Ordinary Differential Equation in MathCad

(Dr. Tom Co 10/23/2008)

Introduction

Several chemical engineering processes are modeled using differential equations. Ordinary differential equations are often described in an explicit form given by

$$\frac{d}{dx}\mathbf{y} = D(x, \mathbf{y}; \alpha_1, \ldots, \alpha_k) \qquad \mathbf{y}(0) = \mathbf{y}_o$$

where x is the independent variable, **y** is the dependent variable/vector of variables, $\alpha_1, \ldots, \alpha_k$ are parameters and $\mathbf{y_o}$ is the initial value of **y**.

Example 1:

$$\frac{d}{dt}C = \frac{1}{\tau}(\,C_{A0} - C_A) - k_0 e^{-\frac{\beta}{T}} C_A$$

$$\frac{d}{dt}T = \frac{1}{\tau}(1+\kappa)(T - T_C) + \left(\frac{-\Delta H_R}{c_{ps}}\right)\left(\frac{k_0 e^{-\frac{\beta}{T}} C_A}{C_{A0}}\right)$$

$$T(0) = T_{init}$$
$$C(0) = C_{init}$$

Then C and T are dependent variables, while t is the independent variable, and ΔH_R, k_0, β, c_{ps}, C_{A0}, κ and C_{A0} are process parameters.

In several cases, the analytical solutions may be too difficult to solve. Numerical solutions often yield acceptable approximate solutions. One of the most popular is the Runge-Kutta method (see Appendix for a more detailed description).

MathCad Procedure : (for **Rkadapt( )**)

1. Rewrite equations such that it contains only first order derivatives.

$$\frac{d}{dx}y_1 = f_1(x, y_1, \ldots, y_n; \alpha_1, \ldots, \alpha_k)$$
$$\vdots$$
$$\frac{d}{dx}y_n = f_1(x, y_1, \ldots, y_n; \alpha_1, \ldots, \alpha_k)$$

2. Gather the initial conditions into an array.

$$\mathbf{y}_{init} := \begin{pmatrix} y_{10} \\ \vdots \\ y_{n0} \end{pmatrix}$$

3. Gather the functions $f_1(\,), \dots, f_n(\,)$ into an array.

$$D(\alpha_1, \dots, \alpha_k, x, \mathbf{y}) := \begin{pmatrix} f_1(x, y_1, \dots, y_n; \alpha_1, \dots, \alpha_k) \\ \vdots \\ f_n(x, y_1, \dots, y_n; \alpha_1, \dots, \alpha_k) \end{pmatrix}$$

4. Solve the differential equations using **Rkadapt( )** ,

$$soln := \mathbf{Rkadapt}\left(y_{init}, x_{init}, x_{final}, \#steps, D\right)$$

5. Extract the columns to the appropriate variables: x is the first column, y_1 is the second column, ... , y_n is the $(n+1)^{th}$ column.

Example 2: (Using equations given in example 1)

FIXED PARAMETERS & FUNCTIONS:

$$\tau := 0.2hr \qquad k_0 := 450 \cdot \frac{1}{hr} \qquad \beta := 1400K \qquad \kappa := 80 \qquad c_{ps} := 30 \frac{J}{mol \cdot K}$$

$$\Delta H_R(T) := \left[-151000 + 2 \cdot \left(\frac{T}{K} - 298.15 \right) \right] \cdot \frac{J}{mol} \qquad C_{A0} := 0.5 \frac{mol}{cm^3} \qquad T_c := 273.15K$$

ARRAY OF DERIVATIVE EQUATIONS:

$$D(t,y) := \begin{bmatrix} \dfrac{\dfrac{1}{\tau} \cdot \left[C_{A0} - \left(y_0 \cdot \dfrac{mol}{cm^3} \right) \right] - \left[k_0 \cdot exp\left(\dfrac{-\beta}{y_1 \cdot K} \right) \cdot \left(y_0 \cdot \dfrac{mol}{cm^3} \right) \right]}{\dfrac{mol}{cm^3 \cdot hr}} \\ \dfrac{\dfrac{1}{\tau} \cdot (1 + \kappa) \cdot \left[T_c - (y_1 \cdot K) \right] + \dfrac{-\Delta H_R(y_1 \cdot K)}{c_{ps}} \cdot \left[k_0 \cdot exp\left(\dfrac{-\beta}{y_1 \cdot K} \right) \cdot \left(\dfrac{y_0 \cdot \dfrac{mol}{cm^3}}{C_{A0}} \right) \right]}{\dfrac{K}{hr}} \end{bmatrix}$$

INITIAL CONDITIONS:

$$C_{A\_init} := 0.3 \frac{mol}{cm^3}$$

$$T_{init} := 500K \qquad y_{init} := \begin{pmatrix} \dfrac{C_{A\_init}}{\dfrac{mol}{cm^3}} \\ \dfrac{T_{init}}{K} \end{pmatrix}$$

RUNGE-KUTTA SOLUTION:

$$soln := Rkadapt\left(y_{init}, 0, 0.5, 200, D\right)$$

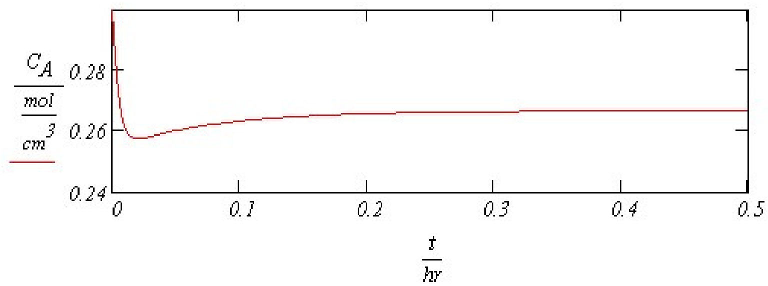
soln =

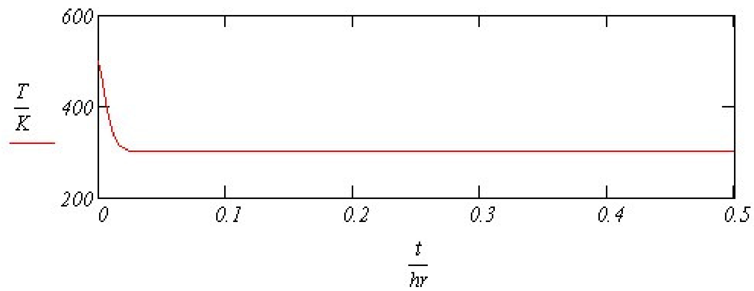
	0	1	2
0	0	0.3	500
1	$2.5\cdot10^{-3}$	0.284	469.572
2	$5\cdot10^{-3}$	0.273	430.841
3	$7.5\cdot10^{-3}$	0.266	392.363
4	0.01	0.262	360.465
5	0.013	0.259	337.413
6	0.015	0.258	322.312

$$t := soln^{\langle 0\rangle}\cdot hr$$

$$C_A := soln^{\langle 1\rangle}\cdot\frac{mol}{cm^3}$$

$$T := soln^{\langle 2\rangle}\cdot K$$





Appendix A: 4th Order Runge-Kutta Method

For a differential equation given by

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

evaluate the following terms:

$$\begin{aligned}
\delta_1 &= \Delta x \cdot f(x_k, y_k) \\
\delta_2 &= \Delta x \cdot f\left(x_k + \frac{1}{2}\Delta x, y_k + \frac{1}{2}\delta_1\right) \\
\delta_3 &= \Delta x \cdot f\left(x_k + \frac{1}{2}\Delta x, y_k + \frac{1}{2}\delta_2\right) \\
\delta_4 &= \Delta x \cdot f(x_k + \Delta x, y_k + \delta_3)
\end{aligned}$$

then the next iterated value of y is given by

$$y_{k+1} = y_k + \frac{1}{6}(\delta_1 + 2\delta_2 + 2\delta_3 + \delta_4)$$

(For an Excel implementation,

link to: **http://www.chem.mtu.edu/~tbco/cm416/RKTutorial.html**)