10b Computational Study of System Dynamics (GIDES)

Software Introduction

STELLA (http://www.hps-inc.com) and Berkeley Madonna (http://www.berkeleymadonna.com) are dynamic modeling programs in which relational diagrams are created using a graphical interface to which numerical values and mathematical functions may be assigned. Free run-time versions of the software (excluding the "Save" and "Help" capabilities) are available for downloading.

There are several other Graphical Interface Differential Equation Solver (GIDES) software programs such as VisSim (Mathcad), Simulink (MATLAB), ModelMaker, and Simile. However, we will consider only STELLA and Madonna. In many respects, both programs are very similar:

> The user interfaces differ slightly. Stella has the mapping, modeling, and equation layers–the modeling layer is used to construct the flow diagram. Madonna has modeling and equation windows–either can be used to directly construct the model and selecting an entry in one window results with the corresponding entry in the other window being highlighted. The equation entries differ slightly in format. The dialog boxes used for entering values, equations, etc. differ only slightly.

> The modeling tools are very similar even though they have slightly different names. Stella has a separate icon for constructing "biflow" processes. The flowchart objects in Madonna are graphically enhanced and various object alignment tools are available.

> Both programs offer graphical and data input. At the mapping level Stella offers "dials" for input and "flight simulation". Stella offers numeric displays of output as well as animation of modeling objects. Madonna automatically opens a graph/table window upon execution which can be easily switched back and forth.

> The execution in Madonna is very fast. Stella offers Euler, RK2, and RK4 whereas Madonna offers Euler, RK2, RK4, auto-stepsize, and Rosenbrock (for stiff systems). Madonna also offers a curve fit routine and handles arrays.

> Using the Shodor-developed "Stella to JAVA", JAVA applets are easily made from Stella models for many models. Madonna does not have this feature.

> The help in Stella is more comprehensive, but Madonna comes with several "How do I" files and examples of its features using systems of interest to chemists.

The directions below are pretty much STELLA-specific, but feel free to use Madonna for any of these modeling exercises.

Once STELLA is opened, there are three different work areas known as "layers" that are available for use. To change from one layer to another, click on the "up" or "down" navigation arrowhead icons at the far left of the screen. The functionality of each layer includes:

> The upper "Mapping" layer is used for placing text; showing output of calculations in various forms; inputting data for calculations using dials, sliders, etc.; and showing photos and QuickTime movies. This level is usually used by those who want to simply run the model once the model has been highly developed and by those not concerned with either the modeling itself or the mathematics involved.

> The center "Modeling" construction layer is used to construct the model using the various "Building Blocks", "Tools", and "Objects" available. Our models will be constructed and run from this layer.

The lower "Equation" layer lists a summary of the initial values of the various "Stocks", the equations representing the time dependence of the "Stocks", and the data within the "Converters". We will use this layer to confirm the accuracy of our model construction by comparing the entries to the known differential equations describing the chemical processes being considered.

The construction of a model is done in the "Modeling" layer. Click the "Globe" icon at the far left of the screen to change it to the "χ^2" icon which is used for modeling entry. The icons at the top of this layer fall into several groups. The ones that we will use primarily include:

1) Building Blocks

Stocks

A "Stock" represents a value undergoing a change. We will use a "Stock" to represent the number of molecules of reactant or product present during a chemical reaction at a given time. Normally, we will set the initial number of reactant molecules at 1000 and the initial number of product molecules at 0.

Flows
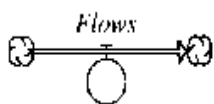
A "Flow" represents a change with respect to time of a "Stock". During the process a "Stock" attached at the left decreases as time passes and one at the right increases. For our study of chemical kinetics, a "Stock" at the left represents a chemical reactant, a "Stock" at the right represents a chemical product, and the "Flow" represents the chemical reaction arrow.

Converters

A "Converter" contains constants and transformation equations. We will use "Converters" to enter values of the rate constants for the chemical reactions being studied. Normally, we set the values of the rate constants in the range of 0 to 100.

Connectors
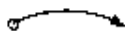
A "Connector" links the various "Building Blocks" within the model.

2) Tools

The Hand

The "Hand" is the general purpose editing tool used for selecting, moving, opening, and editing various objects in the work area.

The Dynamite

The "Dynamite" stick is the delete tool. Not that STELLA does not have an "undo" feature.

3) Objects

Graph Pad

This icon creates a "Graph Pad". Use the "Hand" to double click in the "Graph Pad" to open a dialog box for setting up the graphing parameters. An icon for printing the "Graph Pad" is available at the bottom.

Table Pad

This icon creates a "Table Pad". Use the "Hand" to double click in the "Table Pad" to open a dialog box for setting up the table parameters. The output is very similar to that from a spreadsheet. An icon for printing the "Table Pad" is available at the top.

4) Run Controller

The Run Controller

Opens a dialog box for running the model and obtaining results.

Listed below are some simple directions on using the 'Building Blocks" described above:

1) Drawing a "Stock".
  A) Click the "Stock" icon.
  B) Click in the work area at the desired location. A "Noname" stock appears.
  C) The "Stock" can be named by moving the cursor over the name and typing.
  D) Double clicking the "Stock" opens the dialog box for data entry.

2) Drawing a "Flow" between "Stocks".
  A) Click the "Flow" icon.
  B) Move the cursor to the center of the "Outflow Stock".
  C) Click and drag to center of the "Inflow Stock".
  D) Release. A "Noname Flow" appears.
  E) The "Flow" can be named by moving the cursor over the name and typing.
  F) Double clicking the "Flow" opens the dialog box for data entry.

3) Replacing a "Cloud" on a "Flow" with a "Stock" already in the work area.
  A) Click the "Hand" icon.
  B) Click and move the "Stock" to the "Cloud" until the "Cloud" is highlighted.
  C) Release.

4) Drawing a "Converter".
  A) Click the "Converter" icon.
  B) Click in the work area at the desired location. A "Noname Converter" appears.
  C) The "Converter" can be named by moving the cursor over the name and typing.
  D) Double clicking the "Converter" opens the dialog box for data entry.

5) Drawing a "Connector".
  A) Click the "Connector" icon.
  B) Place the cursor inside the "from Building Block".
  C) Click and drag to the "target Building Block" until the "target" is highlighted.
  D) Release.
  E) The locations of attachments can be adjusted, if desired.

During the execution of a completed model, any differential equations describing the time dependence of the "Stock" *y* are solved using one of three numerical methods based on a Taylor series

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

$$= \; y_m \; + \; \Delta t\; F(t_m,y_m) \; + \; \frac{\Delta t^2}{2}\; F'(t_m,y_m) \; + \; \frac{\Delta t^3}{6}\; F''(t_m,y_m) \; + \; \frac{\Delta t^4}{24}\; F'''(t_m,y_m) \; + \; ...$$

where y_m represents the value of the "Stock" at time $t = t_m$ and $y(t_m+\Delta t)$ represents the value of the "Stock" at time $t_m+\Delta t$. Unless changed, Euler's method is the default method used by STELLA

$$y(t_m+\Delta t) \; = \; y_m \; + \; \Delta t\; F(t_m,y_m)$$

which is based on the first two terms of the series. STELLA also offers "Runge-Kutta 2"

$$y(t_m+\Delta t) \; = \; y_m \; + \; \frac{\Delta t}{2}(\alpha_1 \; + \; \alpha_2)$$
$$\alpha_1 \; = \; F(t_m,y_m)$$
$$\alpha_2 \; = \; F(t_m+\Delta t,y_m+\alpha_1\Delta t)$$

which is based on the first three terms of the series and "Runge-Kutta 4"

$$y(t_m+\Delta t) \; = \; y_m \; + \; \frac{\Delta t}{6}(\alpha_1 \; + \; 2\alpha_2 \; + \; 2\alpha_3 \; + \; \alpha_4)$$
$$\alpha_1 \; = \; F(t_m,y_m)$$
$$\alpha_2 \; = \; F\left(t_m+\frac{\Delta t}{2},y_m+\frac{\alpha_1\Delta t}{2}\right)$$
$$\alpha_3 \; = \; F\left(t_m+\frac{\Delta t}{2},y_m+\frac{\alpha_2\Delta t}{2}\right)$$
$$\alpha_4 \; = \; F(t_m+\Delta t,y_m+\alpha_3\Delta t)$$

which is based on the first five terms of the series. Normally, we will use the "RK4" method because this method produces the most accurate results for our type of calculations. Note that Stella cannot solve systems that are "stiff" but Madonna offers a method for solving these types of problems.

Some of the default settings in STELLA are a little unusual. The following changes are recommended for the following study of chemical kinetics:
   1) Click on "File".
   2) Click on "Default Settings".
   3) Click on "Model" and change the "Variable Name Font Size" to "12 pt".
   4) Click on "Run Specs" and change "To" to "10" and "DT" to "0.1". Also change "Integration Method" to "Runge-Kutta 4".
   5) Click on "OK".