1c /

"Classification of mathematical problems as linear and nonlinear is like classification of the Universe as bananas and non-bananas."

—Author ~~Unknown.~~ Anonymous

2

Review of Ordinary Differential Equations

AU: Relatively rigorous mathematical what?

What can be said about the topic of *ordinary differential equations* (or ODEs) that has not already be said? From the perspective of scientists and engineers, perhaps quite a bit can be said with a focus on developing a better understanding of the material. Almost every engineer, for example, has studied a course on ODEs as part of their undergraduate training. Although ~~usually~~ quite well-intended, these courses are usually taught out of a mathematics department as a service course. As such, the courses are often taught from a relatively rigorous *mathematical* that generally sacrifices clarity for formality and abstraction. Only after one has been fully presented the theory in some general sense is one then invited to think about solving problems. ℓ/

AU: okay as reworded? then / ℓ /

There is nothing, in principle, wrong with such an approach. However, it has been my personal experience that a deeper understanding of mathematics is often realized for scientists and engineers when complex topics are led by example rather than by theory. If one first has a problem in mind that has an obvious physical interpretation, and, potentially, a solution ~~that~~ can be understood on the basis of the same physical interpretation. Layering abstraction and generalization on top of this basic understanding becomes a natural process of extending concepts that are already inculcated. This is the approach that is adopted in these notes.

Our review of ODEs will cover only the following: (1) Linear and (some) nonlinear first-order ODEs, and (2) linear second-order ODEs with constant coefficients. The more general case of linear second-order ODEs with nonconstant coefficients is an intersting topic (and we will encounter those when studying Sturm-Liouville problems), but the topic involves series solutions; these solutions can get a bit tedious without adding substantially to developing new concepts for better understanding ODEs, so the choice has been made to omit them in this review. With a basic understanding of the solution to linear second-order problems with constant coefficients, motivated students can learn to handle problems with nonconstant coefficients fairly readily with a little self-study of the topic. lc / ℓ / ^e^ /

2.1 Terminology

In the study of ODEs, there are a few definitions and vocabulary that are helpful to establish up front. A few key definitions are described here. Some of these are repeated from the review chapter. This is something that will occur routinely in this text. The repetition of ideas when learning is not actually redundant! Most of us do not learn by seeing something a single time. The more fundamental and important an idea or a definition is, the more it may be worth repeating, ideally using slightly different perspective to appeal to different ways of thinking about the topic.

- **Domain.** A *domain* is the set of possible values that can be selected for a particular application. Domains can be represented as either a set of discrete values, or by continuous intervals. Values not in the domain are not generally valid for the application in question. As an example, suppose one conducted an experiment which collected four temperature measurements (whose values were represented by, for example, T_1, T_2, T_3, T_4 at for different times, t_1, t_2, t_3, t_4. Then, the values t_1, t_2, t_3, t_4 represent the domain of the experimental results collected.

- **Range.** The *range* is the set of possible values that is associated with the particular domain in an application. As an example, the range of values from the temperature experiment described above would be the temperatures that were measured: T_1, T_2, T_3, T_4. Each of these temperatures is uniquely associated with a single point from the domain.

- **Independent variable.** An independent variable is one in which represent *causes* or *inputs* to the mathematical description of a process. These variables do not, in principle, depend on any other quantity in other words, one is free to select them from any valid domain. In the temperature experiment example above, the independent variables are the times that were selected to make temperature measurements: t_1, t_2, t_3, t_4. The particular times selected to make measurements are constrained only by factors external to the process itself. These might be governed by convenience, or possibly constrained by physical considerations (e.g., one might not want to make 10,000 measurements over a 4 day period if system reaches a steady condition after 5 minutes). Sometimes the independent variable is "tagged" with the list of dependent variables to keep the relationship clear. So, in the example above, one might indicate that the temperature is considered to be a function of time by writing $T(t)$. Note the relationship between the independent variable and the domain of a function.

- **Dependent variable.** The dependent variable is the one that is computed once the independent variable is specified. In problems of practical interest, the dependent variable is the variable of interest, representing the physical quantity that one wants to predict. Note the relationship between the dependent variable and the range of a function.

- **Derivative.** A derivative is the differential rate of change of a dependent variable variable as one of its independent variables changes. If there is a single dependent variable with a single independent variable, then the derivative corresponds to what we conventionally think of as the slope of a simple function when plotted on two axes (with the vertical axis representing the independent variable, and the horizontal axis representing the dependent variable). In calculus, we all learned that the derivative was given by

$$\frac{dy}{dt} \equiv \lim_{\Delta t \to 0} \frac{\Delta y}{\Delta t} \tag{2.1}$$

$$\equiv \lim_{\Delta t \to 0} \frac{y(t+\Delta t) - y(t)}{\Delta t} \tag{2.2}$$

Note that although the notation $\frac{dy}{dt}$ is in common usage, it is also very common to see the notation for the derivative expressed using the *prime* notation (see 2.1 below), where the derivative is expressed as $y'(t)$. Au: To what does this refer?

The *order of a derivative* is just a count of how many times the derivative of a function has been taken. Thus, when a function has its derivative taken twice, this is denoted $y''(t)$ or $\frac{dy^2}{dt^2}$, and this is also called a *second-order derivative*.

- **Ordinary differential equation.** An *ordinary* differential equation is one in which there is only one independent variable. All derivatives appearing in the equation are taken with respect to the single independent variable. The term ordinary is used in contrast with the term partial differential equation which may be with respect to more than one independent variable. Note that one can have more than one independent variable in the case of coupled systems of equations. For example, consider the conventional multiplicative reaction rate for fully mixed chemical reactors. Suppose there are two chemical species, y_1 and y_2 who must come in contact for the reaction $y_1 \xrightarrow{k_1} y_2$ to happen. The reactions can be represented by that

$$\frac{dy_1}{dt} = -k_1 y_1 y_2 \tag{2.3}$$

$$\frac{dy_2}{dt} = k_1 y_1 y_2 \tag{2.4}$$

Although there are *two coupled* differential equations here, there is still only *one* independent variable. Thus, this set of equations are still ODEs.

- **Order of an ODE.** The *order* of a differential equation is the order of the highest derivative in the equation. Examples. are as follows rom x4

$$y'' + 2y' = 0 \qquad (second\ order ODE) \tag{2.5}$$

$$y''' + 3y = 42 \qquad (third\ order\ ODE) \tag{2.6}$$

$$y^{(iv)} = f(t) \qquad (fourth\ order\ ODE) \tag{2.7}$$

$$\frac{dy^2}{dt^2} + \left(\frac{dy}{dt}\right)^3 = 0 \qquad (second\ order\ ODE) \tag{2.8}$$

Note that in many texts, the prime notation is altered using Roman or Arabic numerals in parentheses to signify derivatives of order four or more. Thus $y''''(t) = y^{(iv)}(t) = y^{(4)}(t)$. You can see why this might be the case writing a 7^{th}-order derivative by $y'''''''(t)$ starts to get to be a bit ridiculous. rom not superscript become

- **Homogeneous ODE.** A *homogeneous* ODE is one in which there are no terms that do not involve the independent variable. For example, examine the following

$$y'' + 3y' + 7y = 0 \qquad \textit{homogeneous} \qquad (2.9)$$

$$y'' + 3y' + 7y = 5t \qquad \textit{nonhomogeneous} \qquad (2.10)$$

$$y''(t) + 3ty'(t) + 7t^2y(t) = 0 \qquad \textit{homogeneous} \qquad (2.11)$$

$$y'(t) + 7y(t) = \pi \qquad \textit{nonhomogeneous} \qquad (2.12)$$

$$(2.13)$$

More generally, a linear homogeneous equation of order n takes the form

$$a_n(t)y^{(n)}(t) + a_{n-1}(t)y^{(n-1)}(t) + \ldots + a_1y(t) = 0 \qquad (2.14)$$

where the $a_n(t)$ are coefficients of the ODE (which may themselves be functions of the independent variable t), and y is the independent variable.

- **Linear ODE.** A *linear ODE* is one which satisfies two properties for the *homogeneous* part of the ODE:
  1. If the function $y(t)$ is a solution to the ODE, then multiplying the solution by any constant α generates a function y_2 that is also a solution; in other words $y_2(t) = \alpha y(t)$ is a solution.
  2. If one has two linearly independent solutions to the ODE, call them y_1 and y_2, then the linear combination of the two is given by $y(t) = y_1(t) + y_2(t)$; this linear combination is also a solution to the ODE.
- **Nonlinear ODE.** Any ODE that is not linear is nonlinear.
- **Analytic function.** An analytic function is one that has a local representation as a convergent power series. In other words, for any point given by the independent variable x, the function $f(x)$ is given by a power series that converges over some radius of convergence.
- **Transcendental function.** A transcendental function is an analytic function that can not be specified by a (finite) polynomial. In other words, it cannot be expressed exactly by a finite sequence of algebraic operations. Such functions are in practice approximated by the appropriate truncation of an infinite series representation.

Note 2.1 (Notation for derivatives!).
There are a number of notations for derivatives in use, and this comes from the long history of the evolution of calculus at nearly the same time but by different people. The two most famous (and rightfully so) names in the development of calculus are Newton and Leibniz (also spelled *Leibnitz*); both developed the fundamental ideas about calculus in the 1660s. Newton preferred to indicate derivatives by a dot over the variable; thus, a derivative of a function $y(t)$ with respect to t would be indicated by $\dot{y}(t)$, or, when the independent variable was obvious in the formulation, just $\dot{y}$. Leibniz adopted a notation that contained more intuitive content, but was a bit more unwieldy; he used the notation $\frac{dy}{dt}$ to indicate the derivative. One of the advantages to this notation was that it was *always* clear what the independent variable was! Despite the fact that this was only notation, there was actually a significant rivalry between mathematicians in England and those in Europe over this topic; it's not clear that there were any fistfights over the topic, but discussions could become heated. To further complicate things, other notations cropped up, including the notation of the French mathematician Lagrange (who introduced the prime to indicate derivatives, as in $y'(T)$) and the Swiss mathematician Euler (who introduced the

notation $Dy(t)$ to indcate the derivative). Much of this problem came to some (minor) resolution in the early 1830s, when at the University of Cambridge (England) a group calling themselves the *Analytical Society* was formed specifically to promote the Leibniz notation for the derivative. Although this may seem somewhat absurd out of context, there was a real point to this transition. Because the Leibniz notation was being used throughout Europe, students in England were not able to easily understand the newest work being done on European mathematicians. This was seen as putting England behind, and thus the Analytical Society was born. The switch to the Leibniz notation helped foster better communication between England and Europe.

In the present day, one finds bot the Lagrange prime notation, and the Leibniz notation used frequently. In addition, in some disciplines such as continuum mechanics and physics one still finds the dot notation used as a nod to the influence that Newton had on the development of these areas.

2.2 First-Order ODEs

First-order differential equations appear in many applications that are familiar to Chemical, Biological, and Environmental Engineers. The *order* of an ODE is simply the order of the highest derivative involved. ~~For example,~~ the classical first-order reaction problem for a fully-mixed batch reactor is an example. If c is the concentration, then we think of the time-history $c(t)$ for the reactor as being specified by an initial configuration (initial condition) c_0, and a rate expression. Together these form the description of the system taking the form

$$\frac{dc(t)}{dt} = -k_1 c(t) \tag{2.15}$$

$$c(0) = c_0 \tag{2.16}$$

In this expression, k_1 is the *first-order reaction rate constant*. The system of equations given by Eqs. (2.15)-(2.16) represents a first-order differential equation for the mass balance of the chemical species c as a function of time t. Equation (2.16) is often called an *initial* condition when the problem has time as an independent variable, or a *boundary* condition when space is the independent variable. For our purposes, we will sometimes simply call them *ancillary* conditions, because these expressions provide additional data about the problem that must be determined from considerations that come from outside of mathematics. We will discuss that in additional detail later.

Note that, by convention, the variable c is called the *dependent* variable because its value is viewed as being a function of time. Similarly, t is called the *independent* variable because its values can be selected freely. Sometimes the dependent variable is "tagged" with the independent variables to keep this dependence clear; hence, one might write $c(t)$ to assure that the relationship between c and t is kept clear.

Although we have not yet discussed how to find solutions, one might recall that the solution to this problem is an exponential function in time

$$c(t) = c_0 exp(-k_1 t) \tag{2.17}$$

We can check to see that this is a solution by noting the following.

1. Taking the derivative of both sides of Eq. (2.17) and then substituting the result for both the derivative and the solution back into Eq. (2.15), we can determine that the equation is *valid*.
2. We also note that at $t = 0$, we have that $exp(0) = 1$, so that $c(0) = c_0$ and thus meets the initial condition. This verifies that the solution given by Eq. (2.17) is both a solution, and meets the ancillary conditions required for the solution.

Below, the steps in this process are detailed

Example 2.1 (Determining if a given solution is a valid one). Often you will want to check to see if a proposed solution is actually a valid one– in other words, that it meets both the ancillary conditions and the ODE itself. The solution may be one that is given to you, or one that you derive yourself. *When working problems, it is always a good idea to check your solutions following the steps below to determine that your solution is correct!*. The steps in checking the solution are the same regardless of the ODE and ancillary conditions. For the problem of the first-order reaction with a single specified initial condition, the steps are as follows.

- **Determine the necessary derivatives for the solution**. In our example, we have a first order equation, so we need derivatives of only order 1.

$$c(t) = c_0 exp(-k_1 t) \tag{2.18}$$
$$c'(t) = -k_1 c_0 exp(-k_1 t) \tag{2.19}$$

- **Substitute the solution and its derivatives into the ODE**. Substituting the solution and its first derivative (computed above) into the ODE, we find

$$-k_1 c_0 exp(-k_1 t) = -k_1 c_0 exp(-k_1 t) \tag{2.20}$$

  Clearly, the two sides of this equation are equal, and this verifies that the proposed solution is indeed correct.

- **Determine if the ancillary conditions are met**. In this case, we have only one ancillary condition (an initial condition). Substituting the value of the independent variable at the time specified in the initial condition ($t = 0$), we find

$$c(t = 0) = c_0 exp(-k_1(0)) \tag{2.21}$$
$$c(t = 0) = c_0 \tag{2.22}$$

  Clearly, the ancillary condition is met for the time specified. Since ODE is validated and the specified condition is met, then Eq. (2.17) is validated as being the particular solution we are looking for.

2.2.1 The solution to separable first-order ODEs

First-oder ODEs represent an interesting case because of their direct link to calculus. You may recall from your first course in calculus the much lauded (but rarely remembered) *fundamental theorem of calculus*. There are a number of presentations for the theorem; two of them are given below.

Theorem 2.1 (Fundamental theorem of calculus). *Suppose f is a continuous function on any open interval I of the real line. Then there exists a function F defined by*

$$F(x) = \int_x f(x)\,dx + C \tag{2.23}$$

called the antiderivative *or* indefinite integral *of f on the interval I. Here, C is usually called a* constant of integration. *The function F has the property that*

$$F'(x) = f(x) \tag{2.24}$$

for all values of x in the interval I.

The primary feature of the fundamental theorem of calculus is that it establishes the idea that differentiation is the inverse operation to integration (hence the term *antiderivative* is often used for indefinite integrals). In a more applied context, there is a corollary that is perhaps more familiar; this corollary relates the indefinite integral to the definite integral (i.e., the area under a curve in a closed interval).

Corollary 2.1 (The definite integral). *If f is a continuous function on the closed interval $[a,b]$ and F is its antiderivative, then the area under the function f in the interval is given by a quantity called the* definite integral, *and it is defined by*

$$\int_{x=a}^{x=b} f(x)\,dx = F(b) - F(a) \tag{2.25}$$

2.2.1.1 First-order separable linear equations

With this tool in hand, we are now ready to consider the solution to the first case of ODEs. The simplest first-order ODEs are linear, directly integrable problems. These problems take the form

$$P(t)\frac{dy(t)}{dt} = Q(t) \tag{2.26}$$

Note that although we are using the independent variable t here, this variable could stand for anything (not necessarily time!). In applications, we will often use the variable t when dealing with problems where the independent variable is meant to represent time, and the variables x in problems where it represents space. However, in the study of ODEs it is understood that there is only *one* independent variable, and the particular symbol used to represent that variable has no inherent significance on its own.

Solving Eq. (2.26) is a straightforward application of the fundamental theorem of calculus. Dividing through by $P(t)$ and integrating both sides of this equation, we find

$$\int \frac{dy(t)}{dt}\,dt = \int \frac{Q(t)}{P(t)}\,dt \tag{2.27}$$

The fundamental theorem of calculus then immediately gives the result

$$y(t) = \int \frac{Q(t)}{P(t)}\,dt + C \qquad (2.28)$$

Where here, we have chosen to put the constant of integration, C, on the right-hand side of the result (N.B., the sign of the arbitrary constant at this juncture is somewhat irrelevant; when it is evaluated on the basis of an ancillary condition, the correct sign will be imposed).

Example 2.2 (First-order separable equations). The conventional problems of computing the position, velocity, and acceleration of an object are usually expressed by systems of first-order, separable ODEs. Recall from your physics classes that, if position is expressed as a function of time, $x(t)$, we have:

$$v(t) = \frac{dx(t)}{dt} \qquad a(t) = \frac{dv(t)}{dt} = \frac{d^2x(t)}{dt^2}$$

We can use these relationships to solve interesting dynamical problems. Consider the following. Suppose we want to determine the velocity as a function of time for a skier starting from a standstill, and accelerating down slope as shown in the figure. We also want to know how long in seconds it takes to get to the bottom of the slope, and the velocity of the skier when they get there.

Assumptions. It is always a good idea to *list your assumptions* when solving problems. That way, it is clear under what circumstances the result you obtain is valid. It also provides you with something to look back on for problem improvement/refinement should your result come out less reasonable than you would have hoped. For this problem, we will make some *very rough* approximations that may not be altogether reasonable. These are (1) the resistance between the skis and the snow will be neglected, and (2) air resistance will be neglected. Note: if we wanted to include such effects, we might hope to find an "overall" drag term that takes the form *drag force* $= \alpha v^2(t)$.

To start the problem, we do a simple force balance on the skier, noting that $v(t=0) = x(t=0) = 0$. The acceleration in the down slope direction is found to be

$$F = ma(t) \Rightarrow a(t) = F/m$$

But, we can compute the force to be

$$F = mg\sin\theta$$

Combining these, we have an expression for the acceleration

$$a(t) = F/m = g\sin\theta$$

Note that, in this case, the acceleration is actually a constant. To find the velocity, we need only integrate. This integration could be done as a definite integral (where the bounds of integration would incorporate the initial condition), or as an indefinite integral (where the integration constant would be determined by using the initial condition as a constraint).

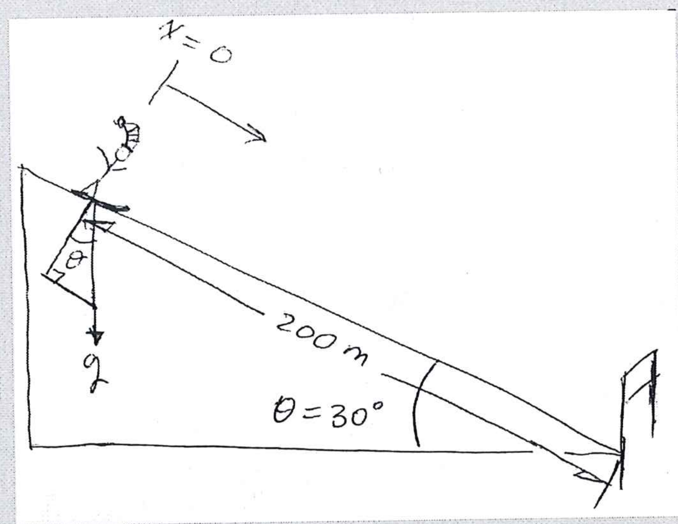


Fig. 2.1: A skier.

$$\text{Recalling} \quad a = \frac{dv(t)}{dt}$$

Upon substititing for a

$$\frac{dv(t)}{dt} = g\sin\theta$$
$$\int_t \frac{dv(t)}{dt}dt = \int_t g\sin\theta\, dt$$
$$v(t) = gt\sin\theta + C_1$$

Using the fact that $v(0) = 0$, then $C_1 = 0$.

$$v(t) = gt\sin\theta$$

The position as a function of time is found by a similar integration.

$$\text{Recalling} \quad v(t) = \frac{dx(t)}{dt}$$

Upon substititing for $v(T)$

$$\frac{dx(t)}{dt} = gt\sin\theta$$
$$\int_t \frac{dx(t)}{dt}dt = \int_t gt\sin\theta dt$$
$$x(t) = \tfrac{1}{2}gt^2\sin\theta + C_2$$

Using the fact that $x(0) = 0$, then $C_2 = 0$.

$$x(t) = \tfrac{1}{2}gt^2\sin\theta$$

or, solving for t

$$t = \left(\frac{x(t)}{\frac{1}{2}g\sin\theta}\right)^{\frac{1}{2}}$$

Au: Delete extra space

With this last expression, we can solve for the time given the final position $x(t_f) = 200$m. Using $g = 9.81$ m/s, the result is $t = 9.0$ s. From the expression for $v(t)$, we can find the velocity at the end of the run to be 44 m/s (equivalent to 99 miles per hour!).

Certainly, this would be the absolute upper limit that one could reach on 200 meters of ski slope pitched at 30°. Note that a 30° slope is equivalent to 67% slope; this actually quite steep!

2.2.1.2 First order separable nonlinear equations

First-order equations that are separable and nonlinear take the form

$$R(y)\frac{dy}{dt} = Q(t) \tag{2.29}$$

Solving these equations is no more difficult than the linear case, but not substantially more difficult; we need only use integration by parts once and the product rule for derivatives once to make the process work effectively. Recall the formula for integration by parts using *indefinite integrals* is

$$\int udv = uv - \int vdu \tag{2.30}$$

And the product rule for derivatives is

$$(uv)' = u'v + uv' \tag{2.31}$$

To start, we note

$$\frac{d}{dt}(R(y)y) = \frac{dR}{dt}y + R\frac{dy}{dt} \tag{2.32}$$

Rearranging this, yields

$$R(y)\frac{dy}{dt} = -\frac{dR(y)}{dt}y + \frac{d}{dt}(R(y)\,y) \tag{2.33}$$

Substituting this result into Eq. (2.29), gives

$$-\frac{dR(y)}{dt}y + \frac{d}{dt}(R(y)\,y) = Q(t) \tag{2.34}$$

Integrating both sides with respect to t we find

$$-\int \frac{dR(y)}{dt}y\,dt + \int \frac{d}{dt}(R(y)\,y)\,dt = \int Q(t)\,dt \tag{2.35}$$

Using the fundamental theorem of calculus on the second term in this equation gives

$$-\int \frac{dR(y)}{dt}y\,dt + R(y)\,y = \int Q(t)\,dt + C \tag{2.36}$$

Conducting integration by parts on the first integral in this last expression and setting $u = y, dv = dR/dt$ yields

$$-\left(yR(y) - \int R(y)dy\right) + yR(y) = \int Q(t)\,dt + C \tag{2.37}$$

Finally, we can simplify this expression to give

$$\int R(y)dy = \int Q(t)\,dt + C \tag{2.38}$$

This last expression allows the direct integration of the problem to generate a solution; however, this solution may not be one that is explicit in the dependent variable, $y(t)$. In the general case, an *implicit* equation is found. Such equations are still useful solutions, but they may require that additional work be done to determine the values of the dependent variable. This is best seen through an example.

Example 2.3 (A first-order, nonlinear equation). Suppose we have the problem

$$y\frac{dy}{dt} = t^2 \tag{2.39}$$

with ancillary condition

$$y(0) = 1 \tag{2.40}$$

What is the explicit solution for $y(t)$?

Solution. We can use the expression given by Eq. (2.38) to solve this problem. Clearly, the solution is given by

$$\int y\,dy = \int t^2\,dt + C \tag{2.41}$$

or, upon computing the integrals

$$y^2(t) - y^2(0) = \tfrac{2}{3}t^3 + C \tag{2.42}$$

Noting the initial condition, this can be expressed

Au: Changes suggested to match format on p. 31

$$y^2(t) = (1 + \tfrac{2}{3}t^3) \tag{2.43}$$

where we must have $C = 0$ (it is easy to verify that this expression matches the ancillary condition at $t = 0$). This is an implicit equation for y, since the expression does not provide us with the value of y, but, rather, the value of y^2. In this case we are lucky– the expression is a quadratic, and we can use the quadratic formula (or, in this case, simply taking the square root of both sides of the expression) to get an explicit expression for y.

$$y(t) = \pm\sqrt{1 + \tfrac{2}{3}t^3} \tag{2.44}$$

The derivative of the solution is

$$\frac{dy}{dt} = \pm\tfrac{1}{2}(1 + \tfrac{2}{3}t^3)^{-\frac{1}{2}}\, 2t^2 \tag{2.45}$$

And with this information, it is easy to verify that the original nonlinear ODE is also met by the solution.

Example 2.4 (Michaelis-Menten kinetics). Michaelis-Menten kinetics describe kinetic processes that are rate-limited by the total number (or amount) of compound that causes the reaction to occur. As an example, reactions due to a catalysts on the surface of a carrier particle (of the form $A \xrightarrow{Catalyst} B$ are sometimes rate-limited because once all of the catalysts sites are occupied by the reactant (A). The reaction rate is given by

$$\frac{dc_A}{dt} = -\frac{kc_A}{c_A + K_A}$$

where k is the rate constant (mol/(L·s) and K_A is the half-saturation constant (mol/L). Michaelis-Menten kinetics are sometimes also called *saturation* kinetics, because the kinetic rate achieves a maximum value as the concentration of the reactant species increases. This is illustrated in Fig. 2.2.

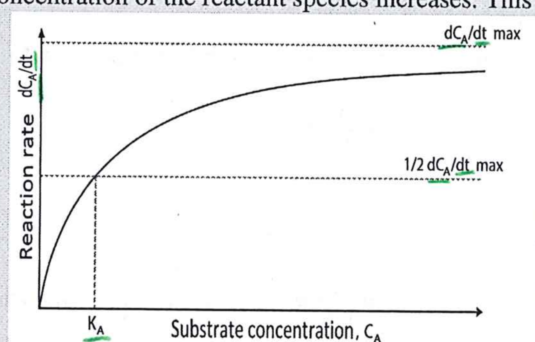


Fig. 2.2: Michaelis-Menten kinetics. Two intersting features about these kinetics can be seen through the geometry of the curve of rate versus concentration. At concentrations that are much larger than the half-saturation constant, K_m, the rate of reaction is approximately equal to the kinetic rate parameter, k. The half-saturation constant, K_A can be found by first finding the rate equal to half of the maximum rate; then, one find the corresponding value on the concentration axis. This value is equal to K_A.

Determine a functional relationship for $c_A(t)$ assuming this rate law and the initial condition $c_A(0) = C_0$. How long does it take for c_A to get to one-half of its initial value?

Solution. Start by doing separation of variables, leading to the form

$$-\frac{c_A + K_A}{c_A} dc_A = kdt$$

$$-\int_{C=c_A(0)}^{C=c_A(t)} \frac{C + K_A}{C} dC = \int_{\tau=0}^{\tau=t} kd\tau$$

(Note that here we have been careful to use variables of integration when writing out the *definite integral*. Sometimes this is helpful to do; it reinforces what the correct bounds for the integration are. However, for compactness and expedience, once one is familiar with indefinite integration, the explicit switching to a separate dummy variable for integration is not necessary. The resulting expression is a bit "sloppy", but as long as it is clear what is being done, it usually causes no problems.)

Performing the integrations, we find

$$-C\Big|_{c_A(0)}^{c_A(t)} - K_A \ln C\Big|_{c_A(0)}^{c_A(t)} = kt$$

Evaluating this result at the bounds and using the properties of logarithms, the final result is

~~Performing the integrations, we find~~ Au: Okay?

$$t = \frac{1}{k}\left[C_0 - c_A(t) + K_A \ln \frac{c_A}{C_0}\right]$$

As a check on this result, note two properties that we would expect from this solution (1) The solution meets the initial condition at $t = 0$ (i.e., for $t = 0$, $c_A(0) = C_0$), and (b) the result is positive for all values of c_A; we expect this latter property because time can not be a negative quantity! Also note that argument of the logarithm is *dimensionless*. It is a good practice to assure that in your *final results* all logarithmic arguments ~~should be~~ dimensionless! They arguments may not be dimensionless during intermediate steps, but if they cannot be made to be free of units at the end of the problem, this may indicate that there has been an error. Generally speaking, it is improper to take the logarithm of a quantity with units.

To solve the second part of the problem, we substitute $c_A(t) = C_0/2$, and solve for time; the result is

$$t = \frac{1}{k}\left[\tfrac{1}{2}C_0 + K_A \ln 2\right]$$

2.2.2 *Separation of variables in differential form*

Au: Equations from this point forward will need to be renumbered

Both the linear and nonlinear cases above have a similar structure. In both cases, the ODEs can be written in a form where the two variables y and t can be put in the forms

$$\frac{dy}{dt} = \frac{Q(t)}{P(t)} \tag{2.46}$$

$$or \tag*{$\cancel{(2.47)}$}$$

$$R(y)\frac{dy}{dt} = Q(t) \tag{2.48}$$

In both cases, the developments above provide a basis for making proper mathematical meaning out of the following representations

$$dy = \frac{Q(t)}{P(t)}dt \tag{2.49}$$

$$R(y)dy = Q(t)\,dt \tag{2.50}$$

To see this, note that integrating both sides of these expressions leads directly to the solutions that we have derived more formally above. In other words, we find

$$y(t) = \int \frac{Q(t)}{P(t)}dt + C \tag{2.51}$$

$$\int R(y)dy = \int Q(t)\,dt + C \tag{2.52}$$

These expressions are each exactly the solutions given by Eqs.(2.28) and (2.38) above. This is an interesting result; it implies that, for first-order ODEs at least, we may treat differentials (i.e., the numerator and denomenator of derivatives, written in the form $\frac{dy}{dt}$) as if they were algebraic quantities. We have essentially proven this above; however, a little thought about what the derivative means in a more fundamental sense will indicate that there should be, in principle, no problem with the treatment of such terms as algebraic quantities. Recall the definition of the conventional derivative

$$\frac{dy}{dt} = \lim_{\Delta t \to 0} \frac{y(t+\Delta t) - y(t)}{\Delta t} \tag{2.53}$$

$$= \frac{\lim_{\Delta t \to 0}(\Delta y)}{\lim_{\Delta t \to 0}(\Delta t)} \tag{2.54}$$

So, in this sense, the quantities dy and dt are well-defined mathematical objects that follow the conventional rules of algebra. Note: This is not the case for second-order and higher derivatives! If one writes out the definition for the second-order derivative, it becomes clear right away why this is not so. Ultimately, then, we can treat differentials appearing in first-order ODEs as algebraic quantities, but we can not, in general, do so for higher-order derivatives.

Usually, this method of "separating" the functions and differentials involving the dependent and independent variables is the way that most people remember how to solve separable first-order ODEs. This can be made more clear by a few examples.

Example 2.5 (Solution to a linear first order ODE by separation of variables). Suppose we have the classical first-order reaction in a completely-mixed reactor problem discussed above, and specified by the set of equations

$$\frac{dy}{dt} = -k_1 y \tag{2.55}$$

$$y(t=0) = c_0 \tag{2.56}$$

What is the solution?

Answer. Separating variables we have

$$\frac{1}{y}\,dy = -k_1\,dt \tag{2.57}$$

Integrating both sides of this immediately yields

$$\int \frac{1}{y}\,dy = -k_1 \int dt \tag{2.58}$$

or

$$\ln(y) = -k_1 t + C \tag{2.59}$$

$$y(t) = C \exp[-k_1 t] \tag{2.60}$$

Substituting the ancillary equation into this result, we find

$$y(0) = C \tag{2.61}$$

$$or \qquad \cancel{(2.62)}$$

$$C = c_0 \tag{2.63}$$

Au: Note need to renumber equations

so that the final result is the familiar exponentially-decreasing function of time

$$y(t) = c_0 \exp[-k_1 t] \tag{2.64}$$

Note that this process works just as well for separable nonlinear equations, as the next example shows.

Example 2.6 (Solution to a nonlinear first order ODE by separation of variables). Suppose instead of the classical first-order reaction in a completely-mixed reactor problem, we have a second-order problem specified by

$$\frac{dy}{dt} = -k_1 y^2 \tag{2.65}$$

$$y(t=0) = c_0 \tag{2.66}$$

What is the solution?

Answer. Separating variables as above, we have

$$\frac{1}{y^2}\,dy = -k_1\,dt \tag{2.67}$$

Au: → (2.68)

Integrating both sides of this immediately yields

$$\int \frac{1}{y^2}\,dy = -k_1 \int dt \tag{2.69}$$

Au: Okay that this "or" differs in placement from the ones above and below?

or

$$-y^{-1} = -k_1 t + C \tag{2.70}$$

Upon solving explicitly for $y(t)$ we have

$$y(t) = -\frac{1}{-k_1 t + C} \tag{2.71}$$

Finaly, substituting the ancillary equation into this result, we find

$$y(0) = -\frac{1}{C} \tag{2.72}$$

or Au: → (2.73)

$$C = -\frac{1}{c_0} \tag{2.74}$$

so that the final result is the following function of time

$$y(t) = \frac{c_0}{k_1 c_0 t + 1} \tag{2.75}$$

Noting that at $t = 0$, we have $y(0) = c_0$, we find that the ancillary condition is met. Also noting that the derivative is given by

$$\frac{dy}{dt} = -\frac{k_1 c_0}{(k_1 c_0 t + 1)^2} \tag{2.76}$$

it is easy to validate that the solution not only meet the initial condition, but it meets the original ODE also.

2.2.3 Non-separable linear first-order ODEs

In the previous sections, first-order ODEs were solved by direct use of the fundamental theorem of calculus. This approach required that the equations be *separable*. However, there are plenty of examples of equations that are not immediately separable. The canonical form for these equations is

$$\frac{dy}{dt} + P(t)y = Q(t) \tag{2.77}$$

There is no obvious way to integrate both sides of this equation to get a solution. Doing so would result in an integral with integrand $P(t)y(t)$; because we do not *know* $y(t)$, we are stuck with an implicit integral solution for $y(t)$. While technically not a disaster, it is not a solution that is easy to compute the values of the dependent variable.

To handle problems of this general form for linear first-order ODEs requires first transforming this problem. This idea is a key element in analytical modeling and in mathematical analysis generally; it is important enough to highlight the idea specifically.

Key Idea 1.1. When encountering a problem that one does not know how to solve, it is worthwhile considering if it is possible to transform the problem into a form that does have a known solution.

This idea behind this statement is simultaneously extremely useful, and potentially frustrating! It suggests what must be attempted, but it provides no information about how this is to be accomplished. This brings up a second key idea that arises in mathematical analysis.

Key Idea 1.2. Mathematical analysis, despite any impressions given to the contrary in conventional presentations of mathematical analysis, often involves the creative use of intuition or experimentation to find solutions.

An example of these two ideas is exactly what is embodied by the following solution to the general first-order linear ODE. It is often most useful to see such developments as an example before stating the more general and abstract result.

Example 2.7. Suppose we have a continuously, stirred tank reactor (CSTR) undergoing a first-order reaction process $A \to B$ with kinetic rate constant k_1. If the flow rate in and out are both equal to Q, the concentration of species A is c_0 at the inlet, and the initial concentration of species A is $y_A(0) = 0$, then the net balance for the concentration of species A reactor is given by the ODE

$$\frac{dy_A}{dt} = \frac{Q}{V}c_0 - \frac{Q}{V}y_A - k_1 y_A \tag{2.78}$$

$$y_A(0) = 0 \tag{2.79}$$

Here, we note that the quantity $\frac{Q}{V}$ is related to the *residence time* for the reactor, τ

$$\frac{Q}{V} = \frac{1}{\tau} \tag{2.80}$$

Au: Fig. 23 not called out in the text.

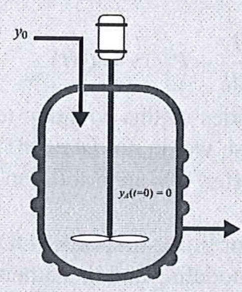


Fig. 2.3: A continuously-stirred tank reactor. The tank initially has zero concentration of species A or B, but does contain a suspended catalyst (as pellets that do not leave the system). At time $t = 0$, species A begins to enter the reactor, and the catalytic reaction proceeds.

To solve this problem, we start by rewriting the equation in the following form

$$\frac{dy_A}{dt} + (\tau^{-1} + k_1)y_A = \tau^{-1}y_0 \tag{2.81}$$

Now, it is clear that this expression is not of the form of one that has been covered in the material above. However, we note that if we set $\beta = (\tau^{-1} + k_1)$, and then multiply this expression through by $e^{\beta t}$, we have

$$\frac{dy_A}{dt}e^{\beta t} + y_A\beta e^{\beta t} = e^{\beta t}\tau^{-1}y_0 \tag{2.82}$$

Although it may not be obvious that this has improved things, it has once we make an observation: The left-hand side of the expression is now a total derivative. In other words, we note

$$\frac{d}{dt}(y_A e^{\beta t}) = \frac{dy_A}{dt}e^{\beta t} + y_A\beta e^{\beta t} \tag{2.83}$$

But this is exactly the left-hand side of the equation above! Thus, we can substitute as follows

$$\frac{d}{dt}(y_A e^{\beta t}) = e^{\beta t}\tau^{-1}y_0 \tag{2.84}$$

Now, we have transformed the original equation into one we know how to solve–this expression is separable in the conventional way that was discussed previously. If this is unclear, we can make the following temporary transformation of variables

$$\psi(t) = y_A e^{\beta t} \tag{2.85}$$

Then, we have

$$\frac{d\psi}{dt} = e^{\beta t}\tau^{-1}y_0 \tag{2.86}$$

Separating variables and integrating, we find

$$\int d\psi = \int e^{\beta t}\tau^{-1}y_0\,dt + C \tag{2.87}$$

This yields

$$\psi(t) = \frac{1}{\beta}e^{\beta t}\tau^{-1}y_0\,dt + C \tag{2.88}$$

Returning to the original variables, we have

$$y_A \exp\left((\tau^{-1}+k_1)t\right) = \frac{1}{(\tau^{-1}+k_1)}\exp\left((\tau^{-1}+k_1)t\right)\tau^{-1}y_0 + C \tag{2.89}$$

Finally, solving for y_A gives the expression

$$y_A(t) = \frac{1}{(1+\tau k_1)}y_0 + \exp\left(-(1+\tau k_1)\frac{t}{\tau}\right)C \tag{2.90}$$

Setting $t = 0$ allows us to use the initial condition to solve for C

$$C = -\frac{1}{(1+\tau k_1)}y_0 \tag{2.91}$$

Thus, the final solution is

$$y_A(t) = \frac{y_0}{(1+\tau k_1)}\left[1 - \exp\left(-(1+\tau k_1)\frac{t}{\tau}\right)\right] \tag{2.92}$$

In Example 2.7, the function $P(t)$ that was incorporated into the exponential was a simple constant, $\beta = \tau^{-1} + k_1$. Recall, however, the general form is

$$\frac{dy}{dt} + P(t)y = Q(t) \tag{2.93}$$

The solution here is actually no more difficult than when $P(t)$ is a constant. For this more general case, take

$$s(t) = \int P(t)\,dt \tag{2.94}$$

This transformation can be done as an indefinite integral. The constant for the indefinite integral can be taken as zero (and **always** will be when we use an integrating factor), because any such constant eventually can be eliminated from the resulting equations. Note that

$$\frac{ds}{dt} = P(t) \tag{2.95}$$

By the fundamental theorem of calculus.

Au: Please update equation numbers here and below.

Now, multiplying Eq. (2.96) through by $\exp[\beta(t)]$ we find

$$\frac{dy}{dt}\exp[s(t)] + P(t)\exp[s(t)]y = \exp[s(t)]Q(t) \tag{2.96}$$

This expression can be rewritten as

$$\frac{d}{dt}(\exp[s(t)]y) = \exp[s(t)]Q(t) \tag{2.97}$$

Now, set $\psi(t) = \exp[s(t)]y$, separate variables, and integrate both sides as *definite* integrals. This results in

$$\int_{\psi(t'=t_0)}^{\psi(t'=t)} d\psi = \int_{t'=t_0}^{t'=t} \exp(s(t'))Q(t')dt' \tag{2.98}$$

Integrating this yields

$$\psi(t) - \psi(t_0) = \int_{t'=t_0}^{t'=t} \exp(s(t'))Q(t')dt' \tag{2.99}$$

Upon returning to the original variables, we find

$$\exp[s(t)]y(t) - \exp[s(t_0)]y(t_0) = \int_{t'=t_0}^{t'=t} \exp[s(t')]Q(t')dt' \tag{2.100}$$

And solving this for $y(t)$ gives us the general formula for the solution to the separable first-order linear ODE

Au: What does the box denote?

$$\boxed{y(t) = \exp[-s(t)]\left[\int_{t'=t_0}^{t'=t} \exp[s(t')]Q(t')dt' + y(t_0)\exp[s(t_0)]\right]} \tag{2.101}$$

that

where recall

$$s(t) = \exp\left(\int P(t)dt\right) \tag{2.102}$$

This expression gives the solution, then, to any linear non-separable first-order ODE.

The entire analysis above can also be done using indefinite integration. The entire process is exactly the same up to Eq. 2.97. From there, we can integrate both sides as indefinite integrals, but remembering to add the appropriate constant of integration. Thus, we would have the result (starting right after Eq. 2.97)

$$\int d\psi = \int \exp(s(t))Q(t)dt \tag{2.103}$$

$$\psi(t) = \int \exp(s(t))Q(t)dt + C_1 \tag{2.104}$$

lc side

Where C_1 is a constant of integration from the integration of the left-hand side. Note that the integral on the right-hand will also generate a constant of integration. However, the two constants can be combined, so we can ignore the constant coming from the remaining integral. Recalling that $\psi(t) = \exp[s(t)]y$, then this can be simplified to give $y(t)$ as follows

$$\exp[s(t)]y(t) = \int \exp(s(t'))Q(t')dt' + C_1 \tag{2.105}$$

Au: Box?

$$\boxed{y(t) = \exp[-s(t)]\left[\int \exp(s(t'))Q(t')dt' + C_1\right]} \tag{2.106}$$

Where, again, remember that *only one constant*, C_1, is generated for this problem in total, which is consistent for the fact that it is a first-order problem. By comparing the two boxed results above, it is clear that $C_1 = y(t_0)\exp[s(t_0)]$. However, some people prefer to use the simpler looking version given by Eq. (2.106), and then simply evaluate the unknown constant using the ancillary data. The results will be the same regardless of which approach is taken.

Example 2.8 (CSTR with catalyst deactivation.). Solid catalysts are used in a huge variety of reactors, from high-tech reactors to make pharmaceuticals to reactors for ion-exchange in the treatment of drinking water. One potential problem with solid catalysts is that they can become deactivated over time. There are any number of deactivation processes (e.g., particle sintering, catalyst poisoning, and catalyst coking are three types of deactivation that are common); all of them reduce catalyst effectiveness, and have significant economic impact.

One model for catalyst inactivation involves an inverse-time function that decreases the net rate of reaction with increasing time. Suppose we have a reaction that proceeds in the presence of a catalyst with the simple form $A \xrightarrow{C} B$, where A is the reactant, B is the product, and C is the catalyst. Returning to the case of a CSTR from the previous example, the molar mass balances for a catalytic reaction with deactivation for chemical species A can be specified by

$$\frac{dy_A}{dt} = \tau^{-1}y_0 - \tau^{-1}y_A - \left(\frac{1}{1+k_d t}\right)k_1 y_A \tag{2.107}$$

$$y_A(0) = 0 \tag{2.108}$$

$$y_B(0) = 0 \tag{2.109}$$

~~(2.110)~~ Au:?

We have assumed that the catalyst concentration is constant in the CSTR (catalyst neither enters nor leaves the reactor). Note that because initially there is no species B in solution, the concentration of species B at any time can be computed from how much of species A has been converted. While it is possible to also get the concentration of species B at any time, for now we will focus only on the balance for species A.

Here, we can see that Eq. (2.107) is identical to Eq. (2.78), except the reaction term includes an additional function of time that multiplies the first-order reaction. This function decreases the net rate of reaction as time increases. This problem would be somewhat intimidating if we had not previously developed the integration factor formula given by Eq. (2.101) (and even with it, it may still be challenging!) Rewriting the mass balance equation, we find

$$\frac{dy_A}{dt} + \left[\tau^{-1} + \left(\frac{k_1}{1+k_d t}\right)\right]y_A = \tau^{-1}y_0 \tag{2.111}$$

In this form, it is clear that we have

$$s(t) = \int \left[\tau^{-1} + \left(\frac{k_1}{1+k_d t}\right)\right] dt \qquad (2.112)$$

or, after completing the integral

$$s(t) = \left[\frac{t}{\tau} + \frac{k_1}{k_d}\ln(1+k_d t)\right] \qquad (2.113)$$

This makes rather short work of writing down the solution; recalling Eq. (2.101)

$$y(t) = y(t_0)\exp[s(t_0)]\exp[-s(t)] + \exp[-s(t)]\int_{t'=t_0}^{t'=t} \exp[s(t')]Q(t')dt' \qquad (2.114)$$

Making the appropriate substitutions (and noting that $y(t_0) = 0$), we have the solution

$$y_A(t) = \exp\left[-\left(\frac{t}{\tau} + \frac{k_1}{k_d}\ln(1+k_d t)\right)\right]\int_{t'=0}^{t'=t} \exp\left[\frac{t}{\tau} + \frac{k_1}{k_d}\ln(1+k_d t)\right]\frac{y_0}{\tau}dt' \qquad (2.115)$$

Computing this last integral is somewhat of a challenge; however, the integral is tabulated in tables, and can be computed by symbolic mathematics programs like Mathematica. The result is

$$y_A(t) = \tau e^{-\frac{1}{k_d \tau}}\left(\frac{1}{k_d \tau}\right)^{-\frac{k_1}{k_d}}\left[\Gamma\left(\frac{k_1+k_d}{k_d}, -\frac{k_d t+1}{k_d \tau}\right) - \Gamma\left(\frac{k_1+k_d}{k_d}, -\frac{1}{k_d \tau}\right)\right] \qquad (2.116)$$

Plots of the solution for species A and B are provided in Fig. 2.5.

The Gamma function, Γ is a transcendental function that corresponds to a generalization of the factorial operation to the real (or complex) numbers. The function is widely used, and is usually an intrinsic function in both symbolic mathematics programs like Mathematica, and in interpreted coding languages like MATLAB.

Au: Fig. 2.4 is not called out in the text

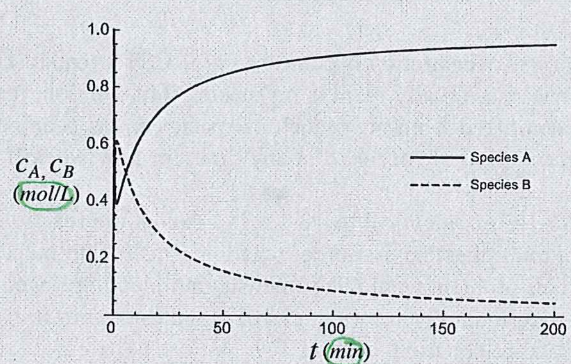


Fig. 2.4: Solutions for species A and species B as a function of time for a catalytic reaction with deactivation. For this solution, $k_1 = 2\,min^{-1}$, $k_d = 0.1\,min^{-1}$, $\tau = 1\,min^{-1}$, $y_0 = 1\,mol \cdot m^{-3}$.

Just for completeness, note that the two Gamma functions are defined by the following integrals

Gamma	$\Gamma_1(x) = \int_{t=0}^{t\to\infty} t^{x-1}e^{-t}dt$	(2.117)
Incomplete Gamma	$\Gamma_2(a,x) = \int_{t=x}^{t\to\infty} t^{a-1}e^{-t}dt$	(2.118)

More information on the Gamma function can be found in many texts. The Gamma function can be evaluated using common computational platforms such as MATLAB or Mathematica, both of which have built-in routines for computing these functions.

2.3 Second-order ODEs

We will cover exactly two kinds of second-order ODEs: (1) directly integrable second-order ODEs, and (2) general second-order ODEs with constant coefficients.

Linear second-order ODEs are functions of a single independent variable that take the form

$$\frac{d^2y}{dx^2} + b(x)\frac{dy}{dx} + c(x)y - g(x) = 0 \tag{2.119}$$

In general, solutions of these equations (where the coefficients are functions rather than constants) require series solution methods which we will not be reviewing. However, there are a few other interesting problems that are solvable. These are the (1) directly integrable problems, and (2) the case of linear second-order ODEs with constant coefficients.

2.3.1 *Directly Integrable Second-Order ODEs*

If a second-order can be put in the form

$$\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right) = h(x) \tag{2.120}$$

then, in principle, it can be solved directly by two integrations through the application of the fundamental theorem of calculus (FTC).

Suppose the ODE above is defined on $x \in [a,b]$, it has two appropriate ancillary conditions imposed, and $p(x) \neq 0$ anywhere in the domain. Then, integrating both sides of Eq. (2.120) gives (using the fundamental theorem of calculus), and then dividing by $p(x)$

Au: Gives what?

$$\frac{dy}{dx} = \frac{1}{p(x)}\int_x h(\xi)d\xi \tag{2.121}$$

where, ~~here~~ we have used a dummy variable of integration to avoid confusion in later developments. A second integration gives a solution for $y(x)$

$$y(x) = \int_x \frac{1}{p(x)} \int_x h(\xi)\,d\xi\,dx \tag{2.122}$$

Note that these two integrations will generate two constants of integration. Au: Not ODEs?

Example 2.9 (Directly Integrable Second-Order ODE.). Suppose we have an ~~integrable~~ of the form integration/

Au: As meant?

$$\frac{d}{dx}\left((x^2+1)\frac{dy}{dx}\right) = 3x^2, \quad x \in [0,1]$$

with

$$y(0) = 0, y(1) = 0$$

What is the solution?

Solution. To start, integrate both sides as an indefinite integral and divide through by x^2+1

$$\frac{dy}{dx} = \int_x \frac{x^3 + c_1}{x^2+1}\,dx$$

Now, this integral is not (at least apparently) easy to do. One could try something like the method of partial fractions (usually introduced in introductory calculus) to integrate it. Alternatively, there are tables of integrals, and various symbolic mathematics languages that can be used to find the value of this integral. We are going to take the latter option here, noting that the integral can be computed as

$$\frac{dy}{dx} = \frac{1}{2}[x^2 + 2c_1 \arctan(x) - \ln(1+x^2)]$$

A second integration yields

$$y(x) = c_1\left(x\arctan(x) - \frac{1}{2}\log\left(x^2+1\right)\right) + \frac{x^3}{6}$$
$$-\frac{1}{2}x\log\left(x^2+1\right) + x - \arctan(x) + c_2$$

Applying the first ancillary condition, $y(0) = 0$, we find $c_2 = 0$. Applying the second ancillary condition $y(1) = 0$ gives

$$0 = c_1\left(\frac{\pi}{4} - \frac{1}{2}\log(2)\right) - \frac{\pi}{4} + \frac{7}{6} - \frac{\log(2)}{2}$$

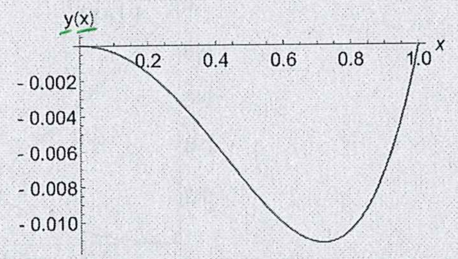
or

$$c_1 = \frac{\frac{\pi}{4} - \frac{7}{6} + \frac{1}{2}\log(2)}{\pi - 2\log(2)}$$

So, the final solution is, somewhat unbelievably, the function

$$y(x) = \left(\frac{\frac{\pi}{4} - \frac{7}{6} + \frac{1}{2}\log(2)}{\pi - 2\log(2)}\right)\left(x\arctan(x) - \frac{1}{2}\log\left(x^2+1\right)\right) + \frac{x^3}{6}$$
$$-\frac{1}{2}x\log\left(x^2+1\right) + x - \arctan(x)$$

ital x2



bf

Fig. 2.5: Plot of solution, $y(x)$

It is possible to verify that $y(0) = y(1) = 0$ for this result, suggesting strongly that it is a correct one.

cap

2.3.2 Thinking about Solutions to Second-order ODEs

Before doing any additional analysis, it is worth doing a little thinking to build our intuitive understanding of problems of this sort. So, let's think about this problem entirely backward for a few moments. To start, consider the function

$$y(x) = \alpha y_1(x) + \beta y_2(x) \quad x \in [0,1] \tag{2.123}$$

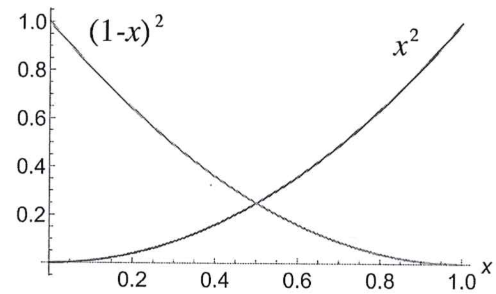
where

$$y_1(x) = x^2$$
$$y_2(x) = (1 - x^2)$$

This function is clearly the sum of two independent functions; these independent functions are plotted in Fig. 2.6

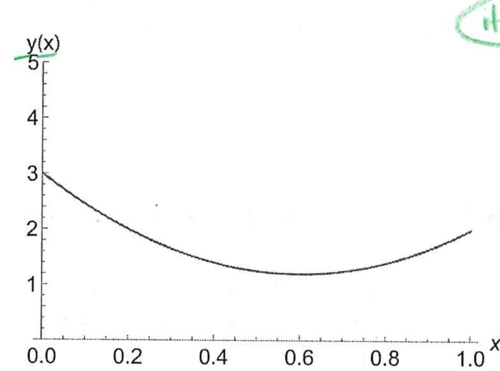
These functions have some interesting features. First, note that y_1 is zero at one end and 1 at the other; y_2 has the same feature but at opposite ends of the domain. Also, the derivative y_1 is zero at $x = 0$, and the derivative of y_2 is zero at $x = 1$. These features give lots of flexibility if one wants to develop new functions by creating linear combinations of these two. For example, suppose I want a function on $[0,1]$ that is (1) a quadradic, (2) has the value 3 on the left-hand side, and has the value of 2 on the right-hand side. A little though will indicate that we can *create* this function by the following linear combination

Fig. 2.6 The functions $y(x) = x^2$ and $y(x) = (1-x)^2$



Au: Okay that Fig. 2.7 appears before its callout?

Fig. 2.7 The functions $y(x)$ composed specifically so that $y(0) = 3$ and $y(1) = 2$.



ital x2

$$
\begin{aligned}
y(x) &= 2y_1(x) + 3y_2(x) \\
&= 2x^2 + 3(1-x)^2 \\
&= 5x^2 - 6x + 3
\end{aligned}
$$

If we want to be really clever, we can even indicate the functional *value* at one end and the *slope* at the other end. To do this, first note

$$y'(x) = 2\alpha x - 2\beta(1-x) \quad x \in [0,1]$$

So, ~~now~~ to meet two conditions (one for the value at one end, one for the slope at the other end) we can solve these two equations simultaneously. For example, suppose we wanted $y(0) = 1$, $y'(1) = 20$. This implies

$$
\begin{aligned}
1 &= 0 + \beta(1-0) & &\to \beta = 1 & &\text{(from the equation for } y(x)\text{)} \\
20 &= 2\alpha + 0 & &\to \alpha = 10 & &\text{(from the equation for } y'(x)\text{)}
\end{aligned}
$$

So far, we have not said a word about the solutions to ODEs. However, the functions that we just examined have relevance here. To see this, we just have to consider the solutions to the following nonhomogeneous problem. This is a directly integrable problem (as described in the previous section) but with a particularly simple form

Au: Fig. 2.8 is not called out in the text.

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ital x2

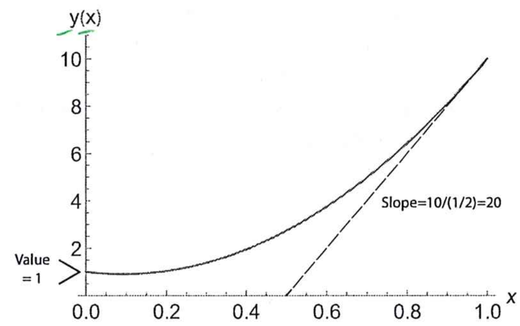

Fig. 2.8 The functions $y(x)$ composed specifically so that $y(0) = 1$ and $y'(1) = 20$.

$$\frac{d^2y}{dx^2} = k_0$$

where k_0 is some specified constant.

Without any ancillary information, we can still solve this problem. To do so, we integrate both sides to give

$$\int_x \frac{d^2y}{dx^2} dx = \int_x k_0 dx \Rightarrow$$
$$\frac{dy}{dx} = k_0 x + C_1$$

and, integrating a second time, we find

$$\int_x \frac{dy}{dx} dx = \int_x (k_0 x + C_1) dx \Rightarrow \tag{2.124}$$
$$y(x) = \frac{k_0}{2} x^2 + C_1 x + C_2 \tag{2.125}$$

It turns out that the function that we examined earlier, $y(x) = \alpha x^2 + \beta(1-x)^2$, is equivalent to this solution. To see this, note that if we expand and regroup Eq. (2.123), we have

$$y(x) = (\alpha+\beta)x^2 - 2\beta x + \beta$$

Comparing the two solutions at the x^2 term, we find that we must have $k_0 = 2(\alpha+\beta)$ for the two solutions to match. Suppose we re-examine the case where we had $y(0) = 3$, $y(1) = 2$. Solving Eq. (2.125) with these constraints gives

$$y(0) = 3 \Rightarrow C_2 = 3$$
$$y(1) = 2 \Rightarrow C_1 = -(1 + k_0/2)$$

The constraint we have on compatibility between the two equations does not allow *any* values for α and β; the value of these are related to k_0 by $2(\alpha+\beta)=k_0$. This means that our problem with $y(0)=3$, $y(1)=2$, which had $\alpha=3$, $\beta=2$, corresponds to $k_0=10$. Thus, we have $C_1=-6$. It is easy to show that this solution is the same solution as plotted in Fig. 2.7. Alternatively, we can say that the first solution that we plotted (where we forced the right-hand value to be 2 and the left-hand value to be 3)

$$y(x)=2x^2+3(1-x)^2$$

Corresponds to the second-order ODE

$$\frac{d^2y}{dy^2}=10$$
$$y(0)=3$$
$$y(1)=2$$

So, why did we bother with this long example? Well, for one thing, it showed us, empirically at least, that we do indeed generate two constants of integration for second-order ODEs. It also showed us that we can think of the solution to such problems as the linear combination of *two linearly independent* solutions. In the example above, we thought of these two solutions as $y_1(x)=x^2$ and $y_2(x)=(1-x)^2$.

2.3.3 Linear Second-Order ODEs with constant Coefficients: Homogeneous Case

Now, let's examine the general case of linear second-order equations with constant coefficients. Recall the general form for a *linear* second-order ODE given by Eq. (2.119). When the term $c(x)\equiv 0$, then the equation is called *homogeneous*. Sometimes, functions like $c(x)$ are called *source* terms. Because functions like this are not dependent on y, and because the entire term is independent from y, the action of these functions can be though of as "sources" or "sinks" that drive the problem.

We will study the particular homogeneous case where the coefficients of the differential equation are constants rather than functions. This means that the equations of interest to us take the form

$$\frac{d^2y}{dx^2}+b\frac{dy}{dx}+cy=0 \tag{2.126}$$

First, we note that *every* homogenous second-order ODE with constant coefficients can be put in this form. Second, we note that the solution to an equation like this must involve two unknown constants. We can think of there being an unknown constant generated for each "integration" that needs to be done to invert the derivatives. Here, we are using the term integration somewhat loosely, but it is a correct interpretation. Because the highest order of derivative is two, this means two integrations need to be done. Finally, because of our previous experience, we might expect that the solution to this equation is the linear combination of two independent solutions. We have not yet proved this (we will offer a proof of sorts later), but this idea is consistent with our observations so far.

Having dispensed with what we know so far we are now at an impasse. We expect that there are two linearly independent solutions to the general homogeneous problem with constant coefficients, and we know that we can make new solutions by making linear combinations of them. However, as to what the solutions actually might be, we have not much to go on. We also know that for the directly integrable homogenous problem

$$\frac{d^2y}{dx^2} = 0 \tag{2.127}$$

the solution must be linear of the form $y(x) = C_1x + C_2$. So, whatever more general solution we find for Eq. (2.126), it must have the linear case as one of the possibilities (we will see, ultimately, that it does).

So, to proceed further, we are going to use a process that is not discussed very often in mathematics: We are going to use our intuition. If we *look* at Eq. (2.126), we note right away that we are looking for some function $y(x)$ such that it is at least possible to take its derivatives, multiply those by constants, and sum them to get zero. In fact, for the case $b = 0$, we even know that we must have a function whose second derivative is some constant multiple of the function that we started with. Clearly all polynomials are out as possibilities. Only a few potential functions that behave this way come immediately to mind. First, we know that functions like $\sin x$ and $\cos x$ behave this way, so those seem like reasonable possibilities. The only other function that comes to mind (unless you know something I don't!) is the exponential function. In fact, because of Euler's identity ($e^{ix} = \cos x + i \sin x$), the exponential function even subsumes the $\sin x$ and $\cos x$ functions. So, as literally a *guess* (albeit, and educated one), trying $y(x) = e^{sx}$ (where s could potentially be a real or a complex number) seems like a good place to start. Trying this, we find the following result

$$\frac{d^2}{dx^2}e^{sx} + b\frac{d}{dx}e^{sx} + ce^{sx} = 0$$
$$s^2e^{sx} + bse^{sx} + ce^{sx} = 0$$

So far, we are off to a good start. Now, we just have to determine under what conditions this last expression might possibly ever be true. Because s^2e^{sx} can never be zero at any point (even if s is complex), then we can safely divide both sides by this value. This simplifies things dramatically

$$s^2 + bs + c = 0$$

We are trying to determine if, given constant (real number) values for b and c, there is a solution to the above equation in terms of s. But the expression is now just a quadratic equation in s, so we can use the quadratic formula to solve it. Recall, the solutions are (noting that for the form $ax^2 + bx + c$, we have $a = 1$)

$$s_1 = \frac{-b + \sqrt{b^2 - 4c}}{2} \tag{2.128}$$

$$s_2 = \frac{-b - \sqrt{b^2 - 4c}}{2} \tag{2.129}$$

This result tells us that, except for the case of a repeated root (which we will cover later), we do indeed have two independent solutions for $y(x)$. These are $y_1(x) = e^{s_1x}$ and $y_2(x) = e^{s_2x}$. We can combine these two solutions linearly to generate the most general solution possible. To do this, we need the *principle of superposition* proved below.

Theorem 2.2 (Principle of Superposition for Second-Order ODES). *Suppose $y_1(x)$ and $y_2(x)$ are solutions to the ODE*

$$\frac{d^2y}{dx^2}+b\frac{dy}{dx}+cy=0$$

Then, the linear combination $y(x)=\alpha y_1(x)+\beta y_2(x)$ is also a solution.

Proof. Let $L=\frac{d^2}{dx^2}+b\frac{d}{dx}+c$. Then $L[\alpha y_1+\beta y_2]=\alpha L[y_1]+\beta L[y_2]$ by linearity. Because $L[y_1]$ and $L[y_2]$ are both solutions, they are both equal to zero. This proves that $L[\alpha y_1+\beta y_2]=0$. ■

Given all the information above, we can now write our general solution to be of the form

$$y(x)=\alpha e^{s_1x}+\beta e^{s_2x} \tag{2.130}$$

A little more thought about this solution indicates that we can actually say a bit more. The possibility for roots in a quadratic equation are as follows.

1. Case 1. The roots s_1 and s_2 are distinct real numbers.
2. Case 2. The roots s_1 and s_2 are real but not distinct ($s_1=s_2$).
3. Case 3. The roots are complex conjugates of the form $s_1=u+i\lambda,\ s_2=u-i\lambda$.

These are the only three options. Because the roots of the equation $s^2+bs+c=0$ basically define the kind of solution you have, this equation is frequently called the *characteristic equation*. The easiest way to proceed from here is to consider each option in sequence.

2.3.3.1 Case 1: The roots are real and distinct

For this case, the solution is relatively uncomplicated; it is just a linear combination of two exponential functions with real exponents. Thus the solution is

$$y(x)=\alpha e^{s_1x}+\beta e^{s_2x} \tag{2.131}$$

where α and β are two constants that are determined by the two ancillary conditions.

Au: Correct?

Example 2.10 (Contaminant Degradation in a River). When organic carbon is dumped into a river, it causes a decrease in oxygen in the river as the carbon is degraded by microorganisms in the river water. Suppose a vegetable processing plant is allowed to put its effluent into a river at a concentration of 20 mg/L of organic carbon (See Figure). Assume that organic carbon is discharged constantly (24 hours a day), mixed immediately, and that the effective concentration in the river of this readily-degradable organic carbon is $u(x=0)=u_0=2$ mg/L at the point of discharge. Also assume that the convection-dispersion-reaction equation is applicable, and that all processes have reached steady state.

How far downstream will the carbon affect oxygen levels? We will interpret the "affecting" oxygen levels, to mean that the organic carbon concentration is equal to or above $u=0.05$ mg/L. Assume that the velocity is $v_0=1.2$ km/h, the dispersion coefficient is $D_0=0.7$ km^2/h, and first-order degradation rate is equal to $k_1=0.3$ h^{-1}. Determine a set of reasonable boundary conditions based on the physical organization of the problem in order to develop a solution.

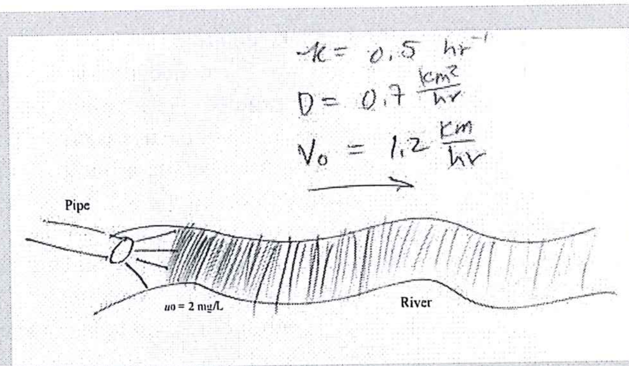

Fig. 2.9: A stream. Carefully drawn by hand.

Solution. The problem statement suggests that the appropriate balance equation takes the form

$$D_0 \frac{d^2u}{dx^2} - v_0 \frac{du}{dx} - k_1 u(x) = 0$$

Or, upon rearranging a bit,

$$\frac{d^2u}{dx^2} - \frac{v_0}{D_0}\frac{du}{dx} - \frac{k_1}{D_0}u(x) = 0$$

Taking $a = 1$, $b = -v_0/D_0$, and $c = -k_1/D_0$. Using the quadratic formula, we have the roots

$$s_1 = \frac{1}{2}\left(\frac{v_0}{D_0} + \sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$

$$s_2 = \frac{1}{2}\left(\frac{v_0}{D_0} - \sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$

The general solution is, then

$$u(x) = \alpha \exp\left(\frac{v_0}{2D_0}x\right) \exp\left(\frac{1}{2}x\sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$
$$+ \beta \exp\left(\frac{v_0}{2D_0}x\right) \exp\left(-\frac{1}{2}x\sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$

In order to determine the solution, we need to impose some ancillary conditions to more fully define the problem (in this case we might call them *boundary* conditions since they apply to space). The condition at $x = 0$ is not too difficult to work out. Clearly, we would like the concentration there to be u_0, so we can set $u(0) = u_0$. For the second ancillary condition, things are not necessarily as clear. However, a little thinking would indicate the following: The concentration downstream from the source can only *decrease* not increase. This is because the problem is essentially one of conservative transport at a constant velocity (with dispersive spreading) plus a decay reaction. Or, more simply, we might impose the condition that our concentration can not become arbitrarily high downstream from the source, although it can go to zero. Both of these conditions are consistent with the idea that the constant for the first exponential term must be zero. Why? Because if it is not zero, then the concentratio will grow exponentially large as one goes downstream from the source this does not make any *physical* sense based on our intuition about the problem. A more "mathematical", but otherwise equivalent statement might be this: we expect the concentration of carbon to become arbitrarily small as x becomes arbitrarily large. Either way, we now have the solution

$$u(x) = \beta \exp\left(\frac{v_0}{2D_0}x\right) \exp\left(\frac{1}{2}x\sqrt{-\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$

$$u(0) = u_0$$

Evaluating this solution at $x = 0$ and using the boundary condition at $x = 0$, we rapidly find the final solution

$$u(x) = u_0 \exp\left(\frac{v_0}{2D_0}x\right) \exp\left(-\frac{1}{2}x\sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$

in Fig. 2.10

A plot of this function appears below.

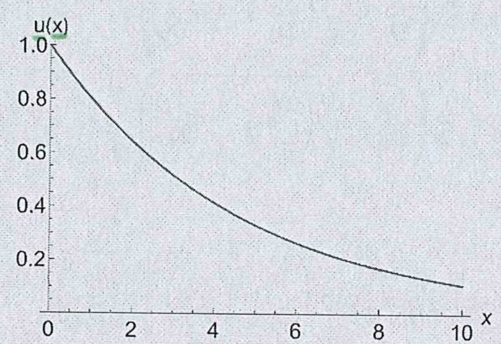

Fig. 2.10: Plot of solution, $u(x)$

The last part of the question asks for the distance at which the carbon content becomes acceptable, i.e., less than 0.05 mg/L. We can determine this by setting

that is,

$$\frac{u(x)}{u_0} = \exp\left(\frac{v_0}{2D_0}x - \frac{1}{2}x\sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$

Or, taking the natural log of both sides

$$\ln\left(\frac{u(x)}{u_0}\right) = \left(\frac{v_0}{2D_0}x - \frac{1}{2}x\sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)$$

Solving for x gives

$$x = \ln\left(\frac{u(x)}{u_0}\right)\left(\frac{v_0}{2D_0} - \frac{1}{2}\sqrt{\left(\frac{v_0}{D_0}\right)^2 + 4\frac{k_1}{D_0}}\right)^{-1}$$

And, substituting in the parameter values from above, we have the solution

$$x = \ln\left(\frac{0.05}{2}\right)\left(\frac{1.2\,km/h}{2\times 0.7\,km^2/h} - \frac{1}{2}\sqrt{\left(\frac{1.2\,km/h}{0.7\,km^2/h}\right)^2 + 4\frac{0.5\,h^{-1}}{0.7\,km^2/h}}\right)^{-1}$$

$$x = 16.62\,km$$

2.3.3.2 Case 2: The roots are real, but not distinct

This is the case where the terms in the radical of the characteristic equation $s^2 + bs + c = 0$, is zero. Or, equivalently, we have that $b^2 = 4c$, so that the only root is $s = -b/2$. This presents a little bit of a problem, because we know that we need *two independent* equations to form the general solution to a second-order ODE.

The resolution to this problem is to find a second solution. Recall, the way that we found the exponential solutions to begin with was somewhat empirical; we thought about what kinds of functions could possibly be combined in a way that the archetype for a second-order homogeneous ODE might possibly be valid. The exponential was a candidate that turned out to work. We do know that the first solution generates exponentials of the form $y_1(x) = \alpha e^{-b/2x}$. Lacking any definite direction, we might hope that our second solution could be one that is proportional to this first solution. For example, we could suggest

$$y_2(x) = f(x)e^{-b/2x}$$

And hope that this works. Well, to be quite honest, this is roughly how the process unfolded. If we are guessing a functions that might work for $f(x)$, we might try the simplest thing we can think of.

$$y_2(x) = xe^{-b/2x}$$

Of course, this suggestion wouldn't have been made if it wasn't going to work. To see that it does, we need only take some derivatives

$$
\begin{aligned}
y_2(x) &= xe^{-xb/2} \\
y_2'(x) &= e^{-xb/2} - x\frac{b}{2}e^{-xb/2} \\
y_2''(x) &= -\frac{b}{2}e^{-xb/2} - \frac{b}{2}e^{-xb/2} + x\left(\frac{b}{2}\right)^2 e^{-xb/2} \\
&= -be^{-xb/2} + x\frac{b^2}{4}e^{-xb/2}
\end{aligned}
$$

Now, substitute this into

$$\frac{d^2y}{dx^2} + b\frac{dy}{dx} + cy = 0 \tag{2.132}$$

To give

$$-be^{-b/2x} + x\frac{b^2}{4}e^{-b/2x} + be^{-b/2x} - x\frac{b^2}{2}e^{-b/2x} + cxe^{-b/2x} = 0$$

And, after simplifying, this is

$$\left[-\frac{b^2}{4} + c\right] xe^{-b/2x} = 0$$

Finally, recalling that for this case we have $b^2 = 4c \Rightarrow -b^2/4 + c = 0$, we have proved that y_2 is a solution.

Example 2.11 (Case 2 Example). Consider the following steady diffusion problem

$$
\begin{aligned}
D\frac{d^2u}{dx^2} &= 0 \\
u(0) &= u_0 \quad \text{(This is a specified concentration boundary condition)} \\
-D\left.\frac{du}{dx}\right|_{x=L} &= 0 \quad \text{(This is a } \textit{no-flux} \text{ boundary condition)}
\end{aligned}
$$

Show that this solution is a special case of the general solution for Case 2.

Solution. For this example, we have $a = 1$ and $b = c = 0$. Therefore the only roots of the characteristic equation are $s_1 = s_2 = 0$. This is a repeated root (even though it is zero), meaning that the general solution is

$$
\begin{aligned}
u(x) &= \alpha e^0 + \beta x e^0 \\
&= \alpha + \beta x
\end{aligned}
$$

Note that this solution is actually a line, which is indeed a special case of the general exponential solution. Using the two boundary conditions, we have

$$
\begin{aligned}
u_0 &= \alpha \\
0 &= \beta
\end{aligned}
$$

Thus, our final solution is

$$u(x) = u_0 \text{ (a constant)}$$

2.3.3.3 Case 3: The roots are complex conjugates

For this case, the characteristic equation $(s^2 + bx + c)$ is such that $b^2 - 4c < 0$; therefore, one is faced with complex roots coming from the quadratic equation, ~~i.e.,~~ that is,

$$
\begin{aligned}
s_1 &= -\frac{b}{2} + \frac{1}{2}\sqrt{b^2 - 4c} \\
s_2 &= -\frac{b}{2} - \frac{1}{2}\sqrt{b^2 - 4c}
\end{aligned}
$$

Because $b^2 - 4c < 0$, the radical generates an imaginary number. For convenience, set $u = -b/2$ and $i\lambda = 1/2\sqrt{b^2 - 4c}$. Then, the two roots can be put in the form

$$
\begin{aligned}
s_1 &= \mu + i\lambda \\
s_2 &= \mu - i\lambda
\end{aligned}
$$

which is a complex conjugate pair $(s_1 = \overline{s_2})$. Our general solution is, therefore

$$
\begin{aligned}
y(x) &= \alpha e^{\mu x + i\lambda x} + \beta e^{\mu x - i\lambda x} \\
&= e^{\mu x}\left(\alpha e^{i\lambda x} + \beta e^{-i\lambda x}\right)
\end{aligned}
\tag{2.133}
$$

Recalling Euler's identity, we can write the two independent solutions as

$$
\begin{aligned}
y_1(x) &= e^{\mu x} e^{ix} = e^{\mu x}\left[\cos(\lambda x) + i\sin(\lambda x)\right] \\
y_2(x) &= e^{\mu x} e^{-ix} = e^{\mu x}\left[\cos(\lambda x) - i\sin(\lambda x)\right]
\end{aligned}
$$

Now, if we were satisfied with solutions that, in general, contained complex numbers (and, in some cases, such as quantum mechanics, we might very well be!), then we would be done. However, for the vast majority of problems in science and engineering, the problems are such that we expect a real number as an answer. This is actually no problem. We can, if we like, construct two new solutions from the existing one by creating linear combinations of them. Recall, that when we make linear combinations, we can multiply either of the two equations by any constant we like- including complex numbers. Suppose, then, that we construct two new independent solutions as follows

$$
\begin{aligned}
y_A(x) &= e^{\mu x}\frac{1}{2}\left[y_1(x)+y_2(x)\right] \\
&= e^{\mu x}\frac{1}{2}\left[(\cos(\lambda x)+i\sin(\lambda x))+(\cos(\lambda x)-i\sin(\lambda x))\right] \\
&= e^{\mu x}\frac{1}{2}(2\cos(\lambda x)) \\
&= e^{\mu x}\cos(\lambda x)
\end{aligned}
$$

and

$$
\begin{aligned}
y_B(x) &= e^{\mu x}\frac{i}{2}\left[y_1(x)-y_2(x)\right] \\
&= -e^{\mu x}\frac{i}{2}\left[(\cos(\lambda x)+i\sin(\lambda x))-(\cos(\lambda x)-i\sin(\lambda x))\right] \\
&= -e^{\mu x}\frac{i}{2}(2i\sin(\lambda x)) \\
&= e^{\mu x}\sin(\lambda x)
\end{aligned}
$$

With a little thought, we might have realized this from the start. Our two independent solutions can be considered to be either $e^{\mu x}\sin x$ and $e^{\mu x}\cos x$ or $e^{\mu x}e^{ix}$ and $e^{\mu x}e^{-ix}$. It actually makes no difference mathematically- one set of solutions can always be constructed from the other. However, for applications where we desire solutions that are real functions (rather than complex functions), we are better off using the trigonometric solutions. Thus, we can take our general solution to be in this case

$$
\begin{aligned}
y(x) &= \alpha y_A(x)+\beta y_B(x) \\
&= \alpha e^{\mu x}\cos(\lambda x)+\beta e^{\mu x}\sin(\lambda x)
\end{aligned}
$$

Or, factoring out the exponential

$$
y(x) = e^{\mu x}(\alpha\cos(\lambda x)+\beta\sin(\lambda x)) \tag{2.134}
$$

Example 2.12 (Harmonic Oscillator). *Harmonic oscillator* is just a very complicated term for describing something that bounces periodically. This could be the pendulum of a clock, a weight on a spring, or the CEO of Pfizer (slogan: "Pfizer Quality!") inexplicably bouncing on a trampoline in the Mojave Desert on a moonless Wednesday night in late August. Suppose we have the weight on a spring version (sorry). Initially, the spring is pulled by the amount 10 *cm*. Suppose the weight has a mass of 1*kg*, and the spring constant for the spring is $K = 3\ N/cm$. Assume that the system is ideal so that it does not ever lose energy (which, admittedly, is impossible; but, it is often very close to reality for short periods of time!). What is the function defining the oscillations of the weight? Assume that the motion takes place on a frictionless horizontal plane (say, on an air hockey table) so that you do not need to worry about gravity.

Au: Fig. 2.11 not called out in the text

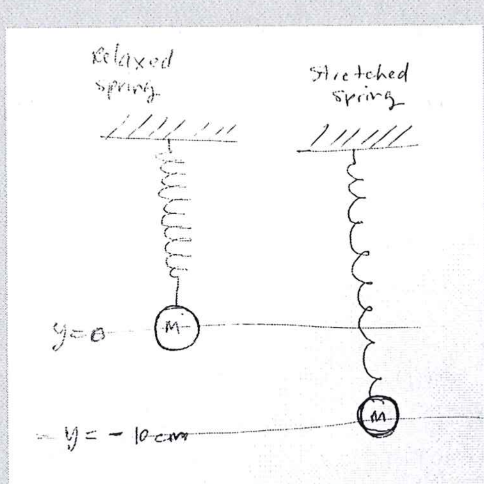

Fig. 2.11: A weight on a spring, with motion in the horizontal plane. On an air hockey table.

Solution. A simple force balance on the mass just as it is let go is as follows

$$m\frac{dv}{dt} = K\Delta y$$

where dv/dt is the acceleration (time rate of change of velocity), g is the gravitational constant ($9.81\, m/s^2$), and Δy is the initial displacement $\Delta y = 0-(-10)\ cm = 10\ cm$. Because the equilibrium position is $y(0)=0$, we have that $\Delta y = -y(t)$. Recall that $v(t) = dy/dt$. With this in mind, our force balance can be written (with two ancillary conditions based on the physical system) as follows:

$$\frac{d^2y}{dt^2} + \frac{K}{m}y(t) = 0$$

condition 1	$y(0) = -10$	initial position at y=-10 cm
condition 2	$y'(0) = 0$	zero initial velocity

The characteristic equation for this problem is $s^2 + K/m = 0$ ($a=1$, $b=0$, $c=K/m$). Thus the two roots are

$$s_1 = 0 + \frac{1}{2}\sqrt{-4\frac{K}{m}} = i\sqrt{\frac{K}{m}}$$

$$s_2 = 0 - \frac{1}{2}\sqrt{-4\frac{K}{m}} = -i\sqrt{\frac{K}{m}}$$

Using the notation established above, we have $\mu = 0$ and $\lambda = \sqrt{K/m}$. Therefore, the solution that we want is

$$y(t) = e^0 \left(\alpha \cos(t\sqrt{K/m}) + \beta \sin(t\sqrt{K/m}) \right)$$

Taking the derivative (for use with the second ancillary condition)

$$y'(t) = \left(-\sqrt{K/m}\alpha \sin(t\sqrt{K/m}) + \sqrt{K/m}\beta \cos(t\sqrt{K/m}) \right)$$

Using the two ancillary conditions, we have

$$-10 = \alpha \cos(0) + \beta \sin(0) \Rightarrow \alpha = -10$$
$$0 = -\sqrt{K/m}\alpha \sin(0) + \sqrt{K/m}\beta \cos(0) \Rightarrow \beta = 0$$

So, our solution is

$$y(t) = -10\cos(t\sqrt{K/m}) \quad (2.135)$$

Does this solution make sense? We can check. First of all, we should check to see if the initial conditions (the two ancillary conditions) are met. Note: $y'(x) = -10\sqrt{K/m}\sin(t\sqrt{K/m})$.

$$y(0) = -10\cos(0)$$
$$y'(0) = -10\sqrt{K/m}\sin(0) = 0$$

So, yes, our solution does meet the initial conditions. It is easy to verify that it also meets the ODE (take derivatives, and substitute back into the original ODE). A plot of the oscillations for $0 < t < 60$ s is given ~~below~~. in Fig. 2.12.

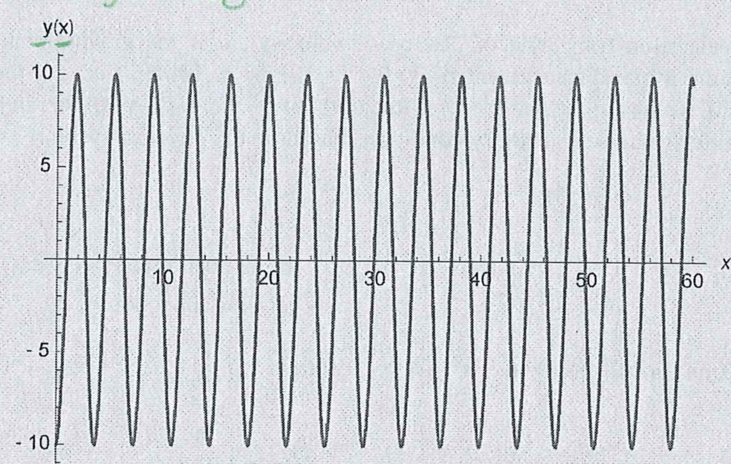

Fig. 2.12: Plot of solution for the weight on a spring.

2.3.4 Nonhomogeneous Solutions for Second-Order ODEs with Constant Coefficients

We will study only one approach for nonhomogeneous second-order ODEs. In particular, we are getting around to solving the problem given by

$$\frac{d^2y}{dx^2} + b\frac{dy}{dx} + cy(x) = g(x) \tag{2.136}$$

As a matter of notation, we call any solution to this problem a *particular* solution, $y_p(x)$.

The method that we are going to use is called *variation of parameters*, and it was developed by two somewhat famous mathematicians: Leonard Euler (of Euler identity fame), and Joseph-Louis Lagrange. The basic idea behind the method is as follows. Suppose we have the two solutions to the homogeneous second-order equation

$$\frac{d^2y}{dx^2} + b\frac{dy}{dx} + cy(x) = 0 \tag{2.137}$$

We call the general solution to this problem the *homogeneous* solution. Because we will make use of $y(x)$ to indicate the solution to Eq. (2.136), we will use $y_h(x)$ to indicate the homogeneous solution

$$y_h(x) = \alpha y_1(x) + \beta y_2(x)$$

Recall that we previously defined the operator notation for general second-order ODEs to be

$$L = \frac{d^2}{dx^2} + b\frac{d}{dx} + c = 0 \tag{2.138}$$

so that $L[y_h] = 0$ gives us Eq. (2.137). This is really nothing but a shorthand notation. So, now we consider the problem $L[y_p] = g(x)$ the nonhomogeneous problem. There are an infinite number of particular solutions, y_p. To see this, suppose we have *any* particular solution to Eq. (2.136). We need only examine the sum

$$\begin{aligned} y(x) &= y_p(x) + \gamma y_h(x) \\ &= y_p(x) + \alpha y_1(x) + \beta y_2(x) \end{aligned}$$

where γ is a constant. Then note

$$L[y(x)] = L[y_p(x)] + \gamma L[y_h(x)]$$

But, by definition $L[y_h] = L[\alpha y_1(x) + \beta y_2(x)] = 0$, and $L[y_p] = g(x)$, so

$$L[y(x)] = g(x)$$

So, if we have any particular solution, we can always add any multiple of the homogeneous solution, and we have a new solution. The specific reason that we might need to add in the homogeneous solution is that the particular solution that we find might not meet the necessary ancillary conditions. However, we know we can find specific values of α and β in the homogeneous solution to meet the possible boundary conditions. Thus, we can use the added homogeneous solution as a way of adjusting our particular solution so that it meets the necessary boundary conditions.

The technique of variation of parameters can be explained in terms of the theory of Green's functions, but we will not be taking that approach here (for one thing, this requires some understanding of distribution theory). Alternatively, let's think about the properties of the solution that we seek, $y(x)$. Clearly $y(x)$ cannot be a constant multiple of either $y_1(x)$ or $y_2(x)$, because then it would be a solution to the homogeneous equation. In other words, we realize that

$$\frac{y(x)}{y_1(x)} \neq C_1 \qquad \frac{y(x)}{y_2(x)} \neq C_2$$

where C_1 and C_2 are constants. The argument at this juncture seems ridiculously trivial. If the ratios above cannot be equal to constants, then they must be equal to functions. Specifically, functions of x, since that is the only independent variable we are considering. Thus we argue

$$\frac{y(x)}{y_1(x)} = u_1(x) \qquad \frac{y(x)}{y_2(x)} = u_2(x)$$

For some (currently unknown) functions u_1 and u_2. This is equivalent to stating that a solution for $y_p(x)$ must be of the form

$$y_p(x) = u_1(x)y_1(x) + u_2(x)y_2(x)$$

Now, if you really think about it, at this juncture we haven't really done much. In fact, if we have any three bounded and continuous functions f, g, and h, it is not difficult to show that we can always find two functions u_1 and u_2 such that $h = u_1 f + u_2 g$. The real brilliance of Eq. (2.3.4) is that we already know that $L[y_1] = L[y_2] = 0$. So, working with Eq. (2.3.4) to find the functions u_1 and u_2 is going to be made much simpler by this fact. This becomes clearer when we actually try to do this. We are looking for the solution

Au: No such equation no.

$$L[y_p] = g(x)$$

or, substituting

$$L[u_1(x)y_1(x) + u_2(x)y_2(x)] = g(x)$$

Or, writing this all out more painfully

$$\frac{d^2}{dy^2}[u_1y_1 + u_2y_2] + b\frac{d}{dy}[u_1y_1 + u_2y_2] + c[u_1y_1 + u_2y_2] = g(x) \tag{2.139}$$

Let's start by noting

$$\frac{d}{dy}[u_1(x)y_1(x)] = u_1'y_1 + u_1y_1'$$
$$\frac{d}{dy}[u_2(x)y_2(x)] = u_2'y_2 + u_2y_2'$$

so that

cap/

$$\frac{d}{dy}[u_1(x)y_1(x)+u_2(x)y_2(x)] = u_1'y_1+u_1y_1'+u_2'y_2+u_2y_2'$$
$$= (u_1'y_1+u_2'y_2)+(u_1y_1'+u_2y_2')$$

and

$$\frac{d^2}{dy^2}[u_1y_1+u_2y_2] = \frac{d}{dy}[(u_1'y_1+u_2'y_2)+(u_1y_1'+u_2y_2')]$$
$$= (u_1'y_1+u_2'y_2)'+u_1'y_1'+u_1y_1''+u_2'y_2'+u_2y_2''$$

Substituting these results back into Eq. (2.139), we have

$$(u_1'y_1+u_2'y_2)'+u_1'y_1'+u_1y_1''+u_2'y_2'+u_2y_2''$$
$$+b[(u_1'y_1+u_2'y_2)+(u_1y_1'+u_2y_2')]$$
$$+c[u_1y_1+u_2y_2] = g(x)$$

From here, we collect all of the terms that are multiplied by u_1 or u_2. This result is

$$u_1(y_1''+by_1'+cy_1)+u_2(y_2''+by_2'+cy_2)$$
$$+u_1'y_1'++u_2'y_2'$$
$$+b(u_1'y_1+u_2'y_2)$$
$$+(u_1'y_1+u_2'y_2)' = g(x)$$

This simplified immediately because y_1 and y_2 are solutions to the homogeneous problem $y''+by'+cy=0$, leaving us with

$$u_1'y_1'++u_2'y_2'+b(u_1'y_1+u_2'y_2)+(u_1'y_1+u_2'y_2)' = g(x)$$

At this juncture, we have one equation but two unknown functions u_1 and u_2. This kind of a problem has an infinite number of solutions; we only need one solution, and any particular solution will do. So, we are free to add any additional equation that we like (as long as it is independent) to make our system solvable. A particularly convenient requirement is to set $u_1'y_1+u_2'y_2=0$; you can see that doing so is reasonably clever because it eliminates *two* groups of terms in the equation above! In summary, then, we have the two equations

$$u_1'y_1+u_2'y_2 = 0$$
$$u_1'y_1'++u_2'y_2' = g(x)$$

are/ which ~~is~~ two equations in the uknowns u_1' and u_2'. In fact, we can arrange this in a matrix

$$\begin{bmatrix} y_1 & y_2 \\ y'_1 & y'_2 \end{bmatrix}\begin{bmatrix} u'_1 \\ u'_2 \end{bmatrix} = \begin{bmatrix} 0 \\ g(x) \end{bmatrix}$$

and then use Cramer's rule to solve for u_1' and u_2'. First note that

$$\begin{vmatrix} y_1 & y_2 \\ y'_1 & y'_2 \end{vmatrix} = y_1 y'_2 - y_2 y'_1$$

So, Cramer's rule gives us

$$\frac{du_1}{dx} = \frac{1}{y_1 y'_2 - y_2 y'_1} \begin{vmatrix} 0 & y_2 \\ g(x) & y'_2 \end{vmatrix} \qquad \frac{du_2}{dx} = \frac{1}{y_1 y'_2 - y_2 y'_1} \begin{vmatrix} y_1 & 0 \\ y'_1 & g(x) \end{vmatrix}$$

or

$$\frac{du_1}{dx} = \frac{-y_2 g(x)}{y_1 y'_2 - y_2 y'_1} \qquad \frac{du_2}{dx} = \frac{y_1 g(x)}{y_1 y'_2 - y_2 y'_1}$$

Although not essential, we can put this in integral form by integrating both sides of this expression with respect to x. Note that because we are looking for *any* particular solution, we can discard any constants of integraiton generated at this point.

$$u_1(x) = \int_x \frac{-y_2 g(x)}{y_1 y'_2 - y_2 y'_1} dx \qquad u_2(x) = \int_x \frac{y_1 g(x)}{y_1 y'_2 - y_2 y'_1} dx$$

This completes our solution. However, to summarize, recall that the two solutions above allow us to generate the following particular solution

$$y_p(x) = u_1(x) y_1(x) + u_2(x) y_2(x)$$

To this particular solution we must add the general form of the homogeneous solution to get our final solution for the nonhomogeneous equation

$$y(x) = y_p(x) + y_h(x)$$

or

$$y(x) = y_p(x) + \alpha y_1(x) + \beta y_2(x)$$

This last step is crucial! Without the addition of the homogeneous solution, we do not have two free constants to specify via two ancillary conditions. As a reminder, because $L[y_h] = 0$, adding the homogeneous solution means that we still meet the nonhomogeneous second order ODE

$$\frac{d^2y}{dx^2} + b\frac{dy}{dx} + cy(x) = g(x)$$

because adding the homogeneous solution does nothing but add zero to this ODE! An example is helpful here.

Example 2.13 (Solution for a nonhomogeneous second-order ODE). The previous example of a harmonic oscillator is an interesting one to use for this example, in part because we already have the homogeneous solution. A *forced* harmonic oscillator is one that is forced to oscillate at a frequency different from its *natural* frequency. Consider the system on the air hockey table described in the previous example. Suppose our weight is made of magnetic material, and we put a giant electromagnetic array under the table that can create a magnetic force which fluctuates in time according to

$$g(x) = -10\cos(10t)$$

This is different from the natural frequency that we found above that was equal to $-10\cos(\sqrt{K/mt}) = -10\cos(\sqrt{3}t)$. What happens when we do this? The system of equations that we want to solve is now

$$\frac{d^2y}{dt^2} + \frac{K}{m}y(t) = -10\cos(10t)$$

condition 1	$y(0) = -10$	initial position at $y = 10$ cm
condition 2	$y'(0) = 0$	zero initial velocity

Recall our homogeneous solution for this case was

$$y(t) = \alpha\cos(t\sqrt{K/m}) + \beta\sin(t\sqrt{K/m})$$

Note that here we have $y_1(t) = \cos(t\sqrt{K/m})$, $y_2(t) = \sin(t\sqrt{K/m})$. Following the example above, we are now seeking a solution to the nonhomogenous problem of the form

$$y_p(t) = u_1(t)\cos(t\sqrt{K/m}) + u_2(t)\sin(t\sqrt{K/m})$$

To find this solution, we need the functions y_1, y_2, y_1', y_2' and $g(t)$. It is also handy to have the combination $y_1y_2' - y_2y_1'$.

$$\begin{aligned}
y_1 &= \cos(t\sqrt{K/m})\\
y_2 &= \sin(t\sqrt{K/m})\\
y_1' &= -\sqrt{K/m}\sin(t\sqrt{K/m})\\
y_2' &= \sqrt{K/m}\cos(t\sqrt{K/m})\\
y_1y_2' - y_2y_1' &= \sqrt{K/m}\cos^2(t\sqrt{K/m}) + \sqrt{K/m}\sin^2(t\sqrt{K/m}) = \sqrt{K/m}\\
g(t) &= -10\cos(10t)
\end{aligned}$$

At this juncture, the solution is a bunch of busy work

$$\frac{du_1}{dt} = \frac{10\sin(t\sqrt{K/m})\cos(10t)}{\sqrt{K/m}}$$
$$\frac{du_2}{dt} = \frac{-10\cos(t\sqrt{K/m})\cos(10t)}{\sqrt{K/m}}$$

These can be integrated using standard trigonometric techniques, or by looking the integrals up on a table. The results are

$$u_1(t) = 10\sqrt{\frac{K}{m}}\left(-\frac{\cos\left(t\left(\sqrt{\frac{K}{m}}-10\right)\right)}{2\left(\sqrt{\frac{K}{m}}-10\right)} - \frac{\cos\left(t\left(\sqrt{\frac{K}{m}}+10\right)\right)}{2\left(\sqrt{\frac{K}{m}}+10\right)}\right)$$
$$u_2(t) = -10\sqrt{\frac{K}{m}}\left(\frac{\sin\left(t\left(\sqrt{\frac{K}{m}}-10\right)\right)}{2\left(\sqrt{\frac{K}{m}}-10\right)} + \frac{\sin\left(t\left(\sqrt{\frac{K}{m}}+10\right)\right)}{2\left(\sqrt{\frac{K}{m}}+10\right)}\right)$$

Well, worse things have happened. Recalling that $K/m = 3$ and simplifying, our final solution is

$$y(t) = \alpha\cos\left(\sqrt{3}t\right) + \beta\sin\left(\sqrt{3}t\right) + \frac{30}{97}\cos(10t)$$

and its derivative is

$$y'(t) = -\sqrt{3}\alpha\sin\left(\sqrt{3}t\right) + \sqrt{3}\beta\cos\left(\sqrt{3}t\right) - \frac{300}{97}\sin(10t)$$

From the first ancillary condition we have

$$-10 = \alpha\cos(0) + \frac{30}{97}\cos(0) \Rightarrow \alpha = -\frac{1000}{97}$$

From the second ancillary condition we have

$$0 = \sqrt{3}\beta\cos(0) \Rightarrow \beta = 0$$

Apparently, the solution we want is

$$y(t) = -\frac{1000}{97}\cos\left(\sqrt{3}t\right) + \frac{30}{97}\cos(10t)$$

Problems

Practice Problems

For the problems below, keep in mind that $y = y(x)$ is the *dependent* variable, and x is the *independent* variable. Note also that the choice of what we call the independent variable is not important. Thus, some problems might be posed in terms of other independent and dependent variables (e.g., $u(t)$ and t).

For the following problems, determine the *general* solution by separating variables. Also list the dependent variable in each case. Please solve explicitly for the dependent variable only if it is both possible, and does not require unusual effort (e.g., it would not be expected that you would solve for the roots of any polynomial solution beyond quadratic).

1. $\frac{dy}{dx} = \frac{x}{y}$
2. $\frac{2y}{y^2+1}\frac{dy}{dx} = \frac{1}{x^2}$
3. $\frac{dy}{dx} = \frac{y}{x}$
4. $\frac{dy}{dx} = \frac{\sin x - \cos x}{y^2+y}$
5. $(y^2-3)\frac{dy}{dx} = 1$
6. $(1+x^2)\frac{dy}{dx} = (1+y^2)$
7. $\frac{1+e^t}{1-e^{-y}}\frac{dy}{dt} + e^{t+y} = 0$
8. $\exp(t+y)\frac{dy}{dt} = \frac{t}{y}$, for $t > 0$, $y(t) > 0$
9. $z^3\frac{du}{dz} = \sqrt{z^2 - u^2z^2}$
10. $u'(t) = 4tu^2(t)$
11. $y'(t) = mc^2t^{\pi}y(t)$, where m and c are constants

For the following problems, determine the *general* solution by whatever method is required. If ancillary conditions are specified, then also find the *particular* solution for those conditions.

12. $\frac{dy}{dx} + \frac{1}{x^2}y = 0, x \in (0,1]$
13. $\frac{dy}{dt} + 2y = 4,\ y(0) = 0,\ x \in [0,2]$
14. $\frac{dy}{dx} - ay = f(x),\ x \in [a,b]$, where $f(x)$ is some integrable function. You will not be able to solve this explicitly! You will have to leave it in integral form.
15. $\frac{dy}{dz} = 2y + z,\ z \in [0,\infty]$
    $y'(0) = 1$
16. $y' + x^5y = x^5$
17. $y'(t) = y(t) + \frac{1}{1-e^{-t}}$
18. $\frac{dy}{dt} + y\cos t = \cos t,\ t \in [0,\infty], y(0) = 5$
19. $\frac{dy(t)}{dt} - y(t) - t\sin(t) = 0$

For the following problems, determine the *general* solution for the second order ODE.

20. $y''(t) - 5y'(t) - 14y(t) = 0$
21. $y''(x) - 25y(x) = 0$
22. $\frac{d^2y}{dx^2} + 2\frac{dy}{dx} - 24y = 0$
23. $\frac{d^2y}{dx^2} - 6\frac{dy}{dx} + 9y = 0$
24. $\frac{d^2y}{dx^2} + 10\frac{dy}{dx} + 25y = 0$
25. $\frac{d^2y}{dx^2} + 2\sqrt{2}\frac{dy}{dx} + 2y = 0$

26. $\frac{d^2y}{dx^2}+3\frac{dy}{dx}+3y=0$

27. $\frac{d^2y}{dx^2}+2\frac{dy}{dx}+5y=0$

28. $6\frac{d^2y}{dt^2}-4\frac{dy}{dt}=0$

29. $6\frac{d^2y(t)}{dt^2}-4y(t)=0$

For the following problems, determine the *particular* solution for the second order ODE and the two given ancillary conditions.

30. $\frac{d^2y}{dx^2}-2\frac{dy}{dx}-15y=0,\ y(0)=1,\ y'(0)=-1,$ $x\in[0,\infty]$

31. $\frac{d^2y}{dx^2}+16y=0,\quad y(0)=3,\quad y'(0)=12,$ $x\in[0,\infty]$

32. $\frac{d^2y}{dx^2}-10\frac{dy}{dx}+25y=0,\ y(0)=0,\ y(1)=0,$ $x\in[0,1]$

33. $4y''(t)-4y'(t)+y(t)=0,\quad y(0)=1,\ y'(0)=0,\ t\in[0,\infty]$

34. Show that if $y_1(x)$ and $y_2(x)$ are each solutions to the ODE

$$\frac{d^2y}{dx^2}+b\frac{dy}{dx}+cy=0$$

then, for any constants C_1 and C_2, the function $y(x)=C_1y_1(x)+C_2y_2(x)$ is also a solution. To start, substitute this last expression for $y(x)$ directly into the ODE. Group terms containing y_1 and terms containing y_2.

For the following problems, determine the solution for the *nonhomogeneous* second order ODE. If ancillary conditions are provided, solve the problem for the unknown coefficients.

35. $y''(t)-y(t)'-2y(t)=2e^{-t},\ y(0)=1,$ $y'(0)=0$

36. $\frac{d^2y}{dx^2}+2\frac{d^2y}{dx^2}+y=3e^{-t},\ y(0)=0,\ y'(0)=1$

37. $\frac{d^2y}{dx^2}-\frac{d^2y}{dx^2}+\frac{1}{4}y=4e^{t/2},\ y(0)=1,\ y'(0)=1$

Applied and More Challenging Problems

1. Repeat the skier problem (Example problem 2.2), but with the following modification. The net drag due to friction from both the interface with the snow and from air resistance will be accounted for by a term proportional to the velocity: $F_{drag}=-\alpha mv(t)$. Add this force into the force balance, and then re-solve the problem using $\alpha=1\ \mathrm{s}^{-1}$.

2. For this problem involving a CSTR with first-order reaction, determine how a sudden change in the influent concentration, y_{in} would be manifest in the CSTR given that it has an initial concentration equal to y_0.

   a. The mass balance and initial condition are given by the following:

$$\frac{dy}{dt}+(\frac{1}{\tau}+k)y=\frac{1}{\tau}y_{in} \tag{2.140}$$

$$y(t=0)=y_0 \tag{2.141}$$

Solve this problem for $y(t)$. You may find it helpful to make the substitution $\beta=(\frac{1}{\tau}+k)$ to simplify the analysis (and prevent mistakes from dealing with complex algebraic computations), but do not forget to convert back to the original variables if you do so.

Au: Text missing here?

b. For the conditions

3. Catalysts are sometimes subject to degradation. This can be for many reasons. Some examples include thermal degradation, poisoning by other reactive chemicals (that changing the oxidation state of catalytic site or bind to the site irreversibly), and fouling by components in the treatment stream (physically altering the catalyst).

Au: open parenthesis missing?

Suppose we have the catalytic reaction $A \xrightarrow{C} B$), where species A is converted to species B in the presence of the active catalyst sites, represented by species C. Assume that the catalysts is being degrades due to the reaction process occurring at a low pH.
We can model a catalytic reaction by creating balances for both the catalyst (y_C) and the chemical being catalysed (A). A possible set of balances for catalytic degradation during the production of the three chemical species (reactant A, product B, and catalyst C) is as follows.

$$\frac{dy_C(t)}{dt} = -k_C y_C(t) \tag{2.142}$$

$$y_C(0) = C_0 \tag{2.143}$$

$$\frac{dy_A(t)}{dt} = -k_A y_A(t) y_C(t) \tag{2.144}$$

$$y_A(0) = A_0 \tag{2.145}$$

$$\frac{dy_B(t)}{dt} = k_B y_A(t) y_C(t) \tag{2.146}$$

$$y_B(0) = B_0 \tag{2.147}$$

We can solve this problem in a step-wise fashion. First, note that the balance for the catalyst, C, does not depend at all on the concentrations of the other two species. Thus, an explicit expression for the concentration $y_C(t)$ is straightforward to evaluate. For the problem, do the following.

a. Solve the balance for the catalyst to determine an expression for $y_C(t)$.
b. Substitute your expression for $y_C(t)$ into the right-hand side of the balance for species A. Solve this expression for $y_A(t)$.
c. With the solution for $y_A(t)$ and $y_C(t)$ determined, the final step is to substitute these into the right-hand side of the balance for species B. Solve the resulting expression for $y_B(t)$. You will probably want to use a symbolic integration software like Mathematica to compute the associated integral.
d. Plot the resulting function on the interval $0 \le t \le 20$ min for the following list of constants. To help make the graph easier to view, plot the normalized values y_A/A_0, y_B/A_0, and y_C/C_0.

$$k_A = 0.2 \text{ min}^{-1} \qquad A_0 = 10 \text{ mmol/L} \tag{2.148}$$

$$k_B = 0.3 \text{ min}^{-1} \qquad B_0 = 0 \text{ mmol/L} \tag{2.149}$$

$$k_C = 0.25 \text{ min}^{-1} \qquad C_0 = 1 \text{ mmol/L} \tag{2.150}$$

4. Sometimes problems are separable, but the resulting solution is *implicit* in the dependent variable. As an example, consider the following problem for degradation of a chemical species by enzyme kinetics in a batch reactor. If Michaelis-Menten type kinetics apply, an initial value problem for a well-stirred batch system can be stated by

$$\frac{dy}{dt} = -\mu \frac{y}{y+K} \tag{2.151}$$

$$y(0) = y_0 \tag{2.152}$$

where y is the concentration of the chemical species (mass/volume), k is the reaction rate parameter (mass/time) and K is the half saturation constant (mass/volume). For this problem, do the following.

a. Solve the problem by simple separation of variables. Include the initial condition by either solving using definite integration, or by evaluating the constant of integration from the initial condition if indefinite integration is used.

b. The result is explicit in the variable t, but implicit in the variable y. Suppose we have $y_0 = 20$ mmol/L, $\mu = 0.1$ mmol·s^{-1}, and $K = 8$ mmol/L. Suppose you wanted to solve the equation for values of the concentration between $0 \le y \le 20$, for the time period of approximately $0 \le t \le 50$ s. How could you do this? *Hint. Try reversing the roles of the dependent and independent variables, treating time as if it were the dependent variable.*

c. Make a plot of your results using whatever plotting software is convenient for you. If you use Mathematica, you may find the plotting command `ParametricPlot` useful. You can read about how to use that in the help pages for Mathematica.

in which /

5. Suppose we have a completely stirred reactor ~~that~~, because of a problem with the pump, the flow rate decreases in time. Specifically, assume

$$Q(t) = \frac{Q_0}{\alpha + \gamma t} \tag{2.153}$$

Assume that the initial condition is $y(0) = 0$. Where α and γ are parameters that control the decrease in flow rate over time. The revised mass balance equation can be taken for this case as

$$\frac{dy}{dt} = \frac{1}{\tau}\left(\frac{1}{\alpha+\beta t}\right) y_{in} - \frac{1}{\tau}\left(\frac{1}{\alpha+\beta t}\right) y(t) - ky(t) \tag{2.154}$$

a. Begin by rewriting this expression so that you have a single term on the left-hand side that can be associated with $P(t)$, and a single term on the right hand side associated with $Q(t)$. Separate from the ODE, write down the explicit functions representing $P(t)$ and Q(t).

b. Determine the integrating factor by first computing $s(t)$ from

$$s(t) = \int P(t)dt \tag{2.155}$$

Then, compute explicit expressions for $e^{s(t)}$ and $e^{-s(t)}$. You should need to use the logarithmic identity $a\ln(x) = \ln(x^a)$.

c. Finally, using Mathematica (or similar symbolic integration software), determine the result

$$y(t) = e^{-s(t)}\left[\int Q(t)e^{s(t)}dt + C_1\right] \tag{2.156}$$

Computing this integral is challenging, and will lead to a solution in terms of the Gamma function that was introduced earlier in the text. Note that in Mathematica, you will want to compute this

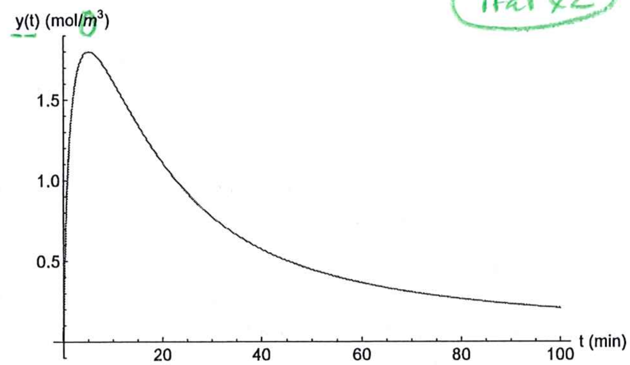

Fig. 2.13 Solution to Applied Problem 5.

integral by putting conditions on the constants and variables, as follows.

```
Integrate[Q(t), {t, 0, t}, Assumptions ->{{t, k, t} ∈ Reals && {t,
k, tau} ≥ 0}]
```

(where, here, you will substitute the appropriate expression for $Q(t)$).

d. Noting the initial condition $y(0) = 0$, find the appropriate value for C_1.

e. Finally, using the values $k = 0.1\ \text{min}^{-1}$ and $\tau = 0.5$ min, $a = 1$ min, and $b = 1$, plot the solution over the range $0 \le t \le 100$ min using whatever software is conveneint. Your solution should look like the plot in Fig. 2.13. Does the resulting function match your intuition about what should happen to the effluent concentration over time? Why or why not?

6. Dispersion is the spreading that occurs during chemical species transport resulting from the variations in the velocity field plus the effects of molecular diffusion. Sometimes for a plug flow reactor, one models the reactor without dispersion; the idea is that for plug flow reactors, this is one of the goals (to reduce spreading).

For this problem, assume we have a 1 m long plug flow reactor that catalyses a reactant A to a product B, and model the system at steady state both with and without the process of hydrodynamic dispersion. Suppose for now we are interested only in the concentration evolution of species A (the reactant). The problem is outlined as follows.
Without hydrodynamic dispersion, the steady state differential mass balance equation is given by the first order expression

$$-u_0 \frac{dy}{dx} = ky(x) \tag{2.157}$$

$$y(0) = y_0 \tag{2.158}$$

Including hydrodynamic dispersion, the steady state differential mass balance equation is given by the first order expression

$$
\begin{aligned}
D\frac{d^2y}{dx^2} - u_0\frac{dy}{dx} &= ky(x)\\
y(0) &= y_0\\
y'(L) &= 0
\end{aligned}
$$

(note, we need one additional ancillary (boundary) condition to determine the constants, because now the problem is second-order).

a. Solve these two problems. For each problem, begin by dividing through by whatever constant makes the coefficient of the *highest derivative* equal to 1. This step often makes problems a bit easier to think about. Please remember not to substitute any numeric values into the solution until the solution is complete.

b. Using $D = 1\times 10^{-9}\ \mathrm{m^2\,s^{-1}}$, $u_0 = 1\times 10^{-8}\ \mathrm{m\,s^{-1}}$, $k = 1\times 10^{-8}\ \mathrm{s^{-1}}$, and $y_0 = 100$ mmol/L, solve this problem over the interval $0 < x < L$, with $L = 1$ m. Plot the two solutions using whatever software is convenient.

c. How do the two solutions compare? Why do you think they are different from one another?

7. Steady state heat transport in a radiator fin, assuming that the fin is thin compared to its length, can be described by the following second-order ODE. Here, we are imposing boundary conditions at the left of a specified temperature ($y(0) = y_0 = 400$ K), and the right boundary as a zero gradient condition.

$$
\begin{aligned}
K\frac{d^2y}{dx^2} - \frac{h}{\ell}y &= -\frac{h}{\ell}y_\infty\\
y(0) &= y_0\\
\left.\frac{dy}{dx}\right|_{x=L} &= 0
\end{aligned}
$$

Physically, this equation represents the temperature, y, in the fin assuming that there is both heat conduction, and convective cooling by an external air source blowing over the radiator fin.
Assume the fin is $L = 0.1$ m long, with thermal conductivity $K = 385\ \mathrm{W\,m^{-1}K^{-1}}$, and with heat transfer coefficient $h = 150\mathrm{W\,m^{-2}K^{-1}}$. The thickness of the fin is $\ell = 0.002$ m. Assume the far-field temperature, y_∞ is 293 K. Solve this problem. Plot the solution over the domain and range $0 < x < L$ and $293 < T < 400$. Please remember not to substitute any numeric values into the solution until the solution is complete.