MODELING TOOLS

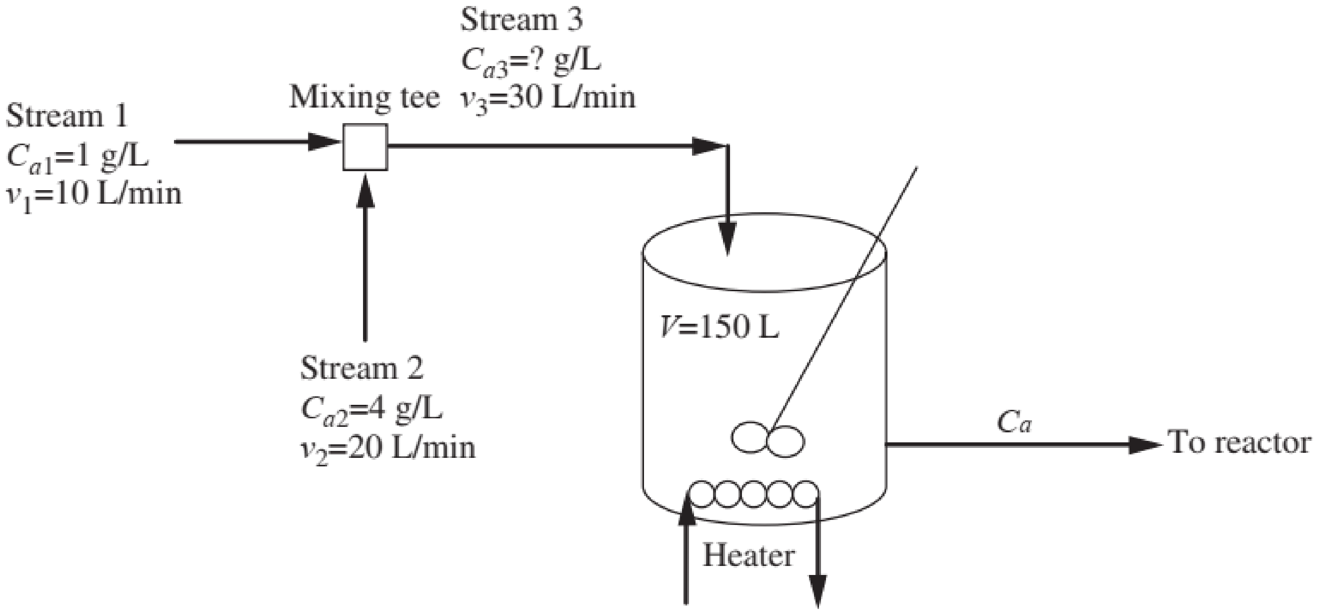
FOR

PROCESS DYNAMICS

- Understanding process dynamics (how process variables change with time) will be very important to our studies of process control.
- explore process dynamics further and review some mathematical tools for solving the resulting process models

PROCESS DYNAMICS—A CHEMICAL MIXING SCENARIO

- Two process streams are mixed to produce one of the feeds for our chemical reactor.
- After mixing, the blended stream is fed to a heating vessel before being sent to the reactor.



- We can model the mixing tee and the blending tank using an unsteady-state mass
  balance to predict the behavior of this part of the process since the shift change and the unfortunate error by the new operator.
- A balance on component *A* around the mixing tee before and after the change

$$\begin{pmatrix} \text{Rate of } A \text{ into} \\ \text{mixing tee} \\ \text{in stream 1 (g/min)} \end{pmatrix} + \begin{pmatrix} \text{Rate of } A \text{ into} \\ \text{mixing tee} \\ \text{in stream 2 (g/min)} \end{pmatrix} = \begin{pmatrix} \text{Rate of } A \text{ leaving} \\ \text{mixing tee} \\ \text{in stream 3 (g/min)} \end{pmatrix}$$

$$v_1 C_{a1} + v_2 C_{a2} = v_3 C_{a3}$$

Before the change, we can calculate the original steady-state concentration into the heating vessel:

$$\left(10\ \frac{\text{L}}{\text{min}}\right)\left(1\ \frac{\text{g}}{\text{L}}\right) + \left(20\ \frac{\text{L}}{\text{min}}\right)\left(4\ \frac{\text{g}}{\text{L}}\right) = \left(30\ \frac{\text{L}}{\text{min}}\right)\left(C_{a3}\ \frac{\text{g}}{\text{L}}\right)$$

$$C_{a3} = 3\ \frac{\text{g}}{\text{L}}$$

After the change, the new feed concentration to the heating vessel is

$$\left(20\ \frac{\text{L}}{\text{min}}\right)\left(1\ \frac{\text{g}}{\text{L}}\right) + \left(10\ \frac{\text{L}}{\text{min}}\right)\left(4\ \frac{\text{g}}{\text{L}}\right) = \left(30\ \frac{\text{L}}{\text{min}}\right)\left(C_{a3}\ \frac{\text{g}}{\text{L}}\right)$$

$$C_{a3} = 2\ \frac{\text{g}}{\text{L}}$$

So the net result of the operator error is to decrease the feed concentration to the heating vessel from 3 to 2 g/L.

- To analyze how the exit from the heating vessel (the feed to the reactor) varies
  with time, we must perform an unsteady mass balance on component *A* around the heating vessel

$$\underbrace{\begin{pmatrix}\text{Rate of } A \text{ into} \\ \text{heating vessel (g/min)}\end{pmatrix}}_{\text{in}} - \underbrace{\begin{pmatrix}\text{Rate of } A \text{ leaving} \\ \text{heating vessel (g/min)}\end{pmatrix}}_{\text{out}} = \underbrace{\begin{pmatrix}\text{Accumulation of } A \text{ in} \\ \text{heating vessel (g/min)}\end{pmatrix}}_{\text{accumulation}}$$

$$v_3 C_{a3} - v_3 C_a = \frac{d}{dt}(V C_a)$$

Volumetric flow rate *v* is constant into and out of the heating vessel at v_3 .
Thus the volume of fluid in the tank *V* is constant.

$$\underbrace{\frac{V}{v_3}}_{\tau} \frac{dC_a}{dt} + C_a = C_{a3}$$

The coefficient of the derivative term is the residence time of the heating vessel
which in this process is 5 min. Substituting the numbers

$$5\frac{dC_a}{dt} + C_a = 2 \qquad C_a(0) = 3\frac{\text{g}}{\text{L}}$$

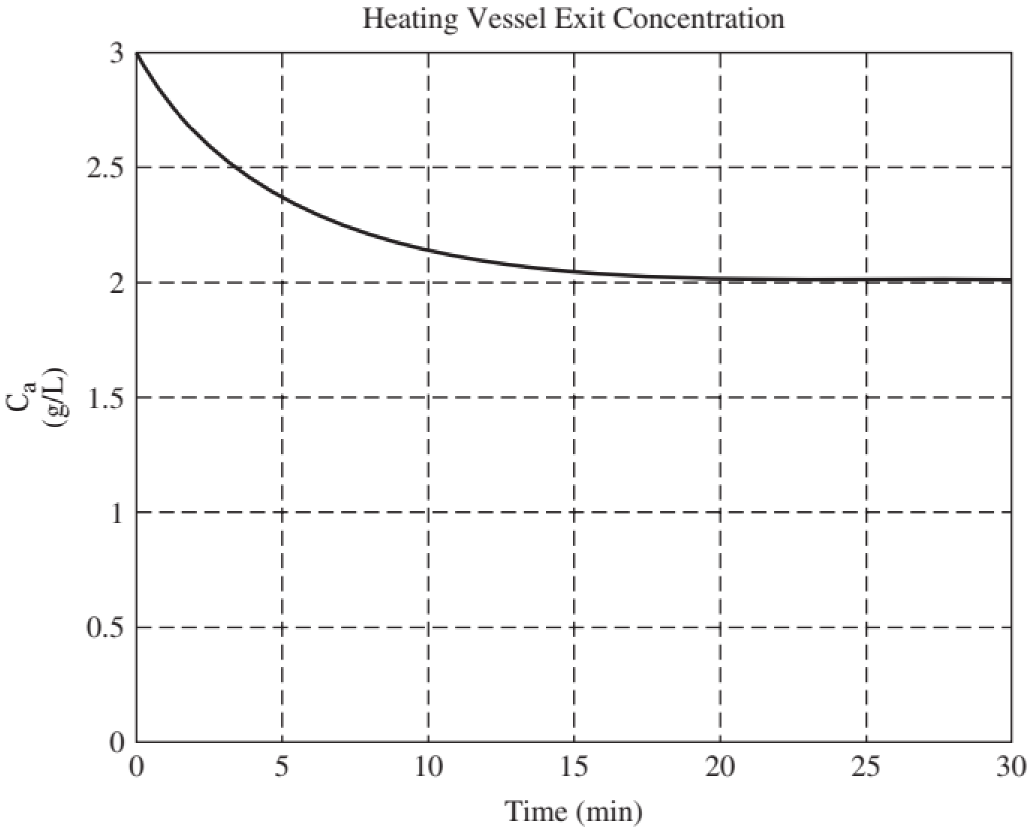
We can rearrange and solve this equation as follows.

$$\int_3^{Ca} \frac{dC_a}{2 - C_a} = \int_0^t \frac{1}{5}\, dt$$

$$-\ln(2 - C_a)\Big|_3^{Ca} = \frac{t}{5}$$

$$\ln\left(\frac{2 - C_a}{2 - 3}\right) = \frac{-t}{5}$$

$$C_a = 2 + e^{-t/5}$$

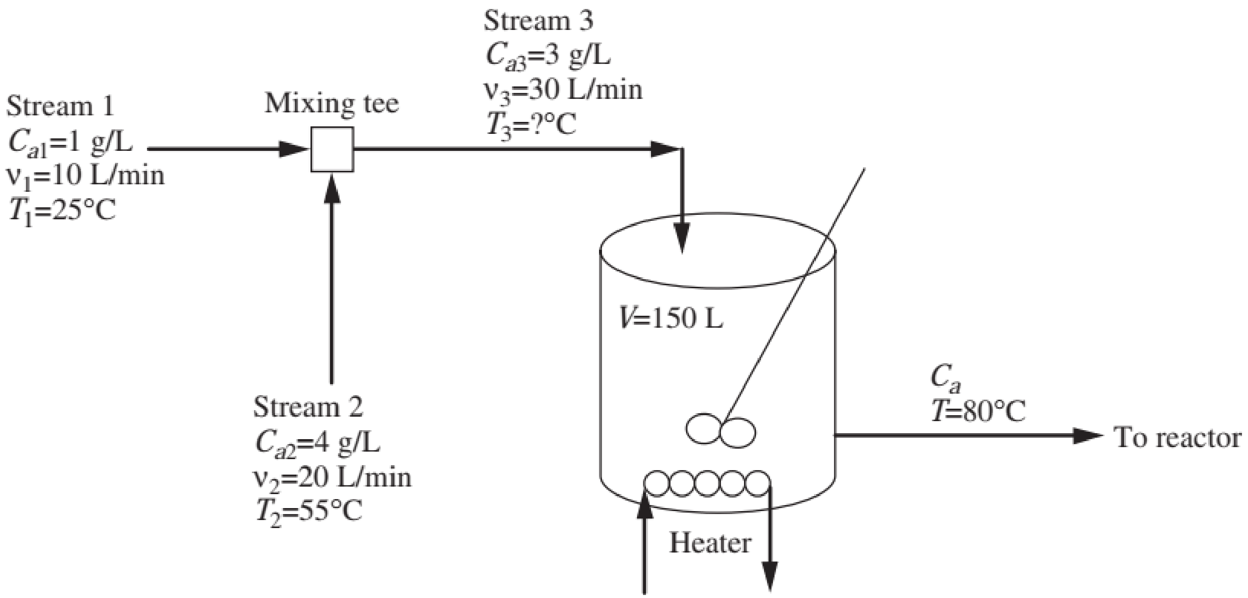


Before we look at the effect of the disturbance caused by the operator, it is necessary to determine the steady-state process conditions prior to the upset.

An energy balance around the mixing tee will enable us to calculate the steady-state feed temperature to the heating vessel T_3.

$$\begin{pmatrix}\text{Rate of}\\ \text{enthalpy into}\\ \text{mixing tee}\\ \text{with stream 1}\end{pmatrix} + \begin{pmatrix}\text{Rate of}\\ \text{enthalpy into}\\ \text{mixing tee}\\ \text{with stream 2}\end{pmatrix} = \begin{pmatrix}\text{Rate of}\\ \text{enthalpy leaving}\\ \text{mixing tee}\\ \text{with stream 3}\end{pmatrix}$$

$$\rho v_1 C_p(T_1 - T_{ref}) + \rho v_2 C_p(T_2 - T_{ref}) = \rho v_3 C_p(T_3 - T_{ref})$$



$$v_1 T_1 + v_2 T_2 = v_3 T_3$$

→ $T_{ref} = 0$

- Note that we have made use of the relation

$$(v_1 + v_2)\, T_{ref} = v_3 T_{ref}$$ to eliminate some terms.

- Solving for T_3 yields

$$T_3 = \frac{v_1 T_1 + v_2 T_2}{v_3} = \frac{(10)(25) + (20)(55)}{30} = 45°\text{C}$$

So, the steady-state inlet temperature to the heating vessel is 45 C.

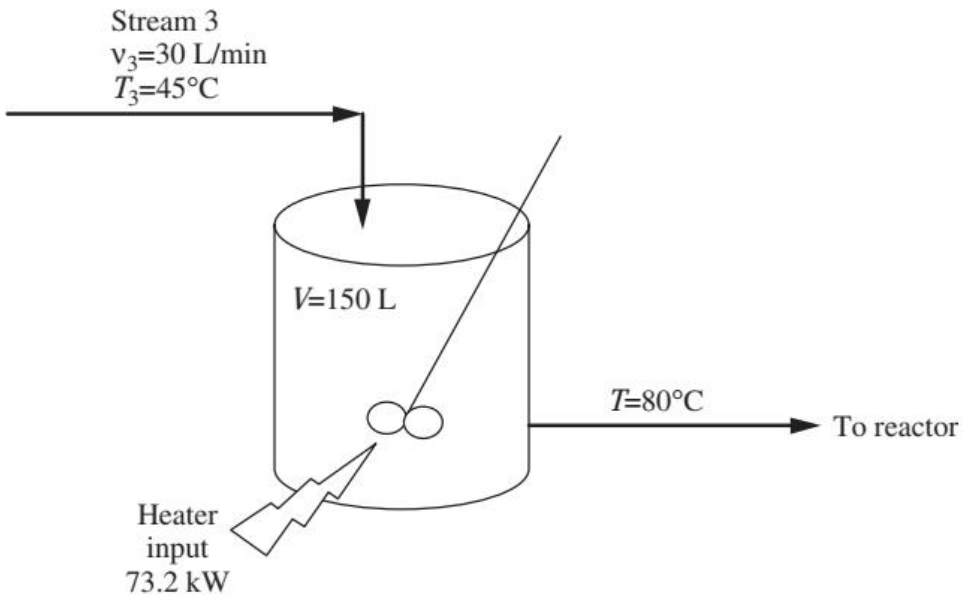
We can now determine the steady-state heat input required from the heater by performing a steady-state energy balance around the heating vessel

$$\begin{pmatrix}\text{Rate of}\\ \text{enthalpy into}\\ \text{heating vessel}\\ \text{with stream 3}\end{pmatrix} + \begin{pmatrix}\text{Rate of}\\ \text{enthalpy into}\\ \text{heating vessel}\\ \text{from heater}\end{pmatrix} = \begin{pmatrix}\text{Rate of}\\ \text{enthalpy leaving}\\ \text{heating vessel}\end{pmatrix}$$

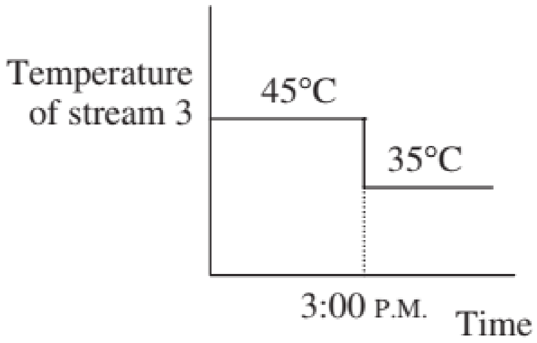
$$\rho v_3 C_p (T_3 - T_{ref}) + Q = \rho v_3 C_p (T - T_{ref})$$

$$Q = \rho v_3 C_p (T - T_3) = \left(1000\ \frac{\text{g}}{\text{L}}\right)\left(30\ \frac{\text{L}}{\text{min}}\right)\left(1\ \frac{\text{cal}}{\text{g}\cdot°\text{C}}\right)(80°\text{C} - 45°\text{C})$$

$$= 1.05 \times 10^6\ \frac{\text{cal}}{\text{min}} = 73.2\ \text{kW}$$



$$T_3 = \frac{v_1 T_1 + v_2 T_2}{v_3} = \frac{(20)(25) + (10)(55)}{30} = 35°C$$



To determine the effect of this inlet temperature disturbance on the feed to the reactor, an unsteady-state energy balance on the heating vessel is required.

$$\begin{pmatrix}\text{Rate of enthalpy}\\ \text{into heating}\\ \text{vessel}\\ \text{with stream 3}\end{pmatrix} - \begin{pmatrix}\text{Rate of enthalpy}\\ \text{leaving heating}\\ \text{vessel}\\ \text{with exit stream}\end{pmatrix} + \begin{pmatrix}\text{Rate of energy}\\ \text{input to}\\ \text{heating vessel}\\ \text{from heater}\end{pmatrix} = \begin{pmatrix}\text{Rate of}\\ \text{accumulation}\\ \text{of enthalpy in}\\ \text{heating vessel}\end{pmatrix}$$

$$\rho v_3 C_p (T_3 - T_{ref}) - \rho v_3 C_p (T - T_{ref}) + Q = \frac{d}{dt}(\rho V C_p (T - T_{ref}))$$

$$\underbrace{\left(\frac{V}{v_3}\right)}_{\tau}\frac{dT}{dt} + T = T_3 + \frac{1}{\rho v_3 C_p}Q$$

$$(5\ \text{min})\ \frac{dT}{dt} + T = 35^\circ\text{C} + \frac{1}{\left(1000\ \frac{\text{g}}{\text{L}}\right)\left(30\ \frac{\text{L}}{\text{min}}\right)\left(1\ \frac{\text{cal}}{\text{g}\cdot{}^\circ\text{C}}\right)}\left(1.05\times10^6\ \frac{\text{cal}}{\text{min}}\right) = 70^\circ\text{C}$$

$$T(0) = 80^\circ\text{C}$$

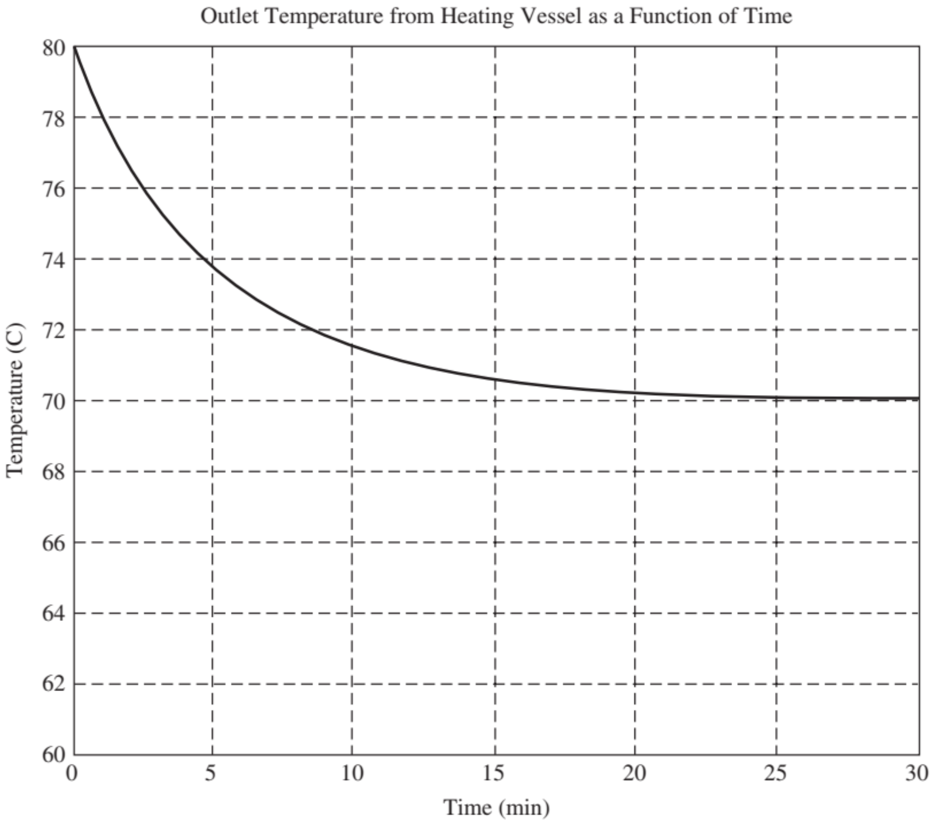
Separating and integrating, we have

$$5\frac{dT}{dt} = 70 - T$$

$$\int_{80}^{T}\frac{dT}{70 - T} = \int_{0}^{t}\frac{dt}{5}$$

$$-\ln\left(\frac{70 - T}{-10}\right) = \frac{t}{5}$$

$$T = 70 + 10e^{-t/5}$$



- 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.

MATHEMATICAL TOOLS FOR MODELING

The unsteady-state material and energy balance models required to solve differential equations

It would be beneficial to review some additional tools available to us for solving our process models.

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

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

We often abbreviate this to

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

Find the Laplace transform of the function

$$f(t) = 1$$

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

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

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

Properties of Laplace function

- 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.*

$$L\{af_1(t) + bf_2(t)\} = \int_0^\infty [af_1(t) + bf_2(t)]e^{-st}\,dt$$

$$= a\int_0^\infty f_1(t)e^{-st}\,dt + b\int_0^\infty f_2(t)e^{-st}\,dt$$

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

Transforms of Simple Functions

The *step function*

This important function is known as the unit-step function and will henceforth be denoted by *u* (*t*)

$$f(t) = \begin{cases} 0 & t < 0 \\ 1 & t > 0 \end{cases} \qquad L\{u(t)\} = \frac{1}{s}$$

- 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,

$f(t) = Au(t)$

$F(s) = A/s.$

The *exponential function*

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

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

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

- The *ramp function*

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

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

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

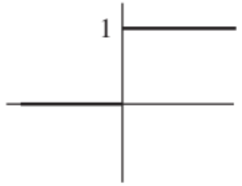
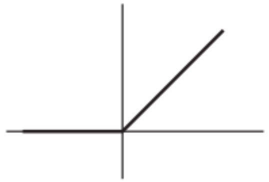
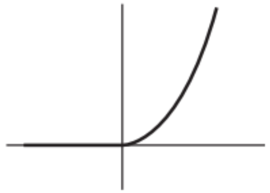
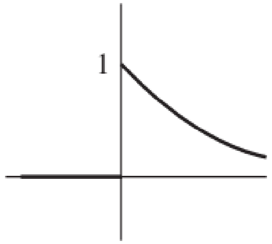
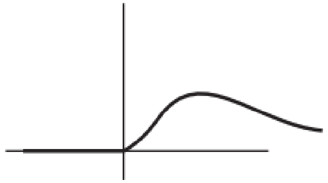
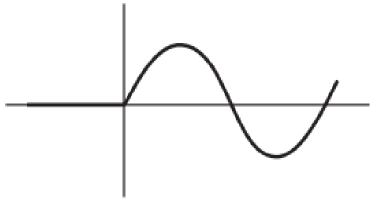
- The *sine function*

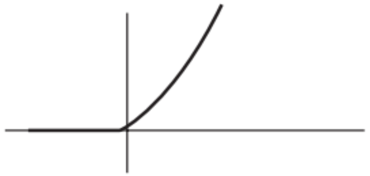
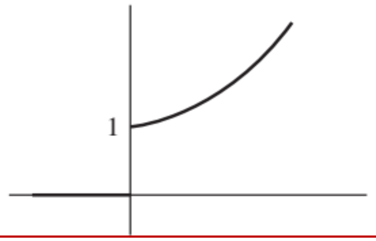
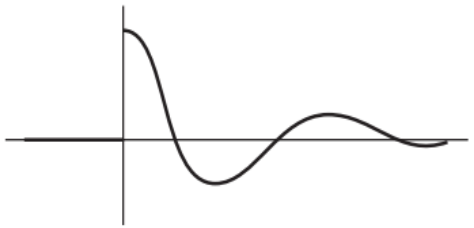
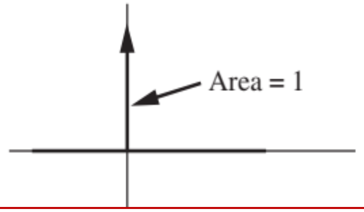
$$f(t) = \begin{cases} 0 & t<0 \\ \sin kt & t>0 \end{cases} = u(t)\sin kt$$

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

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

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

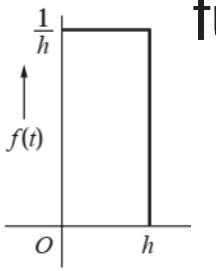
Function	Graph	Transform
$u(t)$		$\frac{1}{s}$
$tu(t)$		$\frac{1}{s^2}$
$t^n u(t)$		$\frac{n!}{s^{n+1}}$
$e^{-at}u(t)$		$\frac{1}{s+a}$
$t^n e^{-at}u(t)$		$\frac{n!}{(s+a)^{n+1}}$
$\sin kt\, u(t)$		$\frac{k}{s^2+k^2}$

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

- New function which is zero everywhere except at the origin, where it is infinite. However, it is important to note that the area under this function always remains equal to unity.
- We call this new function *d* (*t*), and the fact that its area is unity means that

$$\int_{-\infty}^{\infty} \delta(t)\, dt = 1$$

- The function *d* (*t*) is called the unit-impulse function or, alternatively, the fu



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

$$f(t) = \frac{1}{h}[u(t) - u(t - h)]$$

$$f(s) = \frac{1}{h}\frac{1 - e^{-hs}}{s}$$

- Laplace transform of *d* (*t*) can be obtained by letting *h* go to 0 in *L* { *f (t)* }.
- Applying L’Hôpital’s rule, we find

$$L\{\delta(t)\} = \lim_{h\to 0} \frac{1 - e^{-hs}}{hs} = \lim_{h\to 0} \frac{se^{-hs}}{s} = 1$$

- The operation of differentiation with respect to *t* to that of multiplication by *s.*
- Thus, we claim that

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

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

and *f*(0) is *f* (*t*) evaluated at *t* = 0

Proof

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

$$v = f(t)$$

$$dv = \frac{df}{dt} dt$$

$$u = e^{-st}$$

$$du = -se^{-st}\, dt$$

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

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

$$L\left\{\frac{d^2 f}{dt^2}\right\} = L\left\{\frac{d}{dt}\left(\frac{df}{dt}\right)\right\} = sL\left\{\frac{df}{dt}\right\} - \left.\frac{df(t)}{dt}\right|_{t=0}$$

$$= s[sF(s) - f(0)] - f'(0)$$

$$= s^2 F(s) - sf(0) - f'(0)$$

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

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

Example

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

Given

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

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

Inserting the initial conditions and solving for *x* (*s*)

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

SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS (ODES)

- 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.

Solution to the differential equation and initial conditions of Example:

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

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

- Therefore, what is required is a method for expanding the common-denominator form of Eq. to the separated form of Eq..
- This method is provided by the technique of partial fractions

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

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. $$x(s) = \frac{2}{s+3} = 2\frac{1}{s+3}$$
3. $$x(t) = 2e^{-3t}$$