Appendix: Using the MADONNA Language

1 A Short Guide to MADONNA

Computer Requirements

Two unregistered versions of MADONNA are supplied with this book on the CD, one for Windows 95, NT 4.0 and later and one for the Power Macintosh, including OSX. More information with free downloads of this software can be found on the following MADONNA website: http://www.berkeleymadonna.com. The unregistered version does not allow saving new programs but will run any existing program.

Installation

The files are compressed on the CD in the same form as they are available on the Internet. Information on registering MADONNA is contained in the files. Registration is optional since all the examples in the book can be run with the unregistered version. Registration makes available a detailed manual and is necessary for anyone who wants to develop his or her own programs.

Running Programs

To our knowledge, MADONNA is by far the easiest simulation software to use, as can be seen on the Screenshot Guide in this Appendix. Running an example typically involves the following steps:

- Open MADONNA and open a prepared program file.
- Go to Model/Equations on the menu and study the equations and program logic.
- Go to Parameters/Parameter Window on the menu and see how the values are set. They may be different than on the program listing. Those with a* can be reset to the original values. Also, if necessary, here the integration

Chemical Engineering Dynamics: An Introduction to Modelling and Computer Simulation, Third Edition
J. Ingham, I. J. Dunn, E. Heinzle, J. E. Prenosil, J. B. Snape

ISBN: 978-3-527-31678-6

method and its parameters (D_T, $D_{T_{min}}$ and $D_{T_{max}}$, Stoptime, etc.) values can be changed.
- Decide which plot might be interesting, based on the discussion in the text.
- Go to Graph/New Window and then Graph/Choose Data to select data for each axis. All calculated results on the left side of the equations are available and can be selected.
- Run the program and make a graph by clicking Run on the graph window.
- Adjust the graph by setting the legend with the legend button. Perhaps put one of the variables on the right side of the graph with Graph/Choose Data.
- Possibly select the range of the axes with Graph/Axis Settings. Choose colours or line types with the buttons.
- Decide on further runs. It is most common to want to compare runs for different values of the parameters. This is usually done with Parameter/Batch Runs and also with Model/Define Sliders. If the overlay button is set, then more than one set of runs can be graphed on top of the first run. Sometimes more than one parameter needs to be set; this is best done with changes done in the Parameters/Parameter Window, with an overlay graph if desired.

As seen at the end of the Screenshot Guide, Parametric Plots are very useful to display the steady-state values as a function of the values of one parameter. For this, one needs to be sure that the Stoptime is sufficiently long to reach steady-state for all the runs.

When running a program with arrays, as found in the finite-differenced examples, the X axis can be set with [i] and the Y axes with the variables of interest. The resulting graph is a plot of the variable values at the Stoptime in all of the array sections. For equal-sized segments, this is the equivalent of a plot of the variables versus distance. If the steady-state has been reached then the graph gives the steady-state profile with distance. More on running programs is found in Section 1.1.7 and in Section 2 of the Appendix.

Special Programming Tips

MADONNA, like all programming languages, has certain functions and characteristics that are worth noting and that do not appear elsewhere in this book.

Editing Text

The very convenient built-in editor is usually satisfactory. Also the program can be written with a word processor and saved as a text-only file with the suffix ".mmd". MADONNA can then open it.

Finding Programming Errors. Look at a Table Output of the Variables

Sometimes programs do not run because of errors in the program that cause integration problems. Some hint as to the location of the error can often be found by making an output table of all the calculated variables. This is done by going to Graph/New Window and then Graph/Choose Data to select all the variables. Then the program is run and the tabular data button is chosen. Inspection of all the values during the first one or two time intervals will usually lead to an isolation of the problem for those values that are marked in red with NAN (not a number). Also, values going negative can be found easily here and often indicate an integration error.

The Program Does Not Compile. Is a Bracket Missing?

Sometimes variables are not found when the program is compiling. Often this can be due to one of the comment brackets missing, usually on the right side. MADONNA does not presently test for bracket pairs, and a missing bracket means that the whole program will be read as a comment. The error message is usually "Undetermined comment" or expect "=".

Setting the Axes. Watch the Range of Values

Remember that each Y axis can have only one range of values. This means that you must choose the ranges so that similarly sized values are located on the same axis. Choose the right axes in Graph/Choose Variables.

Are There Bugs or Imperfections in MADONNA?

Yes, there are some that we are aware of. You may find some or you may have some special wishes for improvements. The MADONNA developers would be glad to receive your suggestions. See the homepage for the email address.

Making a Pulse Input to a Process

This can be done in two ways: Either use the pre-programmed PULSE function (see the program CSTRPULSE for an example) or use an IF-THEN-ELSE statement to turn a stream on and off (see example CHROM).

Making a More Complex Conditional Control of a Program

In general the IF-THEN-ELSE conditional statement form is used, combined with the inequality and/or possibilities as found in the HELP. This can involve a switching from one equation to another within this statement. Another way is to use flags or constants that take values of 0 or 1 and are multiplied by terms in the equations to achieve the desired results. The programs RUN and RELUY contain such programming. As shown in RUN, nesting of multiple IF statements is possible:

```
V=IF(Disk<1 AND P>1.9)
    THEN 0.85*KV*P/SQRT(TR+273)
        ELSE IF (Disk<1 AND P<=1.9 AND P>1.1)
          THEN KV*P/SQRT(TR+273)*SQRT(1+(1/P)*(1/P))
```

Parameter Estimation to Fit Parameters to Data

For fitting sets of data to one or more parameters the data can be imported as a text file (Import Data Set) found in the window of Parameters/Curve Fitting. The Preferences/Graph Windows provide the possibility of having the data as open circles. See the programs KLAFIT and ESTERFIT for examples of this. Normally this data would be time in the first column and the measured variable in the second column. If the data is available at equal time increments then two sets of data can be used. See also Help/How Do I.

Optimisation of a Variable

There is a real optimisation routine available in MADONNA under Parameters/Optimize. It is actually a minimization and the function needs to be written in the window. It is also useful to check the results by making runs. If it is something simple with one or two parameters, then sliders can be effectively used. If the value of a maximum is sought as a function of a single parameter value, then the Parametric Plot for maximum value should be used.

Finding the Influence of Two Parameters on the Steady State?

A Parametric Plot choosing the "final" value can be used to find the influence of one variable on the steady state. The second parameter can be changed in the Parameter Window and additional parametric runs made and plotted with an overlay plot. Thus it is possible to obtain a sort of contour plot with a series of curves for values of the second parameter. Unfortunately, no automatic contour plot is yet possible.

Nice Looking Results Are Not Always Correct

A warning! It is possible to obtain results from a program that at first glance seems OK. Always make sure that the same results are obtained when D_T is reduced by a factor of 10 or when a different integration method is used. Plotting all the variables may reveal oscillations that indicate integration errors. These may not be detectable on plots of the other variables.

Setting the Integration Method and Its Parameters?

It is recommended to choose the automatic step-size method AUTO and to set a small value of $D_{T_{min}}$ and a large value for $D_{T_{max}}$. If the results are good, try to improve the speed by increasing both parameters. Sometimes the resulting curves are not smooth if $D_{T_{max}}$ is too high. In most cases, good results are obtained with AUTO and $D_{T_{min}}$ set to about 1/1000 of the smallest time constant.

If no success is found with AUTO, then try Rosenbrock (STIFF) and adjust by the same procedure. Oscillations can sometimes be seen by zooming in on a graph; often these are a sign of integration problems. Sometimes some variables look OK but others oscillate, so look at all of them if problems arise. Unfortunately there is not a perfect recipe, but fortunately MADONNA is very fast so the trial-and-error method usually works out.

Checking Results by Mass Balance

For continuous processes, checking the steady-state results is very useful. Algebraic equations for this can be added to the program, such that both sides became equal at steady state. For batch systems, all the initial mass must equal all the final mass, not always in mols but in kg. Expressed in mols the stoichiometry must be satisfied.

What Is a "Floating Point Exception"?

This error message comes up when something does not calculate correctly, such as dividing by zero. This is a common error that occurs when equations contain a variable in the denominator that is initially zero. Often it is possible to add a very small number to it, so that the denominator is never exactly zero. These cases can usually be located by outputing a table of all the variables.

Plotting Variables with Distance and Time

Stagewise and finite-differenced models involve changes with time and distance. When the model is written in array form the variable can be plotted as a function of the array index. This is done by choosing an index variable for the Y axis and the [ ] symbol for the X axis. The last value calculated is used in the plot, which means that if the steady-state has been reached then it is a steady-state profile with distance. An example is given in the "Screenshot Guide" in Section 2 of the Appendix and in many other simulation examples.

Writing Your Own Plug-in Functions or Integration Methods

Information on using C or C++ for this can be obtained by email from Tim Zahnley, the MADONNA programmer-developer, at madonna@kagi.com.

2 Screenshot Guide to BERKELEY-MADONNA

This guide is intended as a supplementary introduction to MADONNA.

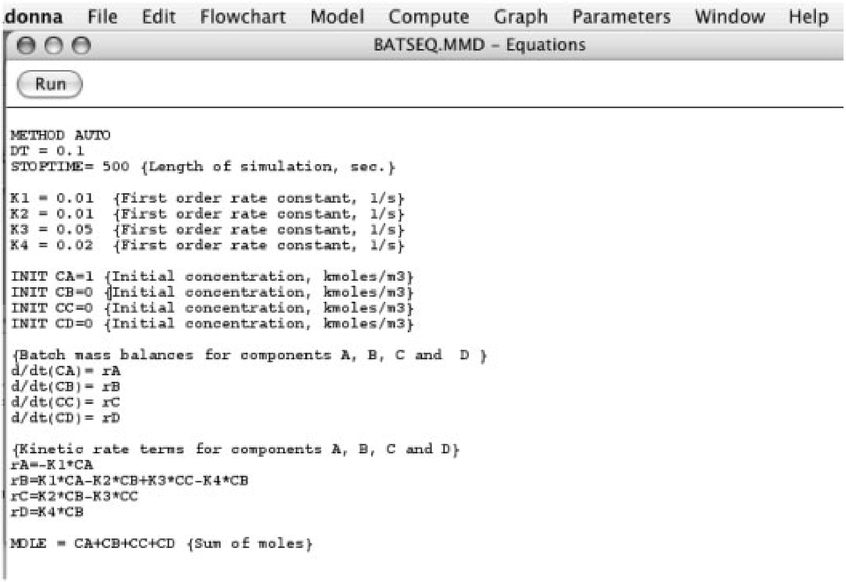

Fig. 1 The example BATSEQ equation window has been opened with Model/Equations.

Fig. 2 The example BATSEQ has been run with the Colors, Data Points and Grid selected. From left: Lock, Overlay, Table, Legend, Parameters, Colors, Dashed Lines, Data Points, Grid, Value Output and Zoom.

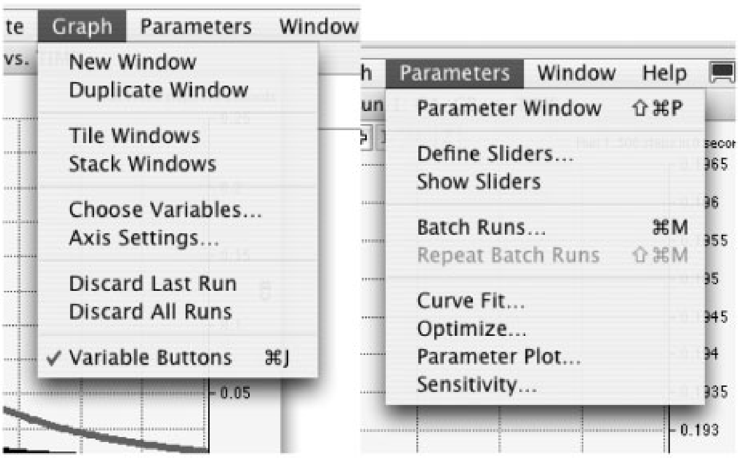

Fig. 3 The menus GRAPH and PARAMETERS are shown above.

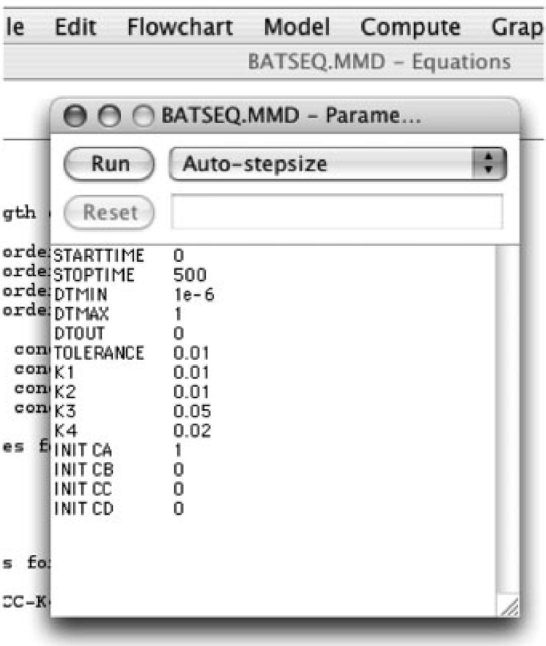

Fig. 4 The MODEL/EQUATIONS was chosen. Seen here is also the PARAMETER WINDOW.

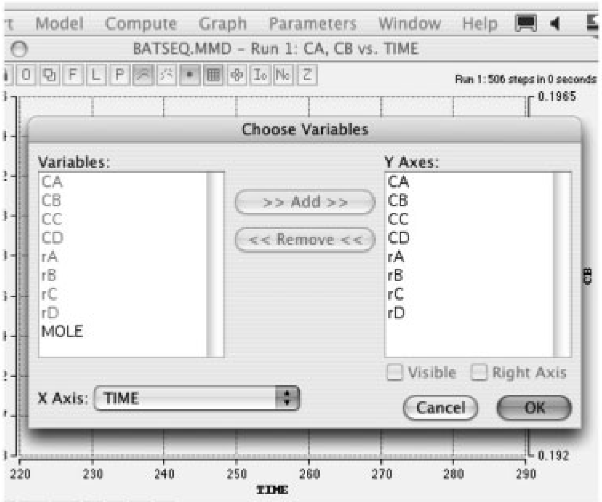

Fig. 5 If a new graph is chosen under GRAPH/NEW WINDOW then the data must be selected under GRAPH/CHOOSE VARIABLES.

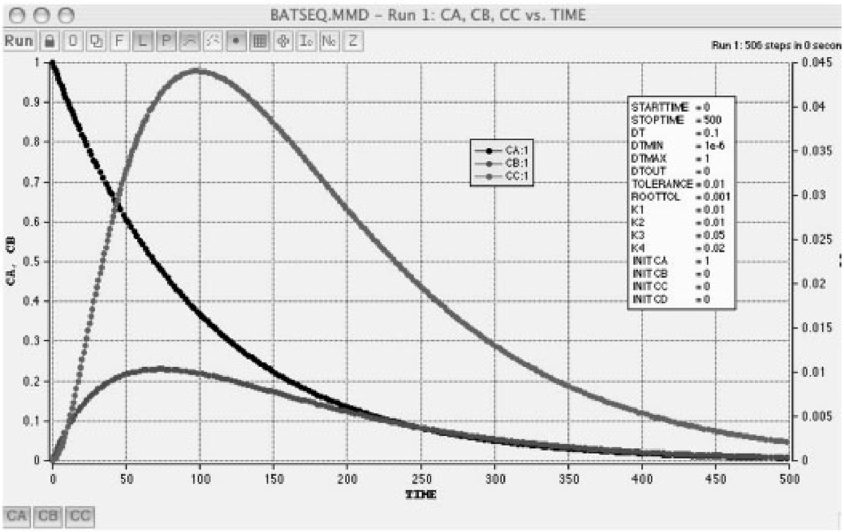

Fig. 6 A graph window with CC on the right-side Y-axis with Legend, Parameter and Data buttons selected.

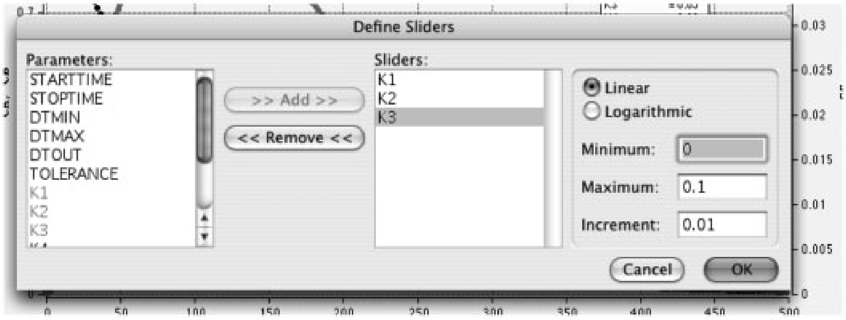

Fig. 7 The window to define the sliders (Parameters/Define Sliders).

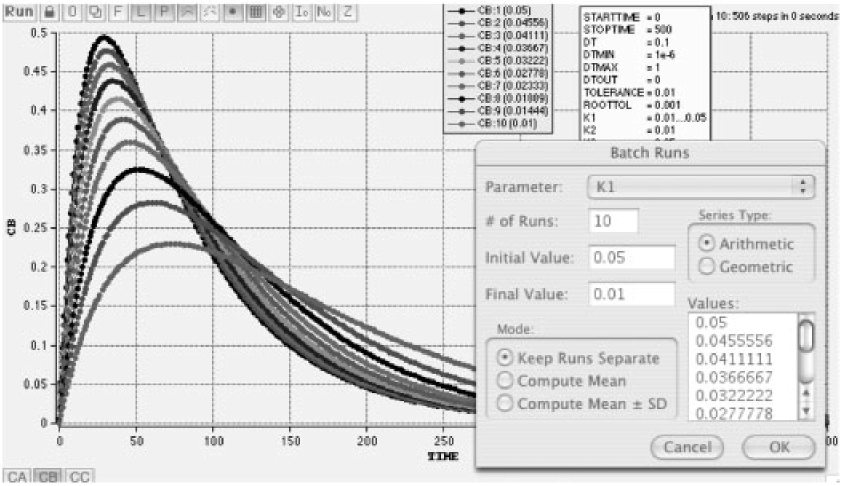

Fig. 8 The Batch Runs window for 10 values of k_1 as shown.

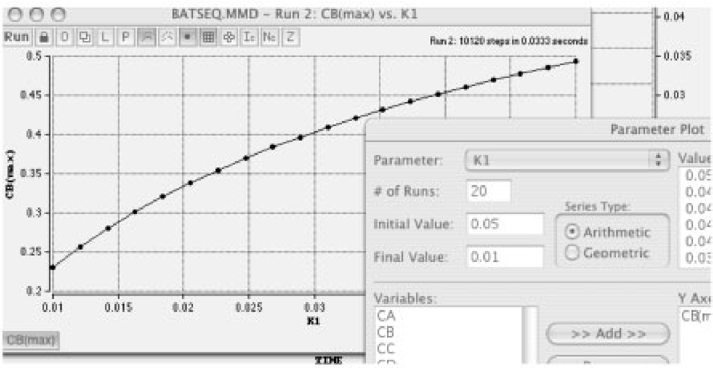

Fig. 9 A Parametric Plot to give the maximum in CB as a function of k_1.

3 List of Simulation Examples