# Chemical and Petroleum Refining Engineering <br> Engineering Analysis / $3^{\text {rd }}$ stage <br> <br> Chapter 3 <br> <br> Chapter 3 <br> Modeling with First-Drder Differential Equations 

### 3.1 Linear Models

## Example (1) Bacterial Growth

Aculture initially has $\mathrm{P}_{0}$ number of bacteria. At $\mathrm{t}=1 \mathrm{~h}$ the number of bacteria is measured to be $\frac{3}{2} P_{0}$, determine the time necessary for the number of bacteria to triple.

$$
\begin{gathered}
\frac{d P}{d t}=k P \quad \text { at } t_{o}=0 \text { and } P(0)=P_{o}, \quad \text { at } t=1 \text { and } P(1)=\frac{3}{2} P_{o} \\
P(t)=c e^{k t} \\
\text { at } t=0 P(0)=P_{o}=c e^{o} \Rightarrow c=P_{o} \\
\text { at } t=1 P(1)=\frac{3}{2} P_{o}=P_{o} e^{k} \Rightarrow k=0.4055
\end{gathered}
$$

## Example 2 Half-Life of Plutonium

A breeder reactor converts relatively stable uranium-238 into the isotope plutonium- 239. After 15 years it is determined that $0.043 \%$ of the initial amount $A_{0}$ of plutonium has disintegrated. Find the half-life of this isotope.

$$
\begin{gathered}
\frac{d A}{d t}=k A \quad A(0)=A_{0} \\
A(t)=A_{0} e^{k t}
\end{gathered}
$$

If $0.043 \%$ of the atoms of $A_{0}$ have disintrgrated, then $99.957 \%$ of the substance remains.

$$
\begin{gathered}
0.99957 A_{0}=A_{0} e^{15 k} \Rightarrow k=-0.00002867 \\
A(t)=A_{0} e^{-0.00002867 t} \\
0.5 A_{0}=A_{0} e^{-0.00002867 t} \Rightarrow t=24,180 y r
\end{gathered}
$$

Note that


Growth $(\mathrm{k}>0)$ and decay $(\mathrm{k}<0)$

## Example 3: Age of a Fossil

Afossilized bone is found to contain $0.1 \%$ of its original amount of $\mathrm{C}-14$. Determine the age of the fossil. The half-life of C-14 was approximately 5730 years

$$
\begin{gathered}
\frac{d A}{d t}=k A \\
A(t)=A_{0} e^{k t} \\
\frac{1}{2} A_{0}=A_{0} e^{5730 k} \Rightarrow k=-0.00012097 \\
0.001 A_{0}=A_{0} e^{-0.00012097 t} \Rightarrow t=57,100 y r
\end{gathered}
$$

## Example 4: Cooling of a Cake

When a cake is removed from an oven, its temperature is measured at $300^{\circ} \mathrm{F}$. Three minutes later its temperature is $200^{\circ} \mathrm{F}$. How long will it take for the cake to cool off to a room temperature of $70^{\circ} \mathrm{F}$ ?

$$
\begin{gathered}
\frac{d T}{d t}=k(T-70), \quad T(0)=300 \\
\frac{d T}{T-70}=k d t \\
T=70+c_{2} e^{k t} \\
T(0)=300=70+c_{2} \Rightarrow c_{2}=230 \\
T(3)=200=70+230 e^{3 k} \Rightarrow k=-0.19018 \\
T=70+230 e^{-0.19018 t}
\end{gathered}
$$



## Example 5: Mixture of Two Salt Solutions

The large tank holds 300 gallons of a brine solution. Salt was entering and leaving the tank; a brine solution was being pumped into the tank at the rate of $3 \mathrm{gal} / \mathrm{min}$; it mixed with the solution there, and then the mixture was pumped out at the rate of $3 \mathrm{gal} / \mathrm{min}$. The concentration of the salt in the inflow, or solution entering, was $2 \mathrm{lb} / \mathrm{gal}$, If 50 pounds of salt were dissolved initially in the 300 gallons, how much salt is in the tank after a long time?


## Example 5 Revisited

If the well-stirred solution in Example 5 is pumped out at a slower rate of $2 \mathrm{gal} / \mathrm{min}$. then liquid will accumulate in the tank at the rate of $r_{i n}-r_{o u t}=(3-2) \frac{\mathrm{gal}}{\mathrm{min}}=1 \mathrm{gal} / \mathrm{min}$. After t minutes,

$$
(1 \mathrm{gal} / \mathrm{min})(t \mathrm{~min})=t \mathrm{gal}
$$

The tank will contain $300+t$ gallons of brine. The concentration of salt

$$
\frac{d A}{d t}=R_{\text {in }}-R_{\text {out }}
$$

$$
\begin{gathered}
\frac{d A}{d t}=\left(2 \frac{l b}{g a l}\right)\left(3 \frac{g a l}{\min }\right)-\left(\frac{A(t)}{300+t} \frac{l b}{g a l}\right)\left(2 \frac{g a l}{\min }\right) \\
\frac{d A}{d t}-\frac{2 A}{300+t}=6, \quad A(0)=50 l b
\end{gathered}
$$

The integrating factor is

$$
e^{\int 2 d t /(300+t)}=e^{2 \ln (300+t)}=(300+t)^{2}
$$

and so after multiplying by the factor the equation is cast into the form

$$
\begin{gathered}
\frac{d}{d t}\left[(300+t)^{2} A\right]=6(300+t)^{2} \\
(300+t)^{2} A=2(300+t)^{3}+c, A(0)=50
\end{gathered}
$$

Solving for A

$$
A(t)=600+2 t-\left(4.95 \times 10^{7}\right)(300+t)^{-2}
$$

### 3.2 Nonlinear Models

## Chemical Reactions

Suppose that a grams of chemical A are combined with b grams of chemical B. If there are M parts of A and N parts of B formed in the compound and $\mathrm{X}(\mathrm{t})$ is the number of grams of chemical C formed, then the number of grams of chemical A and the number of grams of chemical B remaining at time $t$ are, respectively,

$$
a-\frac{M}{M+N} X \quad \text { and } \quad b-\frac{N}{M+N} X
$$

The law of mass action states that when no temperature change is involved, the rate at which the two substances react is proportional to the product of the amounts of A and B that are untransformed (remaining) at time t :

$$
\frac{d X}{d t} \propto\left(a-\frac{M}{M+N} X\right)\left(b-\frac{N}{M+N} X\right)
$$

It factor out $\mathrm{M} /(\mathrm{M}+\mathrm{N})$ from the first factor and $\mathrm{N} /(\mathrm{M}+\mathrm{N})$ from the second factor

$$
\begin{gathered}
\frac{d X}{d t}=k(\alpha-X)(\beta-X) \\
\alpha=\frac{a(M+N)}{M} \text { and } \beta=\frac{b(M+N)}{N}
\end{gathered}
$$

## Example 2: Second-Order Chemical Reaction

A compound C is formed when two chemicals A and B are combined. The resulting reaction between the two chemicals is such that for each gram of A, 4 grams of $B$ is used. It is observed that 30 grams of the compound C is formed in 10 minutes.Determine the amount of C at time t if the rate of the reaction is proportional to the amounts of A and B remaining and if initially there are 50 grams of A and 32 grams of B . How much of the compound C is present at 15 minutes? Interpret the solution as $t \rightarrow \infty$.

$$
\begin{gathered}
\frac{d X}{d t}=k(a-X)(\beta-X) \\
\alpha=(50) \frac{(1+4)}{1}=250, \beta=(32) \frac{(1+4)}{4}=40 \\
\frac{d X}{d t}=k(250-X)(40-X)
\end{gathered}
$$

By separation of variables and partial fractions

$$
\begin{gathered}
\frac{-\frac{1}{210}}{(250-X)} d X+\frac{\frac{1}{210}}{(40-X)} d X=k d t \\
\ln \frac{(250-X)}{(40-X)}=210 k t+c_{1} \\
\frac{(250-X)}{(40-X)}=c_{2} e^{210 k t}
\end{gathered}
$$

At $t=0, X=0 \rightarrow c_{2}=\frac{25}{4}$
At $t=10, X=30 \rightarrow k=0.1258$

$$
X(t)=1000 \frac{1-e^{-0.1258 t}}{25-4 e^{-0.1258 t}}
$$

$$
\begin{aligned}
& X(15)=34.78 \text { grams } \\
& \lim _{t \rightarrow \infty} X(t)=40 \text { grams }
\end{aligned}
$$

### 3.3 Modeling With Systems Of First-Order Des

Mixtures Consider the two tanks: tank $A$ contains 50 gallons of water in which 25 pounds of salt is dissolved. Suppose tank $B$ contains 50 gallons of pure water. Liquid is pumped into and out of the tanks as indicated in the following figure; the mixture exchanged between the two tanks and the liquid pumped out of $\operatorname{tank} B$ are assumed to be well stirred. To construct a mathematical model that describes the number of pounds $x_{1}(t)$ and $x_{2}(t)$ of salt in tanks $A$ and $B$, respectively, at time $t$.


Input rate of salt
Output rate of salt

$$
\begin{gathered}
\frac{d x_{1}}{d t}=\overbrace{\left(\frac{3 g a l}{\min }\right)\left(0 \frac{l b}{g a l}\right)+\left(\frac{1 g a l}{\min }\right)\left(\frac{x_{2}}{50} \frac{l b}{g a l}\right)}-\overbrace{\left(\frac{4 g a l}{\min }\right)\left(\frac{x_{1}}{50} \frac{l b}{g a l}\right)} \\
\frac{d x_{1}}{d t}=-\frac{2}{25} x_{1}+\frac{1}{50} x_{2}
\end{gathered}
$$

Input rate of salt
Output rate of salt

$$
\begin{gathered}
\frac{d x_{1}}{d t}=\overbrace{\left(\frac{4 g a l}{\min }\right)\left(\frac{x_{1}}{50} \frac{l b}{g a l}\right)}-\overbrace{\left(\frac{3 g a l}{\min }\right)\left(\frac{x_{2}}{50} \frac{l b}{g a l}\right)+\left(\frac{1 g a l}{\min }\right)\left(\frac{x_{2}}{50} \frac{l b}{g a l}\right)}^{\frac{d x_{2}}{d t}=\frac{2}{25} x_{1}-\frac{2}{25} x_{2}}
\end{gathered}
$$

The linear system

$$
\begin{aligned}
\frac{d x_{1}}{d t} & =-\frac{2}{25} x_{1}+\frac{1}{50} x_{2} \\
\frac{d x_{2}}{d t} & =\frac{2}{25} x_{1}-\frac{2}{25} x_{2}
\end{aligned}
$$

