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

\[ \frac{d}{dx} y = D(x, y; \alpha_1, ..., \alpha_k) \quad y(0) = y_0 \]

where \( x \) is the independent variable, \( y \) is the dependent variable/vector of variables, \( \alpha_1, ..., \alpha_k \) are parameters and \( y_0 \) is the initial value of \( y \).

Example 1:

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

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

\[ T(0) = T_{init} \]
\[ C(0) = C_{init} \]

Then \( C \) and \( T \) are dependent variables, while \( t \) is the independent variable, and \( \Delta H_R, k_0, \beta, c_{ps}, C_{A0}, \kappa \) 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.

\[ \frac{d}{dx} y_1 = f_1(x, y_1, ..., y_n; \alpha_1, ..., \alpha_k) \]

\[ \vdots \]

\[ \frac{d}{dx} y_n = f_1(x, y_1, ..., y_n; \alpha_1, ..., \alpha_k) \]
2. Gather the initial conditions into an array.

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

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

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

4. Solve the differential equations using \texttt{Rkadapt()}.

\[ \text{soln} := \texttt{Rkadapt}(\mathbf{y}_{\text{init}}, x_{\text{init}}, x_{\text{final}}, \#\text{steps}, D) \]

5. Extract the columns to the appropriate variables: \( x \) is the first column, \( y_1 \) is the second column, \( \ldots \), \( y_n \) is the \((n + 1)^{th}\) column.
Example 2: (Using equations given in example 1)

**FIXED PARAMETERS & FUNCTIONS:**

\[ \tau := 0.2 \text{ hr} \quad k_0 := 450 \frac{1}{\text{hr}} \quad \beta := 1400 \text{K} \quad \kappa := 80 \quad c_{ps} := 30 \frac{J}{\text{mol.K}} \]

\[ \Delta H_R(T) := \left[ -151000 + 2 \left( \frac{T}{K} - 208.15 \right) \right] \frac{J}{\text{mol}} \quad C_{AO} := 0.5 \frac{\text{mol}}{\text{cm}^3} \quad T_c := 273.15 \text{K} \]

**ARRAY OF DERIVATIVE EQUATIONS:**

\[
D(t, \gamma) := \left[ \frac{1}{\tau} \frac{C_A - \left( y_0 \frac{\text{mol}}{\text{cm}^3} \right)}{\text{cm}^3 \cdot \text{hr}} - \frac{k_0 \exp \left( -\frac{\beta}{y_1 \cdot K} \right) \left( y_0 \frac{\text{mol}}{\text{cm}^3} \right)}{\text{cm}^3 \cdot \text{hr}} \right] + \frac{\Delta H_R(y_1 \cdot K)}{c_{ps}} \left[ k_0 \exp \left( -\frac{\beta}{y_1 \cdot K} \right) \left( y_0 \frac{\text{mol}}{\text{cm}^3} \right) \right]
\]

**INITIAL CONDITIONS:**

\[ C_{A, \text{init}} := 0.3 \frac{\text{mol}}{\text{cm}^3} \]

\[ T_{\text{init}} = 500 \text{K} \]
RUNGE-KUTTA SOLUTION:

\[ soln := \text{Readapt}(y_{\text{init}}, 0, 0.5, 200, D) \]

\[
\begin{array}{|c|c|c|c|}
\hline
& 0 & 1 & 2 \\
\hline
0 & 0 & 0.3 & 800 \\
1 & 2.5103 & 0.294 & 433.572 \\
2 & 5.103 & 0.273 & 438.041 \\
3 & 7.5103 & 0.266 & 392.983 \\
4 & 0.01 & 0.262 & 430.485 \\
5 & 0.013 & 0.259 & 337.413 \\
6 & 0.015 & 0.256 & 322.312 \\
\hline
\end{array}
\]

\[ t := \text{soln}(t, \text{hr}) \]

\[ C_A := \frac{\text{soln}(t, \text{mol})}{\text{cm}^3} \]

\[ T := \text{soln}(t, \text{K}) \]
Appendix A: 4th Order Runge-Kutta Method

For a differential equation given by

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

evaluate the following terms:

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

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](http://www.chem.mtu.edu/~tbco/cm416/RKTutorial.html))