can rewrite as

\[
-K \frac{dT}{dx} \bigg|_{x=0} = \sqrt{K \rho c} \frac{(T_0 - T_i)}{\sqrt{\pi t}}
\]  

(87)

where the weighted mean conductivity is given by

\[
\bar{K} = \frac{\pi}{4} K_0 \left( \frac{1}{(T_i - T_0)^2} \left( \frac{dT}{d\eta} \right)^2 \right)_{\eta=0}
\]  

(88)

and \(K_0\) is taken at the boundary, \(K_0=K(T_0) = c \rho D(T_0)\). Crank (Conduction of Heat in Solids, Oxford Press, 1959) did some numerical experiments to determine approximations for \(\bar{K}\), and then explored the solution for various functions \(K(T)\). You can also find some of this in Eagleson (1970).

For example, Crank found that as long as \(K\) and \(D\) increase with \(T\) then the best weighting for increasing temperature cases is given by

\[
\bar{K} = \frac{5}{3} (T_0 - T_i)^{-5/3} \int_{T_i}^{T_0} (T - T_i)^{2/3} K(T) dT
\]  

(89)

One would take experimental data on \(K(T)\), perform this integration (perhaps numerically), and insert into (87) to get the model for heat flux. Similar calculations are done for temperature distribution and total content. Homologous calculations are done for stream bank storage and moisture absorption and infiltration.