Chapter 08.04 Runge-Kutta 4th Order Method for Ordinary Differential Equations-More Examples Chemical Engineering

Example 1

The concentration of salt X in a home made soap maker is given as a function of time by

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

dt

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? **Solution**

$$dx = 37.5 - 3.5x$$

$$f(t,x) = 37.5 - 3.5x$$

$$x_{i+1} = x_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$
For $i = 0$, $t_0 = 0$, $x_0 = 50$

$$k^1 = f(t^0, x^0)$$

$$= f(0,50)$$

$$= 37.5 - 3.5(50)$$

$$= -137.5$$

$$k_2 = f\left(t_0 + \frac{1}{2}h, x_0 + \frac{1}{2}k_1h\right)$$

$$= f\left(0 + \frac{1}{2}1.5,50 + \frac{1}{2}(-137.5)1.5\right)$$

$$= f(0.75, -53.125)$$

$$= 37.5 - 3.5(-53.125)$$

$$= 223.44$$

$$k_3 = f\left(t_0 + \frac{1}{2}h, x_0 + \frac{1}{2}k_2h\right)$$

$$= f\left(0 + \frac{1}{2}1.5,50 + \frac{1}{2}(223.44)1.5\right)$$

$$= f\left(0.75, 217.58\right)$$

$$= 37.5 - 3.5(217.58)$$

$$= 37.5 - 3.5(217.58)$$

08.04.2 Chapter 08.04

$$= -724.02$$

$$k_4 = f(t_0 + h, x_0 + k_3 h)$$

$$= f(0 + 1.5, 50 + (-724.03)1.5)$$

$$= f(1.5, -1036.0)$$

$$37.5 \quad 3.5(\quad 1036.0)$$

$$\equiv 3663.6 \qquad -$$

$$x_1 = x_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$= 50 + \frac{1}{6}(-137.5 + 2(223.44) + 2(-724.02) + (3663.6))1.5$$

$$= 50 + \frac{1}{6}(2525.0)1.5$$

$$= 681.24 \text{ g/L}$$

 x_1 is the approximate concentration of salt at

$$t = t_1 = t_0 + h = 0 + 1.5 = 1.5$$

$$x(1.5) \approx x_1 = 681.24 \text{ g/L}$$
For $i = 1$, $t_1 = 1.5$, $x_1 = 681.24$

$$k_1 = f(t_1, x_1)$$

$$= f(1.5,681.24)$$

$$= -2346.8$$

$$k_2 = f\left(t_1 + \frac{1}{2}h, x_1 + \frac{1}{2}k_1h\right)$$

$$= f\left(1.5 + \frac{1}{2}1.5, 681.24 + \frac{1}{2}(-2346.8)1.5\right)$$

$$= f\left(2.25, -1078.9\right)$$

$$= 37.5 - 3.5(-1078.9)$$

$$= 3813.6$$

$$k_3 = f\left(t_1 + \frac{1}{2}h, x_1 + \frac{1}{2}k_2h\right)$$

$$= f\left(1.5 + \frac{1}{2}1.5, 681.24 + \frac{1}{2}(3813.6)1.5\right)$$

$$= f\left(2.25, 3541.4\right)$$

$$= 37.5 - 3.5(3541.4)$$

$$= -12358$$

$$k_4 = f(t_1 + h, x_1 + k_3h)$$

$$= f\left(1.5 + 1.5, 681.24 + (-12358)1.5\right)$$

$$= f\left(3, -17855\right)$$

$$= 37.5 - 3.5(-17855)$$

$$= 37.5 - 3.5(-17855)$$

=62530

$$\begin{aligned} x_2 &= x_1 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \\ &= 681.24 + \frac{1}{6}(-2346.8 + 2(3813.6) + 2(-12358) + 62530)1.5 \\ &= \frac{1}{6}(43096)1.5 \\ &= 11455 \text{ g/L} \end{aligned}$$

 x_2 is the approximate concentration of salt at

$$t_2 = t_1 + h = 1.5 + 1.5 = 3 \text{ min}$$

 $x(3) \approx x_2 = 11455 \text{ g/L}$

The exact solution of the ordinary differential equation is given by

$$x(t) = 10.714 + 39.286e^{-3.5t}$$

The solution to this nonlinear equation at $t = 3 \min is$

$$x(3) = 10.715 \text{ g/L}$$

Figure 1 compares the exact solution with the numerical solution using Runge-Kutta 4th order method using different step sizes.

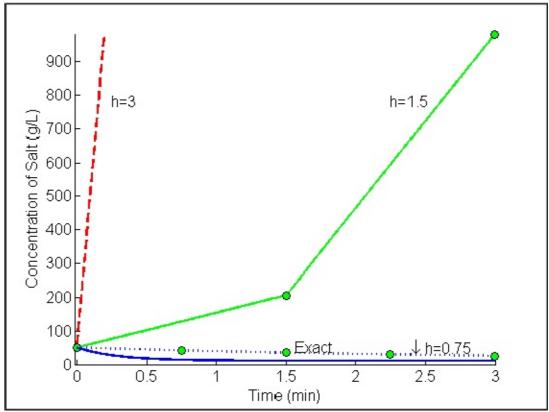


Figure 1 Comparison of Runge-Kutta 4th order method with exact solution for different step sizes.

Table 1 and Figure 2 show the effect of step size on the value of the calculated temperature at t = 3 min.

08.04.4 Chapter 08.04

Table 1 Value of concentration of salt at 3 minutes for different step sizes.

Step size,	x(3)	E_t	€ _t %
3	14120	_14109	131680
1.5	11455	-11444	106800
0.75	25.559	-14.843	138.53
0.375	10.717	-0.0014969	0.013969
0.1875	10.715	-0.00031657	0.0029544

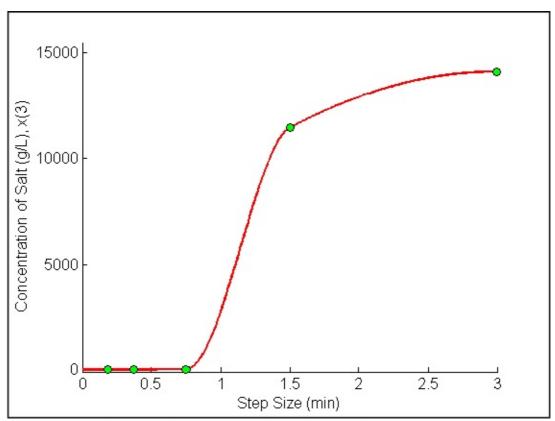


Figure 2 Effect of step size in Runge-Kutta 4th order method.

In Figure 3, we are comparing the exact results with Euler's method (Runge-Kutta 1^{st} order method), Heun's method (Runge-Kutta 2^{nd} order method) and Runge-Kutta 4^{th} order method.

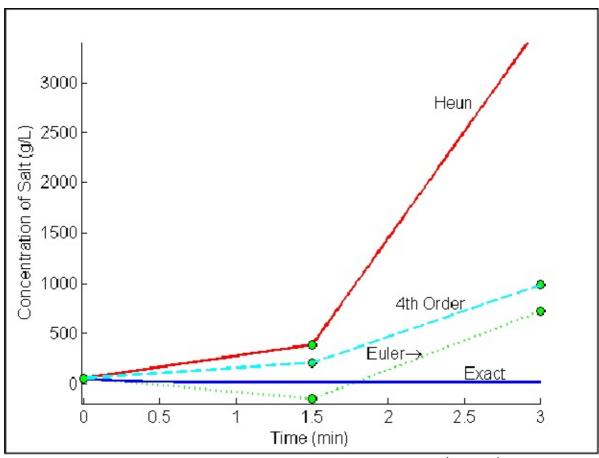


Figure 3 Comparison of Runge-Kutta methods of 1st, 2nd, and 4th order.