Diffusion Equation

- Here is our “heat equation”:

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T, \tag{1}$$

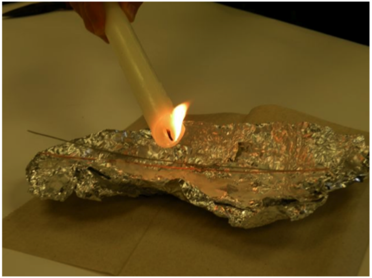
  where $\kappa = k/\rho c_p$ is the heat diffusivity.
- The heat equation describes the heat transfer by conduction.
- The rate of temperature change $\propto$ net flux of heat $\propto$ temperature gradient
  The rate of concentration of a chemical species $\propto$ net flux of the material $\propto$ concentration gradient.
- So, this type of pde can describe the general class of phenomena, called “diffusion.”

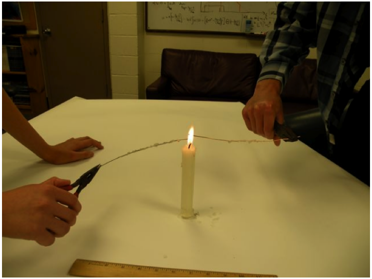
Diffusion Equation

- Let's learn about some qualitative properties of the diffusion equation.
- Note that the r.h.s is the "curvature". So, the equation implies that temperature changes fastest where the "curvature" is the greatest.
- When does the time-dependence vanish? When a temperature distribution is a harmonic function (i.e. functions satisfying the Lapalace equation, r.h.s. = 0). The simplest examples are a constant temperature or a constant gradient of temperature.
- Think about a sinusoidal temperature distribution and qualitatively predict how that temperature profile would change with time.

Diffusion Equation

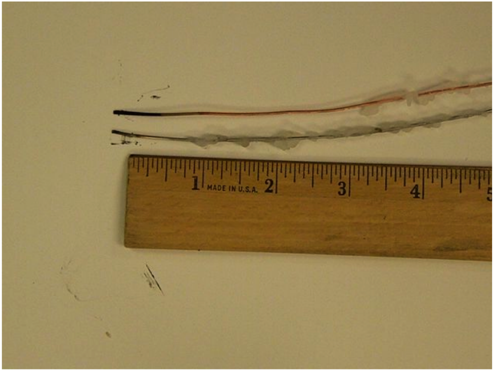
- Recall the unit of heat diffusivity, κ: [m^2/s].
- Purely based on the dimensional analytical argument, we can get a length scale from κ: $\Delta l = \sqrt{\kappa \Delta t}$, called *characteristic thermal diffusion distance*.
- To understand the physical meaning of this relationship, let's look at this experiment.





Diffusion Equation

- $\kappa_{steel} = 7 \times 10^{-6}$ m^2/s, $\kappa_{brass} = 33 \times 10^{-6}$ m^2/s, and the melting front of brass propagated about XX (tbd) times longer distance than that of steel.



- Since both wires were heated for the same Δt, $\Delta l_{brass}/\Delta l_{steel} = \sqrt{\kappa_{brass}/\kappa_{steel}} = \sqrt{33/7} \approx 2.9$.

Diffusion Equation

- It is useful to work out the “fundamental solution” to the diffusion equation at this point.
- The heat (diffusion) equation (1) can be non-dimensionalized by setting $T = T_{ref}u$, $x = Lx'$ and $t = t_{ref}t'$ where u and primed variables are non-dimensional temperature, spatial variable and time, respectively while T_{ref}, L and t_{ref} and the corresponding reference values or “scales”.
- By substituting these definitions into (1), we get (in 1-D case)

$$\begin{aligned} \frac{\partial\left(T_{ref}u\right)}{\partial\left(t_{ref}t'\right)} &= \kappa\frac{\partial^2\left(T_{ref}u\right)}{\partial\left(Lx'\right)^2} \\ \Rightarrow \frac{\partial u}{\partial t'} &= \kappa\frac{t_{ref}}{L^2}\frac{\partial^2 u}{\partial x'^2} \end{aligned} \tag{2}$$

Diffusion Equation

- Since L and t_{ref} can always be chosen such that $\kappa(t_{ref}/L^2) = 1$, we get the following non-dimensional diffusion equation:
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \tag{3}$$
or in the simplified notation,
$$u_t = u_{xx} \tag{4}$$
where variables have been de-primed since there is no risk of confusion.
- The *fundamental solution* to the one dimensional diffusion equation is the solution to the following problem:
$$u_t - u_{xx} = \delta(x)\delta(t), ; -\infty < x < \infty; 0 \leq t < \infty, \tag{5}$$
$$u(x, 0) = 0, \tag{6}$$
$$u(x, t) \to 0 \text{ as } |x| \to \infty. \tag{7}$$

Diffusion Equation

- The solution to this pde is called fundamental because we can use it to solve the following *general* initial-value problem on the infinite domain:

$$u_t - u_{xx} = p(x,t); -\infty < x < \infty; 0 \leq t < \infty, \tag{8}$$

$$u(x,0) = f(x), \tag{9}$$

$$u(x,t) \to f(\pm\infty) \text{ as } x \to \pm\infty. \tag{10}$$

- Assume that we have found the solution of (5)-(7) in the form $u = F(x,t)$. It is possible to use this result to obtain a second solution $u = G(x,t)$ by setting $\bar{x} = \beta x$ and $\bar{t} = \gamma t$ and defining G by

$$G(x,t) \equiv \alpha F(\beta x, \gamma t) = \alpha F(\bar{x}, \bar{t}) \tag{11}$$

for positive constants α, β and γ.

Diffusion Equation

- We compute $G_t = \alpha\gamma F_{\bar{t}}$, $G_{xx} = \alpha\beta^2 F_{\bar{x}\bar{x}}$ and use the fact that for any constant c, we may set

$$\delta(cx) \to \frac{1}{|c|}\delta(x). \tag{12}$$

- The above property is derived from the definition of the Dirac delta function:

$$\int_{-\infty}^{\infty} \delta(cx) f(x) dx = \int_{-\infty}^{\infty} \delta(y) f(y/c) \frac{dy}{c} = \frac{1}{c} f(0).$$

- If $G(x,t)$ is to be a solution of (5)-(7), we must have

$$G_t - G_{xx} = \delta(x)\delta(t),\ G(x,0) = 0,\ G(x,t) \to 0 \text{ as } |x| \to \infty. \tag{13}$$

- Expressing G_t and G_{xx} in terms of $F_{\bar{t}}$ and $F_{\bar{x}\bar{x}}$ and using $\delta(x)\delta(t) = \delta(\bar{x}/\beta)\delta(\bar{t}/\gamma) = \beta\gamma\delta(\bar{x})\delta(\bar{t})$ in the above equation gives

$$\alpha\gamma F_{\bar{t}} - \alpha\beta^2 F_{\bar{x}\bar{x}} = \beta\gamma\delta(\bar{x})\delta(\bar{t}), \tag{14}$$

Diffusion Equation

- Since $F(\bar{x}, \bar{t})$ itself is a solution satisfying $F_{\bar{t}} - F_{\bar{x}\bar{x}} = \delta(\bar{x})\delta(\bar{t})$, $G(x, t)$ can be a solution only if $\beta^2/\gamma = 1$ and $\beta/\alpha = 1$; that is, if $\beta = \alpha$ and $\gamma = \alpha^2$. Thus, $G(x, t)$ must be of the form

$$G(x, t) = \alpha F(\alpha x, \alpha^2 t). \tag{15}$$

- By this, we didn't find any new solution to the diffusion problem (5)-(7). Rather, since the solution should be unique we have only found the ***similarity structure*** of the solution F.

$$G(x, t) = F(x, t) = \alpha F(\alpha x, \alpha^2 t). \tag{16}$$

- That is to say, if we replace x by αx and t by $\alpha^2 t$ in F and then multiply the result by α (for any $\alpha > 0$), ***the resulting expression is identical to F(x,t).***

Diffusion Equation

- This similarity property implies that $F(x,t)$ must be of the form

$$F(x,t) = \frac{1}{\sqrt{t}} f\left(\frac{x}{\sqrt{t}}\right), \text{ or } \frac{1}{\sqrt{t}} g\left(\frac{x^2}{t}\right), \text{ or } \frac{1}{x} h\left(\frac{x}{\sqrt{t}}\right), \ldots. \tag{17}$$

- Any of an infinite number of possibilities that satisfies the similarity condition (16) may be used. Each choice will reduce the diffusion equation to an ***ordinary differential equation***, which, when solved, will give the same result for F.
- Let's pick the form,

$$F(x,t) = \frac{1}{\sqrt{t}} f(\zeta), \; \zeta \equiv \frac{x}{\sqrt{t}}. \tag{18}$$

Diffusion Equation

- We get

$$F_x = \frac{1}{t} f'; \; F_{xx} = \frac{1}{t^{3/2}} f''; \; F_t = -\frac{1}{2t^{3/2}} f - \frac{x}{2t^2} f', \tag{19}$$

  where $' \equiv d/d\zeta$.

- Plugging these into the original diffusion equation (5), we get

$$-\frac{1}{2t^{3/2}} f - \frac{x}{2t^2} f' - \frac{1}{t^{3/2}} f'' = 0, \tag{20}$$

  which is the linear second-order ODE

$$f'' + \frac{\zeta}{2} f' + \frac{1}{2} f = 0 \tag{21}$$

  with the independent variable ζ.

Diffusion Equation

- The ODE (21) is an "exact" equation: i.e. it is a derivative of an ODE of lower order. Specifically,

$$f'' + \frac{\zeta}{2}f' + \frac{1}{2}f = \frac{d}{d\zeta}\left(f' + \frac{\zeta}{2}f\right) = 0. \tag{22}$$

- Integrating this equation once gives

$$f' + (\zeta/2)f = A = \text{constant} \tag{23}$$

  and the solution of this is acquired using the ***integrating factor***.

- *Review of the integrating factor*: All first-order linear inhomogeneous equations are soluble because it is always possible to find an integrating factor which is a function of ζ only. The integrating factor $I(\zeta)$ for

$$f' + p(\zeta)f = q(\zeta) \tag{24}$$

  is $I(\zeta) = \exp\left[\int^{\zeta} p(\xi)d\xi\right]$.

Diffusion Equation

- *Review of the integrating factor* (cont'd): The usefulness of $I(\zeta)$ is in the property

$$I'(\zeta) = p(\zeta)I(\zeta). \tag{25}$$

Multiplying (24) by $I(\zeta)$ gives
$If' + pfI = If' + fI' = (d/d\zeta)(If) = qI$.
So the solution is

$$f(\zeta) = \frac{B}{I(\zeta)} + \frac{1}{I(\zeta)} \int^{\zeta} q(\xi)I(\xi)d\xi, \tag{26}$$

where B is a constant.

Diffusion Equation

- Going back to the similarity solution to the diffusion equation, the integrating factor is

$$I(\zeta) = \exp\left[\int^{\zeta} \frac{\xi}{2} d\xi\right] = e^{\zeta^2/4}, \tag{27}$$

  where integration constant is arbitrarily set to be zero since it doesn't influence the final solution.
- Our $q(\zeta)$ is a constant A so by plugging this and (27) into (26), we get

$$f = B\, e^{-\zeta^2/4} + A\, e^{-\zeta^2/4} \int^{\zeta} e^{s^2/4} ds. \tag{28}$$

Diffusion Equation

- Note that in the end, we are getting a solution representing a temperature field. Thermal energy (or heat content) is the volume integration of temperature multiplied by heat capacity and it cannot be infinite.

$$
\begin{aligned}
H(t) &\equiv \int_{-\infty}^{\infty} F(x,t)dx \\
&= \frac{A}{\sqrt{t}} \int_{-\infty}^{\infty} f_1\left(\frac{x}{\sqrt{t}}\right) dx + \frac{B}{\sqrt{t}} \int_{-\infty}^{\infty} e^{-x^2/4t} dx < \infty.
\end{aligned}
\tag{29}
$$

This constraint requires $A = 0$[1] and we have

$$
F(x,t) = \frac{B}{\sqrt{t}} e^{-x^2/4t}, \ t > 0. \tag{30}
$$

[1] see Sec. 1.2 of *Partial Differential Equations* by Kevorkian [2000, 2nd ed., Springer] for a complete argument.

Diffusion Equation

- To determine B, we turn to the fact that the non-dimensional thermal energy is just the integral of the non-dimensional temperature:

$$H(t) \equiv \int_{-\infty}^{\infty} F(x,t)dx \tag{31}$$

- If we differentiate $H(t)$ with respect to t and use the fact that $F(x,t)$ is the solution to the diffusion equation (5), we obtain

$$\frac{dH}{dt} = \int_{-\infty}^{\infty} F_t(x,t)dx = \int_{-\infty}^{\infty} [F_{xx}(x,t) + \delta(x)\delta(t)]dx, \tag{32}$$

so that

$$\frac{dH}{dt} = F_x(\infty,t) - F_x(-\infty,t) + \delta(t) = \delta(t) \tag{33}$$

because temperature gradients at $x = \pm\infty$ must be zero.

Diffusion Equation

- From (33) we know that $H(t)$ is the Heaviside function, meaning for $t > 0$

$$1 = \int_{-\infty}^{\infty} F(x,t)dx = \int_{-\infty}^{\infty} \frac{B}{\sqrt{t}} e^{-x^2/4t} dx. \tag{34}$$

- We can rewrite the above equation as

$$1 = 2B \int_{-\infty}^{\infty} \frac{e^{-x^2/4t}}{\sqrt{4t}} dx = 2B \int_{-\infty}^{\infty} e^{-\xi^2} d\xi = 2B\sqrt{\pi} \tag{35}$$

or

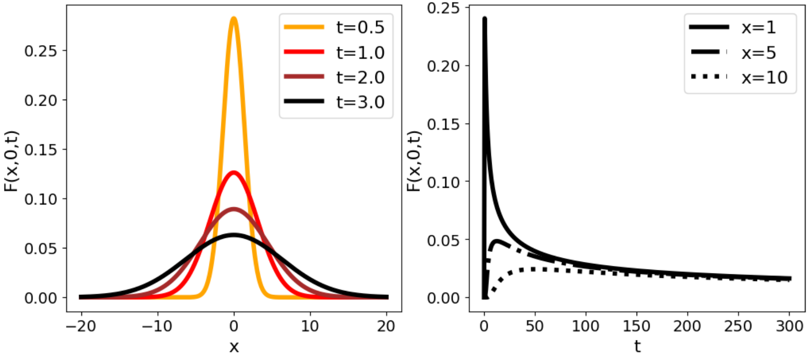
$$B = \frac{1}{2\sqrt{\pi}}. \tag{36}$$

- Finally, we get the *fundamental solution*,

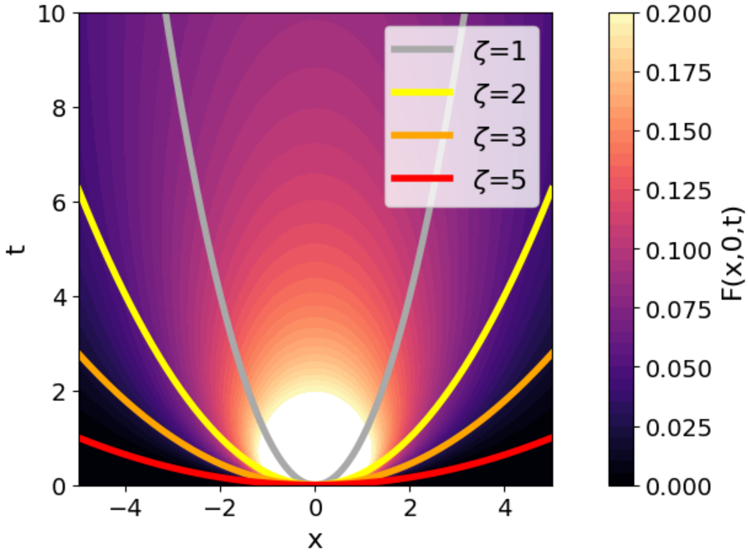
$$F(x,t) = \frac{1}{2\sqrt{\pi t}} e^{-x^2/4t}. \tag{37}$$

- Recall that x and t here are actually non-dimensional (primed) variables $t' = t/t_{ref}$ and $x' = x/L$. Moreover, t_{ref} and L were chosen such that $L^2/t_{ref} = \kappa$.

Diffusion Equation



Diffusion Equation



Diffusion Equation

- Plugging expressions for $F = T(x,t)/T_{ref}$, $t' = t/t_{ref}$ and $x' = x/L$ into

$$F(x',t') = \frac{1}{2\sqrt{\pi t'}} e^{-x'^2/4t'}, \tag{38}$$

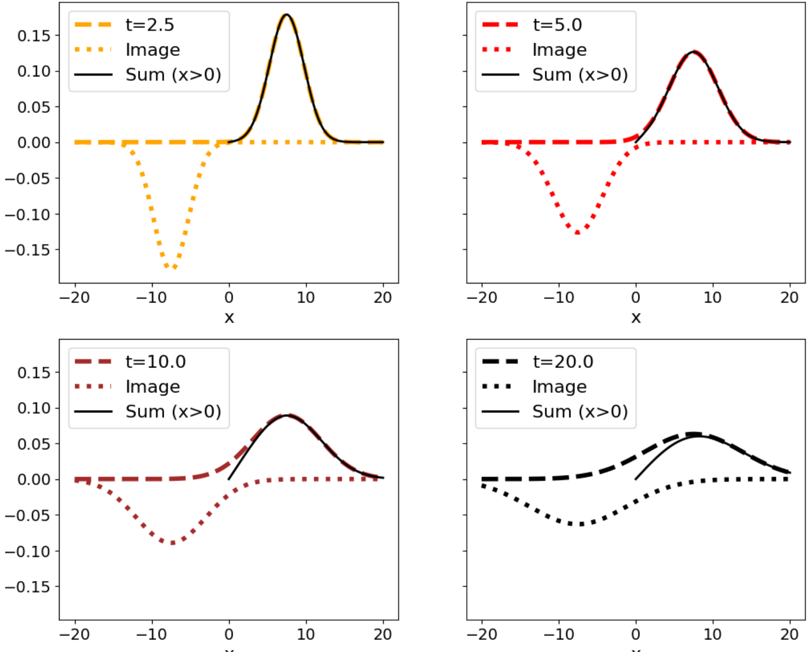
we obtain

$$\begin{aligned} T(x,t) &= \frac{T_{ref}}{2\sqrt{\pi(t/t_{ref})}} e^{-\frac{x^2}{4(L^2/t_{ref})t}} = \frac{T_{ref}\sqrt{t_{ref}}}{2\sqrt{\pi t}} e^{-x^2/(4\kappa t)} \\ &= \frac{T_{ref}L}{2\sqrt{\pi\kappa t}} e^{-x^2/(4\kappa t)} \end{aligned} \tag{39}$$

Diffusion Equation

- The infinite space is not so much relevant to geodynamic problems as the *semi-infinite half-space*.
- The difference between the fundamental solution and the solution for the semi-infinite space is that temperature should be zero at $x = 0$ instead of at $-\infty$.
- The way of making use of the fundamental solution for this case is to put an “image source”.

Diffusion Equation



Diffusion Equation

- Let's formulate this semi-infinite space problem as follows (again, non-dimensional, 1-D):

$$u_t - u_{xx} = \delta(t)\delta(x - \xi), \; 0 \leq x < \infty, \tag{40}$$

$$u(0, t) = 0, \; t > 0, \tag{41}$$

$$u(x, 0) = 0. \tag{42}$$

- As we've seen graphically, the Green's function can be constructed by superposing a fundamental solution for the real source and another for the image source:

$$G(x, \xi, t) \equiv F(x - \xi, t) - F(x + \xi, t) \tag{43}$$

where F is given in (37).

Diffusion Equation

- The "half-space cooling" problem in geodynamics can be similarly formulated as

$$u_t - u_{xx} = 0, \ 0 \le x < \infty, \ 0 \le t, \tag{44}$$

$$u(0,t) = 0, \ t > 0, \tag{45}$$

$$u(x,0) = f(x). \tag{46}$$

- Noting that this problem is equivalent to

$$u_t - u_{xx} = \delta(t) f(x), \ 0 \le x < \infty, \ 0 \le t, \tag{47}$$

$$u(0,t) = 0, \ t > 0, \tag{48}$$

$$u(x,0) = 0. \tag{49}$$

we write the solution in terms of the Green's function

$$\begin{aligned} u(x,t) &= \int_0^\infty \int_0^t \delta(\tau) f(\xi) G(x,\xi,t-\tau) d\tau d\xi \\ &= \int_0^\infty f(\xi) G(x,\xi,t) d\xi. \end{aligned} \tag{50}$$

Diffusion Equation

- When $f(x) = c$ (constant),

$$u(x,t) = \frac{c}{2\sqrt{\pi t}} \left[\int_0^\infty e^{-(x-\xi)^2/4t} d\xi - \int_0^\infty e^{-(x+\xi)^2/4t} d\xi \right]. \tag{51}$$

- Changing the variable of integration from ξ to $\eta = (x-\xi)/2\sqrt{t}$ in the first integral and to $\eta = (x+\xi)/2\sqrt{t}$ in the second gives

$$u(x,t) = \frac{c}{\sqrt{\pi}} \left[-\int_{x/2\sqrt{t}}^{0} e^{-\eta^2} d\eta - \int_0^{-\infty} e^{-\eta^2} d\eta - \int_{x/2\sqrt{t}}^{\infty} e^{-\eta^2} d\eta \right] \tag{52}$$

- Simplifying this expression gives

$$u(x,t) = \frac{2c}{\sqrt{\pi}} \int_0^{x/2\sqrt{t}} e^{-\eta^2} d\eta = c \operatorname{erf}\left(\frac{x}{2\sqrt{t}} \right), \tag{53}$$

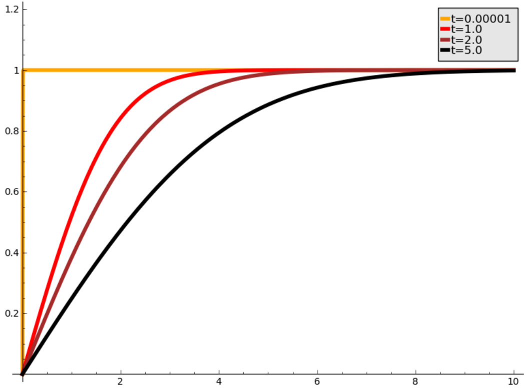
where erf() is the *error function*.

Diffusion Equation

- Again, we can add back dimensions to the variables obtaining

$$T(x,t) = T_{ref}\,\mathrm{erf}\left(\frac{x}{2\sqrt{\kappa t}}\right). \tag{54}$$

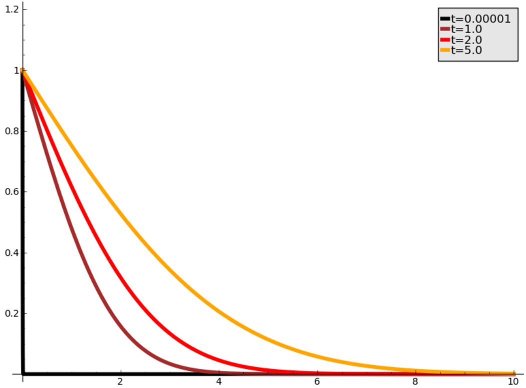
- This is the solution for a temperature field that is initially T_{ref} but equal to 0 at $x = 0$ for $t > 0$. So, this is the problem of *instantaneous cooling* of the half space.



Diffusion Equation

- What about the instantaneous heating? The solution is expressed as the *complementary error function*:

$$T(x,t) = T_{ref}\left(1 - \text{erf}\left(\frac{x}{2\sqrt{\kappa t}}\right)\right) = T_{ref}\,\text{erfc}\left(\frac{x}{2\sqrt{\kappa t}}\right). \quad (55)$$



Diffusion Equation

- It is a trivial matter to adjust the solutions (54) and (55) for non-zero initial or boundary temperature.
- In case of the instantaneous heating (Fig. 4-20 in T&S), the initial temperature is T_1 and the boundary temperature at $x = 0$ is $T_0 (> T_1)$. Then, the “magnitude” of temperature change T_{ref} is equal to $T_0 - T_1$ and also the solution in (55) is shifted by T_1:

$$T(x, t) = (T_0 - T_1)\,\mathrm{erfc}\left(\frac{x}{2\sqrt{\kappa t}}\right) + T_1 . \tag{56}$$

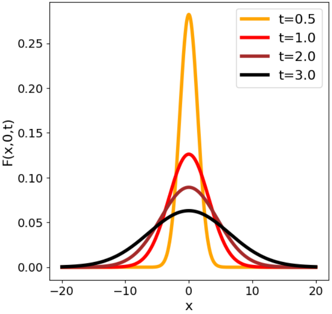
Finally, we get Eq. 4-113 of T&S:

$$\frac{T - T_1}{T_0 - T_1} = \mathrm{erfc}\left(\frac{x}{2\sqrt{\kappa t}}\right) . \tag{57}$$

Half-space cooling model

- Let's review the fundamental solution to the non-dimensional 1D diffusion equation,

$$\mathcal{F}(x,t) = \frac{T_{ref}L}{2\sqrt{\pi\kappa t}} e^{-x^2/(4\kappa t)}.$$



- Note that temperature, except at the source, increases initially and then decrease.
- At a fixed t (> 0), the shape of the fundamental solution is nothing but the bell-shaped curve of the normal or Gaussian distribution.
- This hints us why the solution to the half-space cooling problem involves the "error" function.

Half-space cooling model

- The half-space cooling solution was acquired by the following integration:

$$u(x,t) = \frac{2c}{\sqrt{\pi}} \int_0^{x/2\sqrt{t}} e^{-\eta^2} d\eta.$$

- In statistics, the probability of a random variable with normal distribution of mean 0 and variance 1/2 falling in the rage $[-\eta, \eta]$ is given by

$$\frac{1}{\sqrt{\pi}} \int_{-\eta}^{\eta} e^{-\sigma^2} d\sigma = \frac{2}{\sqrt{\pi}} \int_0^{\eta} e^{-\sigma^2} d\sigma = \text{erf}(\eta) \tag{58}$$

Half-space cooling model

- This probability is related to “error”. For instance, when we ask, “what’s the error bar of those data points?” we are actually asking the range of values measured with (assumed) random error under a certain probability: e.g., 1σ for 67 % probability, 2σ for 95 %, etc.
- Don’t get a wrong idea, though.
  The connection to the normal distribution is only a coincidence. It does NOT mean that our half-space solution is probabilistic!

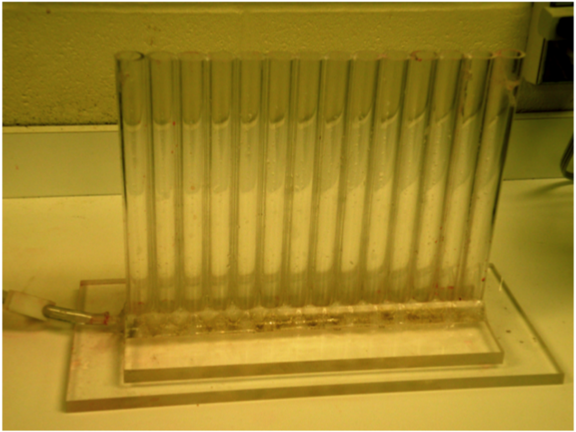
Half-space cooling model

- To understand the generality of the diffusion equation, let's take a look at an example of material diffusion.
- Recall that the heat transport by conduction is described as a diffusion phenomenon because the time rate of change of temperature is proportional to the net flux of the heat energy AND the flux is proportional to the temperature gradient: i.e.,

$$T_t \propto \nabla \cdot \mathbf{f} \text{ and } \mathbf{f} \propto \nabla T. \tag{59}$$

Half-space cooling model

- Let's consider a series of tubes that are going to be filled with a fluid. They are connected by a little pipe going through the near-bottom part.



(Courtesy of Prof. W. Roger Buck, Columbia University)

Half-space cooling model

- If the cross-sectional area of tubes is constant, the rate of change of fluid column's height (h) is proportional to the net flux of fluid in and out of the tube and the flux.
- Furthermore, the flux of fluid from one tube to another ($\mathbf{f}$) is proportional to the pressure gradient between them (∇p).
- Why? Flow rate is velocity times area. In our case, the area is constant. So, velocity should be proportional to the pressure gradient, which is true for flows in pipes. This is one of the first topics we will learn in the fluid mechanics chapter

Half-space cooling model

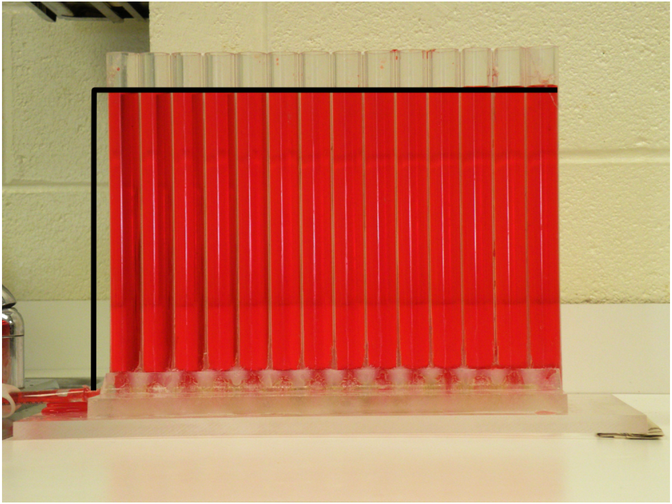
- Since the pressure at the bottom of a tube is $\rho_{fluid} g h$, the pressure gradient is proportional to the gradient of the column height (∇h).
- So, we have the following relationship in this setting:

$$h_t \propto \nabla \cdot \mathbf{f} \text{ and } \mathbf{f} \propto \nabla h, \tag{60}$$

which leads to the conclusion that **the time and spatial variation of the column height, $h(x, t)$, can be described by the diffusion equation.**

Half-space cooling model

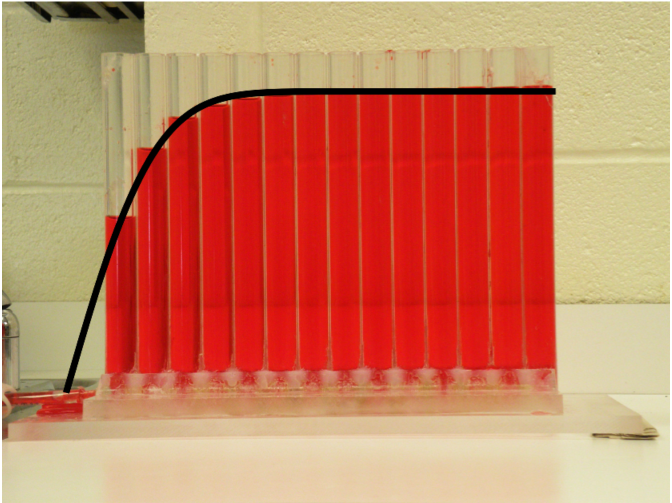
- The instantaneous “cooling” case (1/8):



(Courtesy of Prof. W. Roger Buck, Columbia University)

Half-space cooling model

- The instantaneous “cooling” case (2/8):



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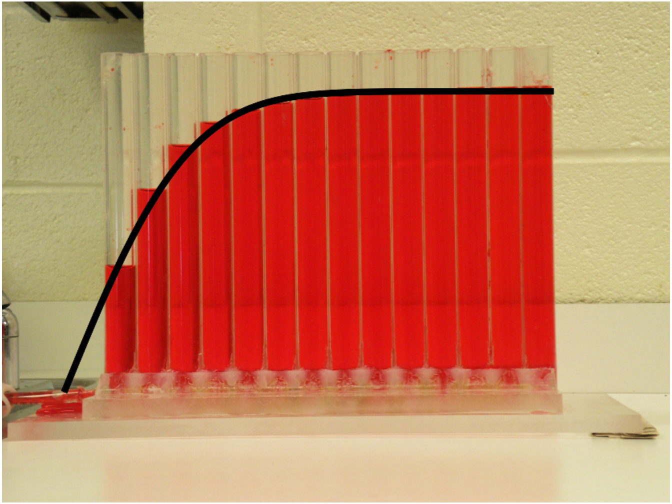
Half-space cooling model

- The instantaneous “cooling” case (3/8):



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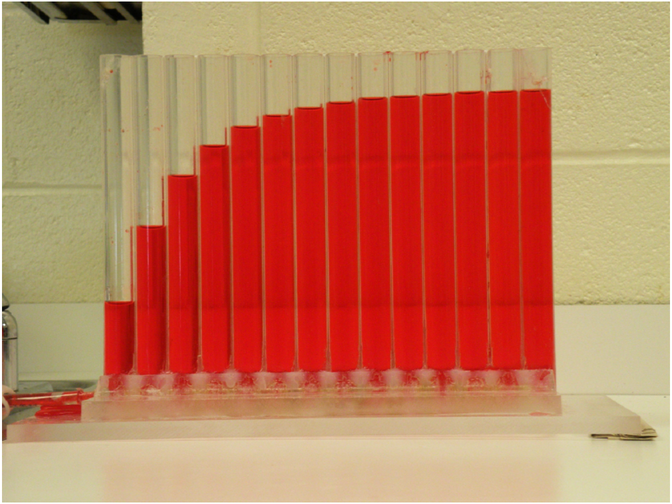
Half-space cooling model

- The instantaneous "cooling" case (4/8):



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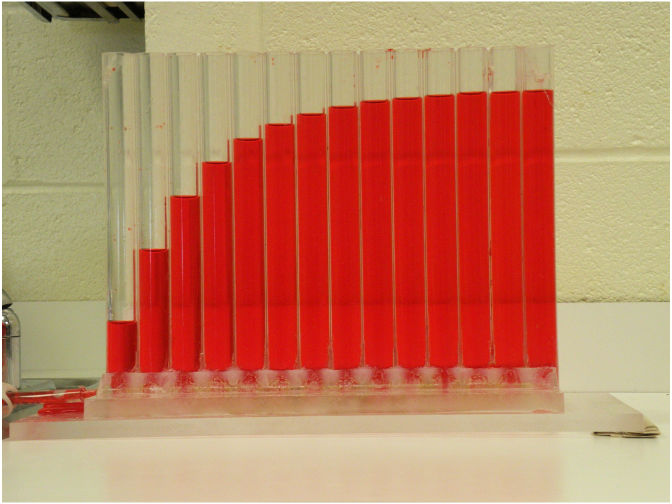
Half-space cooling model

- The instantaneous “cooling” case (5/8):



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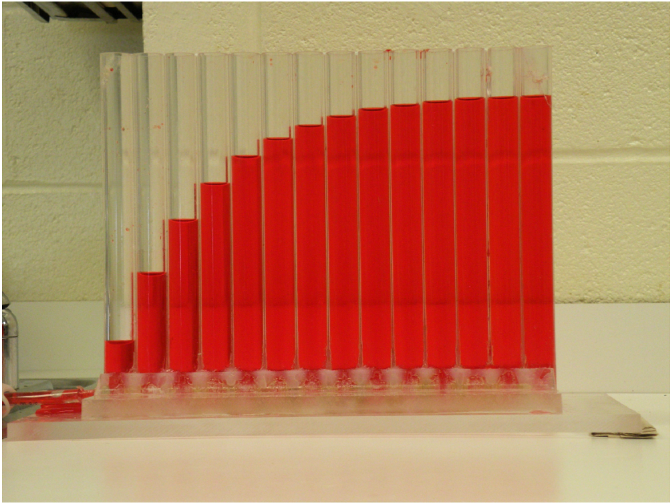
Half-space cooling model

- The instantaneous “cooling” case (6/8):



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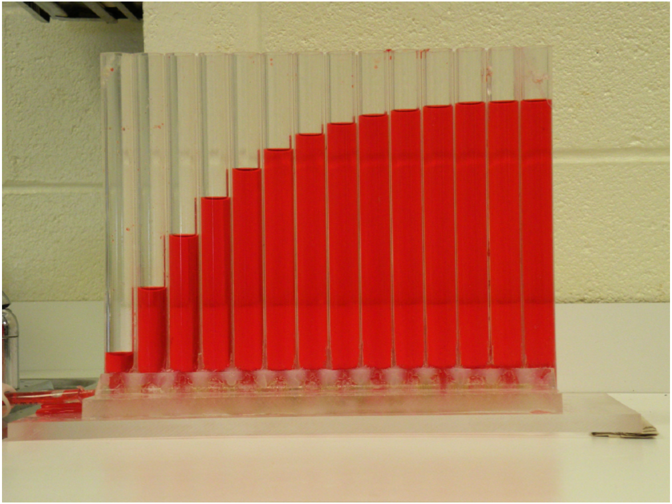
Half-space cooling model

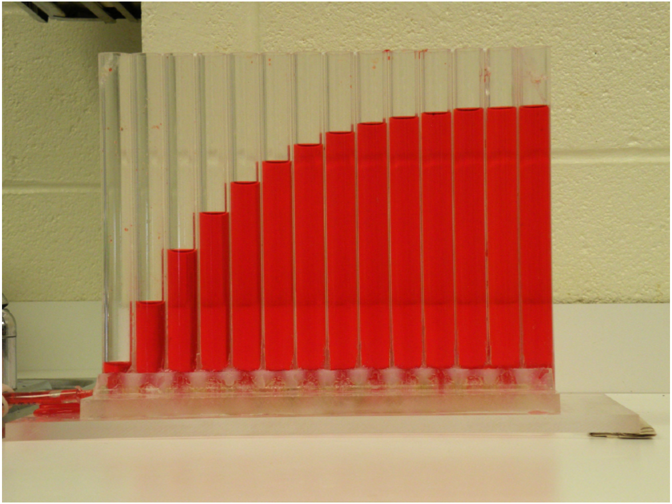
- The instantaneous “cooling” case (7/8):



(Courtesy of Prof. W. Roger Buck, Columbia University)

Half-space cooling model

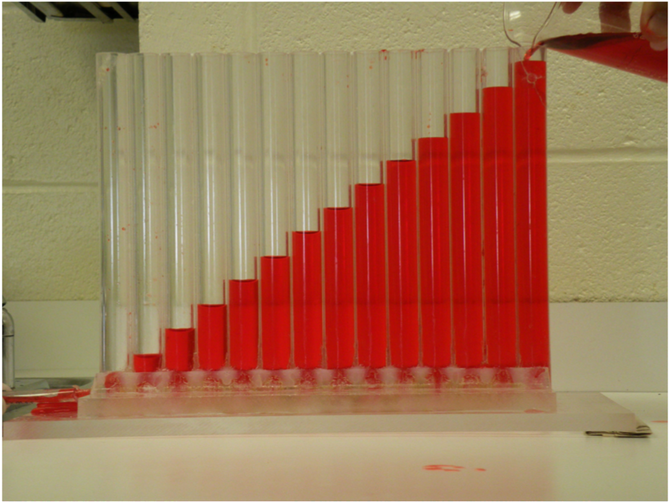
- The instantaneous "cooling" case (8/8):



(Courtesy of Prof. W. Roger Buck, Columbia University)

Half-space cooling model

- The steady-state case:



(Courtesy of Prof. W. Roger Buck, Columbia University)