Chapter 8

Mathematical Modeling of Physical Systems

In many situations a scientist has to form mathematical models of physical processes. The key steps in the process are:

Define the problem: Identify the phenomeon to investigate; identify various factors that influence the outcome; identify the independent and dependent variables; identify the parameters of the system; decide what the model seeks to achieve.

Create the model: Simplify the problem; state the assumptions; formulate mathematical relationships.

Obtain the outcomes of the model: Solve the equations; draw graphs; derive results that can be experimentally or observationally tested.

Test the model: Compare the predictions of the model with reality; Analyze in which aspects the predictions of the model deviates from reality; decide if it is necessary to adjust the model; include factors that you ignored in the earlier cycle; repeat the cycle again.

8.1 Models built from first principles

Often we build models of phenomena by utilizing existing knowledge. Let us illustrate this by trying to obtain the model of the process of cooling of a hot liquid kept in a container, exposed at the top.

Through the mathematical model, what are we trying to achieve? We are trying to obtain how the temperature changes with time. Thus, we seek to obtain a differential equation. The average temperature of the liquid is the variable here. The parameters are the dimensions of the container, the mass and the specific heat of the fluid, etc.

The liquid could dissipate heat by conduction, convection, and radiation. Upon initial investigation, we notice that heat loss happens majorly due to convection; the other components are much smaller than convection so long as the temperature is not too high. So we make the *assumption* that heat loss by conduction and radiation are negligible. Heat dissipation happens through all the sides of the vessel, but we assume that most part of the heat is lost through the top layer that is in contact with air. We may have to abandon these assumptions at a later stage if we find that the predictions of our models do not match with the experiental findings.

Now we set forth to creating the model. Suppose the temperature at the interior of the fluid is Θ_f, that at the surface is Θ_s and that of the air is Θ_a. There will be two stages of convective heat transfer: (i) that from the interior of the fluid to the upper surface, and (ii) that from the surface of the fluid to air. The same amount of heat is transported from the interior to the surface and then from the surface to the air.

It is reasonable to assume that in each case the heat transfer q is proportional to the temperature difference as well as with the surface area of heat transfer. Thus, we may write

$$q = h_f\, A\, (\Theta_f - \Theta_s)$$

and

$$q = h_a\, A\, (\Theta_s - \Theta_a)$$

where h_f and h_a are the corresponding convective heat transfer coefficients. Thus,

$$(\Theta_f - \Theta_s) = \frac{q}{h_f A}, \quad (\Theta_s - \Theta_a) = \frac{q}{h_a A}$$

Eliminating Θ_s we get

$$q = h\, A\, (\Theta_f - \Theta_a)$$

where the overall heat transfer coefficient h is

$$h = \left(\frac{1}{h_f} + \frac{1}{h_a} \right)^{-1}$$

This equation is valid so long as the temperatures are constant. But we had set out to obtain a dynamical equation. So we need to assume that $q(t)$ and $\Theta_f(t)$ are time-varying quantities. The temperature changes by a small amount over a small time δt, and that the heat transfer equation remains valid over this period. Thus, over a time period from t to $t + \delta t$, the rate of heat loss is

$$q(t) = h\, A\, (\Theta_f(t) - \Theta_a)$$

Hence the total heat loss over this period is

$$q(t)\delta t = h\, A\, (\Theta_f(t) - \Theta_a)\, \delta t$$

From the point of view of the fluid, the heat loss due to temperature drop from $\Theta_f(t)$ to $\Theta_f(t + \delta t)$ is

$$\delta E = m\, c\, [\Theta_f(t + \delta t) - \Theta_f(t)]$$

Equating these two quantities of heat, we get

$$m\, c\, [\Theta_f(t + \delta t) - \Theta_f(t)] = -h\, A\, (\Theta_f(t) - \Theta_a)\, \delta t$$

or

$$\frac{\Theta_f(t+\delta t)-\Theta_f(t)}{\delta t} = -\frac{hA}{mc}(\Theta_f(t)-\Theta_a)$$

As δt approaches infinitesimally small values, this equation will become increasingly accurate. Thus, we get

$$\frac{d\Theta_f}{dt} = -\lambda(\Theta_f(t)-\Theta_a)$$

where $\lambda = hA/(mc)$.

This is the model we obtain. But is this model correct? In order to check that, we'll have to obtain a prediction of the model, and for that, we'll have to solve the differential equation. This can be done using the integrating factor method. We leave it to the reader to solve it. We just state that the solution is

$$\Theta_f(t) = \Theta_a + \left(\Theta_f(0)-\Theta_a\right)e^{-\lambda t}$$

where $\Theta_f(0)$ is the initial temperature of the fluid. We see that this relationship is reasonable, because at $t=0$, the fluid temperature is its initial value, and at $t=\infty$, it reaches the air temperature. But is the rate of decay all right? In order to check that, one has to conduct an experiment to obtain the variation of temperature with time, and has to match it with the predicted value. If it does not match, either one has to check the values of h and c used, or one has to relax some of the simplifying assumptions that one used in the first cycle of modeling.

8.2 Dimensional consistency

Any model is basically a relationship between quantities, expressed in the form of equations (algebraic or differential). The resulting equations should be dimensionally consistent, i.e., the left hand side and the right hand side should have the same dimension, when two quantities are added of subtracted, they should have the same dimension, etc.

There are four quantities which are considered to be of fundamental nature in the sense that their dimension cannot be expressed in terms of the dimensions of other quantities. These are mass, length, time, and temperature, denoted at M, L, T, and Θ respectively. The units of all other quantities can be expressed in terms of these base dimensions. We use square brackets to mean 'the dimension of', for example,

$$[\text{speed}] = LT^{-1}$$

Dimensional consistency demands that wherever we write an equation, the dimensions must match. For example, we know that the period τ of small oscillations of a particle of mass m suspended from a fixed point by a light inextensible string of length l is given by

$$\tau = 2\pi\sqrt{\frac{l}{g}}$$

Is this equation dimensionally consistent? To check, we start with the dimension of the right hand side:

$$\left[2\pi\sqrt{l/g}\right] = [2\pi]\left([l]/[g]\right)^{1/2}$$

Now, 2π is an angle in radians, which is dimensionless. The dimensions of l and g are L and LT^{-2} respectively. Substituting, we get the dimension of the RHS as

$$\left(\frac{L}{LT^{-2}}\right)^{1/2} = \left(T^2\right)^{1/2} = T$$

which is the dimension of τ in the LHS.

What should we do when an equation contains functions like exp, ln, sin, cos, etc.? How can one check the dimensional consistency in such cases? The key is to note that these functions take real numbers as their arguments, and return real numbers. Therefore functions like e^x, $\ln x$, $\sin x$, $\cos x$, etc., should be dimensionless, and their arguments should also be dimensionless.

For example, when we write

$$x(t) = A\sin(\omega t + \phi),$$

this is ensured because ϕ (in radians) is non-dimensional, and $[\omega] = T^{-1}$ and $[t] = T$. And, for the whole equation to be dimensionally consistent, the dimension of the constant must be $[A] = L$.

8.3 Modeling using dimensional analysis

It is interesting to note that one can often use dimensional analysis to get some idea about the functional forms describing the dependence of one quantity on others. Suppose you are to find a model to describe the distance a cannonball will go when fired from a cannon. From observation, you notice that the distance traversed depends on the mass m, the initial velocity u, and the angle of firing θ. Physical intuition tells you that this distance should be different on Earth and on Moon, that is, it depends on the acceleration due to gravity g. But suppose you do not know Newton's laws, i.e., you do not know the functional relationships. So your initial model will be

$$D = f(m, u, \theta, g).$$

The dimensions of the quantities in the RHS are $[D] = L$, $[m] = M$, $[u] = LT^{-1}$, $[g] = LT^{-2}$ and θ is dimensionless. What kind of functional form should we assume?

Notice that the transcendental functions like exp, ln, sin, cos, etc. can take only nondimensional numbers as arguments. Therefore any quantity that has a dimension cannot appear in the argument of such a function. Such quantities can only have powers. But since θ is nondimensional, D can have any functional dependence on θ, say, $h(\theta)$.

So let us assume that

$$D = k\, m^{\alpha} u^{\beta} g^{\delta} h(\theta)$$

where k is a dimensionless constant. The problem is then to find the powers α, β, and δ.

Now, dimensional consistency of the above equation demands that

$$\begin{aligned}
[D] &= [k\, m^{\alpha} u^{\beta} g^{\delta}] \\
&= [k]\, [m]^{\alpha} [u]^{\beta} [g]^{\delta} \\
L &= M^{\alpha} \left(LT^{-1}\right)^{\beta} \left(LT^{-2}\right)^{\delta} \\
&= M^{\alpha} L^{\beta+\delta} T^{-\beta-2\delta}
\end{aligned}$$

since k and θ are dimensionless. Equating the powers of M, L, and T, we get

$$\alpha = 0, \quad \beta + \delta = 1, \quad -\beta - 2\delta = 0$$

Solving these equations, we get

$$\alpha = 0, \quad \beta = 2, \quad \delta = -1$$

Thus, we have been able to obtain the unknown parameters simply by dimensional analysis.

Therefore, we get

$$D = h(\theta) \frac{u^2}{g}$$

Dimensional analysis can lead you up to this point. But it cannot give you the functional form $h(\theta)$. You could then design a directed experiment where θ would be varied (while all other parameters remain fixed), and D is measured for different values of θ. From the graph thus obtained, you could guess the functional form (from Newtonian mechanics we know that it will be $h(\theta) = \sin 2\theta$).

In this example, the equations for the powers could be exactly solved. But this may not always be the case. In that case you should obtain these powers in terms of a minimum number of unknown parameters (usually one). Then substitute these powers into the dimensional equation, which will contain the unknown parameter. Then group together the parameters with that unknown power and try to express the LHS in terms of the known powers and an unknown function of a dimensionless group.

Example: By dimensional analysis, try to obtain the distance traversed by a projectile through air (this time include air friction force F).

Solution: In this case D will have an additional term, F, in its functional form, which has a dimension of MLT^{-2}. So we write

$$D = k\, m^{\alpha} u^{\beta} g^{\delta} F^{\epsilon} h(\theta)$$

Dimensional consistency demands that

$$\begin{aligned} [D] &= [k][m]^{\alpha}[u]^{\beta}[g]^{\delta}[F]^{\epsilon}[h(\theta)] \\ L &= M^{\alpha}\left(LT^{-1}\right)^{\beta}\left(LT^{-2}\right)^{\delta}\left(MLT^{-2}\right)^{\epsilon} \\ &= M^{\alpha+\epsilon}\, L^{\beta+\delta+\epsilon}\, T^{-\beta-2\delta-2\epsilon} \end{aligned}$$

Equating the powers of this equation, we get

$$\alpha+\epsilon = 0, \quad \beta+\delta+\epsilon = 1, \quad -\beta-2\delta-2\epsilon = 0$$

Solving these yields $\beta = 2$, but there remains two equations $\alpha+\epsilon = 0$ and $\delta+\epsilon = -1$ with three unknowns. In that case we express the others in terms of one unknown, say, ϵ. Thus, $\alpha = -\epsilon$ and $\delta = -1-\epsilon$. Substituting these into the equation, we get

$$\begin{aligned} D &= k\, m^{-\epsilon}\, u^2\, g^{-1-\epsilon}\, F^{\epsilon} h(\theta) \\ &= k\, \frac{u^2}{g}\left(\frac{F}{mg}\right)^{\epsilon} h(\theta) \end{aligned}$$

Now notice that the quantity $F/(mg)$ is non-dimensional. Since it is non-dimensional, the functional dependence of D on this quantity need not be just a power of ϵ; it could be any transcendental function. Thus, the model needs to be written as

$$D = k\,\frac{u^2}{g}\,h\left(\frac{F}{mg},\theta\right)$$

where h is a function of two variables. In order to complete the model, directed experiments need to be performed to find the character of this function.

8.4 Phenomenological models

A model like this—where you do not try to derive the model from the first principles and do not seek to explain why a specific functional relationship (for example, the dependence on u^2/g in the above model) occurs, but still successfully capture the essential features of a phenomenon by a mathematical relationship—are called phenomenological models. A phenomenological model is a scientific model that describes the relationship between variables appearing in a phenomenon, in a way which is consistent with fundamental theory, but is not directly derived from theory. A phenomenological model does not attempt to explain why the variables interact the way they do. Often phenomenological models are developed first, which then propel theorists to work out the underlying mechanisms of the phenomenon.

8.5 An example of mathematical modeling: The Lotka-Volterra model

It is a common observation of field biologists that, whenever two species occur in some ecological niche—one predator and the other prey—then the number of individuals in each population oscillates. For example, if in a forest there are deer and tiger, then sometimes the deer population would grow and the tiger population would fall, and at some other time the reverse happens. Why do the populations behave in such manner and do not attain equilibrium?

In order to get insight into such issues, one has to build a mathematical model. First we have to identify the variables. These are the prey population and the predator population. Let the number of individuals in the prey population be x and that in the predator population be y. How would these vary with time?

If there is no predator in the forest, the prey population would grow. It is reasonable to assume, as first approximation, that the rate of growth is proportional to the population, i.e., $\dot{x} = ax$, where a if a constant (a parameter of the system). If tigers are present, they will eat up the deer and so will have a negative effect on $\dot{x}$. This will be proportional to the deer-tiger encounters, which can be assumed to be proportional to the product xy as a first approximation. Thus the total equation becomes

$$\frac{dx}{dt} = ax - bxy$$

where b is another parameter of the system.

Now let us see what happens to the predators. If no prey is present, the predators will die. There will be an exponential decay of the predator population, and so we can write $\dot{y} = -cy$. If prey are present, the predator population will rise, and the rate of growth will be proportional to the predator-prey encounters which can be assumed to be proportional to xy. Thus, we get the second equation as

$$\frac{dy}{dt} = -cy + dxy$$

where b is another parameter of the system.

We have thus obtained a very simple model of predator-prey competition. Does it capture the essential features of the phenomenon under consideration?

To check, we notice that the equilibrium points (for which

$\dot{x} = 0$ and $\dot{y} = 0$) are (0, 0) and $(c/d,\ a/b)$. Are these equilibrium points stable? For this, we obtain the Jacobian matrix

$$J = \begin{pmatrix} a - by & -bx \\ dy & -c + dx \end{pmatrix}$$

To explore the stability of the equilibrium point at $(0,0)$, we substitute these values in the Jacobian matrix to obtain

$$J_0 = \begin{pmatrix} a & 0 \\ 0 & -c \end{pmatrix}$$

whose eigenvalues are a and $-c$. A positive eigenvalue implies that this equilibrium point is unstable.

The Jacobian matrix corresponding to the other equilibrium point is

$$J_1 = \begin{pmatrix} 0 & -bc/d \\ ad/b & 0 \end{pmatrix}$$

whose eigenvalues are purely imaginary. This gives rise to sinusoidal solutions, and hence, any initial condition that is not located exactly at the equilibrium point will oscillate.

This explains the bizarre phenomenon of oscillation of wild populations. But is the model accurate? To check, one has to cross-check against the actual data obtained by field biologists. If the amplitude or the frequency of oscillation does not match reality, the model needs to be improved accordingly.

What will be the natural ways of improving the model? For that, let us take stock of the assumptions made.

Assumption 1: We have assumed that the populations are continuous variables. But in reality they are discrete (you cannot have half a tiger). So for small populations, it would incur significant errors. But for large populations, the assumption would be reasonably valid.

Assumption 2: We have assumed that in the absence of predators the prey population increases exponentially. This is reasonably correct for small populations. But if the population is large, food will become scarce, and so the population cannot increase without bound. This is normally accounted for by using the logistic growth model $\dot{x} = ax(x_s - x)$, where x_s is the value at which x 'saturates' if no predator is present.

Assumption 3: We have modelled the predator-prey interactions by a simple product xy. One could think of improving the functional relationship representing various practical situations of predator-prey interactions.

The class of models that can be formulated from such improvements is called the Lotka-Volterra model. These are widely used to understand and to predict variations of wild populations.