



CHE 362

MODELLING AND SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS IN CHEMICAL ENGINEERING PROCESSES

INTRODUCTION

In solving engineering problem (usually of a physical nature), we first have to formulate the problem as a mathematical expression in terms of variables, functions, and equations. Such an expression is known as a mathematical model of the given problem. The process of setting up a model, solving it mathematically, and interpreting the result in physical or other terms is called mathematical modeling or, briefly, modeling.

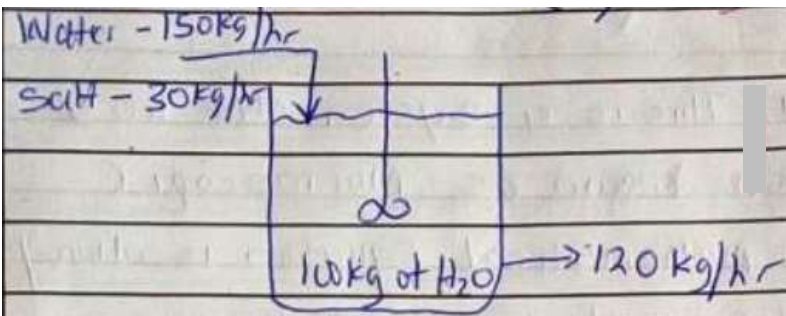
Modeling needs experience, which we shall gain by considering various examples and problems. Computer applications such as MATLAB, MATCAD and others may often help in solving but rarely in setting up models. Many physical problems in chemical engineering usually results into ODEs, therefore its necessary to be able to solve every form of ODEs problem either manually or using computer applications. ODEs can be first, second or higher order and can be solved either by using analytical methods or numerical methods, most of which have been considered in ENG 282, ENG 381 and ENG 382.

Example:

1. A perfectly mixed stirred-tank containing 100 kg of water initially is further filled with 150 kg of water and 30 kg of salt per hour, while the solution is taken out at a rate of 120 kg per hour. Assuming a complete mixing,
 - a. model a differential equation that describes the time rate of change of salt composition in the tank.
 - b. determine the amount of salt in the tank at 9 mins. using MATLAB and MATCAD

Note: use a step value of 0.05 min.

(a)



Total Material balance: $I_N - O_N = \text{Acc}$

$$(150 + 30) - 120 = \frac{dM}{dt}$$

$$\frac{dM}{dt} = 60$$

$$\int_{100}^M dM = 60 \int_0^t dt$$

$$M = 60t + 100$$

\Rightarrow Component Material balance:

$$30 - 120x = \frac{dMx}{dt}$$

$$30 - 120x = M \frac{dx}{dt} + x \frac{dM}{dt}$$

$$30 - 120x = (60t + 100) \frac{dx}{dt} + 60x$$

$$\frac{dx}{dt} = \frac{30 - 180x}{100 + 60t}$$

(b)

i. **MATLAB: Solution using inbuilt function (ode45)**

```
commandwindow
clear
clc
f =@ (t, x) [(30-(180*x))/(100+(60*t))]
tspan=[0:0.05:0.25]
x=0
[t,x] = ode45(f,tspan,x)
plot(t,x)
title('Graph of x against t')
xlabel('t'), ylabel('x')
```

Solution:

f =

@(t,x)[(30-(180*x))/(100+(60*t))]

tspan =

0 0.0500 0.1000 0.1500 0.2000 0.2500

x =

0

t =

0

0.0500

0.1000

0.1500

0.2000

0.2500

x =

0

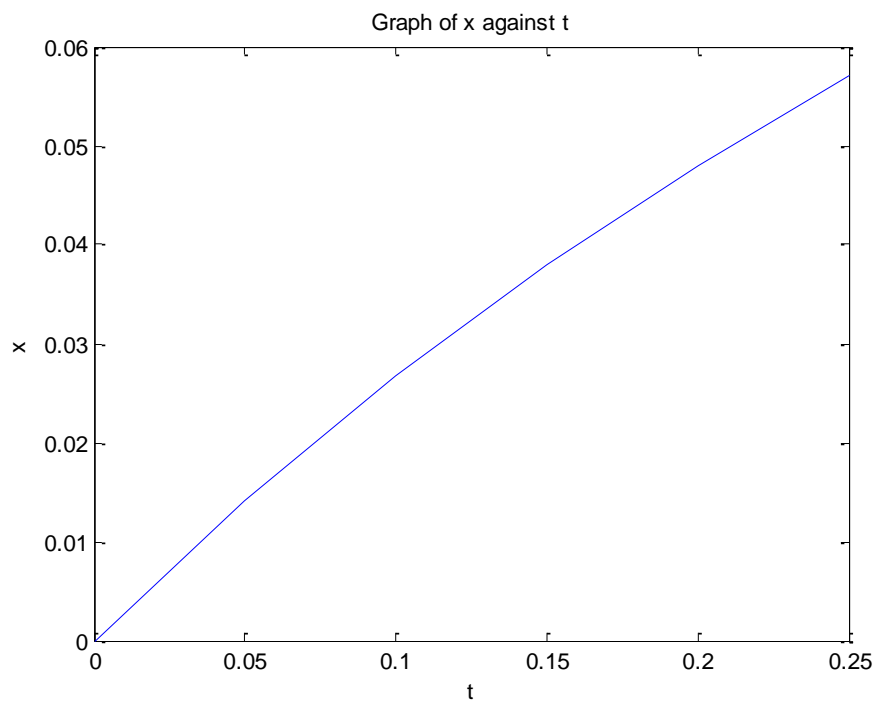
0.0141

0.0267

0.0380

0.0480

0.0571



ii. **MATLAB: Solution using numerical method (euler's method)**

```
commandwindow
clear
clc

t0=0
tn=0.25
h=0.05
t = t0:h:tn
n=length(t)
x(1)=0

for i=1:n-1
    xprime(i+1) = (30-(180*x(i)))/(100+(60*t(i)))
    x(i+1)=x(i)+h*xprime(i)
end
tablo=[x' xprime']
plot(t,x), grid minor
```