## ENGINEERING SYSTEM MODELLING AND SIMULATION <br> Mustafa Kemal SEVINDİR, Ph.D <br> sevindir@yildiz.edu.tr

## Mechanistic Models I: ODEs

Distinguished Role of Differential Equations

Mechanistic models use information about the internal "mechanics" of a system.

The main difference between phenomenological models and mechanistic models lies in the fact that phenomenological models treat the system as a black box, while in the mechanistic modeling procedure one virtually takes a look inside the system and uses this information in the model.

## (Distinguished role of differential equations)

1. Mechanistic models consider the processes running inside a system.
2. Typical processes investigated in science and engineering involve rates of changes of quantities of interest.
3. Mathematically, this translates into equations involving derivatives of unknown functions, i.e. differential equations.

## An Introductory Example

Consider the tank shown in figure where two streams enter the tank, mix, and a single stream exits through a valve.


Mixing tank

## At Steady State condition

$\mathrm{Flow}_{1}+$ Flow $_{2}=$ Flow $_{3}$ or
Flow $_{1}+$ Flow $_{2}-$ Flow $_{3}=0$
$\Sigma$ Flows in $-\Sigma$ Flows out $=0$

$$
\begin{aligned}
& w_{1}=\text { Flow }_{1} ; w_{2}=\text { Flow }_{2} ; w_{3}=\text { Flow }_{3} \\
& w_{1}+w_{2}-w_{3}=0
\end{aligned}
$$

Let us suppose that $w_{1}=20 \mathrm{~kg} / \mathrm{min}$ and $w_{2}=10 \mathrm{~kg} / \mathrm{min}$
$20+10-w_{3}=0$
$w_{3}=30 \mathrm{~kg} / \mathrm{min}$
If $w_{2}$ changes to $20 \mathrm{~kg} / \mathrm{min}$, now $w_{3}=40 \mathrm{~kg} / \mathrm{min}$.
The outlet flow of liquid through the valve depends, among other things, on the height of liquid in the tank, $h$, as indicated in figure, which we often refer to as head of liquid.

This dependence, or relation, may be expressed as

$$
w_{3}=C_{v} \sqrt{h}
$$

$C_{v}$ is the valve coefficient.

For this particular example, assume
$C_{V}=16.67 \mathrm{~kg} / \mathrm{m}^{1 / 2} \cdot \mathrm{~min}$.

$$
w_{1}+w_{2}-16.67 \sqrt{h}=0
$$

For the steady operation, we need height of liquid to deliver the outlet flow,

$$
20+10-16.67 \sqrt{h}=0
$$

$h=3.24 \mathrm{~m}$
If $w_{2}$ becomes $20 \mathrm{~kg} / \mathrm{min}$, the new necessary height to deliver $40 \mathrm{~kg} / \mathrm{min}$ is

$$
20+20-16.67 \sqrt{h}=0
$$

$h=5.76 \mathrm{~m}$

When flow $w_{2}$ changes from 10 to $20 \mathrm{~kg} / \mathrm{min}$ the height in the tank must change from 3.24 to 5.76 m . This change in height, however, is not instantaneous, although the change in inlet flow may be very close to instantaneous.

It takes some amount of time in going from the initial height to the new, or final, height.

If the time to reach the new height is important, then another model is needed.

The new model needs to describe how fast the height in the tank changes when any of the inlet flows, or both, change.
$\sum \begin{gathered}\text { Rate of mass } \\ \text { entering system }\end{gathered}-\sum \begin{aligned} & \text { Rate of mass } \\ & \text { exiting system }\end{aligned}=0$
The expression rate of mass refers to flows in units of mass/time ( $\mathrm{kg} / \mathrm{min}$ in this example).
Equation only refers to the streams entering and exiting the system (the tank in this case); it does not account for the mass inside the system.

Thus, it does not describe what happens to the mass or height of liquid in the tank when the entering and exiting streams are not equal to each other. To account for this mass inside the process, and develop the desired model,
$\sum \begin{gathered}\text { Rate of mass } \\ \text { entering system }\end{gathered}-\sum \begin{gathered}\text { Rate of mass } \\ \text { exiting system }\end{gathered}=\begin{gathered}\text { Rate of change of } \\ \text { mass accumulated } \\ \text { in system }\end{gathered}$
Applying this equation to the tank

$$
w_{1}+w_{2}-w_{3}=\frac{d m}{d t}
$$

The term $\frac{d m}{d t}$ means the rate of change of the mass in the tank ( $m$ ) with respect to time ( $t$ ), or in other words, how fast the mass in the tank changes.

A positive derivative indicates that the mass in the tank is increasing because there is more mass entering the tank than exiting.

A negative derivative indicates that the mass in the tank is decreasing, or depleting, because there is more mass exiting the tank than entering.

The mass of liquid accumulated in the tank is related to the height of liquid by

$$
m=\rho V=\rho A h
$$

$\rho=$ density of fluid, assumed constant at $1000 \mathrm{~kg} / \mathrm{m}^{3}$
$V=$ volume of liquid in tank, $\mathrm{m}^{3}$
$A=$ cross-sectional area of tank, assumed constant at $0.292 \mathrm{~m}^{2}$

$$
\begin{gathered}
\frac{d m}{d t}=\rho A \frac{d h}{d t} \\
w_{1}+w_{2}-C_{v} \sqrt{h}=\rho A \frac{d h}{d t} \\
\rho A \frac{d h}{d t}+C_{v} \sqrt{h}=w_{1}+w_{2}
\end{gathered}
$$

is a differential equation that describes how the height of liquid in the tank varies when either inlet flow, or when both change.

The differential equation describes how the level in the tank changes - in general, we refer to this as the "transient response" or "dynamic response"- and its final steady value.

## Differential Equations

A differential equation is an equation containing one or more derivatives of an unknown function and perhaps the function itself.

$$
\frac{d^{3} x}{d t^{3}}+3 \frac{d^{2} x}{d t^{2}}+4 \frac{d x}{d t}+x=F(t)
$$

$x$ is an unknown function.
The unknown function is called the dependent variable; the variable by which this dependent variable is differentiated by, $t$ is called the independent variable.

The function on the right-hand side of the equal sign, $F(t)$ is called the forcing function because once it changes, it "forces" the dependent variable to change.

It is common in mathematics to use primes (') or dots (v) to represent derivatives.

$$
\begin{gathered}
\frac{d x}{d t}=x^{\prime}=\dot{x} ; \frac{d^{2} x}{d t^{2}}=x^{\prime \prime}=\ddot{x} ; \text { etc. } \\
x^{\prime \prime \prime}+3 x^{\prime \prime}+4 x^{\prime}+x=F(t)
\end{gathered}
$$

$$
\rho A h^{\prime}+C_{v} \sqrt{h}=w_{1}+w_{2}
$$

The order of a differential equation is the highest derivative in the equation.

$$
\left.x\right|_{t=0}=x(0)
$$

This specification is called an initial condition. We call this an initial value problem.
For an $n$ th-order differential equation $n$ initial conditions are needed to complete the model.

The dependent variable in the differential equations discussed so far is a function of only one independent variable; for example, in the example of the mixing tank the height $h$ is only a function of time $t$. These differential equations are called ordinary differential equations or ODEs.

Sometimes the dependent variable may be a function of more than one independent variable. Consider a well-insulated long pipe in which a liquid flows. At the initial steady condition the temperature of the liquid is the same all along the pipe; let us call this temperature $T_{\text {initial }}$, and, of course, at that condition $T_{\text {in }}=T_{\text {initial }}$.


Suppose now that at some time, $t=0$, the inlet temperature $T_{\text {in }}$ increases by $30^{\circ} \mathrm{C}$. The liquid temperature inside the pipe starts increasing at some rate (not instantaneously) to its final value but not at the same time all along the pipe. That is, the temperature next to the entrance starts changing before the temperature at 0.1 L , and this temperature at 0.1 L starts changing before the temperature at 0.2 L , and so on. That means that the temperature along the pipe, call it $T$, is a function of-depends on-time $t$ and distance $x$ down the pipe; we say that $T(t, x)$.

The differential equation in this case will contain partial derivatives of $T(t, x)$ such as $[\partial T(x, t)] / \partial t$ and $[\partial T(x, t)] / \partial x$; these equations are called partial differential equations or PDEs. For a first-order PDE the initial condition is of the form $T(t=0)=T_{\text {initial }}$ for all $x$, and $T(x=0)=T_{\text {initial }}$ for $t$.

## Forcing Functions

An important use of a model is for studying how some variables affect some other variables, or how the forcing functions affect the dependent variables.
For example, the mixing tank may be used to study how the liquid level in the tank responds to different types of forcing functions-changes in $w_{1}(t)$ and/or $w_{2}(t)$.

These changes could be in the form of a ramp, a sine wave, a pulse, a step change, or any other.

The step change is a very common forcing function, and thus it deserves special attention.
To explain its meaning, consider that at some time, $t=$ a, $w_{1}(t)$ changes from 20 to $25 \mathrm{~kg} / \mathrm{min}$ instantaneously;


As the figure shows, the change is in the form of a step. Mathematical modeling requires describing mathematically this change. The term $u(t-a)$ is used to describe a unity step change at time a; that is, the term is a shorthand notation for

$$
u(t-a)= \begin{cases}0 & t<a \\ 1 & t \geq a\end{cases}
$$

Essentially, as long as the argument $(t-a)$ is less than 0 , the function $u=0$.

When the argument $(t-a)$ is equal or greater than 0 , the function $u=1$.

Then, for the example shown in figüre (Step change in flow of stream 1), the mathematical expression $w_{1}(t)=$ $20+5 u(t-a)$ expresses the change of $w_{1}(t)$ from 20 to $25 \mathrm{~kg} / \mathrm{min}$ at time $=\mathrm{a}$.

## Example 1

Consider the forcing function $f(t)$ shown in figure. Develop the mathematical expression for $f(t)$.


There are three step changes in this figure, at times 4, 6 , and 8 ; each change has a magnitude of 3 . The expression is

$$
f(t)=1-3 u(t-4)+3 u(t-6)-3 u(t-8)
$$

At $t<4$, all the $u$ values are zero and $f(t)=1$ as the figure shows. At $t \geq 4$ but less than $6, u(t-4)=1, u(t-$ $6)=u(t-8)=0$, and $f(t)=-2$ as the figure shows. At $t$ $\geq 6$ but less than $8, u(t-4)=u(t-6)=1, u(t-8)=0$, and $f(t)=1$ as the figure shows. On the basis of this presentation, the reader can understand why $f(t)=-2$ after $t \geq 8$.

## Example 2

Consider the forcing function $f(t)$ shown in figure. Develop the mathematical expression for $f(t)$. This is a ramp change starting at 4 min . The expression is $f(t)=5+7 / 4(t-4) u(t-4)$


Forcing function for example 2

## Mass Balances

Example 1

Consider the tank shown in figure. Suppose the liquid is water with a density of $1000 \mathrm{~kg} / \mathrm{m}^{3}$, the area of the tank is $1 \mathrm{~m}^{2}$, the downstream pressure from the valve is 90 kPa , the steady-state flow into the tank is 10 $\mathrm{m}^{3} / \mathrm{min}$, and the valve equation is given by
$w_{1}(\mathrm{~kg} / \mathrm{min})$


$$
f_{2}=1.5 \sqrt{P_{1}-P_{2}} ; \mathrm{m}^{3} / \mathrm{min}
$$

(a)Find the steady-state liquid level.
(b)Develop the model that describes how the level in the tank varies when the inlet volumetric flow changes by $2 \mathrm{~m}^{3} / \mathrm{min}$ or $f_{1}=10+2 u(t)$.
(a) At steady state, the mass flow into the tank must equal the mass flow out of the tank

$$
\begin{gathered}
w_{1}-w_{2}=0 \\
w_{1}=w_{2} \\
w_{1}=w_{2}=f_{1} \cdot \rho=10 \frac{\mathrm{~m}^{3}}{\min }\left(1000 \frac{\mathrm{~kg}}{\mathrm{~m}^{3}}\right)=1 \times 10^{4} \frac{\mathrm{~kg}}{\min }
\end{gathered}
$$

The outlet volumetric flow is

$$
f_{2}=\frac{w_{2}}{\rho}=\frac{1 \times 10^{4} \frac{\mathrm{~kg}}{\mathrm{~min}}}{1000 \frac{\mathrm{~kg}}{\mathrm{~m}^{3}}}=10 \frac{\mathrm{~m}^{3}}{\mathrm{~min}}
$$

In this example, $f_{1}=f_{2}$ because the inlet and outlet densities are equal, $\rho$ is a constant.
To find the pressure that produces this flow, we make use of the valve equation,

$$
f_{2}=10=1.5 \sqrt{P_{1}-P_{2}}=1.5 \sqrt{P_{1}-90} \rightarrow P_{1}=134.44 \mathrm{kPa}
$$

Finally, to find the level to produce pressure $P_{1}$

$$
\begin{gathered}
P_{1}=134.44 \mathrm{kPa}=101.32+\frac{\rho g h}{1000} \\
=101.32+\frac{\left(1000 \frac{\mathrm{~kg}}{\mathrm{~m}^{3}}\right)\left(9.8 \frac{\mathrm{~m}}{\mathrm{~s}^{2}}\right) \mathrm{h}}{1000} \\
\mathrm{~h}=3.38 \mathrm{~m}
\end{gathered}
$$

(b)

$$
\begin{gathered}
\rho f_{1}-1.5 \rho \sqrt{101.32+\frac{\rho g h}{1000}-P_{2}}=\rho A \frac{d h}{d t} \\
\rho f_{1}-1.5 \rho \sqrt{11.32+9.8 h}=\rho A \frac{d h}{d t} \\
\rho A \frac{d h}{d t}+1.5 \rho \sqrt{11.32+9.8 h}=\rho f_{1}=\rho[10+2 u(t)]
\end{gathered}
$$

is a first-order nonlinear differential equation.

## Definition of a Linear Differential Equation

A linear differential equation is one that can be put in the form

$$
a_{n}(x) \frac{d^{n} y}{d x^{n}}+a_{n-1}(x) \frac{d^{n-1} y}{d x^{n-1}}+\cdots+a_{0}(x) y=r(x)
$$

$a_{n}, a_{n-1}, \ldots, a_{0}$, and $r$ are either functions of only the independent variable or constants. They do not have to be linear functions of the independent variable $x$. $r(x)$ is called the forcing function because when it changes it forces the dependent variable $y$ to change.
${ }^{41}$ Consider the following differential equation:

$$
b_{2}(x) y^{\prime \prime}+b_{1}(x) y^{\prime}+b_{0}(x) y=R r(x)+S s(x)
$$

This equation has two forcing functions and obviously could have any number of them. For a linear system, the addition of a solution of

$$
b_{2}(x) y^{\prime \prime}+b_{1}(x) y^{\prime}+b_{0}(x) y=\operatorname{Rr}(x)
$$

plus a solution of

$$
b_{2}(x) y^{\prime \prime}+b_{1}(x) y^{\prime}+b_{0}(x) y=S s(x)
$$

is equal to a solution of above equation.
It is called the Principle of Superposition.

42 If the right-hand side of a differential equation is equal to zero, such as

$$
a_{2}(x) y^{\prime \prime}+a_{1}(x) y^{\prime}+a_{0}(x) y=0
$$

it is called a homogeneous equation; otherwise, it is a nonhomogeneous equation.
The analytical solution of linear differential equations with coefficients that are functions of the independent variable, such as $a_{2}(x), a_{1}(x), \ldots$, and $a_{0}(x)$ is rather difficult. The analytical solutions to linear differential equations with constant coefficients is easy.

$$
a_{2} y^{\prime \prime}+a_{1} y^{\prime}+a_{0} y=r(x)
$$

## Mass Balances

Example 2

Consider the mixing tank shown in figure.


45 In this tank a highly concentrated solution of NaOH and $\mathrm{H}_{2} \mathrm{O}$ (stream 1) is diluted using pure water (stream 2); the concentrated solution contains 0.75 mass fraction of NaOH . The figure shows the steady-state information. The exit stream flows out of the tank by overflow, the tank has a volume of $0.2845 \mathrm{~m}^{3}$, and the density of the liquid accumulated in the tank can be assumed constant at $1200 \mathrm{~kg} / \mathrm{m}^{3}$. Also assume that the contents of the tank are well mixed (meaning that the concentration of NaOH is the same in the entire volume, including the exiting stream).

46 Develop the model that describes how the exit concentration of NaOH varies when the concentration of stream 1 changes in a step change to 0.67 mass fraction of NaOH , or $x_{1}^{\mathrm{NaOH}}=0.75-0.08 u(t)$.
$\sum \begin{aligned} & \text { Rate of mass of } \\ & \text { NaOH entering }\end{aligned}-\sum \begin{aligned} & \text { Rate of mass of } \\ & \text { NaOH exiting }\end{aligned}$
$=\sum \begin{gathered}\text { Rate of change of mass of } \\ \mathrm{NaOH} \text { accumulated in system }\end{gathered}$

$$
\begin{gathered}
w_{1}^{\mathrm{NaOH}}-w_{3}^{\mathrm{NaOH}}=\frac{d m^{\mathrm{NaOH}}}{d t} \\
w_{1} x_{1}^{\mathrm{NaOH}}-w_{3} x_{3}^{\mathrm{NaOH}}=\frac{d m x_{3}^{\mathrm{NaOH}}}{d t} \\
m=\rho V=1200 * 0.2845=341.1 \mathrm{~kg} \\
w_{1} x_{1}^{\mathrm{NaOH}}-w_{3} x_{3}^{\mathrm{NaOH}}=m \frac{d x_{3}^{\mathrm{NaOH}}}{d t}
\end{gathered}
$$

$$
\begin{gathered}
\frac{w_{1}}{m} x_{1}^{\mathrm{NaOH}}-\frac{w_{3}}{m} x_{3}^{\mathrm{NaOH}}=\frac{d x_{3}^{\mathrm{NaOH}}}{d t} \\
\frac{d x_{3}^{\mathrm{NaOH}}}{d t}+0.0799 \cdot x_{3}^{\mathrm{NaOH}}=0.0585 \cdot x_{1}^{\mathrm{NaOH}} \\
12.5 \cdot \frac{d x_{3}^{\mathrm{NaOH}}}{d t}+x_{3}^{\mathrm{NaOH}}=0.73 \cdot x_{1}^{\mathrm{NaOH}} \\
x_{3}^{\mathrm{NaOH}}=0.55-0.05857\left(1-e^{-\frac{t}{12.5}}\right)
\end{gathered}
$$

## Mass Balances

Example 3

50 Consider the same mixing tank. This time develop the model that describes how the exit concentration of NaOH varies when the concentration of stream 1 changes in a step change to 0.67 mass fraction of NaOH , and at the same time the flow of stream 1 changes in a step change to $15 \mathrm{~kg} / \mathrm{min}$.

The model starts in the same manner as previously, that is, with a mass balance on NaOH .

$$
\begin{aligned}
& 341.1 \frac{d x_{3}^{\mathrm{NaOH}}}{d t}+w_{3} x_{3}^{\mathrm{NaOH}}=w_{1} x_{1}^{\mathrm{NaOH}} \\
& 1 \text { equation, } 2 \text { unknowns }\left[w_{3}, x_{3}^{\mathrm{NaOH}}\right] \\
& w_{1}+w_{2}-w_{3}=0 \\
& 2 \text { equations, } 2 \text { unknowns }
\end{aligned}
$$

$$
341.1 \frac{d x_{3}^{\mathrm{NaOH}}}{d t}+\left(w_{1}+w_{2}\right) x_{3}^{\mathrm{NaOH}}=w_{1} x_{1}^{\mathrm{NaOH}}
$$

## Mass Balances

Example 4

53 Consider the gas tank shown in figure. A fan blows air into a tank, and from the tank the air flows out through a valve.


Gas system

54 For purposes of this example, let us suppose that the air flow delivered by the fan is given by

$$
f_{i}(t)=0.453 s_{i}(t)
$$

$f_{i}(t)=$ air flow in $\mathrm{m}^{3} / \mathrm{min}$ at $23^{\circ} \mathrm{C}$ and 101.32 kPa
$s_{i}(t)=$ signal to fan, $0-1$ fraction

55 The flow through the valve is expressed by

$$
f_{o}(t)=2.078 \times 10^{-3} s_{o}(t) \sqrt{p(t)\left[p(t)-p_{1}(t)\right]}
$$

$f_{o}(t)=$ air flow in $\mathrm{m}^{3} / \mathrm{min}$ at $23^{\circ} \mathrm{C}$ and at the pressure of the tank
$s_{o}(t)=$ signal to fan, $0-1$ fraction
$p(t)=$ pressure in tank, kPa
$p_{1}(t)=$ downstream pressure from valve, kPa

56 The volume of the tank is $0.569 \mathrm{~m}^{3}$, and it can be assumed that the process occurs isothermally at $23^{\circ} \mathrm{C}$.

The initial steady-state conditions are the following:

$$
\begin{aligned}
& f_{i}(0)=f_{o}(0)=0.2265 \mathrm{~m}^{3} / \mathrm{min} \\
& p(0)=275.788 \mathrm{kPa} \\
& p_{1}(0)=101.325 \mathrm{kPa} \\
& s_{i}(0)=0.5 \\
& s_{o}(0)=0.1825
\end{aligned}
$$

57 Develop the mathematical model that relates the pressure in the tank to changes in the signal to the fan, $s_{i}(t)$; in the signal to the valve, $s_{o}(t)$; and in the downstream pressure, $p_{1}(t)$.
An unsteady-state mass balance around the system, defined as the fan, tank, and outlet valve, provides the starting relation. That is,

$$
w_{i}(t)-w_{o}(t)=\frac{d m(t)}{d t}
$$

or

$$
\rho_{i} f_{i}(t)-\rho_{o} f_{o}(t)=\frac{d m(t)}{d t}
$$

${ }^{58}$ Because the pressure and temperature of the inlet air are known, its density is also known and given as (the molecular mass of air is $28.9 \mathrm{~g} / \mathrm{mol}$ ),

$$
\begin{aligned}
& \rho_{i}=\bar{\rho}_{i} \cdot \text { molecular mass }=\frac{p_{i} \cdot \text { molecular mass }}{R T_{i}} \\
& =\frac{(101325 \mathrm{~Pa})\left(28.9 \frac{\mathrm{~g}}{\mathrm{~mol}}\right)}{\left(8.314 \mathrm{~Pa} \cdot \frac{\mathrm{~m}^{3}}{\mathrm{molK}}\right)(296 \mathrm{~K})}
\end{aligned}
$$

$$
\rho_{i}=1189.85 \mathrm{~g} / \mathrm{m}^{3}
$$

The exit density,

$$
\rho_{o}=\overline{\rho_{o}} \cdot \text { molecular mass }=\frac{p(t) \cdot \text { molecular mass }}{R T}
$$

2 equations, 5 unknowns $[p(t)]$
The fan provides another equation:

$$
f_{i}(t)=0.453 s_{i}(t)
$$

3 equations, 5 unknowns
${ }^{60}$ The valve provides still another equation:

$$
f_{o}(t)=2.078 \times 10^{-3} s_{o}(t) \sqrt{p(t)\left[p(t)-p_{1}(t)\right]}
$$

4 equations, 5 unknowns
Because the pressure in the tank is low, the ideal gas equation of state can be used to relate the moles in the tank to the pressure.

$$
p(t) V=n(t) R T
$$

5 equations, 6 unknowns $[n(t)]$

$$
n(t)=\frac{m(t)}{\text { molecular mass }}
$$

6 equations, 6 unknowns
This set of equations constitutes the mathematical model for this process. The solution describes how the pressure in the tank responds to changes in $s_{i}(t), s_{o}(t)$, and $p_{1}(t)$.
The resulting equation will be a first-order ordinary nonlinear differential equation.

## Thermal Systems

Conservation of Energy

${ }^{63}$ If we restrict ourselves to processes that do not involve atomic fission, energy, like mass, is conserved.
$\sum_{\text {Entering System }}^{\text {Rate of Energy }}-\sum \begin{aligned} & \text { Rate of Energy } \\ & \text { Exiting System }\end{aligned}=$
$\sum$ Rate of Change of Energy
$\sum$ Accumulated in System
$\dot{q}=-k A \frac{d T}{d x} \quad$ Heat Conduction (Fourier's Law)
$\dot{q}=h A\left(T-T_{f}\right)$ Heat Convection (Newton's Law of Cooling)
$E=m C\left(T-T_{r e f}\right)$ Stored Internal Energy (non-reactive, single phase, solid material)

Rate of change of energy accumulated in system = $d E / d t=m C d T / d t$

# Thermal Systems 

Example 1: Convective Heat Transfer
${ }^{66}$ Spherical steel pellets at a high initial temperature $T_{0}$ are quenched by dropping them into a very large cooling bath containing a fluid that is at temperature $T_{f}$. Develop an expression for the temperature $T$ of a pellet as a function of time after it is dropped into the cooling bath.
We will make two assumptions in solving this problem:

1. The bath temperature $T_{f}$ remains constant.
2. The temperature within the pellet is uniform-it depends on time but not on radial position within the pellet. This is equivalent to treating the pellet as a lumped parameter system.

Energy Accumulated = Energy Entering in Pellet

$$
\begin{aligned}
m C \frac{d T}{d t} & =0-h A\left(T-T_{f}\right) \\
\frac{d T}{d t} & =-\alpha\left(T-T_{f}\right)
\end{aligned}
$$

is a first-order equation, so we need one initial condition.
$T(0)=T_{0}$

$$
\alpha=\frac{h A}{m C}
$$

$$
\int \frac{d T}{\left(T-T_{f}\right)}=-\int \alpha d t
$$

Integrating yields

$$
\ln \left(T-T_{f}\right)=-\alpha t+C_{1}
$$

Applying the initial condition $T(0)=T_{0}$

$$
\ln \left(T_{o}-T_{f}\right)=C_{1}
$$

Rearranging, yields

$$
\ln \left(\frac{T-T_{f}}{T_{o}-T_{f}}\right)=-\alpha t
$$

$$
T=T_{f}+\left(T_{o}-T_{f}\right) \exp (-\alpha t)
$$

This solution is called a decaying exponential because of the exponential to a negative power.

In particular, we note here that the quantity $\alpha$ is simply the reciprocal of the time constant $\tau$.

The time constant provides information about how long it takes for a first-order process to occur.

70 A couple of useful points to consider are the values of $T$ at zero time and at infinite time. At $t=0$, the exponential goes to unity and equation simply becomes

$$
T(0)=T_{f}+T_{o}-T_{f}=T_{o}
$$

Hopefully, this was no surprise because it was our initial condition.
As $t$ approaches infinity, the exponential goes to zero and equation becomes

$$
T(\infty)=T_{f}
$$

71 The exact graph of $T$ versus $t$ depends on the value of $\alpha=\frac{h A}{m c}$. However, it will have the general characteristic of starting at $T_{0}$ and decaying to $T_{f}$, approaching it asymptotically, as shown in figure for two different values of $\alpha$.


Increasing the value of $\alpha$ (decreasing the time constant) will simply make the decay happen faster. Practically, the decay will be complete after $t=5 \tau$.

# Thermal Systems 

Example 2: Heating of a Liquid in a Jacketed, Stirred Vessel

74 A stirred tank (see figure) contains $30 \mathrm{~m}^{3}$ of water, originally at $25^{\circ} \mathrm{C}$.


Heating of water in a jacketed, stirred vessel

75 The water is heated by saturated steam condensing at $100^{\circ} \mathrm{C}$ in the jacket surrounding the vessel. The heat transfer area of the jacket is $80 \mathrm{~m}^{2}$ and the overall heat transfer coefficient between the condensing steam and the water in the vessel is $500 \mathrm{~J} / \mathrm{m}^{2} \mathrm{~s}^{\circ} \mathrm{C}$, The density and heat capacity of water are $1000 \mathrm{~kg} / \mathrm{m}^{3}$ and $4200 \mathrm{~J} / \mathrm{kg}^{\circ} \mathrm{C}$, respectively. Determine how long it will take for the water in the vessel to reach a temperature of $50^{\circ} \mathrm{C}$.

We begin our development of a mathematical model by writing an energy balance for the water in the vessel:
$\sum \begin{aligned} & \text { Rate of Change of Energy } \\ & \text { Accumulated in the Water }\end{aligned}$
$=\sum_{\text {Rate of Energy }}^{\text {into the Water }}-\sum \begin{aligned} & \text { Rate of Energy } \\ & \text { out of the Water }\end{aligned}$

$$
\dot{q}_{i n}=U A\left(T_{s}-T\right)
$$

$A$ is the area of the jacket, $T_{s}$ is the temperature of the condensing steam, $T$ is the temperature of the water in the vessel.

$$
m C \frac{d T}{d t}=U A\left(T_{S}-T\right)
$$

The initial condition is $T(0)=T_{0}=25^{\circ} \mathrm{C}$.

$$
\begin{gathered}
\alpha=\frac{U A}{m C} \\
\frac{d T}{d t}=-\alpha\left(T-T_{s}\right)
\end{gathered}
$$

$$
\int \frac{d T}{\left(T-T_{s}\right)}=-\int \alpha d t
$$

Integrating yields

$$
\ln \left(T-T_{s}\right)=-\alpha t+C_{1}
$$

Applying the initial condition $T(0)=T_{0}$

$$
\ln \left(T_{o}-T_{s}\right)=C_{1}
$$

Rearranging, yields

$$
\ln \left(\frac{T-T_{S}}{T_{o}-T_{S}}\right)=-\alpha t
$$

79 The mass $m$ is equal to the product of density $\rho$ and volume $V$ and evaluate $\alpha$ by

$$
\begin{aligned}
& \alpha=\frac{U A}{\rho V C} \\
& =\left(\frac{500 \mathrm{~J}}{\mathrm{~s} \cdot \mathrm{~m}^{2} \cdot{ }^{\circ} \mathrm{C}}\right)\left(\frac{80 \mathrm{~m}^{2}}{1}\right)\left(\frac{\mathrm{m}^{3}}{1000 \mathrm{~kg}}\right)\left(\frac{1}{30 \mathrm{~m}^{3}}\right)\left(\frac{{ }^{\circ} \mathrm{C} \cdot \mathrm{~kg}}{4200 \mathrm{~J}}\right) \\
& =0.00032 \mathrm{~s}^{-1}
\end{aligned}
$$

The initial temperature $T_{0}$ is $25^{\circ} \mathrm{C}$, that the steam temperature $T_{S}$ is $100^{\circ} \mathrm{C}$, and that we wish to find the time needed for the temperature $T$ to reach $50^{\circ} \mathrm{C}$.

$$
\ln \left(\frac{50-100}{25-100}\right)=-0.00032 t
$$

Solving for $t$ indicates that 1270 s (or approximately 21 min ) are required for the water in the vessel to reach a temperature of $50^{\circ} \mathrm{C}$.

