Introduction to Berkeley Madonna

Commerical Products

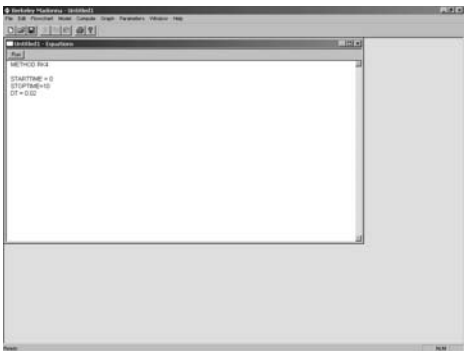
Graphical Interface Differential Equation Solvers (GIDES)

- Berkeley Madonna
  - Download demo version
  - Solves “stiff” differential equations
- STELLA
  - Java conversion available from Shodor
- VisSim (Mathcad)
- Simulink (Matlab)
- Simile
- Model Maker

Madonna Interface

Equation Window

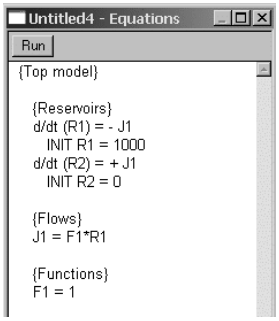
- Initial opening window
- Can enter differential equations directly



Madonna Interface

Sample Equation Window Entries

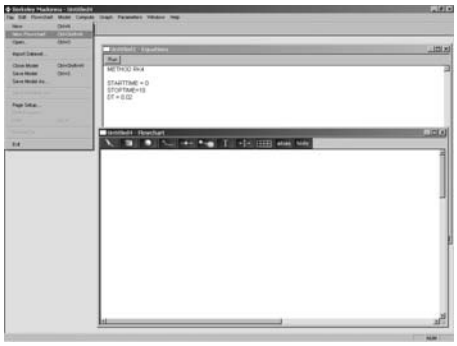
- Differential equation
  - Begins with d/dt
  - R1 is a variable that changes
  - INIT is the initial value of R1
- Flow
  - Differential equation expression
- Function
  - Constants, conversions, values, etc.



Madonna Interface

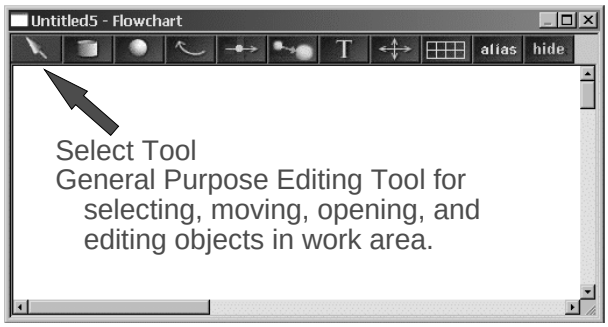
Flowchart Window

- Select
  - File
  - New Flowchart
- Note that Madonna uses Java 1.1.8



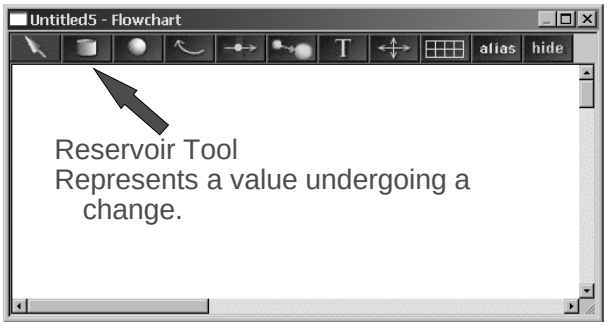
Madonna Interface

Flowchart Window - Icons



Madonna Interface

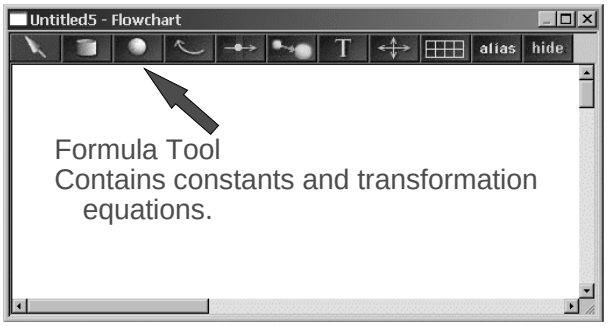
Flowchart Window - Icons



Reservoir Tool
Represents a value undergoing a change.

Madonna Interface

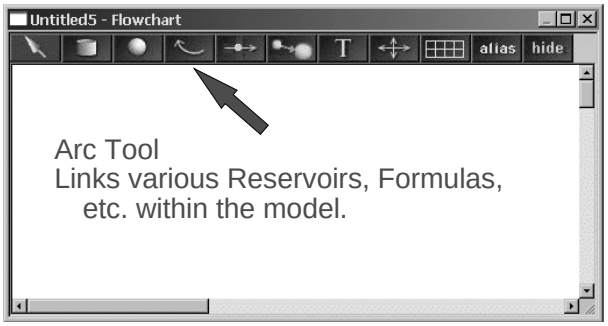
Flowchart Window - Icons



Formula Tool
Contains constants and transformation equations.

Madonna Interface

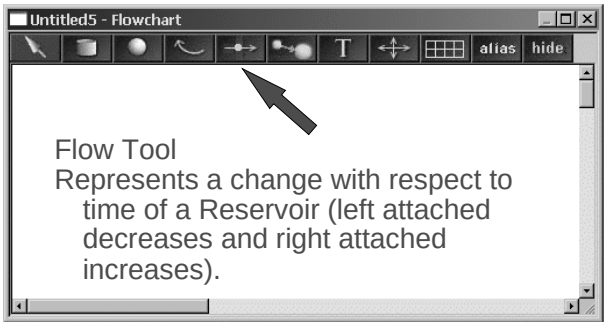
Flowchart Window - Icons



Arc Tool
Links various Reservoirs, Formulas, etc. within the model.

Madonna Interface

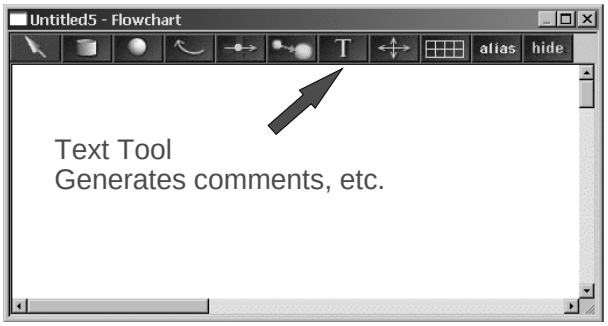
Flowchart Window - Icons



Flow Tool
Represents a change with respect to time of a Reservoir (left attached decreases and right attached increases).

Madonna Interface

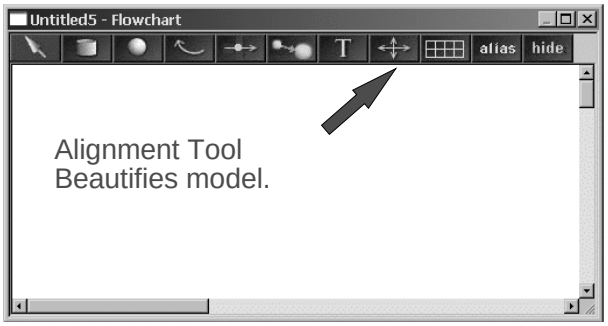
Flowchart Window - Icons



Text Tool
Generates comments, etc.

Madonna Interface

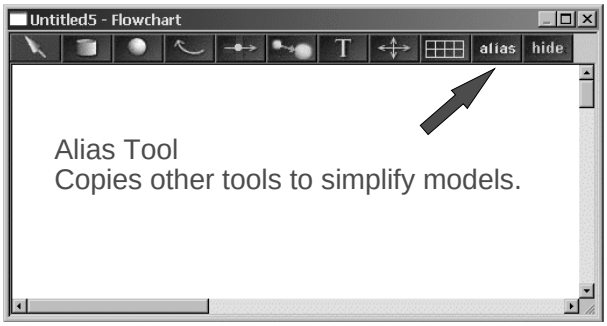
Flowchart Window - Icons



Alignment Tool
Beautifies model.

Madonna Interface

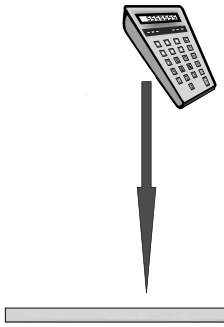
Flowchart Window - Icons



Alias Tool
Copies other tools to simplify models.

Simple Model – Falling Calculator

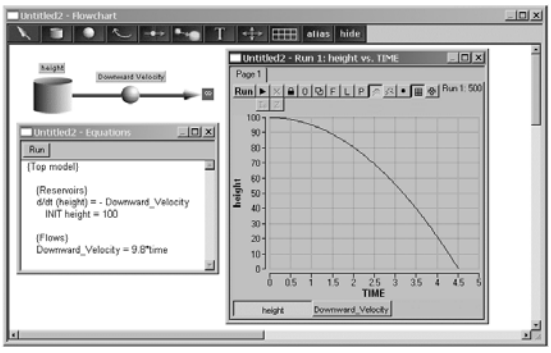
System

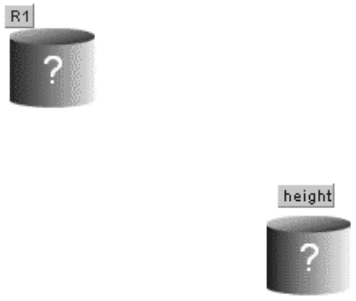


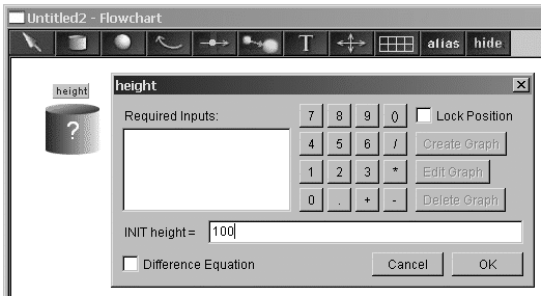
y = height
y' = velocity
= (acceleration)(time)
y'' = acceleration
= g = 9.8 m s^{-2}

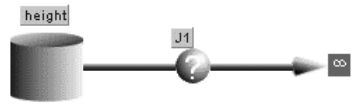
Simple Model – Falling Calculator

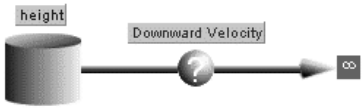
Madonna Model

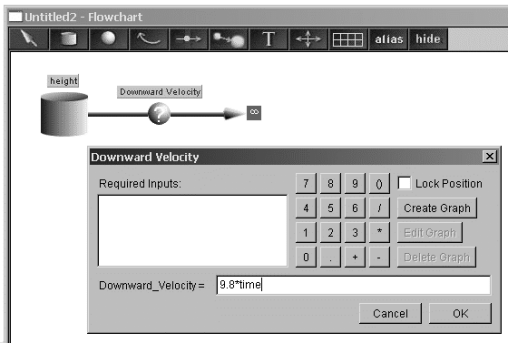



R1
?
height
?

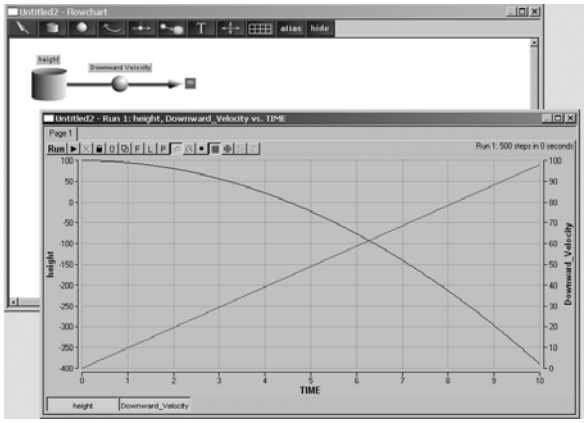

Untitled2 - Flowchart
atlas
hide
height
height
?
Required Inputs:
7
8
9
0
Lock Position
4
5
6
/
Create Graph
1
2
3
*
Edit Graph
0
.
+
-
Delete Graph
INIT height =
100
Difference Equation
Cancel
OK

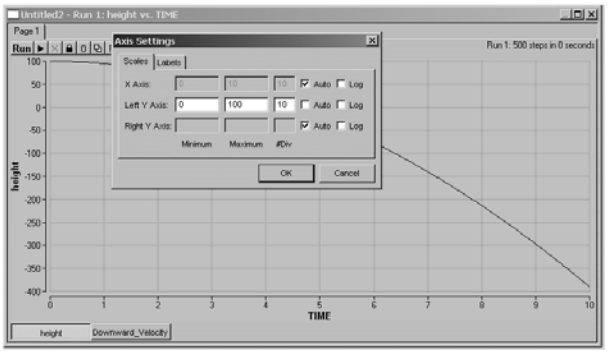

height
J1
?
∞

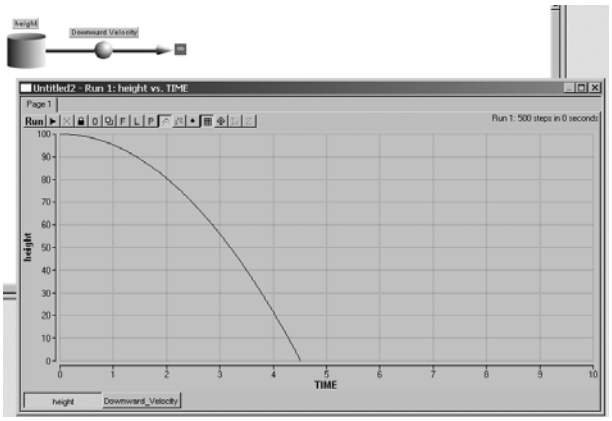

height
Downward Velocity
?
∞

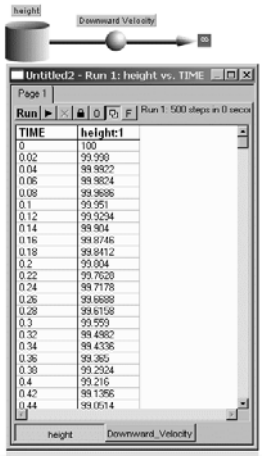

Untitled2 - Flowchart
alias
hide
height
Downward Velocity
Downward Velocity
Required Inputs:
7 8 9 0
Lock Position
4 5 6 /
Create Graph
1 2 3 *
Edit Graph
0 . + -
Delete Graph
Downward_Velocity =
9.8*time
Cancel
OK

Model / Run

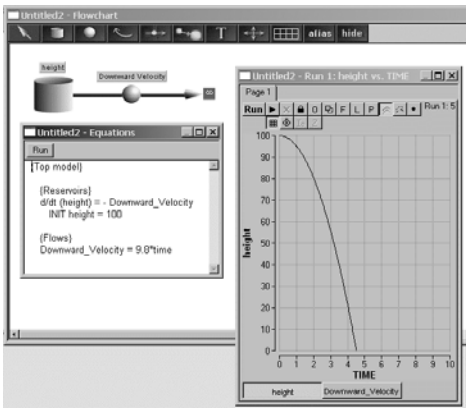

Untitled2 - Flowchart
Untitled2 - Run 1: height, Downward_Velocity vs. TIME
Page 1
Run
Run 1: 500 steps in 0 seconds
height
Downward_Velocity
TIME


Untitled2 - Run 1: height vs. TIME
Page 1
Run
Axis Settings
Scales
Labels
X Axis:
Left Y Axis:
Right Y Axis:
Auto
Log
Minimum
Maximum
#Div
OK
Cancel
Run 1: 500 steps in 0 seconds
height
TIME
height
Downward_Velocity





Model / Equations



Simple Model – Falling Calculator

Madonna Model – Accuracy

- Air Friction
- Bounce

Solving of Differential Equations

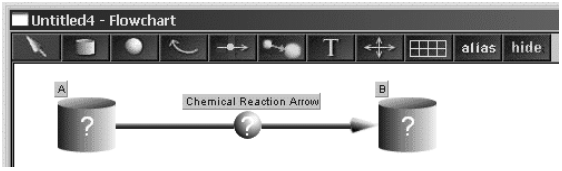
Taylor Series

$$y(t_m \quad t) \quad y_m \quad \frac{t}{1!}\frac{dy}{dt}_{t\ t_m} \quad \frac{t^2}{2!}\frac{d^2y}{dt^2}_{t\ t_m} \quad \frac{t^3}{3!}\frac{d^3y}{dt^3}_{t\ t_m} \quad \frac{t^4}{4!}\frac{d^4y}{dt^4}_{t\ t_m} \quad \ldots$$

- 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

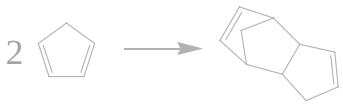
Chemical Kinetics

Sure looked like a natural fit to me!!



Kinetics Model

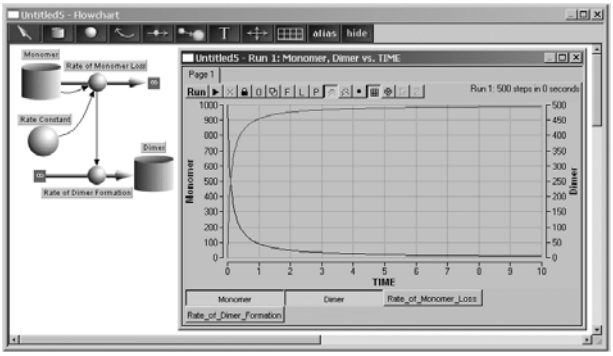
Dimerization of Cyclopentadiene
2nd Order Diels-Alder Reaction

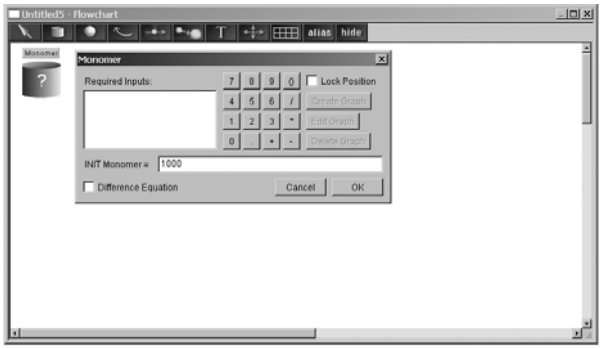


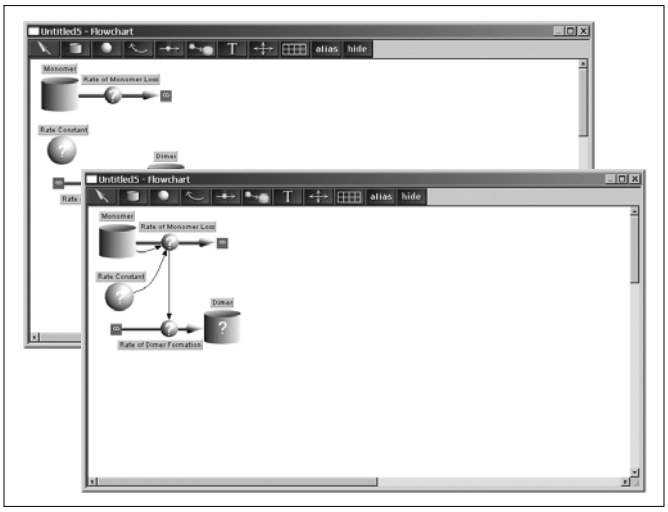
$$\frac{dC}{dt} = -kC^2$$

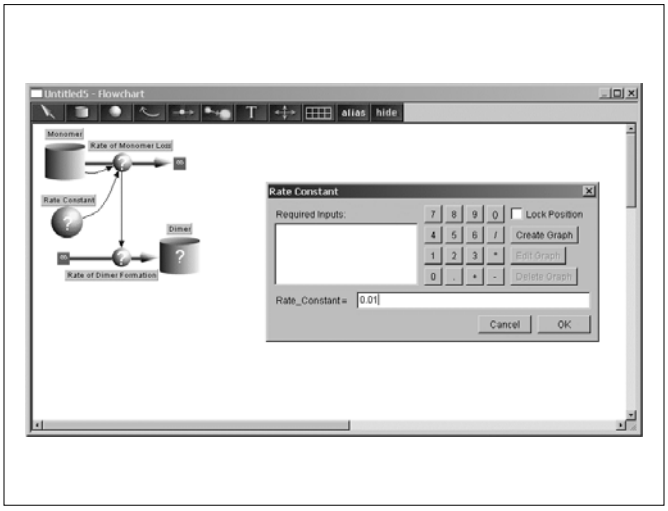
$$\frac{1}{C} = \frac{1}{C_o} + kt$$

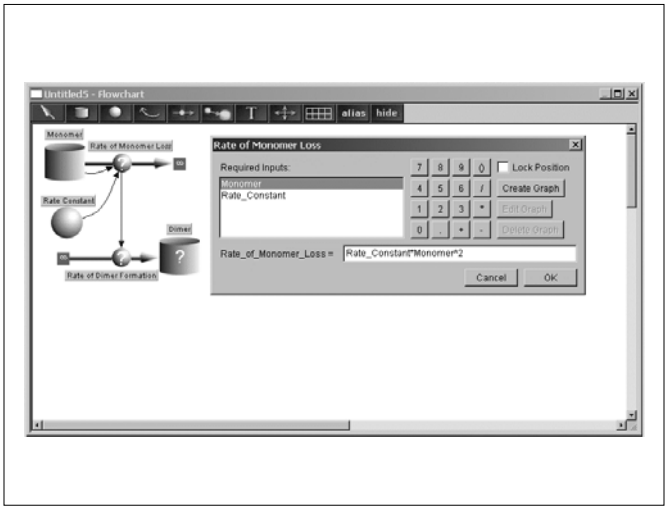
Kinetics Model

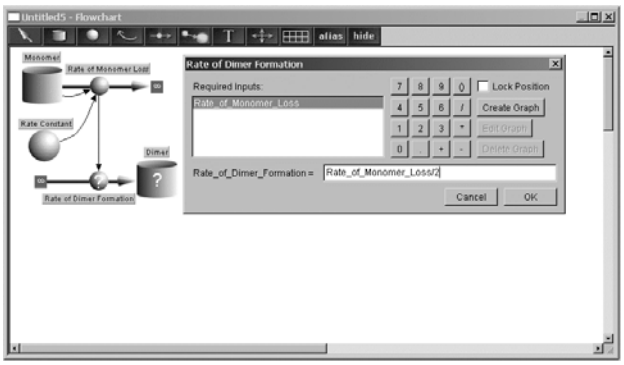


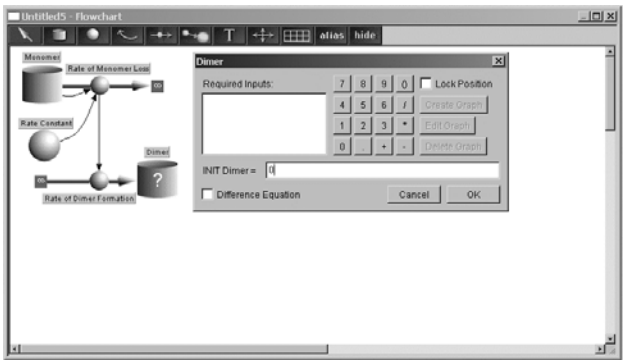



Untitled5 - Flowchart
alias
hide
Monomer
Rate of Monomer Loss
Rate Constant
Dimer
Rate of Dimer Formation

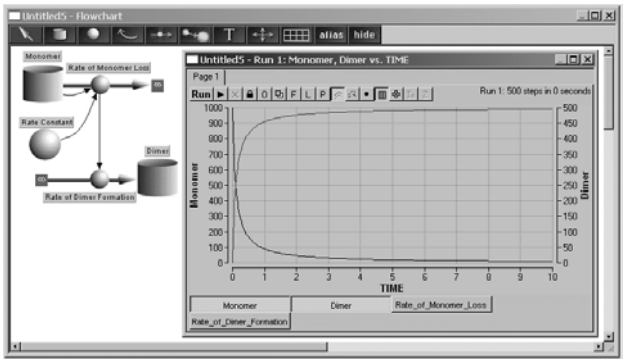

Untitled5 - Flowchart
alias
hide
Monomer
Rate of Monomer Loss
Rate Constant
Dimer
Rate of Dimer Formation
Rate Constant
Required Inputs:
Lock Position
Create Graph
Edit Graph
Delete Graph
Rate_Constant =
0.01
Cancel
OK

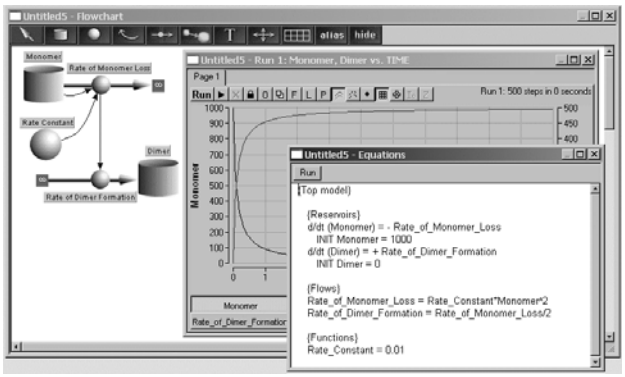

Untitled5 - Flowchart
alias
hide
Monomer
Rate of Monomer Loss
Rate Constant
Dimer
Rate of Dimer Formation
Rate of Monomer Loss
Required Inputs:
Monomer
Rate_Constant
Lock Position
Create Graph
Edit Graph
Delete Graph
Rate_of_Monomer_Loss =
Rate_Constant*Monomer^2
Cancel
OK


Untitled5 - Flowchart
alias
hide
Monomer
Rate of Monomer Loss
Rate Constant
Dimer
Rate of Dimer Formation
Rate of Dimer Formation
Required Inputs:
Rate_of_Monomer_Loss
Lock Position
Create Graph
Edit Graph
Delete Graph
Rate_of_Dimer_Formation =
Rate_of_Monomer_Loss/2
Cancel
OK


Untitled5 - Flowchart
alias
hide
Monomer
Rate of Monomer Loss
Rate Constant
Dimer
Rate of Dimer Formation
Dimer
Required Inputs:
Lock Position
Create Graph
Edit Graph
Delete Graph
INIT Dimer =
Difference Equation
Cancel
OK

Model / Run


Untitled5 - Flowchart
alias
hide
Monomer
Rate of Monomer Loss
Rate Constant
Dimer
Rate of Dimer Formation
Untitled5 - Run 1: Monomer, Dimer vs. TIME
Page 1
Run
Run 1: 500 steps in 0 seconds
Monomer
Dimer
TIME
Monomer
Dimer
Rate_of_Monomer_Loss
Rate_of_Dimer_Formation

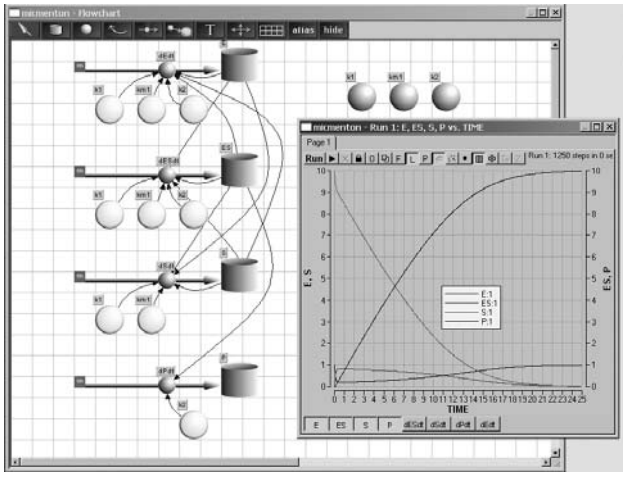


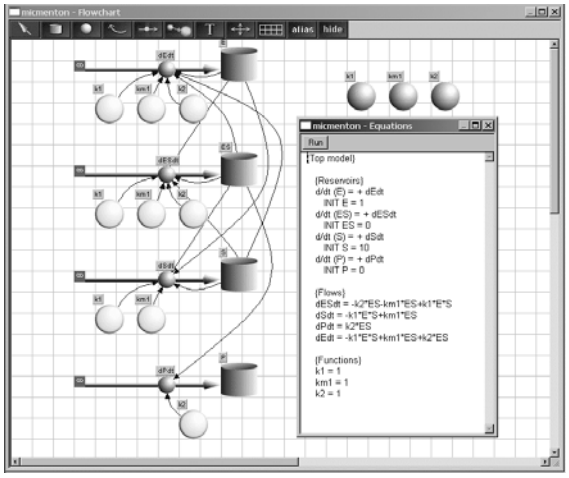
Michaelis-Menton

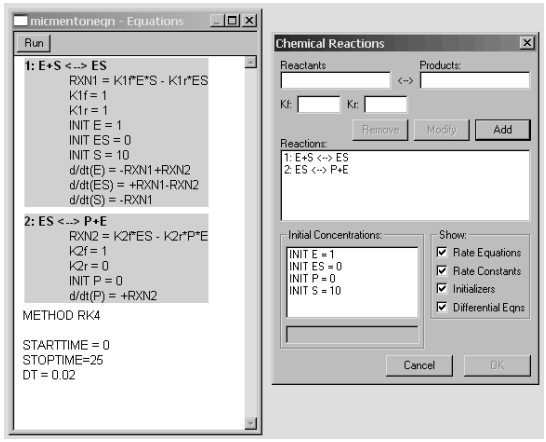
After Len Soltzberg (Simmons College)

$$E + S \rightleftharpoons (ES)$$

$$(ES) \rightarrow P + E$$







Oscillating Reactions

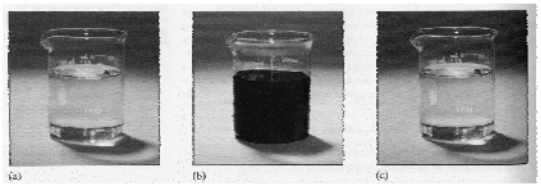
Criteria

- Two or more coupled reactions
- Autocatalytic

Oscillating Reactions

Briggs-Rauscher

- H_2O_2
- KIO_3 and H_2SO_4
- $HOOCCH_2COOH$, $MnSO_4$, starch



Oscillating Reactions

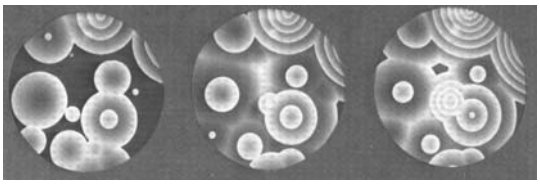
Belousov-Zhabotinskii

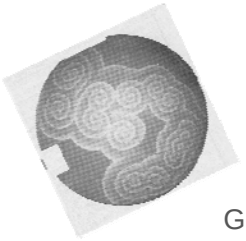
$$BrO_3^- + HBrO_2 + H_3O^+ \rightarrow 2\ BrO_2 + 2\ H_2O$$

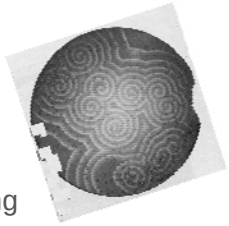
$$2\ BrO_2 + 2\ Ce^{3+} + 2\ H_3O^+ \rightarrow 2\ HBrO_2 + 2\ Ce^{4+} + 2\ H_2O$$

- 18 reversible steps
- 21 different chemical species

~60 s intervals





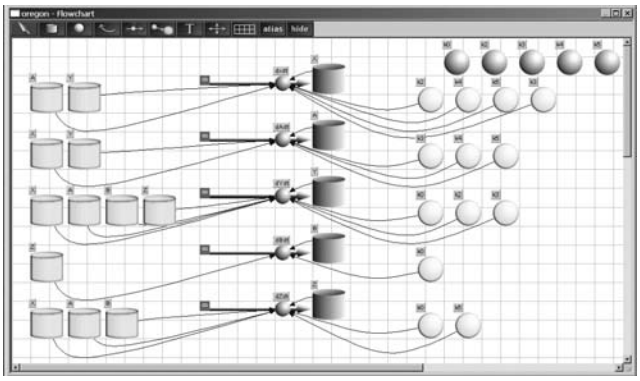


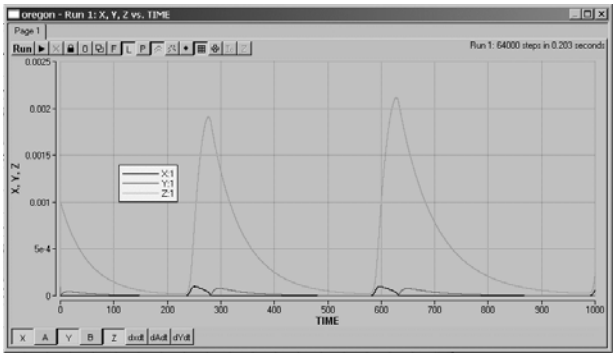
Gentle Stirring

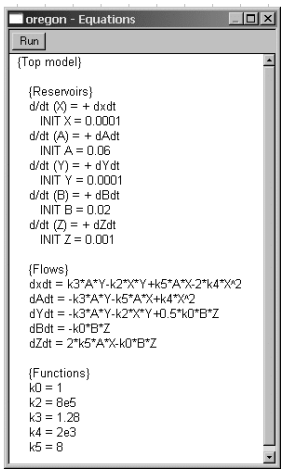
Oregonator after Len Soltzberg (Simmons College)

$A + Y \rightarrow X + P$
$X + Y \rightarrow 2P$
$A + X \rightarrow 2X + 2Z$
$2X \rightarrow A + P$
$B + Z \rightarrow (f/2)\ Y$

where
$A = BrO_3^-$
$X = HBrO_2$
$Z = Ce^{4+}$
$P = HOBr$
$B =$ organic
$Y = Br^-$


oregon - Flowchart
atlas
hide


oregon - Run 1: X, Y, Z vs. TIME
Page 1
Run
Run 1: 64000 steps in 0.203 seconds
0.0025
0.002
0.0015
0.001
5e-4
0
X, Y, Z
X:1
Y:1
Z:1
0
100
200
300
400
500
600
700
800
900
1000
TIME
X
A
Y
B
Z
dXdt
dAdt
dYdt


oregon - Equations
Run
{Top model}
{Reservoirs}
d/dt (X) = + dxdt
INIT X = 0.0001
d/dt (A) = + dAdt
INIT A = 0.06
d/dt (Y) = + dYdt
INIT Y = 0.0001
d/dt (B) = + dBdt
INIT B = 0.02
d/dt (Z) = + dZdt
INIT Z = 0.001
{Flows}
dxdt = k3*A*Y-k2*X*Y+k5*A*X-2*k4*X^2
dAdt = -k3*A*Y-k5*A*X+k4*X^2
dYdt = -k3*A*Y-k2*X*Y+0.5*k0*B*Z
dBdt = -k0*B*Z
dZdt = 2*k5*A*X-k0*B*Z
{Functions}
k0 = 1
k2 = 8e5
k3 = 1.28
k4 = 2e3
k5 = 8

Other Applications

Debye Theory for Monatomic Crystals

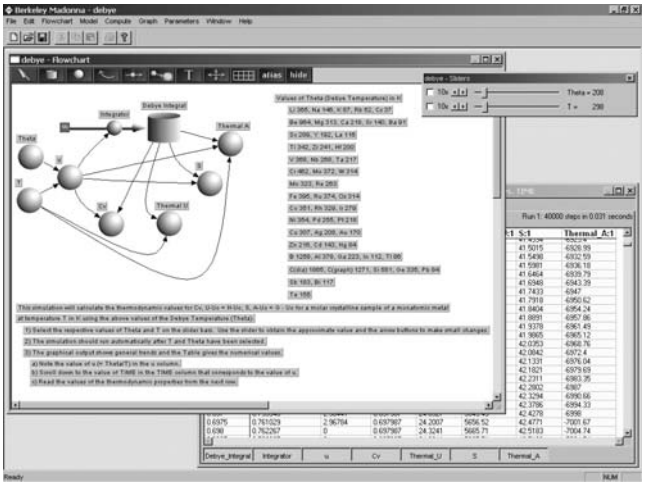
$$D(\ _D / T)\quad \frac{3}{u^3}\quad \frac{x^3}{e^x\quad 1}dx$$

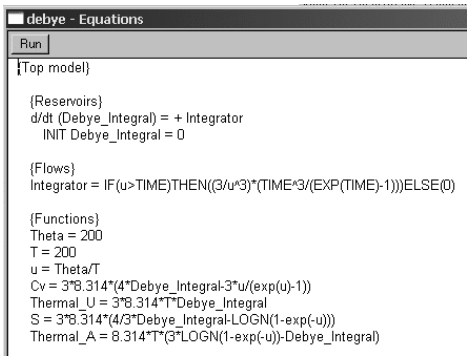
$$U\quad U_0\quad 3RTD$$

$$C_v\quad 3R\ \ 4D\quad 3\frac{u}{e^u\quad 1}$$

$$S\quad 3R\ \frac{4}{3}D\quad \ln 1\quad e^{\ u}$$

$$A\quad U_0\quad RT\ 3\ln 1\quad e^{\ u}\quad\quad D$$




debye - Equations
Run
{Top model}
{Reservoirs}
d/dt (Debye_Integral) = + Integrator
INIT Debye_Integral = 0
{Flows}
Integrator = IF(u>TIME)THEN((3/u^3)*(TIME^3/(EXP(TIME)-1)))ELSE(0)
{Functions}
Theta = 200
T = 200
u = Theta/T
Cv = 3*8.314*(4*Debye_Integral-3*u/(exp(u)-1))
Thermal_U = 3*8.314*T*Debye_Integral
S = 3*8.314*(4/3*Debye_Integral-LOGN(1-exp(-u)))
Thermal_A = 8.314*T*(3*LOGN(1-exp(-u))-Debye_Integral)