# Mathematical Methods for Engineers

by

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# Chapter 1

# Introduction

## 1.1 Why Do We Need Mathematical Methods?

To understand any natural phenomenon or process, scientists and engineers routinely construct simplified model experiments in laboratories. By varying different parameters that may influence the phenomenon, these experiments can be used to measure certain quantities and collect data. The data is then interpreted and simple correlations are developed to understand and potentially predict the behavior of a system under different conditions. The data set is also used to construct mathematical theory and help explain the behavior in more detail. For example, the Wright brothers, inspired by bird flight, used observations, intuition, and wind-tunnel experiments to design and build the first airplane capable of maintaining flight. Thus, constructing clever physical experiments in the laboratory, collecting data, and interpreting the data can help understand several natural phenomena, help build aircrafts without actually requiring the need to solve any complicated mathematical equations. However, such an approach, although extremely valuable and necessary, has its limitations. For example, if an experiment is constructed to observe a certain phenomenon under specified conditions, would the results remain the same if the conditions changed drastically? Would the same set of data be useful to explain/predict the behavior of the system? To help understand this, let us look at a simple case study.

## 1.2 A Simple Water Delivery System

Consider a water tank and delivery system as shown in Figure 1.1. Let the water tank be a simple cylinder of diameter, $D = 5$ m, and height, $H = 4$ m. Let there be a drain pipe of diameter, $d = 20$ cm, draining the water from the bottom of the tank. The goal is to find out how the height of the water column within the tank changes with time, provided that the tank is filled with water initially, that is, at $t = 0$, $h = h_0 = 4$ m.

This is an actual (albeit simplified) real world problem describing the water delivery system of some home. One way to solve this is through the above approach of "experimental measurements". To do this, we setup the water tank to the exact size specifications and have water drained from the tank. We can let the water system work and we "measure" the height of the water column at some time intervals, say every 10 seconds. We can use a simple scale or a ruler to measure the height of the water column periodically. Our physical experiment will yield a data set of $h$ at different times, $t$, starting with the initial height, $h_0$. The height of the water column will decrease over time as water escapes

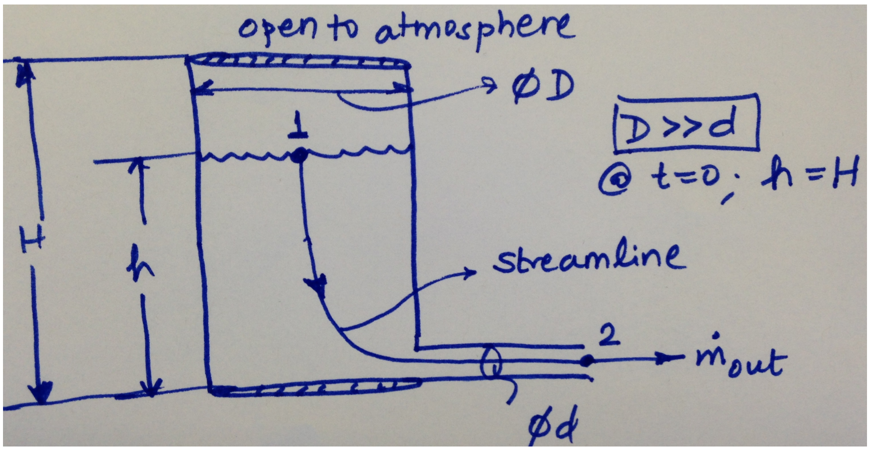



Figure 1.1: Schematic of a simple water delivery system.

the tank. Figure 1.2 shows the measured data with the dependent variable, $h$, plotted on the $y$-axis, and the independent variable, $t$, plotted on the $x$-axis. As expected the data points are *discrete* based on the frequency of the measurement. We can connect two consecutive data points by straight lines, approximating the height between measurement points by a *piecewise linear function*. Now knowing this data, we can estimate the height within the water tank at any time either through interpolation or extrapolation of the curve.

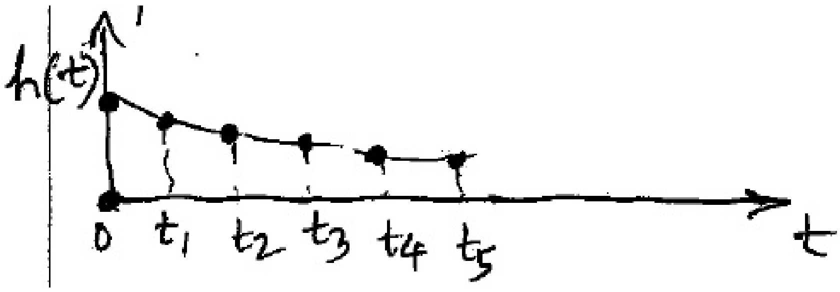



Figure 1.2: Water height, $h$, as a function of time, $t$.

Now let us say, someone else wants to use this water system, but needs much larger water tank for a bigger household. If either of the system's parameters such as the tank height, its diameter, or the pipe diameters is changed, the above data set will no longer be valid. One would have to setup a new experiment with the exact geometry specifications, and collect new data to predict how the height of the water column changes with time. Obviously, this is not an ideal case, as any small change in any parameter will yield different results, which may not be easily predicted from the previous data set. Setting up such experiments with precise measurements for complicated systems can be very challenging, expensive, and time consuming. In addition, any single data set will also involve uncertainty in it due to measurements, precision of measuring equipments, among other reasons. Thus, the experimental data are not always free of errors, and each data point will have some uncertainty (error bar) associated with it.

Mathematical/theoretical approach allows us to overcome some of the drawbacks in the experimental approach. More specifically, a mathematical model representing the above system, if developed, will lead to a solution in terms of general values for the different parameters. Thus, changing any or all parameters would not affect the predictive capability of the model.

### 1.2.1 Formulating a Mathematical Model

For the above problem, a simple mathematical model can be easily formulated by using laws of physics, namely, the conservation of mass and also conservation of energy. Let us consider a control volume (a rectangular prism) surrounding the water tank. Then, by using simple laws of *conservation of mass* applied to this control volume, one can write,

$$\frac{\text{Change of water mass in tank}}{\text{Time interval for the change}} = \text{Inflow rate of water} - \text{Outflow rate of water.} \quad (1.2.1)$$

Let $m$ be the total mass of water (in [kg]) in the tank at time $t$ (in [s]). Let $\dot{m}_{in}$ and $\dot{m}_{out}$ be the inlet and outlet mass flow rates (in [kg/s]). Then the conservation of mass can be written as,

$$\frac{dm}{dt} = \cancelto{0}{\dot{m}_{in}} - \dot{m}_{out} = -\dot{m}_{out}, \quad (1.2.2)$$

as in the present problem $\dot{m}_{in} = 0$. Let $\rho_{\text{water}}$ be the density of water and $\mathcal{V}_{water}$ be the volume of water in the tank. Let $A_{tank}$ be the cross-sectional area of the tank. For the cylindrical tank, $A_{tank} = \pi D^2/4$. Then, one can write,

$$m = \rho_{water}\mathcal{V}_{water} \quad (1.2.3)$$

$$m = \rho_{water}A_{tank}h \quad (1.2.4)$$

$$m = \rho_{water}\frac{\pi}{4}D^2h. \quad (1.2.5)$$

Since water is incompressible, and the tank dimensions are fixed, $\rho_{water}$ and $A_{tank}$ are fixed numbers and do not change with time. This helps simplify the above equation as,

$$\therefore \frac{dm}{dt} = \rho_{water}A_{tank}\frac{dh}{dt} \quad (1.2.6)$$

$$\therefore \rho A_{tank}\frac{dh}{dt} = -\dot{m}_{out}. \quad (1.2.7)$$

The rate of outlet mass flux, however, is not known, and it may depend on the height of the water column inside the tank, the dimensions of the tank and the exit pipe dimensions. In order to obtain an actual expression for the outlet mass flux, one can resort to the energy equation used in Fluid Mechanics and commonly known as the Bernoulli's equation. In order to use this equation, however, we have to invoke certain assumptions. This equation is valid for steady flows, flows where the mass within the control volume does not change with time. The above problem is not a steady flow, the mass of the water in the tank is changing with time (unsteady). However, if we assume that the tank size (diameter) is very large compared to the exit pipe diameter, i.e. $D >> d$, then one can make the assumption of quasi-steadiness. That is, even though the mass of water inside the control volume is changing, we assume that the rate at which the height of the water column is changing is very small compared to the speed at which water is leaving the tank. This is possible if area of the tank is large and the pipe cross-sectional area is small. In that case, the processes within the tank are changing at such a slow rate that we can assume that for each instant the mass within the control volume is nearly constant. This is a sound 'engineering approximation' invoked to make the equation lot easier. Note that, it is possible to write a general energy conservation equation for the unsteady problem. In addition, we assume that water is incompressible, and there are no frictional losses, heat transfer, or work done within the control volume. Under these approximations, one can apply the *Bernoulli's equation*, a simplified form of conservation of energy, along a streamline between two points 1 and 2 as shown in figure 1.1. Note that the point 1 is at the free surface of the water, which is assumed exposed to the atmosphere, and point 2 which is the exit of the pipe and open to atmosphere as well. The Bernoulli's equation between these two points basically states that the total head consisting of the pressure head, the potential head and the kinetic energy heads at point 1 are same as those at point 2:

$$\frac{P_1}{\rho_{water} g} + \overset{\approx 0}{\cancel{\frac{V_1^2}{2g}}} + z_1 = \frac{P_2}{\rho_{water} g} + \frac{V_2^2}{2g} + z_2 \tag{1.2.8}$$

$$\therefore \cancel{\frac{P_{atm}}{\rho_{water} g}} + 0 + h = \cancel{\frac{P_{atm}}{\rho_{water} g}} + \frac{V^2}{2g} + 0 \tag{1.2.9}$$

$$\therefore \frac{V^2}{2g} = h, \tag{1.2.10}$$

where $P_1$ and $P_2$ are the pressures at the two points (equal to the atmospheric pressure $P_{atm}$), $V_1$ and $V_2$ are the average velocities of water at the two points, and $z_1$ and $z_2$ are the elevations of the two points from same datum. If we use point 2 as the datum, $z_2 = 0$ and $z_1 = h$. In addition, using our assumption of quasi-steady, we find that $V_1 \approx 0$, which is a small value compared to $V_2 = V$. This gives us an expression for the exit average velocity at any time $t$ when the height of the water column in the tank is $h$, is given by,

$$V = \sqrt{2gh}. \tag{1.2.11}$$

Then the exit mass flow rate is obtained as

$$\dot{m}_{out} = \rho_{water} A_{pipe} V = \rho_{water} \left(\frac{\pi}{4} d^2\right) V. \tag{1.2.12}$$

Then, one can write an equation for the rate of change of height of the water column as,

$$\rho_{water} A_{tank} \frac{dh}{dt} = -\rho_{water} A_{pipe} \sqrt{2gh} \qquad \text{(conceptual model)} \tag{1.2.13}$$

$$\therefore \frac{dh}{dt} = -\frac{d^2}{D^2}\sqrt{2gh}. \tag{1.2.14}$$

The above equation can be rewritten as

$$\boxed{\frac{dh}{dt} = -C\sqrt{h}}, \tag{1.2.15}$$

where $C = \sqrt{2g}\ d^2/D^2$, is a constant. Equation 1.2.15 represents the conceptual or mathematical model describing the above problem. It is a first-order, non-linear, homogeneous, ordinary differential equation. To solve this equation, we need one condition for $h$, the initial condition which is $h = h_0$ at $t = 0$. By separating the variables, and integrating, one can solve the above differential equation to obtain $h$ as a function of $t$, with $D$, $d$, $\rho_{water}$, and $g$ as the parameters. Changing any one or more of these parameters is straightforward and one can still use the mathematical formulation and its solution, *as long as all approximations invoked in deriving the formulation are valid.*

$$\frac{dh}{dt} = -C\sqrt{h} \tag{1.2.16}$$

$$\therefore \int \frac{dh}{\sqrt{h}} = -C\int dt + \alpha \text{ (integration constant)} \tag{1.2.17}$$

$$\therefore 2\sqrt{h} = -Ct + \alpha. \tag{1.2.18}$$

To find $\alpha$, one can use the initial condition. At $t = 0$, $h = h_0$. Then

$$\alpha = 2\sqrt{h_0}. \tag{1.2.19}$$

Then the height of the water column can be obtained as,

$$\sqrt{h} - \sqrt{h_0} = -\frac{Ct}{2} = \sqrt{\frac{g}{2}\frac{d^2}{D^2}}t. \tag{1.2.20}$$

$$\therefore \boxed{h = \left(\sqrt{h_0} + \sqrt{\frac{g}{2}\frac{d^2}{D^2}}t\right)^2} \tag{1.2.21}$$

This gives us a closed form solution for $h$ as a function of $t$. One can again generate a plot similar to the one given in figure 1.2, but obtained from the above mathematical analysis. This equation, however, can be used for any *cylindrical* water tank of any diameter and height and having any drain pipe of any size. This makes the mathematical prediction very powerful as once a solution is obtained, it is very efficient to do variations in parameters. However, the above approach is not free of any errors. Note that, in arriving at the above solution, we used laws of physics. One has to make sure that these laws of physics are valid for the problem of interest. In addition, we made the assumption that $D/d >> 1$. What if that is not the case? Then, the equation 1.2.15 derived above is no longer valid. Instead, one would have to resort to a general, unsteady energy equation, which will give rise to a differential equation that can be complicated to solve, and under some cases, one may not be able to solve the problem using the above analytical approach. One can 'test' if our mathematical model indeed predicts the correct values for $h$ at different times, by setting up an experiment for a certain condition and comparing the mathematical prediction to the experimentally observed data (validation). As long as the two are close to each other, one can say that the mathematical model is capable of predicting the height at different times within a certain accuracy (determined by the deviations from the experimental data).

Note that in this example, the differential equation is simple enough that one can obtain an exact and closed form solution using analytical methods. However, in many applications of practical interest this is not the case. In fact, it is more often the case that the governing equations for complex physical phenomena are also complex, non-linear, and coupled equations that cannot be solved by analytical techniques. The only option then is to use some numerical approximations to the equation and solve it numerically in a discrete form. The solution obtained is not a closed form solution, and will always have errors in it due to approximations made in evaluating the derivatives/integrations in the equation. Nevertheless, by carefully choosing the parameters in the numerical approximation, one can obtain a solution that closely matches the exact solution in this problem. Similarly, one hopes to predict the solution accurately enough for problems where exact solution is not possible. For those problems, one needs to have a systematic procedure where one can evaluate the uncertainty and the level of accuracy of the predicted numerical solution. Later on, we will learn about different numerical methods, differencing approximations (such as forward, backward, central), order of accuracy of the numerical approximations and how to use these to solve the differential equations of interest. For completeness, let us look at one simple numerical approximation commonly termed as Forward Differencing or Explicit Euler method to solve the above differential equation. For the above problem we know that,

$$\frac{dh}{dt} = -C\sqrt{h} \tag{1.2.22}$$

$$h|_{t=0} = h_0 \quad \text{(the initial condition).} \tag{1.2.23}$$

The goal is to find $h(t)$ at different times given that $h(0) = h_0$. Starting with the initial condition, if we can approximately write the derivative $\frac{dh}{dt}$ in terms of the $h$ values at two different times, one can potentially solve this equation numerically. To do this, let us first define a computational grid for the independent variable, time $t$ in this case. The grid basically involves uniformly[1] placed points on the time-line with a step size of $\Delta t$, termed as time step. These represent the times at which we want to evaluate the height of the water column. If we start from $t = 0$, then we can represent all of the points as

$$t_n = n\Delta t, \text{ where } n = 0,\ 1,\ 2,\ 3, .....\text{(a positive integer).} \tag{1.2.24}$$

From this notation, it follows that $t_{n+1} = (n+1)\Delta t = n\Delta t + \Delta t = t_n + \Delta t$. Given this grid, the numerical approximation for the derivative in the equation can be obtained in different ways. Here, $dh/dt$ represents the first derivative of $h$ with respect to $t$. It also represents the *slope* of the curve $h$ versus $t$ at a given point. The slope of this curve can be approximated by choosing two points on the curve and drawing a straight line between the two points and taking the slope of that line. This is linear approximation. Depending upon the point at which we evaluate this slope, one gets different numerical approximations. Let us say we want to approximate the slope or $dh/dt$ at $t = 0$. We can do that choosing the points $t = 0$ and $t = \Delta t$ or by choosing $t_0$ and $t_1$ on the time line and evaluating the slope using a straight line equation. Let the value of $h$ at any time $t_n$ be denoted by $h_n$. Thus, $h_0$ is the value at $t = 0$, $h_1$ is the value at $t = \Delta t$, etc. Then, the slope at $t = 0$ can be approximated as,

$$\left.\frac{dh}{dt}\right|_{t=0} \approx \frac{h_1 - h_0}{t_1 - t_0} = \frac{h_1 - h_0}{\Delta t - 0} = \frac{h_1 - h_0}{\Delta t}. \tag{1.2.25}$$

Note that, the above evaluation of the slope is an *approximation* and not the real value. In general, there will be error in approximating the slope of a curve by slope of a straight line, unless the curve happens to be a straight line. But, from the governing equation 1.2.23, we know that $dh/dt$ at $t = 0$ must be equal to $-C\sqrt{h}|_{t=0} = -C\sqrt{h_0}$. Using this, and the above equation we can get the value of $h_1$ or $h$ at $t_1$ as

$$\frac{h_1 - h_0}{t_1 - t_0} = -C\sqrt{h_0} \tag{1.2.26}$$

$$\therefore h_1 = h_0 - (t_1 - t_0)\cdot C\sqrt{h_0} \tag{1.2.27}$$

$$\therefore h_1 = h_0 - C\Delta t\sqrt{h_0} \tag{1.2.28}$$

[1] Note that it is not necessary to use uniformly spaced grid points. Non-uniform spacing is possible and in fact is preferred to save computational time.

Once we have the solution at $t = t_1$, we can use that to build the solution for $t = t_2$ and so on.

$$\begin{aligned} h_2 &= h_1 - C\Delta t\sqrt{h_1} & (1.2.29)\\ h_3 &= h_2 - C\Delta t\sqrt{h_2} & (1.2.30)\\ . & & (1.2.31)\\ . & & (1.2.32)\\ h_{n+1} &= h_n - C\Delta t\sqrt{h_n} & (1.2.33) \end{aligned}$$

The finite difference approximation for the conceptual model (equation 1.2.15)

$$\boxed{h_{n+1} = h_n - C\Delta t\sqrt{h_n}}, \quad n = 0, 1, 2, 3, ...... \qquad (1.2.34)$$

Using the above approximations, one can obtain $h(t)$ at discrete points. It is clear that the solution will depend on the time-step. If the time-step ($\Delta t$) is large, the approximations used will yield large errors and the predictions may not be very accurate. But, using small step sizes, one can get a fairly accurate prediction. Since the above discrete equation 1.2.34 is repetitive, one can write a computer program to solve this starting from $n = 0$ to some large $n$ value to obtain $h(t)$. The numerical prediction can be compared with the analytical solution for accuracy. This process is called verification of the computational model. In addition, one can also compare the analytical and numerical predictions to the experimental data for a specific case. This process is called validation. Both are important in computational physics. The difference between verification and validation is explained below.

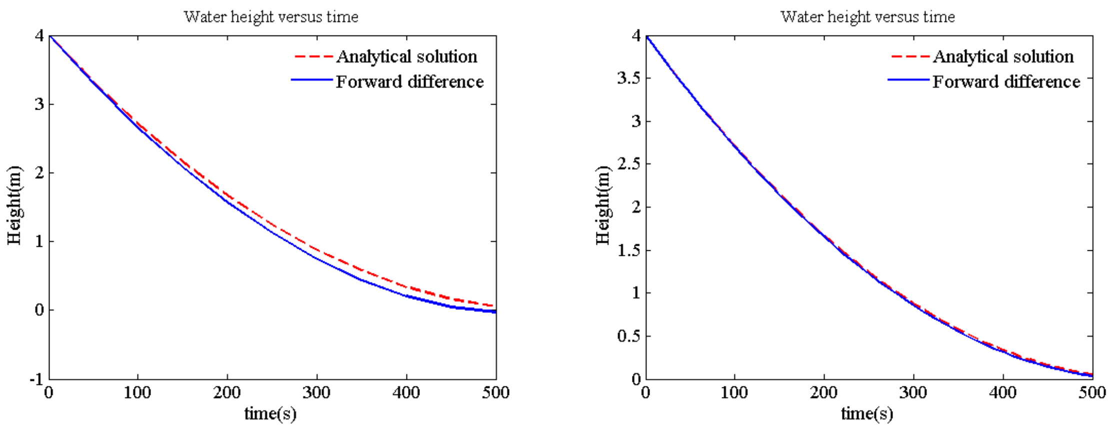
### 1.2.2 Matlab Code for Water Delivery System

```
%-----------------------------------
%Water Delivery System
%-----------------------------------
close all
clc
clear all
set(0,'defaultaxesfontname','times new roman')
set(0,'defaulttextfontname','times new roman')
set(0,'defaultaxesfontsize',14)

%% input parameter
D = 5; %diameter of tank in [m]
d = 0.2; % diameter of pipe [m]
h0 = 4 ; % initial height of water column [m]
g = 9.81; % gravitational acceleration
c = sqrt(2*g)*(d/D)^2;
h_num(1) = h0;
h_anl(1) = h0;
dt = 50; % stepsize
t = [0:dt:500];
```

```
%% exact solution
for i=2:length(t)
h_anl(i) = (sqrt(h_anl(1)) - 0.5*c*t(i))^2;
end

%% forward Difference scheme
for i=1:length(t)-1
h_num(i+1) = h_num(i) - c*dt*sqrt(h_num(i));
end

%% plot
plot(t,h_anl,'r--','linewidth',1.5)
hold on; %grid on
plot(t,h_num,'linewidth',1.5)


xlabel('time(s)','fontsize',14);ylabel('Height(m)','fontsize'
    ,14)
legend('Analytical solution','Forward difference')
legend('boxoff')
title('Water height versus time','fontsize',12)
```

### 1.2.3 Numerical Solution of Water Delivery System

The solution of the above Matlab routine will involve a plot comparing the analytical solution and the numerically obtained solution. The difference between the two solutions is shown in figure 1.3 for two different step sizes. As can be seen, as the step size ($\Delta t$) is reduced, the error between the analytical solution and the numerical solution reduces. With sufficiently small step sizes, one can get numerical results indistinguishable from the exact analytical solution. This *verifies* that the numerical solution, the computer model,




(a) $\Delta t = 50$ s (b) $\Delta t = 10$ s

Figure 1.3: Water height as a function of time for two different step sizes. Here $D = 5$ m, $d = 0.2$ m, $H = h_0 = 4$ m.

and the finite differencing approach are done properly and represent the conceptual model accurately.

## 1.3 Conceptual and Computerized Model

The above example shows that a real world problem can be solved by constructing a physical experiment, collecting the necessary data, and correlating/analyzing the data to understand the problem. Alternatively, a mathematical model that closely represents the real world problem can be constructed. The model can then be solved, under certain assumptions and approximations, to obtain the solution for conditions of interest. In the real world, both these approaches are typically used as they are complementary to each other. The following terminology is developed by the Society of Computer Simulation (SCS) in 1979 in an effort to standardize the process of understanding a natural system with certain confidence level (for further reading refer to Oberkampf & Roy (2010)).

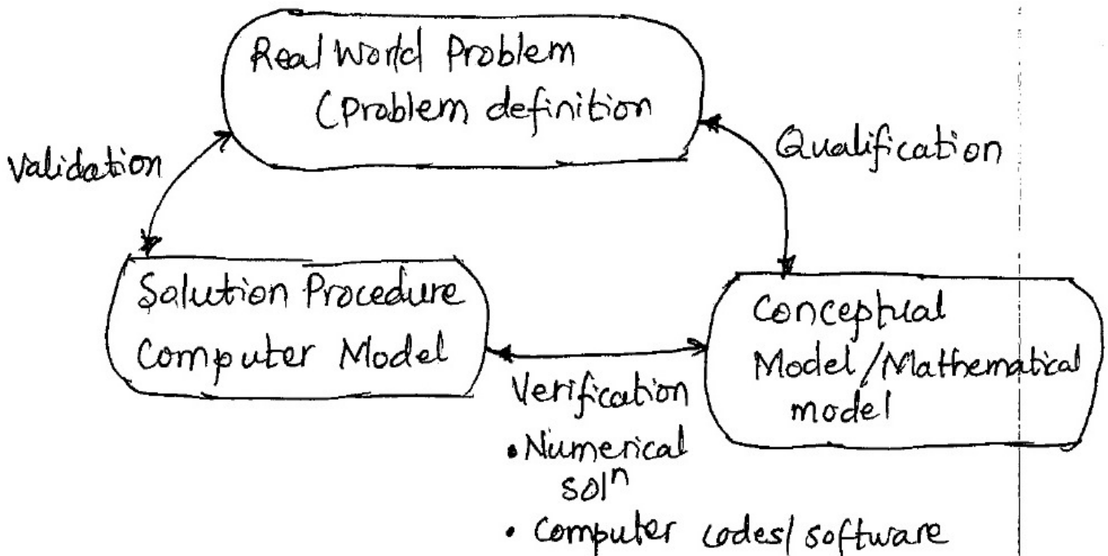



Figure 1.4: Qualification, verification, and validation.

The figure 1.4 identifies two types of models: (i) conceptual model, and (ii) computerized model. The conceptual model is composed of all the mathematical equations that are assumed to govern the natural system or problem of interest. These are the equations (either Partial Differential or Ordinary Differential equations or other relations) that are based on the conservation laws of physics (such as conservation of mass, momentum, and energy) together with any additional auxiliary equations such as constitutive models for materials (e.g. an ideal gas law), turbulence closures, boundary and initial conditions, amongst others. These equations can be simplified by taking into account the type of problem or material (for example, incompressible versus compressible flow, ideal versus real gas, reacting versus non-reacting flows, constant versus variable properties etc.).

Formulating such a conceptual model is a key step toward understanding the natural system from first principles. This is the most critical step and can involve substantial effort and 'analysis' to come up with an accurate model representing the situation at hand. This process of determining whether a mathematical model is adequate to represent the reality is called *qualification.* Using wrong governing laws to describe a process, can never yield the correct answers, no matter how accurately the equations are solved using either analytical or numerical techniques. For example, if one is interested in studying shock waves and interactions of shock waves with objects, using incompressible flow equations that treat density of fluid as a constant would be completely wrong and meaningless.

### 1.3.1 Qualification

Qualification can be defined as 'determination of adequacy of the conceptual model to provide an acceptable level of agreement for the domain of intended application'. This is in other words the scientific confirmation of the theories/hypotheses used in the conceptual model.

Once a conceptual model is formulated, the goal is to solve this problem to get the answer that is of interest for certain conditions and parameters. In the example of the water delivery system, we used conservation of mass and conservation of energy to formulate an ordinary differential equation to solve for the height of the water column as a function of time. This equation is our conceptual model. To come up with this simple model, we did make assumptions such as no heat transfer, no viscous effects, no losses, no piston work, no compressibility, steady flow among others. In addition, we assumed that the diameter of the tank was much larger than the diameter of the exit pipe. The formulation developed is only valid under these assumptions. If we violate these, the conceptual model will not represent the reality and an error will be involved even before solving the problem.

Once the mathematical model is formulated, we have to solve the problem. If the mathematical equation is relatively simple, we may be able to solve it "analytically" and obtain a closed form solution, similar to the example of water delivery system where we integrated the equation to obtain an analytical solution. Then, the solution is exact and introduces no additional errors than that present in the conceptual model.

### 1.3.2 Verification

In most cases (especially most of the real world problems); however, it may not be possible to solve the mathematical model analytically. We resort to numerical methods to solve such problems. Numerical methods, however, <u>do not</u> give "exact" solutions to the conceptual model, but only an approximate solution. There are inherent errors present in numerical differentiations and integrations. One can always minimize these errors, but they still are not capable of giving exact solutions. To use numerical methods, one generates a 'computerized model' (or commonly known as the 'code'), which is an operational computer program that implements instructions for the computer to solve the conceptual model. Once such an implementation is carried out in the form of a computer code, it is important to make sure (verify) that the code represents the conceptual model accurately and has no errors or bugs. This process is called verification.

Verification can be defined as 'the process of determining that a model implementation accurately represents the developer's description of the conceptual model and its solution'. Verification basically substantiates that the code is a true representation of the conceptual model within certain and prescribed ranges of application and accuracy. The methodologies used for code verification include comparing a numerical solution with an analytical solution or with a numerical solution from other verified codes. Most complex codes used to represent very complex phenomena, can only be verified within a certain range of parameters and within a certain range of accuracy. The same code may be applied to conditions and parameters other than the one for which it is verified, however, caution must be used in interpreting the results and their correctness. Verification provides evidence that the conceptual model is solved correctly by the discrete numerical approximations. It deals with the question: *Are we solving the mathematical equations correctly?*. In this sense, verification does not address whether the conceptual model has any relation to the real world problem. The main strategy behind verification is to identify, quantify, and reduce errors in the computational model and its approximation.

A computational model is a discrete approximation of the conceptual model. It involves choosing a step size (in space and time), choosing an appropriate discretization to approximate the derivatives/integrations in the conceptual model (for example, forward difference, backward difference, central difference, etc.), formulating a difference equation (either using concepts of finite-difference, finite volume, or finite elements etc.), and programming the discrete approximation. These various steps can obviously lead to errors which in turn lead to uncertainties in model predictions. Verification process involves identification and quantification of these different errors. To do this, a benchmark test case is typically chosen which relies on the same equations as the real world problem we actually want to solve. However, we either have an analytical solution for the benchmark problem or we have solution that can be obtained from another high fidelity (or verified) software. The prediction from the computational model is then compared with the solution of the benchmark problem, and errors are assessed thoroughly by changing the parameters of the computational model (viz. the time step or grid step etc.). In addition, stability and robustness of the computational model is assessed for these different step sizes.

Typical sources of error in a computational model are: (i) insufficient or inappropriate step sizes (either spatial or temporal or both), (ii) lack of convergence to a specified tolerance level for iterative methods, (iii) computer round-off errors, and (iv) errors/bugs in computer programming. Assessing these errors involves knowledge of computational physics as well as software engineering. The verification process once completed to a certain standard (errors within certain tolerance), the computational model is called a verified model for the range over which it was tested. The verified model simply indicates that the governing equations that we want to solve are solved correctly or to within a permissible error bound. However, this does not necessary tell us about the accuracy of the solution to the real world problem we wanted to solve. To do that, we need to do validation of the computational and conceptual model against available experimental data.

### 1.3.3 Validation

Validation is the process of determining the degree to which a model is an accurate representation of the real world problem from the perspective of the intended use of the model. Validation involves identifying and quantifying the error and uncertainty in the conceptual and computational models, quantifying the uncertainty in the experimental data, and comparing the computational and experimental data to assess the deviations between them. Thus for validation, we need both the experimental observations and computational model predictions. It does not necessarily assume that one is more accurate or representative of reality than the other. By quantifying errors in conceptual and computational models together, validation tries to answer the question, *are we solving the right equations?* and are we doing that accurately enough. The deviations between the numerical and experimental data indicate (i) the capability of the numerical and conceptual models to represent reality, and (ii) precision/accuracy with which we can 'predict' reality.

Once verification and validation (V & V) are performed, we have a numerical tool (software) that can be applied to other similar problems in a "predictive" mode and can be used to conduct parametric studies for improvements to the design of the system under investigation. This is the method of choice in all major industries these days as it saves significant amount of time and money in building a prototype for every design modification one wants to try.

### 1.3.4 V&V of Water Delivery System

In the example problem discussed earlier, getting the equation 1.2.15 was the process of qualification. It involved approximations to make the conceptual model simple. Solving the conceptual problem numerically using the Forward Difference Approximation method and comparing the prediction with an exact analytical solution of the model was the process of verification. This process simply verified that our computer model (involving numerical approximation, program to solve the approximation, implementation) was done correctly and the conceptual model was solved correctly (see figures 1.3a,b). It, however, does not tell us whether the prediction (analytical as well as numerical) are what we are going to get in reality. To confirm this, one can construct a physical model of a water delivery system and measure the height of the water with time for a given $h_0$, $H$, $D$, and $d$. Comparing the the measured values to the numerical or analytical solutions is called the validation. All these processes are critical in design and building complex systems. Validation then tells us that we are indeed solving the correct equations that represent the reality and we are solving them correctly as well. Figure 1.5 shows the verification and validation plot for the water delivery system using the analytical solution of the conceptual model, forward difference method to predict a numerical solution, and experimental data together with error bars. If on the other hand, we apply the conceptual model to a small test tube with a large hole in it at the bottom ($D \sim d$), then we will be ignoring one of our major assumptions, namely that the process within the tank is quasi-steady, and one would get a much larger deviation between the measured $h$ values and numerical or analytical $h$ values.

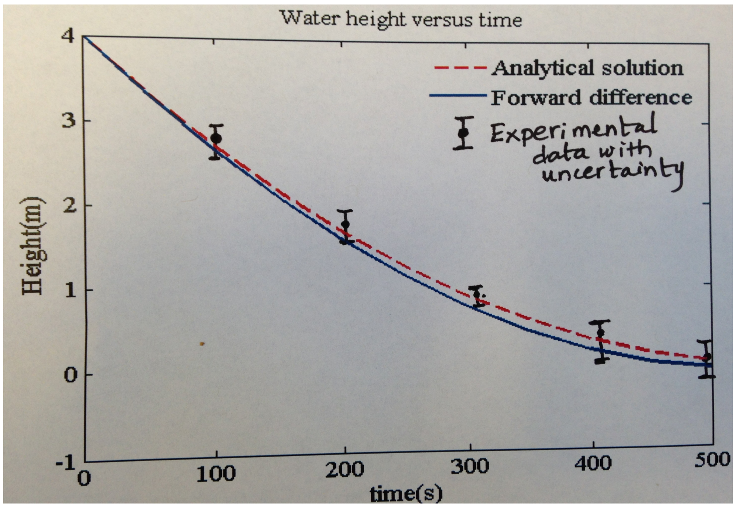



Figure 1.5: Verification and validation of the conceptual and computerized model for the water delivery system.

## 1.4 Pros and Cons of Numerical Methods

The numerical or computational model has following advantages over the experimental procedure:

1. Low cost in building and running the model (compared to full scale experiments).
2. Speed can be very fast compared to setting up experiments and collecting data. However, some advanced computational models can also run for long periods of time for many complex problems such as turbulent flows, unsteady problems, among others.
3. Detailed spatio-temporal information (otherwise not possible from observations) $\phi(x, y, z, t)$.
4. Ability to simulate "realistic conditions."
5. Ability to simulate "ideal conditions."
6. Ability to easily perform parametric studies.

Some disadvantages of the numerical problems are:

1. For some complex problems (such as turbulent flows, wave transport, dynamical systems), the numerical approach can be very costly as well.
2. Representing real world configurations (e.g. flow through complex geometries), realistic physics (e.g. combustion, radiation, multiphase transport etc.) is very difficult and generally limit ability of numerical methods. But, for such problems numerical approach is the only true option. Other experimental approaches are also limited due to various instrumentation issues.

## 1.5 Overview of the course

As an engineer, it is critical to realize the limitations of numerical schemes used in any software you plan to use. It is also important to know in general, the capability of representing particular physics accurately using certain software. It is important to conduct verification as well as validation studies of the software before applying it to the problem of interest. Your new design or modifications/improvements to the current design depend on these systematic procedures employed in computational physics.

In the following chapters, we will look at problems commonly encountered in mechanical engineering; viz. dynamics, vibrations, heat transfer, fluid mechanics, mass transport, chemical reactions as well as other fields of science such as weather prediction, ecosystems, chaos, among others. For most of these problems, one can obtain an analytical solution. However, we will also use these problems to develop different numerical methods to solve them. The analytical solution will then be used to *verify* the numerical prediction of a particular approximation. We will also look at how to quantify errors, how to estimate, whether the step sizes we used are sufficient for an accurate solution, how to know a priori whether a certain numerical scheme is going to provide us a stable numerical scheme by applying linear stability theory. Focus will be on initial and boundary value problems of first and second order for the ordinary differential equations, coupled system of first order ordinary differential equations, and first and second order partial differential equations.

The learning outcomes for this course are listed below. At the completion of this course, students are expected to be able to:

1. Formulate and solve mechanical engineering initial value problems of practical interest represented by first and second order differential equations using both analytical and explicit numerical methods.
2. Formulate and solve mechanical engineering boundary value problems of practical interested represented by first and second order differential equations using both analytical and implicit numerical methods.
3. Formulate and numerically solve partial differential equations.
4. Identify and implement the most appropriate numerical method for solving a specific type of engineering problem. In addition, be able to recognize the advantages, disadvantages and limitations of numerical methods.

*As numerical analysts and engineers you will use advanced software to design a product or improve an existing design. It essential to be very skeptical about the answers obtained using any numerical software and emphasize. Being aware of concepts of stability, accuracy, verification and validation and applying those to your problem will help you design complex systems.*

# Bibliography

Oberkampf, William L & Roy, Christopher J 2010 *Verification and validation in scientific computing*. Cambridge University Press.