

1

Diffusion

These notes contain a lot of challenging material. This chapter contains mostly analytical concepts and techniques for solving problems and serves as a compliment to the lectures and labs. Some sections are listed as “an aside”. If you do not understand these sections, do not be discouraged; however, try and read through them anyway. Go spiral learning!

1.1 INTRODUCTION

Diffusion processes are important in many applications in science and engineering. Diffusion occurs when a system is not in equilibrium and random molecular motion tends to bring everything toward uniformity. Most commonly, we think of diffusion of mass or heat. Heat flowing from hot to cold, or red fluid and blue fluid mixing to make purple. We think of diffusion when we cool a hot pizza on the counter-top to room temperature or mix the steamed milk into our espresso to make cappuccino.

In the examples given, however, diffusion is not the dominant mechanism. Bulk motion of the fluid is often responsible for most of the mixing effects that we experience in liquids and gases. While diffusion is important in the detail of these processes, convection is what we most often experience. Were it not for convective motions in the air it would take us one year to smell our feet after taking off our shoes due to molecular diffusion! (Squires and Quake 2005) Likewise, it is the stirring of the milk in the coffee that mixes it; molecular diffusion would take so long that the drink would long spoil and evaporate before it was mixed.

The most common example of diffusion in our everyday experience, and the one that we will use throughout this chapter, is the diffusion of heat in a solid. On a cold New England winter day, the heat of our homes is transported through the walls by diffusion, or conduction. When we touch the outside of the oven and feel its warmth, that is due to diffusion of heat through the oven walls. Convection is what makes the house smell good when that oven is filled with cookies.

Another common form of diffusion in our normal experience is viscosity. Viscosity determines how momentum diffuses in a fluid flow. While we are familiar with the concept of viscosity, it is a relatively small effect compared to fluid inertia in our everyday experience of breathing and swimming. Very small organisms live in a world where viscous diffusion is the dominant effect; and it is a strange world that results in many counterintuitive effects. We recommend reading the article “Life at Low Reynolds Number” to learn more about this world (Purcell 1976).

Diffusion processes are intimately connected to entropy, irreversibility, and probability. All diffusion processes are irreversible and cannot be run backwards. Place a hot object and a cold object in contact with each other and they will equilibrate to the same temperature, never to spontaneously become hot and cold again. If the process could run backward, there would be a decrease in the entropy of the universe and the second law of thermodynamics

would be violated. Nobody has ever found an experiment that violated the second law. You will learn more about the second law in later courses.

If we consider a box of still gas (no convection) and the molecules on the right are tagged as red and the molecules on the left are tagged blue, what will happen? Even a still gas that is not moving in bulk is moving at the molecular level. Over time the random molecular motions of the gas will lead to a uniform box of purple gas. One answer as to why it must be purple is that it is the most probable state. After a long time of molecules whizzing and bouncing off each other we are equally as likely to find any particle on either side of the box. A particles location is completely random. Once the particles are mixed the randomness of the motion would never lead us to find to all the red on the left and all the blue on the right (you may make your own analogy with red and blue states if you wish). If we threw a million pennies into the air inside a room, there is no chance that the left half would come up all heads and the right half would be all tails.

1.2 HEAT CONDUCTION

In our last course we discussed heat transfer and temperature when we studied the hot wire anemometer. In that case we characterized the temperature of the hot-wire as a single value. This idealization works when the body is small and has a high thermal conductivity, but in many cases we want to understand a system that cannot be characterized by a single temperature. We can use the concepts of the previous course to develop a model for such a system. The example we will analyze is a hot object at constant temperature taken out of the oven and placed on the counter to cool in the air. We will first review the lumped model (single temperature) of this system and then we will use the same techniques to analyze the temperature distribution inside the object.

1.2.1 Lumped model

The change in the amount of thermal energy stored in a solid object, ΔQ , as we change its temperature from T_0 to T is

$$\Delta Q = mC_p(T - T_0), \quad (1.1)$$

where m is the mass, and C_p (J/kg K) is the specific heat. We are assuming that the object is at a single temperature.

When a fluid is in contact with a hot surface, heat is carried away by a process called convection. The fluid takes energy from the surface and then carries it away through bulk fluid motion. The law, often called Newton's law of cooling, is given as

$$q'' = h(T - T_{air}). \quad (1.2)$$

where q'' is the heat flux (W/m^2), h is the convection coefficient, and T_{air} is the temperature of the air. The convection coefficient is a quantity that can be measured or determined theoretically with much effort.

Conservation of energy dictates that the rate of change of energy stored in a body must equal to the net amount of power that is dissipated to the air. The rate that energy is stored is simply the time derivative of 1.1. The rate the heat leaves the object is the heat flux multiplied by the surface area,

$$mC_p \frac{dT}{dt} = -hA(T - T_{air}). \quad (1.3)$$

Simple rearranging of the constants results in

$$\frac{dT}{dt} = -\frac{T - T_{air}}{\tau}, \quad (1.4)$$

where the constant $\tau = mC_p/hA$ is the time constant; you should confirm that the quantity does in fact have units of time. We analyzed this system in detail in the previous course when building the hot-wire anemometer. We found that the temperature will decay as a classic first order system, starting at the initial temperature and then decaying to the air temperature. The time constant of that decay is τ .

1.2.2 Coupled model

The lumped model will work fine when the object is small as in the hot wire anemometer. When we have a large object we can have significant temperature variations inside the solid object. We can analyze this case with a model not much different than the lumped model, only we will break the object into several small blocks.

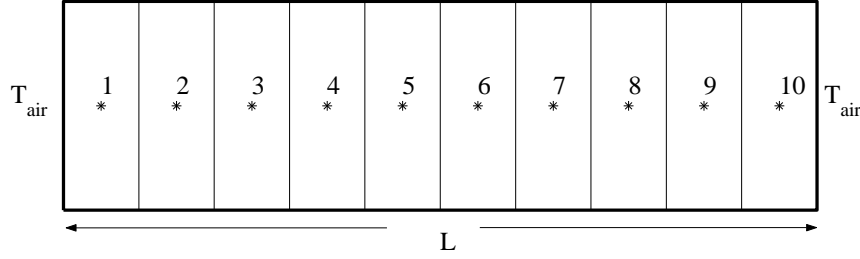


Fig. 1.1 Computational grid for discretized continuum problem. The slab is of thickness L , we break the bar into 10 elements each of equal width. The ends of the bar are exposed to the ambient air. The elements 2-9 transfer heat by conduction with their nearest neighbor only. The two end elements transfer heat with their interior neighbor and the outside air. The slab extends to infinity in the vertical directions and into the page.

To make our task simpler let's look at the problem in a one-dimensional slab. The slab is very large in two of the dimensions (that we don't care about), with respect to its thickness (the dimension we do care about). We will analyze a similar problem as in the last section, a hot object at uniform temperature is placed in cold air. Both sides of the slab are exposed to the fluid and we want to model temperature gradients inside the slab. Instead of representing the body as one thermal mass, we will represent it by a collection of 10 coupled thermal masses. The system model is shown in Figure 1.1.

As we have done in the previous lumped model, we can conduct an energy balance on each element. The change in the amount of stored thermal energy contained in any element i , ΔQ_i , is

$$\Delta Q_i = mC_p(T_i - T_0) \quad (1.5)$$

where m is the mass, C_p is the specific heat, T_i is the temperature of element i , and T_0 is the initial reference temperature. We assume that the size, mass, and specific heat of each element is constant and the elements are the same size. For an interior element, the heat flux, q'' , (W/m^2) that flows from element i to element $i + 1$ is given by Fourier's conduction law,

$$q'' = k \frac{T_{i+1} - T_i}{\Delta x}, \quad (1.6)$$

where k is the thermal conductivity of the material and Δx is the distance between the two points, $\Delta x = L/N$ where N is the number of elements. We are assuming that each block is the same size and therefore Δx is the same for the each point. Using Fourier's law assumes that the temperature gradient is linear between elements i and $i + 1$. Likewise the heat flux leaving the element i to $i - 1$ is

$$q'' = k \frac{T_i - T_{i-1}}{\Delta x} \quad (1.7)$$

Conservation of energy on any region says that the rate of change of energy stored inside the region must equal the net rate that energy leaves/enters the region.

$$\frac{d\text{Energy Stored}}{dt} = \dot{E}_{\text{in}} - \dot{E}_{\text{out}} \quad (1.8)$$

Note the sign; when energy input is greater than the output the energy stored increases. Applying this energy balance on an interior element i .

$$mC_p \frac{dT_i}{dt} = kA \frac{T_{i+1} - T_i}{\Delta x} - kA \frac{T_i - T_{i-1}}{\Delta x}. \quad (1.9)$$

where A is the cross-sectional area normal to the direction of heat flow (area of the wall). Since the mass of the element is dependent on its size, Δx , we can rewrite the equation as

$$\Delta x A \rho C_p \frac{dT_i}{dt} = kA \frac{T_{i+1} - T_i}{\Delta x} - kA \frac{T_i - T_{i-1}}{\Delta x}. \quad (1.10)$$

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where ρ is the material density. Assuming that the density, thermal conductivity, and specific heat do not change from element to element and using the definition of thermal diffusivity as $\alpha = k/\rho C_p$ (this property is tabulated for most materials, e.g. copper = $1.17 \text{ cm}^2/\text{s}$ and building insulation $0.001 \text{ cm}^2/\text{s}$) we obtain

$$\frac{dT_i}{dt} = \alpha \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}. \quad (1.11)$$

Since the material properties are constant this equation is valid for any interior node. The property α is a material property that has units of m^2/s . At the edges exposed to the air and the heat is lost by convection

$$q'' = h(T_1 - T_{air}). \quad (1.12)$$

For the first node the equation becomes

$$\Delta x A \rho C_p \frac{dT_1}{dt} = -hA(T_1 - T_{air}) + kA \frac{T_2 - T_1}{\Delta x} \quad (1.13)$$

which reduces to

$$\frac{dT_1}{dt} = -\frac{h}{\Delta x \rho C_p} (T_1 - T_{air}) + \alpha \frac{T_2 - T_1}{\Delta x^2}. \quad (1.14)$$

The other node has a similar relationship, namely

$$\frac{dT_{10}}{dt} = -\frac{h}{\Delta x \rho C_p} (T_{10} - T_{air}) + \alpha \frac{T_9 - T_{10}}{\Delta x^2}. \quad (1.15)$$

The boundary expression can also be written as

$$\frac{dT_1}{dt} = -\frac{hk}{k\Delta x \rho C_p} (T_1 - T_{air}) + \alpha \frac{T_2 - T_1}{\Delta x^2}. \quad (1.16)$$

or equivalently

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2} (-Bi(T_1 - T_{air}) + (T_2 - T_1)). \quad (1.17)$$

where $Bi = h\Delta x/k$ is called the Biot number in the classical heat transfer literature. The final expression is more useful as it shows that the dimensionless Biot number can be used to understand the influence of the boundary condition. If the Biot number is large, then the system will tend to have the boundary nodes equal to the air temperature. A large Biot number means that convection is much faster than conduction; heat leaves the surface to the fluid quickly but it takes time for heat to leave the interior region. The effect of large Biot number can be seen in the governing equations; a strong tendency to equilibrate T_1 with T_{air} . When Bi is small, convection is slow and conduction is fast. Heat leaves the body slowly, but once it leaves at the fluid surface the interior “corrects” itself instantaneously. If the Biot number is small when we are only using one grid point (i.e. $Bi = hL/k$) the lumped model is sufficiently accurate. When the Biot number is zero, the boundary is insulated and there is no heat transfer out of the body. The effect of the Biot number will be shown in the next section in the simulations.

You should not overlook this simple but important point about dimensionless numbers. The usefulness of dimensionless numbers is one of the great ideas in science and engineering. Nature does not care that man has defined seconds, meters, and kilograms. Nature has no idea if something is big or small, fast or slow. We must always talk of something being fast with respect to something else. One of the great dimensionless numbers is the Reynolds number, attributed to Osbourne Reynolds in a paper he wrote in 1883. Before Reynolds there were numerous tables and charts that showed the relationship between pressure drop and flow rate in a pipe for different sized pipes and different fluids. For each fluid and pipe there was a separate chart. Reynolds showed that by using a dimensionless numbers that all these charts could be collapsed into one single curve. He showed all pipe flows were the same if one used “Nature’s” units rather than man’s units. The key parameter is, the Reynolds number, and physically it is the ratio of inertial force to viscous force.

1.2.3 Modeling and implementation

Below we provide a sample program that will perform a simulation of the slab with the two ends exposed to the exterior flowing air. The equations that we will be solving were derived in the previous section, but are summarized

below.

$$\frac{dT_i}{dt} = \frac{\alpha}{\Delta x^2}(T_{i+1} - 2T_i + T_{i-1}), \quad (1.18)$$

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2}(-Bi(T_1 - T_{air}) + (T_2 - T_1)), \quad (1.19)$$

$$\frac{dT_{10}}{dt} = \frac{\alpha}{\Delta x^2}(-Bi(T_{10} - T_{air}) + (T_9 - T_{10})), \quad (1.20)$$

where i indicates the index for the interior nodes, 2-9. In the above equations, the Biot number is dimensionless and α has units of Length²/time. The quantity $\Delta x^2/\alpha$ has units of time and can be considered a conduction τ for each grid-block. The equations are dimensionally correct which is always a necessary condition for our analysis to be correct!

This system of ordinary differential equations can be solved using many of the techniques for solving any system of ordinary differential equations. We will choose to solve the equations using Euler's method for simplicity. Also, note in the program below that I am using MATLAB's whole array operations to write a single compact expression for the time rate of change of the temperature of each interior node. The end points are treated independently. You could also have an loop that runs through all the interior nodes, however the formulation below is nice and compact.

```

N = 10;           %% number of boxes
dt = 0.0001;     %% time step size
T = ones(N,1)    %% initial temperature
x = linspace(0,1,N); %% grid points
dT = zeros(size(T)); %% initial dT/dt vector
dx = 1/N;       %% distance between grid pointd
Bi = 10;        %% Biot number
a = 1;          %% alpha (cm^2/s)
time = 0;      %% initial time

while time < 1
    time = time+dt;

    dT(2:end-1) = a/dx^2*(T(1:end-2) - 2*T(2:end-1) + T(3:end)); %% dT eqns
    dT(1) = a/dx^2*(-Bi*(T(1) - 0) + (T(2) - T(1))); %% boundary
    dT(end) = a/dx^2*(-Bi*T(end) - 0) + (T(end-1) - T(end)); %% boundary

    T = T + dt*dT; %% integrate forward in time using Euler

    %% plot and set axis
    plot(x,T,'r')
    axis([0 1 0 1])
    pause(0.01)
end

```

The results of this model for different Biot are shown in Figure 1.2. It is clear from this picture that if the Biot number is below 0.1 then the temperature inside the object can be considered uniform. As the Biot number becomes large, it is clear that the object has significant temperature variations. As the Biot number increases the object also cools faster. This increased speed in cooling is due to the increase in the convection coefficient.

We can easily change the boundary conditions in the simulation. If we would like to maintain a fixed temperature on one wall, we simply set the temperature of that wall in the initial condition and change the boundary condition in the governing differential equations to be $dT(1) = 0$. If we would like to assume that the wall is adiabatic, that means that no heat can escape, then we simply set $dT(1) = -a*(T(1) - T(2))/1^2$ since there is only heat flow into the body from its nearest neighbor.

We see in figure 1.2 that the boundary is not well resolved when we only use a small number of points. If you increase the resolution, the result will get "better". You should experiment with this simulation to make sure that the solution converges as you increase the number of sub-blocks you use to represent the solution. If you continue to increase the resolution in the simulation, you will find that at some point, the simulation gives you a jumbled looking solution and there is an apparent instability. The cause of this instability is well known.

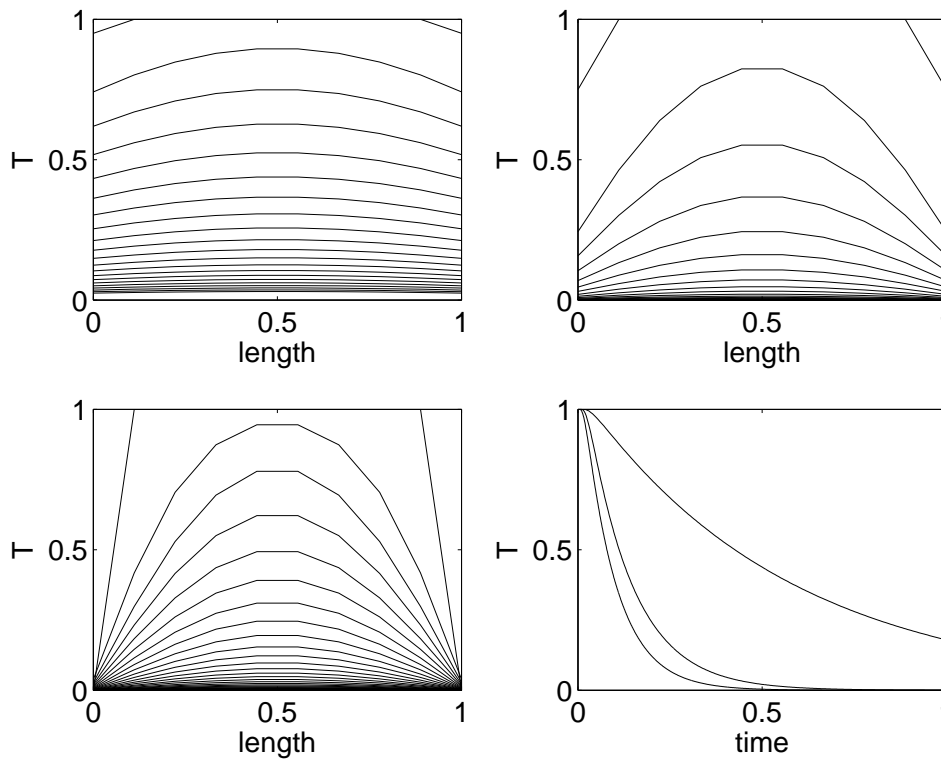


Fig. 1.2 Solutions to the cooling problem as generated by the code provided. Going left to right then down, the first three figures show the temperature inside the solid for $Bi = 0.1, 1, 10$ respectively at different instances in time. The figure in the lower right shows the center temperature as a function of time for the three cases. The Biot number increases the object cools faster. Also note that for small Biot numbers that we could probably get away with the lumped analysis. The non-uniformity in the first figure where $Bi = 0.1$ is small enough that the lumped model would predict similar results; the agreement becomes stronger as Bi decreases.

1.2.4 Stability

Through analysis that is not very complicated, but will not be presented here, the equations are unstable when integrated with Euler's method and the time step is such that $\Delta t \alpha / \Delta x^2 > 0.5$. You can explore this behavior with the code provided by changing the time step size. In general, when solving these diffusion problems numerically we must use a small enough time step.

Physically this criteria means that we must take steps small enough that there is not significant diffusion across one grid block during one time step. The number $\Delta t \alpha / \Delta x^2 > 0.5$ has no units and can be interpreted as the ratio of the time step taken in the integration and the time it takes heat to "move" across one grid point.

For different methods of integration where the derivative is evaluated based on current knowledge of the state (explicit methods) there will always be some similar criteria as stated above. The criteria will change with the method of time integration, but there will be a stability criteria. Methods where the derivative is based on future knowledge (implicit methods) are always stable.

1.3 ANALYSIS

1.3.1 Continuous equations

In this section we will use Taylor series to understand the discrete equations that we derived in the previous section. At this point, if you do not remember the Taylor series you should perhaps review the concept in your Calculus textbook.

Consider the temperature of the bar at one of the nodes, T_i , in the simulation. The temperature at a neighboring node which is located a distance Δx to the right, T_{i+1} , can be approximated by the Taylor Series.

$$T_{i+1} = T_i + \frac{dT_i}{dx} \Delta x + \frac{d^2 T_i}{dx^2} \frac{\Delta x^2}{2} + \frac{d^3 T_i}{dx^3} \frac{\Delta x^3}{3!} + \frac{d^4 T_i}{dx^4} \frac{\Delta x^4}{4!} \quad (1.21)$$

Likewise, the temperature to the left of node i may be written as

$$T_{i-1} = T_i - \frac{dT_i}{dx} \Delta x + \frac{d^2 T_i}{dx^2} \frac{\Delta x^2}{2} - \frac{d^3 T_i}{dx^3} \frac{\Delta x^3}{3!} + \frac{d^4 T_i}{dx^4} \frac{\Delta x^4}{4!} \quad (1.22)$$

Adding these two expressions together results in

$$T_{i+1} + T_{i-1} = 2T_i + 2\frac{d^2 T_i}{dx^2} \frac{\Delta x^2}{2} + 2\frac{d^4 T_i}{dx^4} \frac{\Delta x^4}{4!} \quad (1.23)$$

which can be written as

$$\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} = \frac{d^2 T_i}{dx^2} + 2\frac{d^4 T_i}{dx^4} \frac{\Delta x^2}{4!} \quad (1.24)$$

If the spacing between nodes is small and Δx is taken to zero, the term with the fourth derivative is negligible. In the limit as Δx goes to zero the equation becomes

$$\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} \approx \frac{d^2 T_i}{dx^2} \quad (1.25)$$

If we refer back to our numerical approximation to the conduction in the bar we find that the discrete equation is an approximation to the continuous equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}. \quad (1.26)$$

This result is the one-dimensional diffusion equation. This equation is well-known in physics and governs a variety of different phenomena.

Let's think about this expression for a moment. It states that the time rate of change of the temperature at a point is proportional to the second spatial derivative. The second derivative of a function is the curvature. If we have a location where the temperature curves upward the temperature increases, when the curvature is negative the temperature at that point decreases. This effect can be visualized by looking at Figure 1.3. In the figure we show three possible temperature distributions. In each case let us consider the rate of change of temperature at the center point. When we have positive curvature, the neighboring points (circles) pull the temperature of the center up. When we have negative curvature, the neighboring points pull the temperature of the center down. When we have a linear temperature gradient the center is pulled equally up and down and therefore does not change!

1.3.2 Non-dimensionalization

Let's start with the diffusion equation from the previous section over a slab of total length L . We introduce a non-dimensional spatial coordinate $\hat{x} = x/L$ so that the diffusion equation becomes,

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial (L\hat{x})^2}. \quad (1.27)$$

Since L is a constant we can pull it outside the derivative to obtain

$$\frac{\partial T}{\partial t} = \frac{\alpha}{L^2} \frac{\partial^2 T}{\partial \hat{x}^2}. \quad (1.28)$$

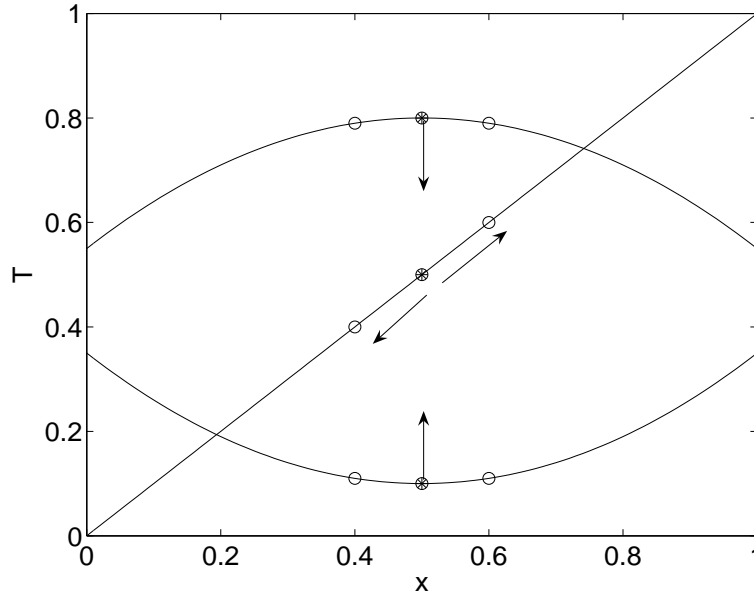


Fig. 1.3 Three different temperature distributions with positive, negative, and zero curvature. When we have positive curvature, the neighboring points pull the temperature of the center up. When we have negative curvature, the neighboring points pull the temperature of the center down. When we have a linear temperature gradient the center is pulled equally up and down.

We can also define a non-dimensional time as $\hat{t} = t/t_0$ where t_0 is an arbitrary (for now) time scale; the new equation is

$$\frac{\partial T}{\partial(t_0 \hat{t})} = \frac{\alpha}{L^2} \frac{\partial^2 T}{\partial \hat{x}^2}, \quad (1.29)$$

which is rearranged as

$$\frac{\partial T}{\partial \hat{t}} = \frac{\alpha t_0}{L^2} \frac{\partial^2 T}{\partial \hat{x}^2}. \quad (1.30)$$

Nothing is stopping us from arbitrarily setting $t_0 = L^2/\alpha$ so that the diffusion equation becomes

$$\frac{\partial T}{\partial \hat{t}} = \frac{\partial^2 T}{\partial \hat{x}^2}. \quad (1.31)$$

We can also scale the temperature as appropriate for the boundary conditions. Consider the problem where the body is of uniform temperature and the left and right boundaries are held at T_0

$$T(t = 0, x) = T_{init}; \quad T(x = 0, t > 0) = T_0; \quad T(x = 1, t > 0) = T_0 \quad (1.32)$$

We can introduce the function

$$\hat{T} = \frac{T - T_0}{T_{init} - T_0} \quad (1.33)$$

This scaling changes the boundary conditions to

$$\hat{T}(t = 0, x) = 1; \quad \hat{T}(x = 0, t > 0) = 0; \quad \hat{T}(x = 1, t > 0) = 0 \quad (1.34)$$

The scaling for temperature does not effect the governing partial differential equation either.

While it may not seem so, this result is very powerful; it says all diffusion problems are the same. We simply scale the geometry to have a length that ranges from zero to one. The combination of the size and the thermal diffusivity tell give us the appropriate time unit. On the scaled domain and in the proper time units, problems of different size and material property will have the same solution. Regardless of the size, material or temperatures

involved, if you solve the diffusion equation for one set of boundary conditions you have solved it for all cases once and for all. Once we have our solution we simply use the definitions above to move from the dimensionless solution to physical units by multiplying by the appropriate constants.

Suppose we have a slab of copper that is one centimeter thick, the appropriate time scale is $t_0 = L^2/\alpha = 1^2/1.17$ seconds. If we then double the thickness to 2 centimeters the time scale changes to $t_0 = 2^2/1.17$ seconds. This means that temperature field will be the same in the second case at a physical time that is four times longer. If you are cooking two steaks and one is twice as thick as the other, the thicker one will need to cook four times longer to achieve the same center temperature. The scaling also shows that the cooling of an object from 200 C to 25 C is the same as cooling from 30 C to 25 C. This result is truly remarkable.

1.3.3 Separation of variables

The partial differential equation that governs diffusion processes is one that we can solve analytically. If the boundary conditions are simple we can compute this solution readily, if the conditions are complicated we can still solve the problem but we will not consider those complicated situations in this course.

Take the standard diffusion equation

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, \quad (1.35)$$

and assume that the solution is composed of the product of two functions one that is a function of x and the other is a function of t .

$$T(x, t) = \Theta(t)X(x). \quad (1.36)$$

Substitution into the governing equation becomes

$$\frac{d\Theta(t)}{dt}X(x) = \Theta(t)\frac{d^2X(x)}{dx^2}, \quad (1.37)$$

which is rewritten as

$$\frac{1}{\Theta(t)}\frac{d\Theta(t)}{dt} = \frac{1}{X(x)}\frac{d^2X(x)}{dx^2} \quad (1.38)$$

Since everything on the left side of the equation is a function of time only, and everything on the right side of the equation is a function of space only, the only possible solution is that both sides of the equation equal a constant;

$$\frac{1}{\Theta(t)}\frac{d\Theta(t)}{dt} = \frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = -\lambda^2. \quad (1.39)$$

The minus sign and the power of two are put in the equation arbitrarily. This will not effect the answer but they will make the answer come out a little nicer in the end. The reason for the negative sign will be apparent shortly. Since I know the answer ahead of time I will include these factors now. We can now solve each of the problems independently;

$$\frac{1}{\Theta(t)}\frac{d\Theta(t)}{dt} = -\lambda^2. \quad (1.40)$$

which is easily rearranged

$$\frac{d\Theta(t)}{\Theta} = -\lambda^2 dt. \quad (1.41)$$

which is integrated to yield

$$\log(\Theta) = -\lambda^2 t + C \quad (1.42)$$

where C is a constant of integration.

$$\Theta = e^{-\lambda^2 t + C} = e^C e^{-\lambda^2 t} \quad (1.43)$$

and since C is an arbitrary constant

$$\Theta = C e^{-\lambda^2 t} \quad (1.44)$$

It is clear why the negative sign was needed when choosing the constant. If the constant was positive, the solution would grow out of control with positive feedback. The negative sign allows a nice gentle decay as we would expect from physical reasoning.

Now we turn to the equation that was a function of x ;

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} = -\lambda^2. \quad (1.45)$$

We have seen this equation several times and can integrate it directly or simply go straight to the answer

$$X(x) = A \sin(\lambda x) + B \cos(\lambda x) \quad (1.46)$$

where A and B are constants of integration. You may now see why we chose λ^2 as our constant. Combining our expressions for X and Θ are

$$T(x, t) = e^{-\lambda^2 t} (A \sin(\lambda x) + B \cos(\lambda x)) \quad (1.47)$$

Note that the constant of integration C is absorbed with A and B . You can verify that this expression satisfies the governing equations by simple substitution.

To find the constants of integration, we need to apply initial and boundary conditions to the equation. We will solve the problem where T is initially uniform and at $t > 0$ the boundaries are held fixed at zero;

$$T(x = 0, t > 0) = 0; \quad T(x = 1, t > 0) = 0; \quad T(0 < x < 1, t = 0) = 1. \quad (1.48)$$

When $x = 0$,

$$T(x = 0, t) = e^{-\lambda^2 t} B = 0 \quad (1.49)$$

can only be satisfied when $B = 0$. When $x = 1$

$$T(x = 1, t) = e^{-\lambda^2 t} A \sin(\lambda) = 0 \quad (1.50)$$

The only way this equation can be satisfied is that $A = 0$ or when $\lambda = n\pi$ where n is an integer; $n = 0, 1, 2, \dots$. The second option is the only interesting solution. Since the solution is linear, any combination of solutions corresponding to any acceptable value of n is a solution to the governing equation and satisfies the boundary conditions.

At this point our solution looks like,

$$T(x, t) = \sum_{n=0}^{\infty} A_n e^{-(n\pi)^2 t} \sin(n\pi x). \quad (1.51)$$

To get our final solution, we need to apply the initial condition.

$$T(x, t = 0) = \sum_{n=0}^{\infty} A_n \sin(n\pi x) = 1 \quad (1.52)$$

We now need a way to compute the A_n so that the above expression holds true. This method will seem odd at first, however, just bear through the solution and convince yourself that it works. To find the coefficients A_n you can use the following integral properties. These properties can be derived or you can look them up in a calculus textbook, but we will just state the result here:

$$\int_0^1 \sin(n\pi x) \sin(m\pi x) dx = 0; \quad \text{n and m are integers, and } n \neq m \quad (1.53)$$

$$\int_0^1 \sin(n\pi x) \sin(n\pi x) dx = 1/2; \quad \text{n is an integer} \quad (1.54)$$

Using these properties of integrals allows us to extract the coefficients. We multiply 1.52 by $\sin(m\pi x)$ and integrate the function across the domain;

$$\int_0^1 \sum_{n=0}^{\infty} A_n \sin(n\pi x) \sin(m\pi x) dx = \int_0^1 \sin(m\pi x) dx \quad (1.55)$$

The sum results in many terms, however they are all zero except for the one where $n = m$. Using the fact that most terms in the sum are zero under this operation, we are left with,

$$\int_0^1 A_m \sin(m\pi x) \sin(m\pi x) dx = \int_0^1 \sin(m\pi x) dx. \quad (1.56)$$

Both sides of this expression can be integrated analytically such that

$$A_m = \frac{4}{m\pi} \quad \text{when } m = 1, 3, 5, 7 \quad (1.57)$$

and

$$A_m = 0 \quad \text{when } m = 0, 2, 4, \quad (1.58)$$

While the expression is difficult to visualize, it is easy to plot. The sum is taken to infinity, however in practice it need not be. The smoother the function, the fewer terms are needed to represent the solution. The convenient aspect of this solution is that we can find the temperature profile at any instant in time without finding the solution at any earlier times.

1.3.4 How are we finding A_n ; an aside

Consider the sample problem we just worked with the same boundary condition, but take the initial condition is an arbitrary function, $f(x)$, we would need to solve the following equation

$$T(x, t = 0) = \sum_{n=0}^{\infty} A_n \sin(n\pi x) = f(x) \quad (1.59)$$

The technique we used to extract the coefficients A_n certainly seems strange the first time through; however, it is not at all strange as we will now show through analogy with a simpler example.

An ordinary vector, F , has components in three dimensional space; x, y , and z . The vector can be represented with a basis set of the three units vectors, \hat{e}_x , \hat{e}_y and \hat{e}_z , pointing in three dimensions. Each of the units vectors are perpendicular (or orthogonal) to each other. To describe the vector F , each unit vector has some magnitude, A , that represents the projection (shadow) of the F in that direction.

$$A_x \hat{e}_x + A_y \hat{e}_y + A_z \hat{e}_z = \mathbf{F}. \quad (1.60)$$

If F is a known and I asked you to find the coefficient A_x , you would tell me that it is trivial. To find any of the A coefficients, we simply take the inner (or dot) product of the whole expression with each of the unit vectors in turn. When F is known, we find A_x by

$$(A_x \hat{e}_x + A_y \hat{e}_y + A_z \hat{e}_z = \mathbf{F}) \cdot \hat{e}_x. \quad (1.61)$$

Since the inner product of any two of the different unit vectors is zero, and the inner product of like unit vectors is one we obtain

$$A_x = \mathbf{F} \cdot \hat{e}_x \quad (1.62)$$

This example may seem rather trivial and obvious given that it is so familiar. The procedure is so simple since the original basis vector set had the nice property that the inner product of any two unlike units vectors is zero.

Now consider our functional expression

$$A_1 \sin(\pi x) + A_2 \sin(2\pi x) + A_3 \sin(3\pi x) + A_4 \sin(4\pi x) + \dots = f(x) \quad (1.63)$$

and let us find the coefficients in the exact same way. Think of each function $\sin(n\pi x)$ as a basis “vector”. In this function space the operation, $\int_0^1 f(x) \sin(n2\pi x) dx$ will serve as the inner product of our “vector” f with the n^{th} basis “vector” $\sin(n\pi x)$. The inner product operation satisfies the same conditions as our usual operation with three dimensional basis vectors. We get zero for the inner product of any combination of basis functions, except when we take the inner product with itself. For example,

$$\int_0^1 \sin(\pi x) \sin(2\pi x) dx = 0; \quad (1.64)$$

$$\int_0^1 \sin(\pi x) \sin(\pi x) dx = 1/2; \quad (1.65)$$

This expression is analogous to saying the $\hat{e}_x \cdot \hat{e}_y = 0$ and $\hat{e}_x \cdot \hat{e}_x = 1$. If we were going to be more precise we would define the basis functions such that the inner product with itself was unity, but the factor of $1/2$ gives us no problem at this time.

So now, following our analogy to find the coefficients in front of each basis function we take the inner product of the whole expression with the first basis function ($n = 1$) just like in equation 1.60

$$\int_0^1 [A_1 \sin(\pi x) + A_2 \sin(2\pi x) + A_3 \sin(3\pi x) + A_4 \sin(4\pi x) + \dots = f(x)] \sin(\pi x) dx \quad (1.66)$$

Since the basis functions are orthogonal, the inner product is zero for any combination of unlike functions. Our analogous expression to 1.62

$$A_1 = 2 \int_0^1 f(x) \sin(\pi x) dx. \quad (1.67)$$

For any coefficient, n , we would obtain

$$A_n = 2 \int_0^1 f(x) \sin(n\pi x) dx. \quad (1.68)$$

The term on the right $\int f(x) \sin(n\pi x) dx$ is the inner product of the first basis function with the known function $f(x)$. Just like $\mathbf{F} \cdot \hat{e}_x$ gives the projection of F in the x direction, $\int_0^1 f(x) \sin(\pi x) dx$ gives the projection of $f(x)$ on $\sin(\pi x)$.

It turns out that the analogy between the functions and vectors and all the talk of inner products is more than an analogy; it turns out to be precisely the same thing! These ideas are explained only to introduce you to this idea and hopefully spark some interest. You will likely see these ideas in a later math course and would need to talk to a “real” mathematician to get the ideas precise. If this seems utterly confusing, don’t worry, these ideas are only presented as an aside.

1.3.5 Vector calculus: an aside

Thus far we have considered the diffusion equation in one-dimension. In two or three dimensions we can use our knowledge of vector calculus to obtain a compact notation for heat diffusion. Consider an arbitrary “blob” of material in our solid of interest. We can apply the energy balance laws with our more generalized notation.

The local heat flux vector in a conducting solid is given by Fourier’s law as,

$$\mathbf{q}'' = -k\nabla T. \quad (1.69)$$

This expression says that heat flows down a temperature gradient from hot to cold. If we know the temperature field we can use this expression to find the local heat flux (magnitude and direction).

The change in the total thermal energy stored inside a solid control volume as we move from temperature T_0 to T is

$$\int \rho C_p (T - T_0) dV. \quad (1.70)$$

Since T is a function of x and t , the spatial dependence is removed by integrating over the volume. Equation 1.70 is a function of time only. Therefore, the rate of change of the total energy inside a control volume follows as

$$\frac{d}{dt} \int \rho C_p (T - T_0) dV. \quad (1.71)$$

We can find the total amount of heat leaving our control volume by taking the dot product of the heat flux vector and the normal vector at the surface bounding the control volume. The total heat loss leaving our volume is found by integrating over the surface area,

$$\int \mathbf{q}'' \cdot \mathbf{n} dA \quad (1.72)$$

Considering conservation of energy, we know that the rate of change of energy stored inside the control volume must equal the rate that energy is leaving the control volume at the surface,

$$\frac{d}{dt} \int \rho C_p (T - T_0) dV = - \int \mathbf{q}'' \cdot \mathbf{n} dA \quad (1.73)$$

Using the 1.69 and Gauss's theorem and we have the equality

$$\int q'' \cdot n dA = \int \nabla \cdot q'' dV. \quad (1.74)$$

Using Fourier's law

$$- \int \nabla \cdot q'' dV = \int \nabla \cdot k \nabla T dV. \quad (1.75)$$

These equalities transform our integral expression for the energy balance to

$$\frac{d}{dt} \int \rho C_p (T - T_{ref}) dV = \int \nabla \cdot k \nabla T dV \quad (1.76)$$

Since the object is solid, the control volume is fixed and does not change with time, we can move the time derivative operator inside the integral. Also assuming the material properties are constant (a pretty good assumption) we can simplify our expression to become

$$\int \rho C_p \frac{\partial T}{\partial t} dV = \int \nabla \cdot k \nabla T dV \quad (1.77)$$

which is written as

$$\int \left(\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot k \nabla T \right) dV \quad (1.78)$$

Since the control volume is arbitrary, the only way that the expression holds true is if the differential expression inside the integral is satisfied everywhere, namely,

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T \quad (1.79)$$

when the thermal conductivity is constant we obtain

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T \quad (1.80)$$

In setting up the diffusion equation, we saw that the energy balance could be stated as

$$\frac{\partial \text{Energy Stored}}{\partial t} = -\nabla \cdot \mathbf{q} \quad (1.81)$$

or stated in words

$$\nabla \cdot \mathbf{q} = \text{rate of heat out per unit volume.} \quad (1.82)$$

When a system is at steady state

$$\nabla \cdot \mathbf{q} = 0 \quad (1.83)$$

In electrostatics we found that when the divergence of the electric field was zero, there was no charge inside the volume of interest. In conduction problems when the divergence of the heat flux vector is zero, the system is at steady state; the energy in the body is no longer changing.

1.4 MASS DIFFUSION

The laws we have described in the context of heat are found when we analyze the inter-diffusion of molecules. Imagine a container of two gases separated at the center by a partition. If the partition is removed, the two gases will mix. They can mix by convection, if the gas is disturbed and flows around inside the contained. If the partition is removed carefully and the gas is not disturbed the two fluids will mix due to molecular diffusion. Even though there is no fluid velocity in the bulk, the gas molecules are always moving. The molecules will whiz around inside the box, knocking each other around and over time the particles of both gases will be intermixed. How long does it take for such a process to happen?

Just like in heat flow, we can show (but we won't) that when we have a gradient in the number density of a particular gas that there is a resulting mass flux that moves down this gradient.

$$\mathbf{j} = -D \nabla n, \quad (1.84)$$

where D is the mass diffusivity and \mathbf{j} is the mass flux vector. This law is known as Fick's law of diffusion and is identical to Fourier's law of conduction. Conservation of mass states that the rate of change of mass inside a arbitrary control volume is equal to the amount leaving. The amount of particles crossing a particular surface is the dot product of the mass flux vector and the normal to the surface. The conservation of mass can be written as

$$\frac{d}{dt} \int n dV = \int \mathbf{j} \cdot \mathbf{n} dA \quad (1.85)$$

Using Gauss's theorem

$$\int \left(\frac{\partial n}{\partial t} = \nabla \cdot D \nabla n \right) dV \quad (1.86)$$

As before, we get the following partial differential equation when take the mass diffusivity to be constant

$$\frac{\partial n}{\partial t} = D \nabla^2 n. \quad (1.87)$$

When this equation is cast into non-dimensional form it looks identical to the problems that we solved for heat diffusion. The analysis is the same. The analogy is perfect.

We have discussed diffusion as a continuous problem. We consider that the number density has a value that is distributed in space and that mass flux can be taken as the gradient of this field. If we get a microscope out we find that there are little particles that are moving about inside the container. The gas is not continuous, so how is this understanding of continuous diffusion linked to the randomness of molecular motion.

When we imagine the case of tagging the molecules on the left of our container blue (blue states) and the right of our container red (red states), what is happening to each particle? Each particle undergoes a wayward path. It is constantly colliding with other particles which causes the particle to change direction and speed often. As the processes proceeds the red particles push their way, bouncing around, through to the blue part of the container and vice versa. The path of any and all particles is very random and cannot be predicted. We can however, speak of a statistical average of the random motion.

This random walk is often called the drunken sailor problem. The drunk sailor walks out of the bar has no idea where he is going, does not remember where he has been, and does not know where he is going. Every step is taken at complete random. I do not know why we are so quick to stereotype sailors, but that is beside the point. Some of his steps will be small, some long; some to the left, some to the right. A simulation of this situation is easy to do. Simply start at known x, y coordinate location and with each time step, move a random distance in both x and y . In doing so we use the Gaussian, or normal, distribution to determine the direction and magnitude of each step. Every time we run the simulation we will get something different, a sample is shown in figure 1.4.

Since each simulation is different we can repeat the experiment many time and ask the question, on average how far away from the bar is the sailor? If we plot the total distance from the bar versus time for one situation and the average of many simulations on log-log coordinates we obtain a result as shown in Figure 1.5. We find that in this case that an individual sailor gets further from the bar in a random way, but that on average r^2 increases linearly with time. To go twice the distance takes 4 times as long. This is the same result we found in the diffusion problem, it takes four time longer to cook a steak that is twice as thick.

The situation that we have just discussed is also known as Brownian motion. In 1828 Robert Brown noticed that small pollen grains in a liquid had paths as shown in Figure 1.4. Einstein considered this problem in 1905 (the same year that he wrote the special theory of relativity) and put the motion of such particles on a theoretical basis. He considered the motion of the particles to be due to collisions of molecules with the small particles. He derived an expression that allowed one of the first accurate measurements of Avogadro's number and other molecular properties. It turns out that a French mathematician, Louis Bachelier, considered the diffusion of probabilities in 1900 (before Einstein) for his PhD thesis which was done on the supervision of Poicare (a famous mathematician who you may come across). The thesis was titled "Theory of Speculation" and dealt with a theory for options pricing.

1.4.1 Analysis of the random walk: an aside

It is easy to show that the distance traveled by the particles increases as the square root of the time as we observed in our simulations. Consider the equations of motion for a small particle; it obeys Newtons law and the forces acting

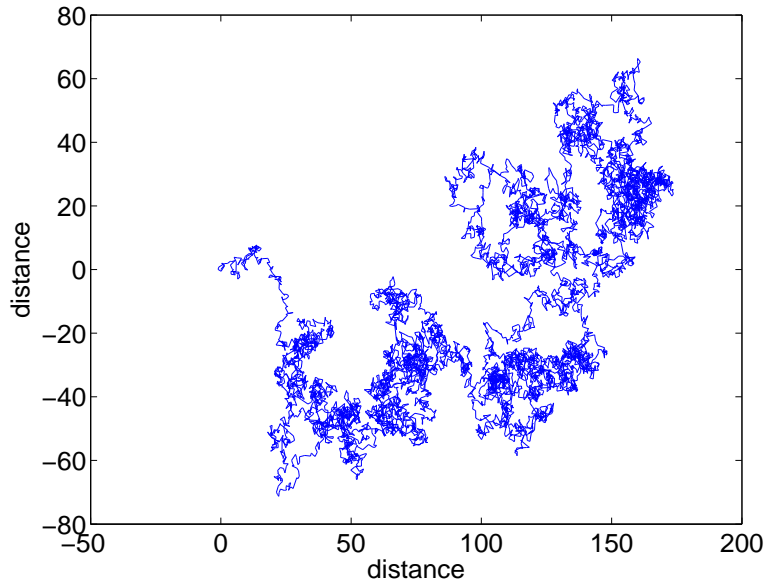


Fig. 1.4 Example of a random path taken by the drunken sailor. The sailor starts at zero,zero and at each instant in time takes a step that has random direction and magnitude.

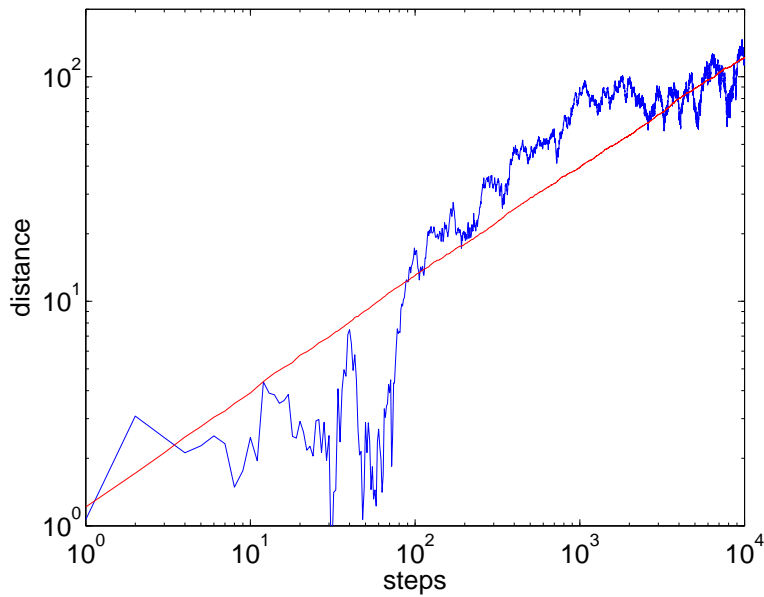


Fig. 1.5 Distance traveled in a random walk. The jagged line represent one particles motion. The smooth line represents the average of 1000 particles. The smooth line follows increases with the square root of the time, just like the diffusion problem.

on the particle are a random external force due to molecular collisions and a viscous drag

$$m \frac{d^2x}{dt^2} + \mu \frac{dx}{dt} = F_{ext} \tag{1.88}$$

where m is the mass, x is the position, μ is a constant, and F_{ext} is the external force. The constant μ could be found experimentally by finding how past the particle settles in a constant gravity field.

We introduce the notation $\langle \rangle$ to denote time averaging; $\langle x^2 \rangle$ is the time average of the displacement squared. What we want to know is how does the mean squared displacement vary with time;

$$\frac{d\langle x^2 \rangle}{dt} = ? \quad (1.89)$$

Let's start the analysis by noting that

$$\frac{dx^2}{dt} = 2x \frac{dx}{dt} \quad (1.90)$$

Now we multiply equation 1.88 by x to obtain

$$mx \frac{d^2x}{dt^2} + \mu x \frac{dx}{dt} = xF_{ext} \quad (1.91)$$

note that

$$x \frac{d^2x}{dt^2} = \frac{d(x dx/dt)}{dt} - \left(\frac{dx}{dt} \right)^2 \quad (1.92)$$

$$m \left(\frac{d(x dx/dt)}{dt} - \left(\frac{dx}{dt} \right)^2 \right) + \mu x \frac{dx}{dt} = xF_{ext} \quad (1.93)$$

Now we take time average of the whole equation

$$\left\langle m \frac{d(x dx/dt)}{dt} \right\rangle - \left\langle m \left(\frac{dx}{dt} \right)^2 \right\rangle + \left\langle \mu x \frac{dx}{dt} \right\rangle = \langle xF_{ext} \rangle \quad (1.94)$$

If we computed the frequency with which the particle in the fluid is colliding with molecules, we would find that the particle is hit about 10^{14} times a second. If we time average over any scale with which we can observe, this jitter is extremely fast. We expect that since the jitter is completely random that certain terms in the equation disappear with time averaging. The external force is just as likely to push to the left as to the right. Therefore, averaged over time and this force is zero. The velocity is just as likely to be to the left or the right, therefore the term xv is time averaged to zero. All that is left is

$$-\langle mv^2 \rangle + \frac{\mu}{2} \left\langle \frac{dx^2}{dt} \right\rangle = 0 \quad (1.95)$$

It is known from kinetic theory that the time averaged kinetic energy is proportional to the temperature through Boltzmann's constant, k . So we have that

$$\frac{d\langle x^2 \rangle}{dt} = \frac{2kT}{\mu} \quad (1.96)$$

Therefore the time time rate of change of the square of the displacement is a positive constant, and therefore grows linearly with time.

2

Diffusion Labs and problem sets

2.1 WEEK 1: RC CIRCUITS AND SIMULATION

This week you will build an “analog” computer to solve a discrete set of equations similar to those that you saw in Chapter 1. In Chapter 1 we derived a model based on energy conservation for a series of coupled, lumped thermal masses. We showed that as fineness of the discretization increased, that the equation set becomes that of a partial differential equation governing heat flow.

In this lab you will use a network of resistors and capacitors to simulate the diffusion equation in one dimension. The circuit is a perfect representation of the discrete heat equation that we derived in chapter 1. Through a series of simulations and experiments you will explore the behavior of the diffusion equation.

2.1.1 Introduction to circuit modeling

You may have seen in physics that the charge of a capacitor is related to the voltage across the plates as

$$Q = CV. \quad (2.1)$$

We will make the analogy that the total charge, Q , is like thermal energy and the voltage, V , is like temperature. Taking the time derivative of the above expression yields

$$i = C \frac{dV}{dt}. \quad (2.2)$$

Here, the current i will be analogous to the heat flux. If current flows in, the voltage increases just as when heat flows into a body the temperature increases.

Now, consider the simple RC circuit shown in figure 2.1. The voltage is initially 0 everywhere. A switch is flipped such that the voltage at V_0 is suddenly set to 1. The current that flows through the resistor is given by Ohm’s law as

$$i = \frac{V_0 - V_1}{R}. \quad (2.3)$$

Since the current is conserved, the current that flows through the resistor must also flow through the capacitor. Using equation 2.2 we obtain a differential expression for the voltage, V_1 ,

$$\frac{dV_1}{dt} = \frac{V_0 - V_1}{RC}. \quad (2.4)$$

Note that combination of RC has units of time. You can make the analogy to the lumped model of heat and you will see that this equation is precisely the same. You could solve the equation by hand, numerically, or with Simulink

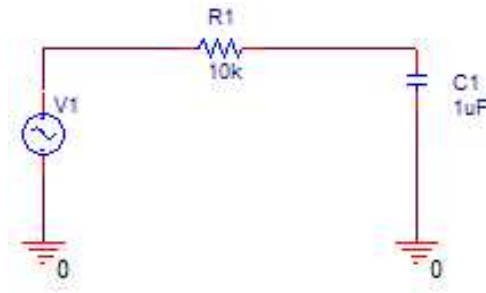


Fig. 2.1 Simple RC circuit. In the equations V_0 is the voltage coming from the voltage source and V_1 is the voltage across the capacitor.

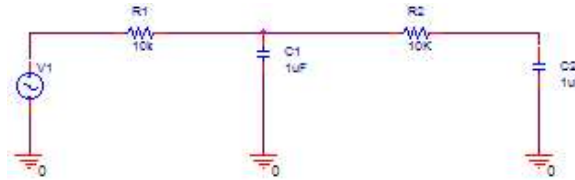


Fig. 2.2 Simple RC circuit. In the equations V_0 is the voltage coming from the voltage source and V_1 is the voltage across the first capacitor and V_2 is the voltage across C_2 .

and you would find a classic first order response. The voltage on the capacitor would increase from 0 to 1 with a time constant of RC.

Now consider the circuit shown in figure 2.2 with two resistors and two capacitors. Working from right to left on the circuit, we can conduct a similar analysis as with the lumped model. The current flowing through R_2 is

$$i_{R2} = \frac{V_1 - V_2}{R_2} \quad (2.5)$$

and the current flowing through R_1 is

$$i_{R1} = \frac{V_0 - V_1}{R_1}. \quad (2.6)$$

Since the current is conserved that amount flowing through R_1 is equal to the amount flowing through R_2 and C_1 . Therefore the current flowing through the capacitor C_1 , when $R_1 = R_2$, is

$$i_{c1} = i_{R1} - i_{R2} = \frac{V_0 - 2V_1 + V_2}{R}. \quad (2.7)$$

Due to the voltage/current relationship of a capacitor we obtain

$$\frac{dV_1}{dt} = \frac{V_0 - 2V_1 + V_2}{RC}. \quad (2.8)$$

Problems

2.1 Build the circuit shown in Figure 2.3. Using the function generator set to the square wave, the frequency set around 1 Hz, and the amplitude between 0 and 1 volt. Measure the time response of the voltage across each capacitor with the oscilloscope and download the scope data to your laptop. You should now be experienced enough with the scope, function generator, and protoboard that you can make progress without detailed instructions on how to build the circuit and take data. Please do not be afraid to ask for help if you need it during the lab time. Using

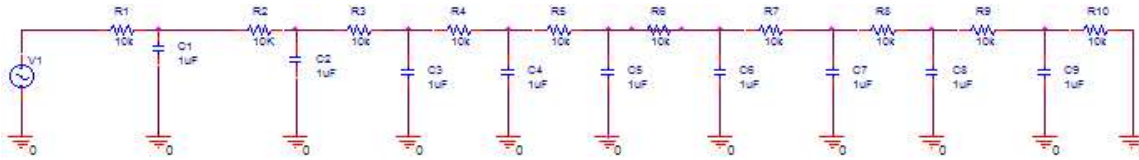


Fig. 2.3 Networked RC circuit. Consider the voltage across each capacitor when deriving your equations. Use the notation V_i as the voltage across capacitor C_i . V_0 is the voltage coming from the source.

the downloaded data, plot the time history of the voltage at each even node (by node we mean the voltage across the capacitor).

2.2 Using the same circuit, plot the steady state voltage of each measured node as a function of node number. Use the scope to measure the steady state voltage and write the numbers down by hand; you need not download all the data. Create the plot. Using the same circuit, remove the final resistor that terminates the RC chain. The circuit should now end with the ninth capacitor going to ground. Investigate the steady state voltage at each node for this configuration and compare to the results of the two circuits.

2.3 Modify the circuit built for the first problem, however reduce the number of resistors and capacitors so that you have 4 capacitors instead of 9. Repeat the experiment as in problem 1, measuring the voltage response at each node. Compare the results to the previous problem. Plot the results in the same way as in previous problem Using the information from these two experiments can you predict what would happen in the case of twenty nodes, without running the experiment?

2.4 Consider the circuit shown in figure 2.3. Show that the governing differential equations for the voltage at each node are identical to the discrete model of coupled thermal masses that was presented in the Diffusion Chapter 1, section 1.2.

Derive the differential equation for the voltage at each node in the circuit; the interior nodes will follow a generic form so you will not need to derive an equation for each node. You should consider the voltage at the final node. State which physical parameters are “equivalent” in the thermal and electrical systems. Considering the leftmost and rightmost node of the circuit; what is the boundary condition that is being imposed?

2.5 Write a MATLAB simulation (similar to the one provided in section 1.2 of the reading on Diffusion) to model the circuit that you have built. The equations were derived in the previous problem. The equations are similar to the ones presented in Chapter 1; note the difference in the boundary conditions (i.e. the voltage at nodes 0 and 10). Create plots of the voltage of each even node as a function of time, as well as the steady state voltage as a function of node number. Use the same RC value as in your experiments. Compare the simulation to the recorded data.

2.6 Use the previous simulation to plot the steady state profile of voltage as a function of node number. Modify the code to model the boundary conditions when the last resistor is pulled from the circuit. Plot the steady state profile for that case and compare to the experiments. What is the equivalent thermal boundary condition to in this configuration?

2.7 Test the stability criteria for the simulation provided in the notes, i.e. $\Delta t \alpha / \Delta x^2 > 0.5$, however decide what the appropriate parameter for the circuit model to determine the stability. Does this make physical sense? Plot the voltage of the center node versus time for a time step size a bit above and below the stability threshold to confirm the stability criteria.

2.2 WEEK 2: MODELING AND COMSOL

This week you will experiment with Comsol (FEMLAB) software for a variety of virtual diffusion experiments. You will also gain experience solving one-dimensional diffusion problems by implementing simple numerical methods. We will demonstrate Comsol during class and lab time.

2.8 Consider the scaled diffusion equation

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \quad (2.9)$$

with boundary and initial conditions,

$$T(x = 0, t > 0) = 0; \quad T(x = 1, t > 0) = 0; \quad T(0 < x < 1, t = 0) = 1. \quad (2.10)$$

Modify your circuit simulation from last time or the example problem in the reading to model these equations and the boundary condition.

2.9 Solve the previous problem using Comsol. Select the transient diffusion problem in 1-dimension. Draw your domain as a line between 0 and 1. Leave the default constants in the “physics; sub-domain settings” to one or zero. Set the initial concentration to 1. You can check the equation at the top of the window to confirm that your constants are set to solve the diffusion equation. Under “Physics->boundary conditions” set the left and right boundary to have a concentration of 0. Mesh the line and refine twice to get nice resolution. Run the simulation. Under “post-processing” run the animation and plot the solutions at various times. You may need to adjust the “solver parameters” to output the solution at relevant times. After you experiment with this problem a little bit, make comparisons to the solution that you obtained in the previous problem.

2.10 Consider 1-D heat conduction in a domain that is 100 mm wide. The left half ($0 < x < 50$) is made of copper, $k = 400 \text{ W/mK}$, and the right half ($50 < x < 100$) is made of glass, $k = 1.5 \text{ W/mK}$. Initially, the entire system is at room temperature, $T = 25^\circ\text{C}$. Suddenly, the left edge is raised to 100°C and the right edge is lowered to 0°C .

Rescale this problem so the domain and temperatures are all bounded between zero and one and there are no coefficients. Modify your simulation from the previous problem to solve this problem numerically. Observe the development of the temperature field as the system evolves to steady state. Plot the steady state temperature distribution. Could you have found this steady state without solving the entire transient problem numerically? When the temperature distribution is steady, compute the heat flux at the left ($x = 0$) and right ($x = 1$) edge of the domain. Convert the answer to W/m^2 .

2.11 Solve the previous problem using Comsol. Check that you can compute the same results.

2.12 Solve the following one-dimensional, transient diffusion problem in Comsol. Start a new 1-D simulation of diffusion. Draw your line to solve the problem on between -1 and 1. Leave the default constants in the “physics; sub-domain settings” to one or zero. You can check the equation at the top of the window to confirm that your constants are set to solve the diffusion equation. Under the “init” tab, set your initial condition to the following expression $\exp(-(x^2) * 50)$. Set the boundary conditions to be insulating. Run the simulation. Watch the animation of the solution. You may need to adjust the “solver parameters” to output the solution at relevant times. Explain how you could predict the solution when the problem has come to steady state without running the simulation.

2.13 Modify your 1-D MATLAB simulation to solve the previous problem. You should only need to change a few lines from the simulation that you already developed in earlier problems. Again, compare your results with Comsol to make sure you are getting the same answer.

2.14 Solve a two-dimensional transient diffusion problem using Comsol. Draw a square box between -1 and 1 in both the x and y coordinate directions. Set the constants in the “physics; sub-domain settings” so you are solving the plain diffusion equation with unity constants. Set the initial condition to 0. Set one horizontal wall to have a boundary condition of $c=1$. Set one vertical wall to have a boundary condition of $c=0$. Set the other two walls to be insulating. Mesh and solve the problem. Using the post-processing, plot animations of the development of the temperature field. Note that under solver parameters you will want to save only 10-20 snapshots of the data or else your animator is likely to crash. Plot the vector plot to show the heat flux vectors at the final time. Confirm that heat flows from hot to cold. Change the length of the simulation such that the final solution appears to be at steady state.

2.15 Solve a radial, steady state problem in Comsol. You may need to read through the help section on asymmetric problems. In this problem consider a copper pipe with an inner diameter of 20 mm and an outer diameter of 20 mm. The inner surface of the pipe is held at 400 K and the outer surface is held at 300 K. Solve for the steady state temperature distribution. Is it linear? Does the steady state temperature distribution change if you change the material? What is the heat flux (W/m^2) leaving the surface of the pipe? Does the heat flux change if you change the material of the pipe?

2.16 Solve a two-dimensional steady state heat transfer problem using Comsol. Create a 3 by 3 grid of square boxes that are 50 cm on each side. The total region will be 150 cm by 150 cm, however the 50 cm boxes should each be separate regions. Under “physics; sub-domain settings”, set the material (using the load button) to be concrete or copper. Set the boxes such that you have a checkerboard of concrete and copper. Set the initial temperature to 298 Kelvin. Set the boundary conditions such that the left is held fixed at 400 K and the right is held fixed at 298 K. Solve the problem. Plot the temperature field and the heat flux vectors on the same plot. Provide a qualitative explanation of the heat flow. This problem is constructing a simple model of heat transfer in a composite material.

2.17 Create a two dimensional region that consists of alternating plates of glass and copper. Make the regions have a 50/50 area ratio. Using the steady state mode of Comsol, design an experiment to “measure” the effective thermal resistance of the structure. The thermal resistance would be defined for a single plate as $R = L/k$ where L is the length and k is the material property the thermal conductivity. The definition of resistance comes from Fourier’s law of conduction and the analogy to Ohm’s law in circuits; $q'' = k/L(T_1 - T_2) = (T_2 - T_1)/R$. Test if the effective thermal conductivity is now anisotropic. Namely, is the effective thermal conductivity different in the direction aligned with or across the alternating plates of different material?

2.3 WEEK 3: ANALYSIS AND BROWNIAN MOTION

2.18 Consider the diffusion equation

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \quad (2.11)$$

with boundary and initial conditions,

$$T(x = 0, t > 0) = 0; \quad T(x = 1, t > 0) = 0; \quad T(0 < x < 1, t = 0) = 1. \quad (2.12)$$

The problem was solved using separation of variables in the reading (and class). The series solution is presented in the chapter. For the solution to this problem, plot the temperature distribution at time = 0.2 using 1 term, 2 terms, 3 terms, 4 terms, and 5 terms in the sum. On a separate plot, show the temperature distribution at different instances in time ($t = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9,$ and 1) on the same plot. Comment on how many terms are needed for the solution to converge to within a reasonable amount. Test the convergence early in the solution and at later times. You can do this problem by writing a short MATLAB script. The script should be fairly short; approximately 10 lines. Compare the simulation in the previous problem to the analysis. If they do not agree something is incorrect.

2.19 Use separation of variables to solve the problem $\partial T / \partial t = \partial^2 T / \partial x^2$, $T(x = 0, t) = 1$, $T(x = 1, t) = 0$, $T(x, t = 0) = 0$. Plot the temperature at locations $x = 0, 0.2, 0.4, 0.6, 0.8, 1.0$ as a function of time. Plot the temperature distribution at steady state. Look back and make comparisons to the results from the circuit experiment. Last week you modified your simulation that solves the heat equation with finite differences to model these boundary conditions. Compare the results to show that your analysis is in agreement with the simulation.

2.20 In MATLAB, implement the simple random walk model in two dimensions. Start by locating 1000 particles at the origin. Take 1000 time steps. At each time step, move each particle by a normally distributed random number in the x and y direction multiplied by 0.01 (for now). Use the command `randn(1000, 1)` to generate a list of 1000 random numbers. The factor of 0.01 will keep the particles moving only a mean distance of 0.01 between each iteration. At each iteration plot the x and y position of each particle as a point. After plotting all the particle positions at each time step, issue the following commands; `axis([-1 1 -1 1])` and `pause(0.01)`. These two commands will hold the axis fixed so MATLAB will not scale the axis with each time iteration and the pause command allows you to see the location of the particles for an instant before moving to the next time iteration. Just watch and have fun with this simulation. You need not turn in any results for this problem.

2.21 Starting with the above simulation, compute the distance from the origin of each particle and take the average over all particles. Create a plot of the mean squared distance r^2 versus time. Confirm that the plot is linear. What is the slope of the line? How does that slope relate to the constant of 0.01 used in the previous problem? If you are not sure, try experimenting by changing the value in the simulation and recreating this result.

2.22 In this problem you will create a simulation of a simple diffusion problem using the random walk model that you have developed in the previous problems.

- Imagine a box that extends from 0 to 1 in the x and y direction. Using your random walk model of 1000 particles, modify your code such that the particles are uniformly distributed inside the left half of the box ($0 < x < 1/2$). initially and no particles are in the right half ($1/2 < x < 1$).
- Modify your code in a way that makes the boundaries insulating. It is probably not crucial the exact method you use to keep all the particles inside the bounding box. Try a few ideas, stick with one that seems to work.
- Run the simulation. You should “animate” a histogram of all the particles x location as a function of time. A similar simulation was demonstrated in class, you are modifying that result. Wait to print the results until you complete the next problem.

2.23 Solve the previous problem using separation of variables instead of the “molecular” simulation. The governing equation is

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}, \quad (2.13)$$

where C is the concentration (particles/Volume). The boundary conditions are

$$\left. \frac{\partial C}{\partial x} \right|_{x=0} = 0 \quad (2.14)$$

$$\left. \frac{\partial C}{\partial x} \right|_{x=1} = 0, \quad (2.15)$$

and the initial condition is

$$C(t = 0, 0 < x < 1/2) = 1, \quad (2.16)$$

$$C(t = 0, 1/2 < x < 1) = 0. \quad (2.17)$$

$$(2.18)$$

Follow the separation of variables procedure outlined in the reading and the lecture notes. Determine the series solution using this method. Use MATLAB to plot the result when you are done. Compare the results qualitatively to the molecular simulation that you performed in the previous problem. Adjust the molecular simulation such that that the histogram makes dimensional sense, i.e. you can interpret time and the concentration. Plot the concentration from the molecular simulation and the analytical solution derived from separation of variables on the same plot at a few instances in time.

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