

FASTSTART

This section is for people who do not read or even scan the main documentation. If you still cannot run your model after following the below short procedure then you should read the tutorial in the first section of the documentation.

- 1) Go into command mode (on the Windows start button select RUN, type “command” and press the <ENTER> key) and create a file named MODEL.DAT. If you have Excel97/2000/XP or Sun Microsystem's FREE Star-Office you can use the *blank Kintecus_workbook.xls* or *Enzyme_Regression_Fitting.xls* or *GRI_MECH_30.xls* EXCEL Visual Basic graphical interface modules and click the **MODEL tab** located at the bottom. If you use a text editor than enter your reactions like so:

```
1.323e-4, A- + Widget-- + C==>G+++ + F---+H2O
3.2      , E+F ==> G + DNA_A_Replicated
54.34    , G = A
END ( <==-- Make sure this END is here)
```

If you have Arrhenius expressions, then do your reactions like this (make sure you specify the correct Energy of Activation units in the parm.dat spreadsheet, look for the Ea Units field and type either Calories, Cal, Joules, J, KJ, KCAL or Kelvin:

```
1.323e-4, -1.2, 3000, A- +Widget-- + C==>G+++ + F---+H2O
3.2      , 0.3, 2000, E+F == > G + DNA_A_Replicated
54.34    , 2.1,5430, G = A
END ( <==-- Make sure this END is here)
```

- 2) Run Kintecus with the following switch: >Kintecus -c
(EXCEL: click the "**Make Species Worksheet from Model**" button located on the **CONTROL** worksheet)
- 3) Now copy the created ADDSPEC.TXT file as a SPECIES.DAT file
(ie. >COPY ADDSPEC.TXT SPECIES.DAT)
- 4) Edit the Initial concentration fields in species.dat for your model and type "Y" in the DISPLAY field for species' concentrations you want to save. (EXCEL: click the **species tab** located near the bottom and then edit the same fields in the species worksheet)
- 5) Run kintecus: >KINTECUS -ig:mass -show. (EXCEL: click the **CONTROL tab** located near the bottom and then click the **RUN button** to start your model!)
- 6) If you are using the EXCEL modules, on the **CONTROL** worksheet, click the **Plot Results** button to plot your results!

- 7) **OPTIONAL:** If you wish to do include thermodynamics (temperature and reverse rate autocalculations), just use the –THERM switch on the command line.
- 8) **OPTIONAL:** If you wish to do sensitivity analysis just use the –SENSIT:1 on the command line.
- 9) **OPTIONAL:** If you wish to FIT experimental data to a model, have your data in a text file named, FITDATA.TXT with Time(s) as the first column, first row. The species names should follow the Time(s) heading on the same row. Place your species/temperature data under the appropriate species column (if a species is missing data for a time point, place an “N” in the cell). Append a question mark, "?", to the end of ***any number*** you wish for Kintecus to regress/fit. Run Kintecus with –FIT:2:3:FITDATA.TXT. You can also try –FIT:1:3:FITDATA.TXT , -FIT:1:1:FITDATA.TXT and –FIT:2:1:FITDATA.TXT .