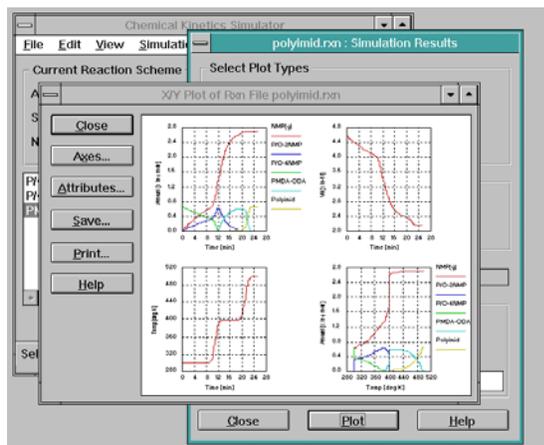


Dynamics Methods

Chemical Kinetics Simulator
<http://www.almaden.ibm.com/st/msim>

- CKS does not integrate differential equations
- CKS performs general, rigorously accurate stochastic algorithm to propagate reaction
- Speed
 - Comparable in efficiency to integration for simple
 - Significantly faster for “stiff” systems
- Models complex reactions
 - Explosions
 - Changing volumes
- High learning curve
- Research quality

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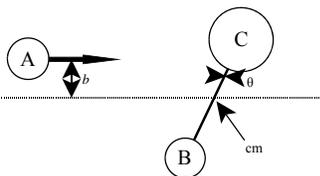


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Dynamics Methods

A+BC: General Trajectory
<http://qcpe.chem.indiana.edu/cgi-bin/catalog/view.pl>

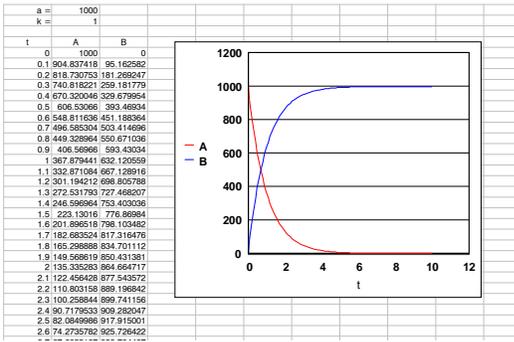
- LEPS diagram
- Monte Carlo Collisions



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Mathematics Methods--Integral

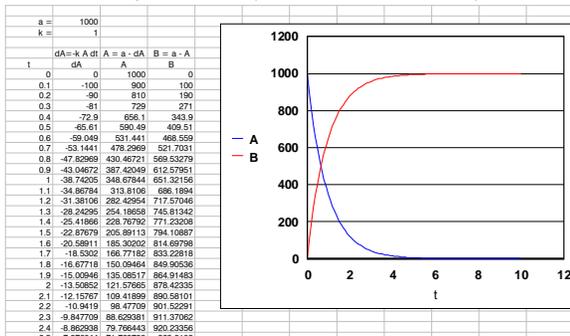
Spreadsheet



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Mathematics Methods--Differential

Spreadsheet (Based on Euler's Rule)

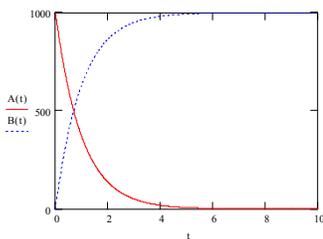


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Mathematics Methods--Integral

Mathcad

a := 1000
k := 1
 $A(t) := a \cdot e^{-k \cdot t}$ $B(t) := a \cdot (1 - e^{-k \cdot t})$



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Mathematics Methods--Differential

Mathcad

k1:=1 k2:=1
a:=1000 b:=0 c:=0
T:=10

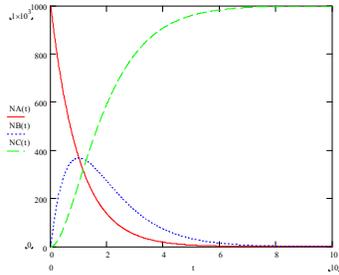
Given

$$\frac{d}{dt}A(t) = -k_1 A(t) \quad A(0) = a$$

$$\frac{d}{dt}B(t) = k_1 A(t) - k_2 B(t) \quad B(0) = b$$

$$\frac{d}{dt}C(t) = k_2 B(t) \quad C(0) = c$$

$$\begin{pmatrix} NA \\ NB \\ NC \end{pmatrix} := \text{Odesolve} \left(\begin{pmatrix} A \\ B \\ C \end{pmatrix}, t, T \right)$$



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Graphical Interface Differential Equation Solvers

General

- Model differential rate law
- Software solves differential equations
 - Watch "stiff"
- Tables and Graphs

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Solving of Differential Equations

Taylor Series

$$y(t_m + \Delta t) = y_m + \frac{\Delta t}{1!} \left(\frac{dy}{dt} \right)_{t=t_m} + \frac{\Delta t^2}{2!} \left(\frac{d^2 y}{dt^2} \right)_{t=t_m} + \frac{\Delta t^3}{3!} \left(\frac{d^3 y}{dt^3} \right)_{t=t_m} + \frac{\Delta t^4}{4!} \left(\frac{d^4 y}{dt^4} \right)_{t=t_m} + \dots$$

- y_m = value of reservoir at time $t = t_m$
- $y(t_m + \Delta t)$ = value of reservoir at time $t = t_m + \Delta t$
- Methods
 - Euler retains first two terms
 - Runga-Kutta 2 retains first three terms
 - RK4 retains first five terms

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