Métodos numéricos en Excel (III):
Ecuaciones diferenciales

Problema:

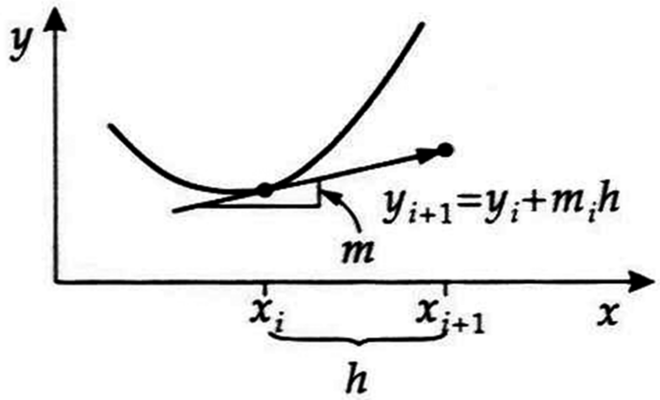
Se quiere resolver $\dfrac{dy}{dx} = f(x)$, considerando determinadas condiciones de borde, $y(x=0)=y_0$.

Solución:

Se divide la región de interés *L* en *n* intervalos de dimensión h=*L*/N y se encuentran formulas aproximadas para calcular $y_n=y(x_0+nh)$ como una función de $\{y_{n-1},y_{n-2}$, etc.}

Método de Euler
Método de Runge-Kutta

Método de Euler sencillo



Euler method, h is step size,
m_i is slope

Geometric interpretation: The new function value is approximated by the tangent at the old function value.

$$y' = f(x, y) \quad \rightarrow \quad \frac{y(x_i + h) - y(x_i)}{h} \approx f(x_i, y(x_i)) + O(h)$$

$$\rightarrow \quad y(x_i + h) \approx y(x_i) + f(x_i, y(x_i)) \cdot h \ .$$

Ejemplo: Reacción de primer orden por método de Euler simple.

$$A \rightarrow B$$

$$\frac{d[A]}{dt} = -k[A] \qquad [A]_t = [A]_0 \, e^{(-kt)}$$

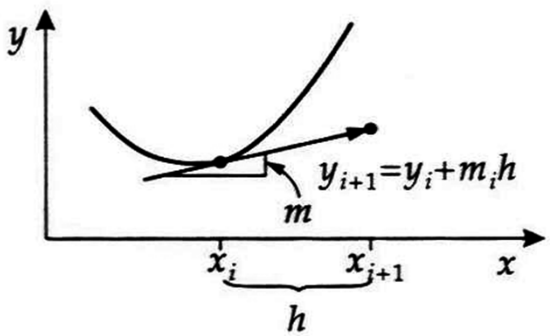
$C_0 = 0.2000$ mol L^{-1}

$K = 5 \cdot 10^{-3}$ s^{-1}

Calcular [A] desde t=0 a t s.

$$[A]_n = [A]_{n-1} + \Delta[A]$$

$$\Delta[A] = k[A]_{n-1} \cdot \Delta t$$



Euler method, *h* is step size, m_i is slope

Error del método de Euler

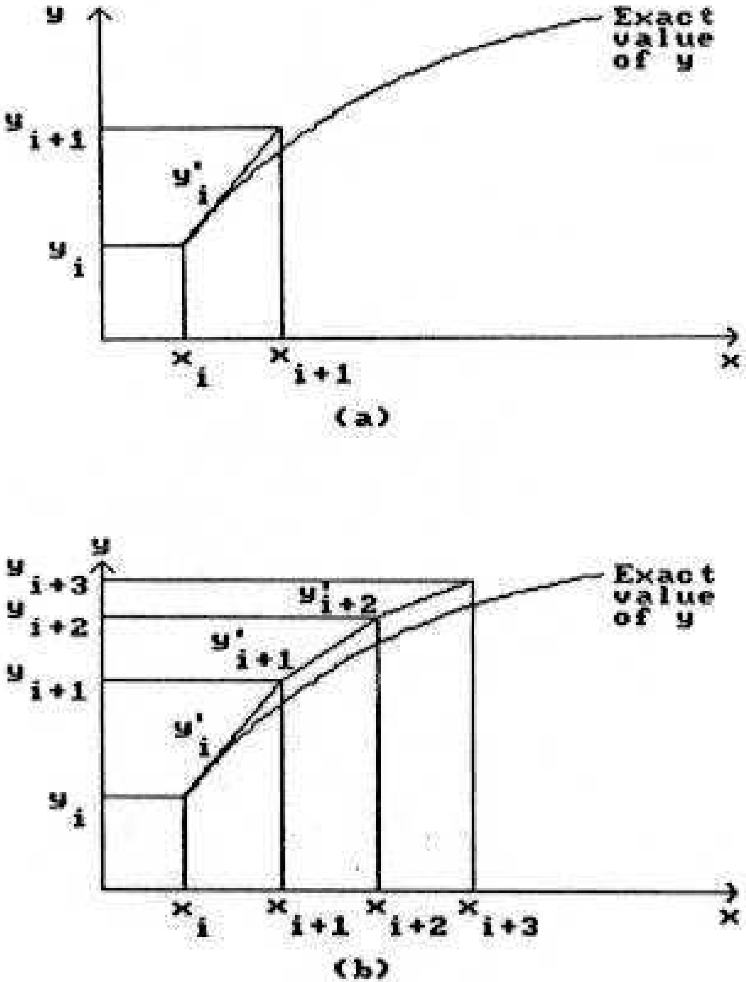
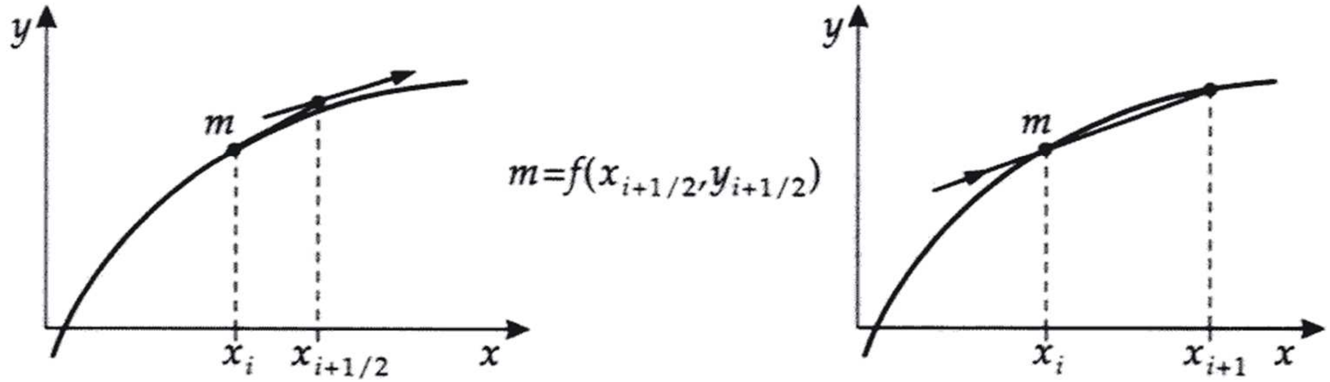


Figure 5-9 The explicit Euler method of integration: (*a*) single step, (*b*) several steps.

Método de Euler modificado

Geometric interpretation: To calculate the next function value, use the slope at intermediate point $x_{i+1/2}$ instead of the slope at point x_i.



Modified Euler method; m = slope

$$y_{i+1/2} = y_i + h \cdot f(x_i, y_i)$$
$$y'_{i+1/2} = f(x_{i+1/2}, y_{i+1/2})$$
$$y_{i+1} = y_i + h \cdot f(x_{i+1/2}, y_{i+1/2})$$

Runge-Kutta

THE RUNGE–KUTTA METHODS

The Runge–Kutta methods for numerical solution of the differential equation $dy/dx = F(x, y)$ involve, in effect, the evaluation of the differential function at intermediate points between x_i and x_{i+1}. The value of y_{i+1} is obtained by appropriate summation of the intermediate terms in a single equation. The most widely used Runge–Kutta formula involves terms evaluated at x_i, $x_i + \Delta x/2$ and $x_i + \Delta x$. The *fourth-order Runge–Kutta* equations for $dy/dx = F(x, y)$ are

$$y_{i+1} = y_i + \frac{T_1 + 2T_2 + 2T_3 + T_4}{6} \tag{9-9}$$

where

$$T_1 = F\,(x_i, y_i)\,\Delta x \tag{9-10}$$

$$T_2 = F\left(x_i + \frac{\Delta x}{2}, y_i + \frac{T_1}{2}\right)\Delta x \tag{9-11}$$

$$T_3 = F\left(x_i + \frac{\Delta x}{2}, y_i + \frac{T_2}{2}\right)\Delta x \tag{9-12}$$

$$T_4 = F\,(x_i + \Delta x, y_i + T_3)\,\Delta x \tag{9-13}$$

Runge-Kutta / Implementación

$$T_1 = -k[\mathrm{A}]_t \, \Delta x$$

$$T_2 = -k([\mathrm{A}]_t + T_1/2) \, \Delta x$$

$$T_3 = -k([\mathrm{A}]_t + T_2/2) \, \Delta x$$

$$T_4 = -k([\mathrm{A}]_t + T_3) \, \Delta x$$

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=-k*F6*DX

=-k*(F6+TA1/2)*DX

=-k*(F6+TA2/2)*DX

=-k*(F6+TA3)*DX

=F6+(TA1+2*TA2+2*TA3+TA4)/6.
```

Sumario del método RK de cuarto orden

Summary of Steps to Implement the RK Method

1. Write down the differential equations that describe the system.
2. From the set of differential equations, enter formulas in spreadsheet cells using Euler's method, **Fill Down** and make sure that the results make sense.
3. Insert five columns to the right of each variable. Label them TA1,..., TA4 and A(t), TB1,...,TB4 and B(t), etc.
4. **Copy** the Euler's method formula from the formula bar and **Paste** it into the four cells for TA1,...,TA4. The Euler's method formula should be of the form $= y_0 + F^*y_0{}^*\Delta x$. Edit it to leave only the $= F^*y_0{}^*\Delta x$ part. Modify the formulas to produce the formulas for TA1,···, TA4. TA1 remains $F^*y_0{}^*\Delta x$, TA2 becomes $F^*(y_0 + TA1/2)^*\Delta x$, TA3 becomes $F^*(y_0 + TA2/2)^*\Delta x$, TA4 becomes $F^*(y_0 + TA3)^*\Delta x$.
5. Enter the formula for y(m): ym + (TA1 +2*TA2 + 2*TA3 + TA4)/6
6. **Fill Down** the TA1,...,TA4 and y(m) cells. y(m) should agree approximately with the Euler's method column.
7. **Delete** the columns containing the Euler's method values.

Reacciones consecutivas

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \underset{k_4}{\overset{k_3}{\rightleftharpoons}} C$$

$$\frac{d[A]}{dt} = -k_1[A] + k_2[B]$$

$$\frac{d[B]}{dt} = k_1[A] - k_2[B] - k_3[B] + k_4[C]$$

$$\frac{d[C]}{dt} = k_3[B] - k_4[C]$$

Reacciones consecutivas (II)

which lead to the following expressions for the concentrations:

$$[\mathrm{A}]_t = [\mathrm{A}]_0\, e^{-k_1 t} \qquad (23\text{-}12)$$

$$[\mathrm{B}]_t = [\mathrm{A}]_0 \frac{k_1}{k_2 - k_1}\left[e^{-k_1 t} - e^{-k_2 t}\right] \qquad (23\text{-}13)$$

$$[\mathrm{C}]_t = [\mathrm{A}]_0 \left[1 - \frac{k_2}{k_2 - k_1} e^{-k_1 t} + \frac{k_1}{k_2 - k_1} e^{-k_2 t}\right] \qquad (23\text{-}14)$$

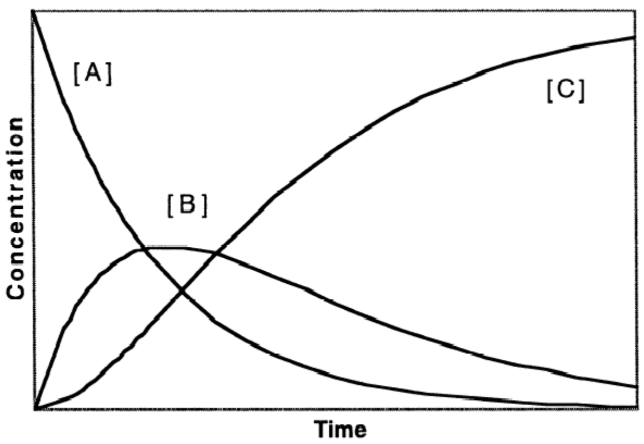

Figure 23-4. Concentration vs. time for consecutive first-order reactions.