Tikrit University

College of Petroleum Processes Engineering

Petroleum Systems Control Engineering Department

Petroleum Systems Control

Lecture 2

"Mathematical Tools for Systems Modelling"

By

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Chapter 2

PART I

MODELING FOR PROCESS DYNAMICS

Notice the shape of the temperature response is the same as the shape of the concentration response that we saw previously. By appropriate modeling of the process, we can predict how the system will respond to changes in the operating conditions. Our ability to model the process will be extremely valuable as we design controllers to automatically control the process variables at their desired settings.

2.2 MATHEMATICAL TOOLS FOR MODELING

As we just saw in our analysis of the chemical mixer, the unsteady-state material and energy balance models that we wrote required us to solve differential equations to obtain the concentration and temperature versus time behavior for the process. This will be a common occurrence for us as we continue our studies of process dynamics and control. It would be beneficial to review some additional tools available to us for solving our process models. In Sec. 2.1, we solved the equations by separation and integration. A couple of other useful tools for solving such models are Laplace transforms and MATLAB/Simulink. In the next several sections, we will review the use of these additional tools for solving our model differential equations.

Definition of the Laplace Transform

The Laplace transform of a function $f(t)$ is *defined* to be $F(s)$ according to the equation

$$F(s) = \int_0^\infty f(t)e^{-st}\,dt \tag{2.5}$$

We often abbreviate this to

$$F(s) = L\{f(t)\}$$

where the operator L is defined by Eq. (2.5).

Example 2.1. Find the Laplace transform of the function

$$f(t) = 1$$

According to Eq. (2.5),

$$F(s) = \int_0^\infty (1)e^{-st}\,dt = -\frac{e^{-st}}{s}\bigg|_{t=0}^{t=\infty} = \frac{1}{s}$$

Thus,

$$L\{1\} = \frac{1}{s}$$

There are several facts worth noting at this point:

1. The Laplace transform $F(s)$ contains no information about the behavior of $f(t)$ for t, 0. This is not a limitation for control system study because t will represent the time variable and we will be interested in the behavior of systems only for positive time. In fact, the variables and systems are usually defined so that $f(t)$ 0 for t , 0. The time we designate as $t = 0$ is arbitrary. We shall generally define $t = 0$ as the time when the process is disturbed from steady state (i.e., when an input is changed). Our usual starting point will be a steady-state system or process, and we will be interested in examining what happens when the system is disturbed. This will become clearer as we study specific examples.

2. Since the Laplace transform is defined in Eq. (2.5) by an improper integral, it will not exist for every function $f(t)$. A rigorous definition of the class of functions possessing Laplace transforms is beyond the scope of this book, but readers will note that every function of interest to us *does* satisfy the requirements for possession of a transform [see Churchill (1972)].

3. The Laplace transform is linear. In mathematical notation, this means

$$L\{af_1(t) + bf_2(t)\} = aL\{f_1(t)\} + bL\{f_2(t)\}$$

where a and b are constants and f_1 and f_2 are two functions of t.

Proof. Using the definition, we have

$$\begin{aligned} L\{af_1(t) + bf_2(t)\} &= \int_0^\infty [af_1(t) + bf_2(t)]e^{-st}\,dt \\ &= a\int_0^\infty f_1(t)e^{-st}\,dt + b\int_0^\infty f_2(t)e^{-st}\,dt \\ &= aL\{f_1(t)\} + bL\{f_2(t)\} \end{aligned}$$

4. The Laplace transform operator transforms a function of the variable t to a function of the variable s. The t variable is eliminated by the integration.

Transforms of Simple Functions

We now proceed to derive the transforms of some simple and useful functions. We shall see these common functions repeatedly during our future studies.

1. The *step function* is

$$f(t) = \begin{cases} 0 & t < 0 \\ 1 & t > 0 \end{cases}$$

This important function is known as the unit-step function and will henceforth be denoted by $u(t)$. From Example 2.1, it is clear that

$$L\{u(t)\} = \frac{1}{s}$$

As expected, the behavior of the function for $t < 0$ has no effect on its Laplace transform. Note that as a consequence of linearity, the transform of any constant A, that is, $f(t) = Au(t)$, is just $F(s) = A/s$. Notice in the chemical mixing example that we just discussed that the inlet concentration and temperature are described by a step function initiated at time zero (3 P.M. in the example).

2. **The *exponential function* is**

$$f(t) = \begin{cases} 0 & t<0 \\ e^{-at} & t>0 \end{cases} = u(t)e^{-at}$$

where $u(t)$ is the unit-step function. Again proceeding according to definition, we have

$$L\left\{u(t)e^{-at}\right\} = \int_0^\infty e^{-(s+a)t}\,dt = -\frac{1}{s+a}e^{-(s+a)t}\bigg|_0^\infty = \frac{1}{s+a}$$

provided that $s + a > 0$, that is, $s > -a$. In this case, the convergence of the integral depends on a suitable choice of s. In case s is a complex number, it may be shown that this condition becomes

$$\mathrm{Re}(s) > -a$$

For problems of interest to us it will always be possible to choose s so that these conditions are satisfied, and the reader uninterested in mathematical niceties can ignore this point.

3. **The *ramp function* is**

$$f(t) = \begin{cases} 0 & t<0 \\ t & t>0 \end{cases} = tu(t)$$

$$L\{tu(t)\} = \int_0^\infty te^{-st}dt$$

Integration by parts yields

$$L\{tu(t)\} = -e^{-st}\left(\frac{t}{s} + \frac{1}{s^2}\right)\bigg|_0^\infty = \frac{1}{s^2}$$ Homework 1

4. **The *sine function* is**

$$f(t) = \begin{cases} 0 & t<0 \\ \sin kt & t>0 \end{cases} = u(t)\sin kt$$

$$L\{u(t)\sin kt\} = \int_0^\infty \sin kt\, e^{-st}\,dt$$

Integrating by parts, we have

$$L\{u(t)\sin kt\} = \frac{-e^{-st}}{s^2 + k^2}(s \sin kt + k \cos kt)\bigg|_0^\infty$$ Homework 2

$$= \frac{k}{s^2 + k^2}$$

TABLE 2.1

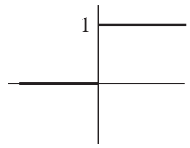
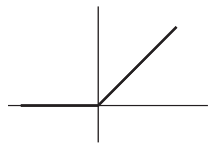
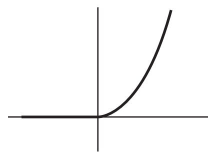
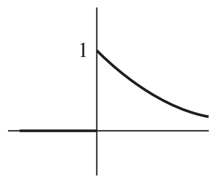
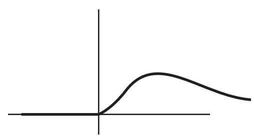
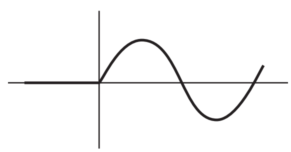
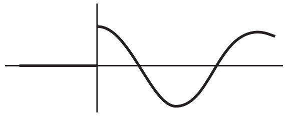
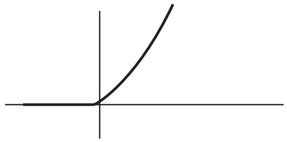
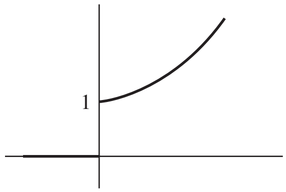
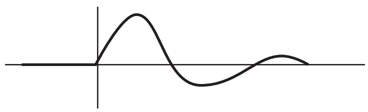
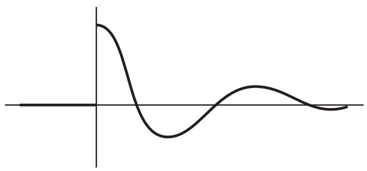
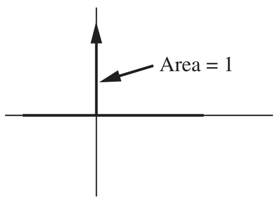
Function	Graph	Transform
$u(t)$		$\frac{1}{s}$
$tu(t)$		$\frac{1}{s^2}$
$t^n u(t)$		$\frac{n!}{s^{n+1}}$
$e^{-at}u(t)$		$\frac{1}{s+a}$
$t^n e^{-at}u(t)$		$\frac{n!}{(s+a)^{n+1}}$
$\sin kt\, u(t)$		$\frac{k}{s^2+k^2}$

TABLE 2.1 ***(Continued)***

Function	Graph	Transform
$\cos kt\, u(t)$		$\dfrac{s}{s^2 + k^2}$
$\sinh kt\, u(t)$		$\dfrac{k}{s^2 - k^2}$
$\cosh kt\, u(t)$		$\dfrac{s}{s^2 - k^2}$
$e^{-at} \sin kt\, u(t)$		$\dfrac{k}{(s + a)^2 + k^2}$
$e^{-at} \cos kt\, u(t)$		$\dfrac{s + a}{(s + a)^2 + k^2}$
$\delta(t)$, unit impulse		1

In a like manner, the transforms of other simple functions may be derived. Table 2.1 is a summary of transforms that will be of use to us. Those which have not been derived here can be easily established by direct integration, except for the transform of $\delta(t)$, which will be discussed in detail in the Appendix at the end of Chap. 3.

Using MATLAB for Symbolic Processing—Laplace Transforms

MATLAB is capable of symbolic processing. To prepare MATLAB for symbolic operations, some variable names will be declared symbolic (rather than numeric) using the `syms` command.

```
syms a x y z t k s
```

We can also define *u* as the Heaviside function (the unit step):

```
u=sym('Heaviside(t)')
u=
Heaviside(t)
```

Now we can determine the transform of the simple functions we have just discussed:
The step function:

```
laplace(u)
ans=
1/s
```

The exponential function:

```
laplace(exp(-a*t))
ans=
1/(s+a)
```

The ramp function:

```
laplace(t)
ans=
1/s^2
```

The sine function:

```
laplace(sin(k*t))
ans=
k/(s^2+k^2)
```

Transforms of Derivatives

At this point, the reader may wonder what has been gained by introduction of the Laplace transform. The transform merely changes a function of t into a function of s. The functions of s look no simpler than those of t and, as in the case of $A \rightarrow A/s$, may actually be more complex. In the next few paragraphs, the motivation will become clear. It will be shown that the Laplace transform has the remarkable property of transforming the operation of differentiation with respect to t to that of multiplication by s. Thus, we claim that

$$L\left\{\frac{df(t)}{dt}\right\} = sF(s) - f(0) \tag{2.6}$$

where

$$F(s) = L\{f(t)\}$$

and $f(0)$ is $f(t)$ evaluated at $t = 0$. If $f(t)$ is discontinuous at $t = 0$, $f(0)$ should be evaluated at $t = 0^+$, that is, just to the right of the origin. Since we will seldom want to differentiate functions that are discontinuous at the origin, this detail is not of great importance. However, the reader is cautioned to watch carefully for situations in which such discontinuities occur.

Proof

$$L\left\{\frac{df(t)}{dt}\right\} = \int_0^\infty \frac{df}{dt} e^{-st}\, dt$$

To integrate this by parts, let

$$u = e^{-st} \qquad dv = \frac{df}{dt}\, dt$$

Then

$$du = -se^{-st}\, dt \qquad v = f(t)$$

Since

$$\int u\, dv = uv - \int v\, du$$

we have

$$\int_0^\infty \frac{df}{dt} e^{-st}\, dt = f(t)e^{-st}\Big|_0^\infty + s\int_0^\infty f(t)e^{-st}\, dt = -f(0) + sF(s)$$

The salient feature of this transformation is that whereas the function of t was to be differentiated with respect to t, the corresponding function of s is merely multiplied by s. We shall find this feature to be extremely useful in the solution of differential equations.

To find the transform of the second derivative we make use of the transform of the first derivative twice, as follows:

$$\begin{aligned} L\left\{\frac{d^2 f}{dt^2}\right\} = L\left\{\frac{d}{dt}\left(\frac{df}{dt}\right)\right\} &= sL\left\{\frac{df}{dt}\right\} - \frac{df(t)}{dt}\bigg|_{t=0} \\ &= s[sF(s) - f(0)] - f'(0) \\ &= s^2F(s) - sf(0) - f'(0) \end{aligned}$$

where we have abbreviated

$$\boxed{\left.\frac{df(t)}{dt}\right|_{t=0} = f'(0)}$$

In a similar manner, the reader can easily establish by induction that repeated application of Eq. (2.6) leads to

$$L\left\{\frac{d^n f}{dt^n}\right\} = s^n F(s) - s^{n-1} f(0) - s^{n-2} f^{(1)}(0) - \cdots - sf^{(n-2)}(0) - f^{(n-1)}(0)$$

where $f^i(0)$ indicates the ith derivative of $f(t)$ with respect to t, evaluated for $t = 0$.

Thus, the Laplace transform may be seen to change the operation of differentiation of the function to that of multiplication of the transform by s, the number of multiplications corresponding to the number of differentiations. In addition, some polynomial terms involving the initial values of $f(t)$ and its first $n - 1$ derivatives are involved. In later applications we usually define our variables so that these polynomial terms will vanish. Hence, they are of secondary concern here.

Example 2.2. Find the Laplace transform of the function $x(t)$ that satisfies the differential equation and initial conditions

$$\frac{d^3x}{dt^3} + 4\frac{d^2x}{dt^2} + 5\frac{dx}{dt} + 2x = 2$$

$$x(0) = \frac{dx(0)}{dt} = \frac{d^2x(0)}{dt^2} = 0$$

It is permissible mathematically to take the Laplace transforms of both sides of a differential equation and equate them, since equality of functions implies equality of their transforms. Doing this, we obtain

$$s^3x(s) - s^2x(0) - sx'(0) - x''(0) + 4[s^2x(s) - sx(0) - x'(0)] \\ + 5[sx(s) - x(0)] + 2x(s) = \frac{2}{s}$$

where $x(s) = L\{x(t)\}$. Use has been made of the linearity property and of the fact that only positive values of t are of interest. Inserting the initial conditions and solving for $x(s)$, we have

$$x(s) = \frac{2}{s\left(s^3 + 4s^2 + 5s + 2\right)} \tag{2.7}$$

This is the required answer, the Laplace transform of $x(t)$.

2.3 SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS (ODEs)

There are two important points to note regarding this last example. First, application of the transformation resulted in an equation that was solved for the unknown function by *purely algebraic means.* Second, and most important, if the function $x(t)$, which has the Laplace transform $2/s(s^3 + 4s^2 + 5s + 2)$, were known, we would have the solution to the differential equation and initial conditions. This suggests a procedure for solving differential equations that is analogous to that of using logarithms to multiply or divide. To use logarithms, one transforms the pertinent numbers to their logarithms and then adds or subtracts, which is much easier than multiplying or dividing. The result of the addition or subtraction is the logarithm of the desired answer. The answer is found by reference to a table to find the number having this logarithm.

In the Laplace transform method for solution of differential equations, the functions are converted to their transforms, and the resulting equations are *algebraically* solved for the unknown function. This is much easier than solving a differential equation. However, at the last step the analogy to logarithms is not complete. We obviously cannot hope to construct a table containing the Laplace transform of every function $f(t)$ that possesses a transform. Instead, we will develop methods for expressing complicated transforms, such as $x(s)$ in Example 2.2, in terms of simple transforms that can be found in Table 2.1. For example, it is easily verified that the solution to the differential equation and initial conditions of Example 2.2 is

$$x(t) = 1 - 2te^{-t} - e^{-2t} \tag{2.8}$$

The Laplace transform of x, using Eq. (2.8) and Table 2.1, is

$$x(s) = \frac{1}{s} - 2\frac{1}{(s+1)^2} - \frac{1}{s+2} \tag{2.9}$$

Equation (2.7) is actually the result of placing Eq. (2.9) over a common denominator. Although it is difficult to find $x(t)$ from Eq. (2.7), Eq. (2.9) may be easily inverted to Eq. (2.8) by using Table 2.1. Therefore, what is required is a method for expanding the common-denominator form of Eq. (2.7) to the separated form of Eq. (2.9). This method is provided by the technique of partial fractions, which is developed in Chap. 3.

Using MATLAB for Symbolic Processing—Inversion of Laplace Transforms

Remember that we have previously declared some variables symbolic (a, k, x, y, z, t and s). Let's have MATLAB invert Eq. (2.3) for us and determine $x(t)$.

```
x=ilaplace(2/s/(s^3+4*s^2+5*s+2))
x=
1-exp(-2*t)-2*t*exp(-t)
```

which is the same as Eq. (2.8).

Using MATLAB for Symbolic Processing—Solution of Differential Equations

MATLAB can solve differential equations symbolically using the DSOLVE command. The derivatives are represented as Dx (first derivative), D2x (second derivative), etc.

```
x=dsolve('D3x+4*D2x+5*Dx+2*x=2','x(0)=0','Dx(0)=0','D2x(0)=0')
x=
1-exp(-2*t)-2*t*exp(-t)
```

same result

which, again, is the same as Eq. (2.8).

Now, let's return to our chemical mixing scenario from earlier in the chapter.

Example 2.3. Transform the differential equations resulting from the mass and energy balances for the chemical mixer to determine the transform of the exit concentration and temperature.

$$\tau \frac{dC_a}{dt} + C_a = C_{a3} \qquad \text{mass balance}$$

$$\tau \frac{dT}{dt} + T = T_3 + \left(\frac{1}{\rho v_3 C_p}\right) Q \qquad \text{energy balance}$$

For the mass balance,

$$\tau[sC_a(s) - C_a(0)] + C_a(s) = C_{a3}(s)$$

Rearranging and solving for $Ca(s)$, we have

$$C_a(s) = \frac{C_{a3}(s) + \tau C_a(0)}{\tau s + 1}$$

After the disturbance, C_{a3} has a constant value of 2 g/L. Therefore, C_{a3} (s) = 2/s. Also, from the process description, we know that $C_a(0)$ = 3g/L [this is the initial concentration of A in the tank at time 0 (3 P.M.)] and that τ, the time constant, is 5 min. Substituting these values into the expression for Ca yields

$$\boxed{C_a(s) = \frac{2/s + 5(3)}{5s + 1} = \frac{2}{s(5s + 1)} + \frac{15}{5s + 1}} \tag{2.10}$$

For the energy balance,

$$\tau[sT(s) - T(0)] + T(s) = T_3(s) + \frac{1}{\rho v_3 C_p} Q(s)$$

Rearranging and solving for $T(s)$, we find

$$T(s) = \frac{T_3(s) + \left[1/(\rho v_3 C_p)\right]Q(s) + \tau T(0)}{\tau s + 1}$$

After the disturbance, T_3 is constant at 35°C, so $T_3(s) = 35/s$. The initial temperature in the tank $T(0)$, at 3 P.M. is 80°C. The heater input Q is constant at 1.05×10^6 cal/min. The time constant τ is 5 min. Substituting these values into the expression for $T(s)$ gives

$$T(s) = \frac{\dfrac{35}{s} + \left(\dfrac{1}{\left(1000\,\dfrac{g}{L}\right)\left(30\,\dfrac{L}{\min}\right)\left(1\,\dfrac{\text{cal}}{g\cdot{}^\circ\text{C}}\right)}\right)\dfrac{\left(1.05 \times 10^6\,\dfrac{\text{cal}}{\min}\right)}{s} + 5(80)}{5s + 1}$$

Simplifying yields

$$\boxed{T(s) = \frac{70/s + 5(80)}{5s + 1} = \frac{70}{s(5s + 1)} + \frac{400}{5s + 1}} \tag{2.11}$$

If we can invert these expressions for $C_a(s)$, Eq. (2.10), and $T(s)$, Eq. (2.11), we will obtain the time domain solutions for the exiting concentration and temperature. We will address this topic in Chap. 3.

To summarize, we have reviewed a procedure using Laplace transforms for solving *linear, ordinary, differential equations (ODEs) with constant coefficients*.

The procedure is as follows:

1. Take the Laplace transform of both sides of the equation. The initial conditions are incorporated at this step in the transforms of the derivatives.
2. Solve the resulting equation for the Laplace transform of the unknown function algebraically.
3. Find the function of t that has the Laplace transform obtained in step 2. This function satisfies the differential equation and initial conditions and hence is the desired solution. This third step is frequently the most difficult or tedious step and will be developed further in Chap. 3. It is called inversion of the transform. Although there are other techniques available for inversion, the one that we will develop and make consistent use of is that of partial fraction expansion.

A simple example will serve to illustrate steps 1 and 2 (we'll save step 3 until Chap. 3).

Example 2.4. Solve

$$\frac{dx}{dt} + 3x = 0$$
$$x(0) = 2$$

We number our steps according to the discussion in the preceding paragraphs:

1. $\underbrace{[sx(s) - 2]}_{sx(s)-x(0)} + 3x(s) = 0$

2. $x(s) = \dfrac{2}{s+3} = 2\dfrac{1}{s+3}$

3. $x(t) = 2e^{-3t}$

SUMMARY

In this chapter we discussed the importance of process modeling and worked through a chemical mixing example that led to two differential equations that described the process (one from the mass balance and one from the energy balance). We solved those relatively simple equations by separating and integrating. We also discussed using Laplace transforms for solving differential equations and presented a table of common transforms. We concluded by demonstrating the use of MATLAB for symbolically solving differential equations. In Chap. 3 we will discuss the method of partial fractions for inverting the solutions we obtained by using transforms to the time domain.

PROBLEMS

2.1. Transform the following:

(a) $\sin(2t + \frac{\pi}{4})$

(*b*) $e^{-t}\cos 2t$

(*c*) Use the formula for the Laplace transform of a derivative to find $L\{\sinh(kt)\}$ if you are given that $L\{\cosh(kt)\} = s/(s^2 - k^2)$.

2.2. Invert the following transforms.

(*a*) $\dfrac{3}{s}$

(*b*) $\dfrac{3}{s+2}$

(*c*) $\dfrac{3}{(s+2)^2}$

(*d*) $\dfrac{3}{s^3}$

(*e*) $\dfrac{\frac{1}{2}}{s^2+9}$

(*f*) $\dfrac{3}{s^2+4s+8}$

(*g*) $\dfrac{s+4}{s^2+4s+8}$

(*h*) $\dfrac{1}{(s+2)^2}$

2.3. Find *x(s)* for the following differential equations.

(*a*) $\dfrac{d^2x}{dt^2} + 4\dfrac{dx}{dt} + 3x = u(t) \quad x(0) = x'(0) = 0$

(*b*) $\dfrac{d^2x}{dt^2} + 2\dfrac{dx}{dt} + x = u(t) \quad x(0) = x'(0) = 1$

(*c*) $\dfrac{d^2x}{dt^2} + 2\dfrac{dx}{dt} + x = u(t) \quad x(0) = x'(0) = 0$

2.4. Solve Prob. 2.1 using the MATLAB `laplace` command.

2.5. Solve Prob. 2.2 using the MATLAB `ilaplace` command.

2.6. Solve Prob. 2.3 using the MATLAB `dsolve` command, and then use `ezplot` to graph the solutions.

2.7. Use the MATLAB `dsolve` command to solve the differential equations that we developed for the mass and energy balances for the chemical mixing scenario, and then use `ezplot` to graph the solutions. Compare the results with those presented in the text.

2.8. Use the MATLAB `ilaplace` command to invert Eqs. (2.10) and (2.11), and then use `ezplot` to graph the solutions. Compare the results with those presented in the text.

2.9. Rework the chemical mixing scenario if at 3 P.M. the operator mistakenly increases the flow rate of stream 1 to 20 L/min while stream 2 and the heater input remain unchanged.

CHAPTER 2

CAPSULE SUMMARY

Definition of the Laplace transform: $L\{f(t)\} = f(s) = \int_0^\infty f(t)e^{-st}\,dt$

Linearity: $L\{af_1(t) + bf_2(t)\} = aL\{f_1(t)\} + bL\{f_2(t)\}$

Transform of first derivative: $L\left\{\dfrac{df(t)}{dt}\right\} = sf(s) - f(0)$

Transform of *nth* derivative:

$$L\left\{\frac{d^n f}{dt^n}\right\} = s^n f(s) - s^{n-1} f(0) - s^{n-2} f^{(1)}(0) - \mathrm{n} - sf^{(n-2)}(0) - f^{(n-1)}(0)$$

Transforms of some simple functions: See Table 2.1.

The following procedure uses Laplace transforms for solving *linear, ordinary, differential equations (ODEs) with constant coefficients:*

1. Take the Laplace transform of both sides of the equation. The initial conditions are incorporated at this step in the transforms of the derivatives.
2. Solve the resulting equation for the Laplace transform of the unknown function algebraically.
3. Find the function of t that has the Laplace transform obtained in step 2. This function satisfies the differential equation and initial conditions and hence is the desired solution. This third step is frequently the most difficult or tedious step. We will make consistent use of partial fraction expansions to accomplish this (see Chap. 3).

Useful MATLAB Commands:
`syms`—declares variables to be symbolic
`laplace`—takes the Laplace transform of a symbolic expression
`ilaplace`—inverts a symbolic Laplace transform expression
`dsolve`—solves a differential equation symbolically