1.2 Runge-Kutta Method

To find numerical solution to the initial value problem $\frac{dy}{dx} = f(x,y),\ y(0) = y_0$ using Runge-Kutta method we have the following consideration (This method gives more accurate result compared to Euler's method):

$$k_1 = f(x_n, y_n)$$
$$k_2 = f(x_n + h/2, y_n + hk_1/2)$$
$$k_3 = f(x_n + h/2, y_n + hk_2/2)$$
$$k_4 = f(x_{n+1}, y_n + hk_3)$$
$$y_{n+1} = y_n + \frac{h}{6}\cdot(k_1 + 2k_2 + 2k_3 + k_4)$$

Exercise 3: Simple first order ODE

Consider the following initial value problem:

$$\frac{dx}{dt} = t^2 + t$$

With the initial condition: x (0) = 0.5 write a code to solve this equation using Runge-Kutta integration method.

```
t_in=0; t_fin=2; nsteps=10; dt=(t_fin-t_in)/nsteps;
t(1)=t_in; x(1)= 0.5;
f=inline('t^2+t') ;
for n=1:nsteps
t(n+1)=t(n)+dt ;
k1 = f(t(n));
k2 = f( t(n)+dt/2);
k3 = f( t(n) + dt/2);
k4 = f( t(n) + dt);
x(n+1)=x(n)+(1/6)*dt*(k1 +2*k2 + 2*k3 +k4);
end
x_analytical=t.^3/3+t.^2/2+0.5;
plot (t,x,'k*:',t,x_analytical,'k+-')
xlabel('Time (t)'),ylabel('x(t)')
legend('Runge Kutta integration','analytical integration')
```

The results of this program are plotted in Figure (4), the error between analytical and Runge- Kutta integration method is too small.

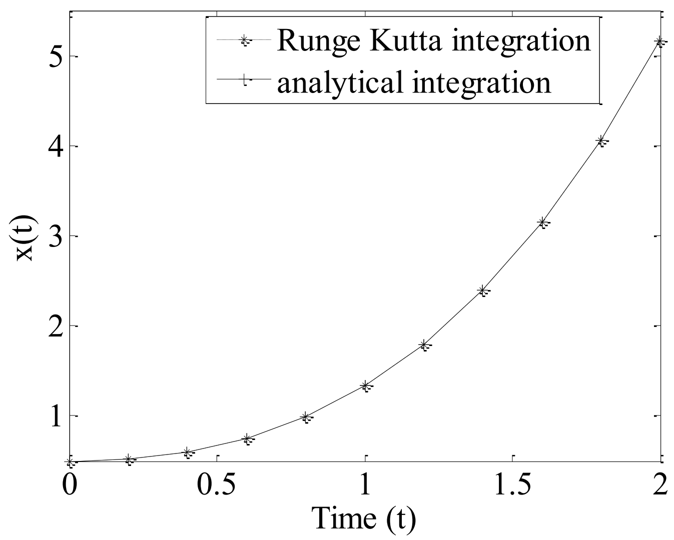

Figure (4): analytical and Runge-Kutta integration for $\frac{dx}{dt} = t^2 + t$ function

Exercise 4:

Solve the following equation using both Eular and Runge-Kutta method and to approximate the solution of the initial value problem $\frac{dy}{dx} = x + y, \quad y(0) = 1$ with step size h = 0.1.

Solution:

Eular	Runge Kutta
clear all, clc,format short x(1)=0; y(1)=1; h=0.5 for i=1:5 x(i+1)=x(i)+h; dy=x(i)+y(i); y(i+1)=y(1)+h*dy; end y_exact= -1-x+2*exp(x); error=y_exact-y table=[x',y',y_exact',error']	**clear all, clc,format short x(1)=0; y(1)=1; h=0.1; f=inline('-0.5*x/y'); % f(x,y) = x+y for i=1:6 x(i+1)=x(i)+h; k1 = f(x(i),y(i)); k2 = f(x(i)+h/2,y(i)+k1*h/2); k3 = f(x(i) + h/2,y(i)+k2*h/2); k4 = f(x(i) + h,y(i)+k3*h); y(i+1)=y(i)+(1/6)*h*(k1 +2*k2 + 2*k3 +k4); end y_exact= -1-x+2*exp(x); error=y_exact-y table=[x',y',y_exact',error']**

table =				table =			
0	1.0000	1.0000	0	0	1.0000	1.0000	0
0.1000	1.1000	1.1103	0.0103	0.1000	1.1103	1.1103	0.0000
0.2000	1.1200	1.2428	0.1228	0.2000	1.2428	1.2428	0.0000
0.3000	1.1320	1.3997	0.2677	0.3000	1.3997	1.3997	0.0000
0.4000	1.1432	1.5836	0.4404	0.4000	1.5836	1.5836	0.0000
0.5000	1.1543	1.7974	0.6431	0.5000	1.7974	1.7974	0.0000

Note: compare the results of both two methods (Eular and Runge Kutta) with the results of modified Eular method that supported in Exercise 3.

1. Integration two or more coupled first-order ODE's

Consider the following system of first-order ODE's describing the dependence of two dependent variables y and z on one independent variable x:

$$\frac{dy}{dx} = f(x, y, z)$$

$$\frac{dz}{dx} = g(x, y, z)$$

These two differential equations are coupled and must be integrated simultaneously because both equations involve both dependent variables.

Initial conditions are required giving the values of y and z at the initial value of x. The algorithm for 4th-order Runge-Kutta integration of two coupled ODEs is:

$$y_{i+1} = y_i + (h/6)[(k_{11} + 2k_{12} + 2k_{13} + k_{14}]$$

$$z_{i+1} = z_i + (h/6)[(k_{21} + 2k_{22} + 2k_{23} + k_{24]}$$

$$k_{11} = f(x_i, y_i, z_i)$$

$$k_{21} = g(x_i, y_i, z_i)$$

$$k_{12} = f(x_i + 0.5h, y_i + 0.5hk_{11}, z_i + 0.5hk_{21})$$

$$k_{22} = g(x_i + 0.5h, y_i + 0.5hk_{11}, z_i + 0.5hk_{21})$$

$$k_{13} = f(x_i + 0.5h, y_i + 0.5hk_{12}, z_i + 0.5hk_{22})$$

$$k_{23} = g(x_i + 0.5h, y_i + 0.5hk_{12}, z_i + 0.5hk_{22})$$

$$k_{14} = f(x_i + h, y_i + hk_{13}, z_i + hk_{23})$$

$$k_{24} = g(x_i + h, y_i + hk_{13}, z_i + hk_{23})$$

Examples include exothermic reaction in an unsteady-state continuous stirred tank reactor and exothermic reaction in a plug flow reactor with heat exchange through the reactor walls.

From the one and two ODE examples, you can extend the method to integration of three coupled ODE's. Three coupled ODE's would be encountered, for example, for reaction of gases in a steady-state non-isothermal plug flow reactor with significant pressure drop (dC/dx =, dT/dx =, and dP/dx=).

MATLAB Built-In Routines for solving ODES

MATLAB have several sub programs (Routines) to solve ODES;

- ode113:Variable order solution to non-stiff system
- ode15s:Variable order, multistep method for solution of stiff system
- ode23: Lower order adaptive step size routine for non-stiff systems
- ode23s:Lower order adaptive step size routine for stiff systems
- ode45: Higher order adaptive step size routine for non-stiff system

To solve the same example using MATLAB Routine, We just have to write a function which returns the rate of change of the vector x.

```
function dx = example(t,x)
dx(1,1) = t^2+t;
```

The above file named example.m must be saved in default MATLAB folder then the following code must run.

```
t_in=0;t_fin=2; nsteps=10;
dt=(t_fin-t_in)/nsteps;
Vspan = t_in:dt:t_fin;
x0=0.5;
 [t,x] = ode45('example',Vspan,x0);
plot (t,x,'k*:')
xlabel('Time (t)'),ylabel('x(t)')
legend('Runge Kutta integration')
```

The numerical solution, computed using ODE45 is given below in Figure (5)

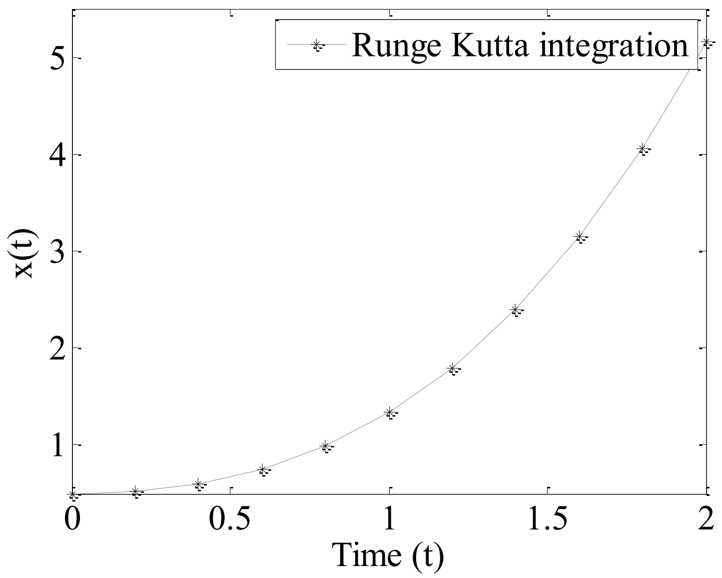

Figure (5): Solution produced by ODE45.

Exercise 4:

Let's consider a simple example of a model of a plug flow reactor that is described by a system of ordinary differential equations. A plug flow reactor is operated as shown in Figure (6) below.

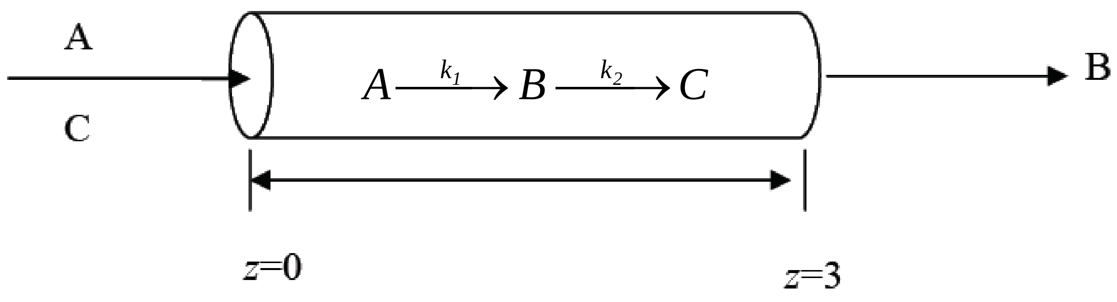

Figure (6) Isothermal plug flow reactor

The plug flow initially has only reactant A, the components A react to form component B. The mole balance for each component is given by the following differential equations

$$u\frac{dC_A}{dz} = -k_1 C_A$$
$$u\frac{dC_B}{dz} = k_1 C_A - k_2 C_B$$
$$u\frac{dC_C}{dz} = k_2 C_B$$

With the following initial values

C_A (z=0) =1 kmol/m^3 C_B (z=0) =0 C_C (z=0) =0   and k_1=2 k_2=3

If u=0.5 m/s and reactor length z=3 m. Solve the differential equations and plot the concentration of each species along the reactor length

Solution:

We'll start by writing the function defining the right hand side (RHS) of the ODEs. The following function file 'example2' is used to set up the ode solver.

```
function dC= Exercise4 ( z, C)
u = 0.5;k1=2; k2=3;
dC(1,1) = -k1 *C(1) / u;
dC(2,1) = (k1 *C(1)-k2 *C(2)) / u;
dC(3,1) = k2 *C(2)/ u;
```

Now we'll write a main script file to call ode45. CA, CB and CC must be defined within the same matrix, and so by calling CA as C(1), CB as C(2) and CC as c(3), they are listed as common to matrix C.

The following run file is created to obtain the solution:

```
clear all, clc
C0 = [1 0 0];
txspan = [0 3];
[z , C] = ode45('Exercise4', txspan, C0)
plot (z,C(:,1),'k+-',z,C(:,2),'k*:',z,C(:,3),'kd-.')
xlabel ('Length (m)');
ylabel ('Concentrations (kmol/m^3) ');
legend ('A', 'B', 'C');
```

The produced plot is as in Figure (7)

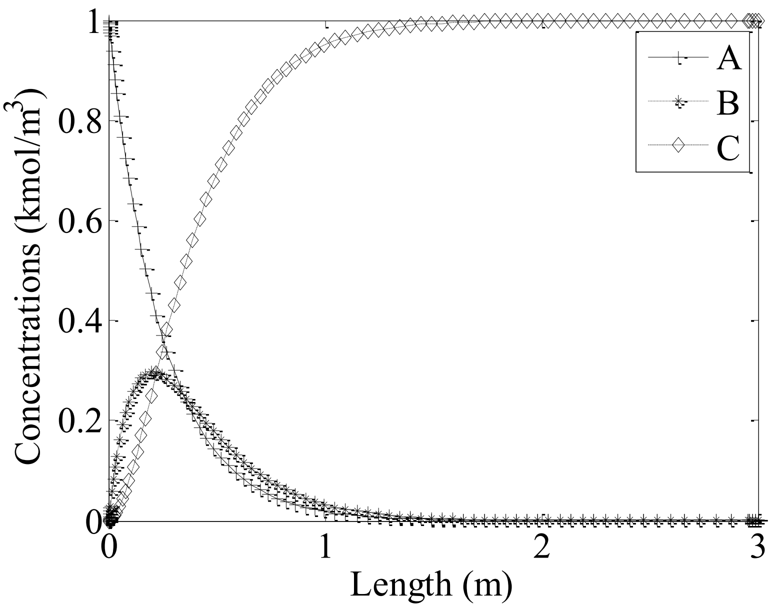

Figure (7): A, B and C concentrations along plug flow reactor

Practice Problems

1) A ball initially at 1200 K is allowed to cool down in air at an ambient temperature. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{dT}{dt} = -2.2067\times10^{-12}\,(T^4 - 81\times10^8)$$

Where T is in K and t in seconds.

Plot the temperature at time range $0 \le t \le 480$ seconds using fourth order Runge-Kutta ode45 method.

2) The concentration of salt x in a homemade soap maker is given as a function of time by

$$\frac{dx}{dt} = 37.5 - 3.5x$$

At the initial time, $t = 0$, the salt concentration in the tank is 50 g/L.

Using Runge-Kutta 4th order method and a step size of, $h = 1.5$ min, what is the salt concentration after 3 minutes (compare the numerical integration result with exact solution result)?

3) Consider two interacting tanks in series, shown in Figure (8) with outlet flow rates that are a function of the square root of tank height. Notice that the flow from tank 1 is a function of $\sqrt{h_1 - h_2}$, while the flow rate out of tank 2 is a function of $\sqrt{h_2}$.

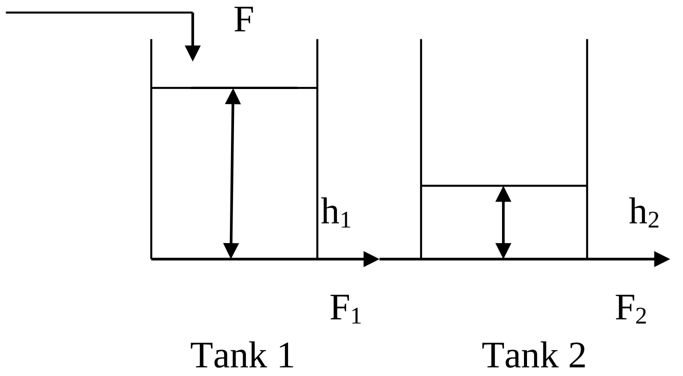

Figure (8): Interacting tanks.

The following differential equations (DE's) describe this system.

$$\frac{dh_1}{dt} = \frac{F}{A_1} - \frac{\beta_1}{A_1}\sqrt{h_1 - h_2}$$

$$\frac{dh_2}{dt} = \frac{\beta_1}{A_2}\sqrt{h_1 - h_2} - \frac{\beta_2}{A_2}\sqrt{h_2}$$

Use the following parameter values:

$$\beta_1 = 2.5\frac{ft^{2.5}}{min} \quad \beta_2 = \frac{5}{\sqrt{6}}\frac{ft^{2.5}}{min} \quad A_1 = 5ft^2 \quad A_2 = 10ft^2$$

And the input flow rate: F= 5 ft^3/min.

Solve these two DE's numerically using ***ode45*** with the initial conditions $h_1(0) = 12$ and $h_2(0) = 7$. Then plot $h_1(t)$ and $h_2(t)$ over the time range 0 to 100.