

# Manual for gmkim

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# Introduction

The R add-on package `gmkIn` provides a browser based graphical interface for performing kinetic evaluations of degradation data using the `mkIn` package. While the use of `gmkIn` should be largely self-explanatory, this manual may serve as a functionality overview and reference.

For system requirements and installation instructions, please refer to the `gmkIn` homepage.

## Starting gmkIn

As gmkIn is an R package, you need to start R and load the gmkIn package before you can run gmkIn. The latter can be achieved by entering the command

```
library(gmkIn)
```

into the R console. This will also load the packages that gmkIn depends on, most notably gWidgetsWWW2 and mkin. Loading the package only has to be done once after you have started R.

Before you start gmkIn, you should make sure that R is using the working directory that you would like to keep your gmkIn project file(s) in. If you use the standard R GUI application on windows, you can change the working directory from the File menu ('File' -> 'Change dir...').

Once you are sure that the working directory is what you want it to be, gmkIn can be started by entering the R command

```
gmkIn()
```

## Three column layout

Since version 0.6.1, gmkin adheres to a three column layout. To the left, there are explorer areas for the available projects, datasets, kinetic models and the completed fits.

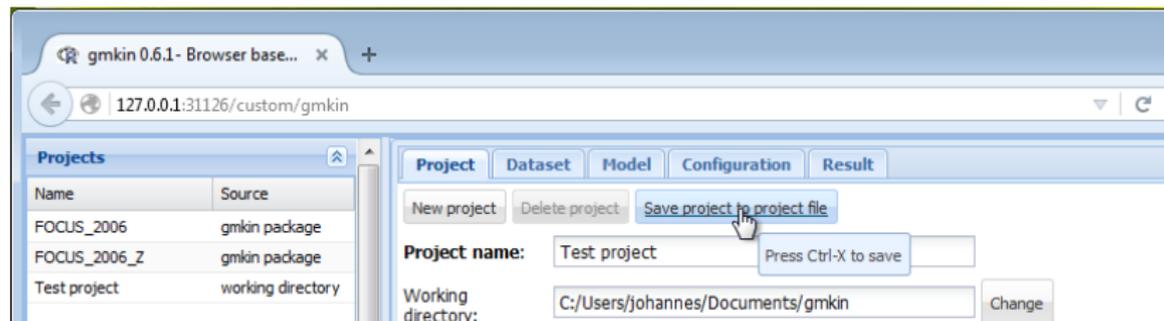
In the central, tabbed area, the projects, datasets, models and fits are defined. The area to the right is mainly for showing information intended to support the user, and results. However, it also contains a tab 'Data' for editing kinetic data.

## Project file management

At startup, the project explorer to the left shows the two project workspaces 'FOCUS\_2006' and 'FOCUS\_2006\_Z' delivered with the package. The project management area in the center gives the possibility to save these projects under a new name, or to start a new, empty project.

A gmkin project workspace contains datasets, kinetic models for fitting, and so-called fits, i.e. the results of fitting models to data. The project area also shows the current working directory, where project workspace files are saved using the file extension `.gmkinws`.

Once a project has been saved by the user, the project explorer to the left will show it in the project list.



The screenshot shows the gmkin 0.6.1 web interface. The browser address bar displays '127.0.0.1:31126/custom/gmkin'. The interface is divided into several sections:

- Projects:** A table on the left lists existing projects.
- Project Management:** A central area with tabs for 'Project', 'Dataset', 'Model', 'Configuration', and 'Result'. It contains buttons for 'New project', 'Delete project', and 'Save project to project file'. A tooltip 'Press Ctrl-X to save' is visible over the 'Save project to project file' button.
- Project name:** A text input field containing 'Test project'.
- Working directory:** A text input field containing 'C:/Users/Johannes/Documents/gmkin' with a 'Change' button next to it.

Name	Source
FOCUS_2006	gmkin package
FOCUS_2006_Z	gmkin package
Test project	working directory

# Dataset editor

When you select one of the datasets in the dataset explorer to the left, some summary information about the dataset is shown in the center, and the data itself is loaded into the data editor to the right.

The screenshot shows the gmskin dataset editor interface. The left sidebar contains a 'Projects' section with 'Datasets' and 'Models'. The 'Datasets' section shows 'FOCUS example dataset Z'. The 'Models' section lists 'Z.2a.ff', 'Z.FOCUS', and 'Z.mkn.1'. The 'Configuration' section shows 'FOCUS example dataset Z' as the current model. The 'Results' section is empty.

The main area is divided into two panes. The top pane is titled 'Dataset' and contains the following information:

- Project: FOCUS example dataset Z
- Dataset title: FOCUS example dataset Z
- Sampling times: 0, 0.04, 0.125, 0.29, 0.54, 1, 2, 3, 4, 7, 10, 14, 21, 42, 61, 96, 1
- Unit: [empty]
- Replicates: 1
- Observed: Z0, Z1, Z2, Z3
- Unit: [empty]

Below this information is a section for 'Generate grid for entering kinetic data' with an 'Upload text file' button and a 'Browse...' button. An 'Upload' button is also present.

The bottom pane is titled 'Kinetic data' and contains a table with the following columns: name, time, value, override, and err. The table displays data for various time points (Z0, Z1, Z2, Z3) and replicates (1, 2, 3, 4).

name	time	value	override	err
Z0	0.00000	100.00000	NA	1.00000
Z0	0.04000	81.70000	NA	1.00000
Z0	0.12500	70.40000	NA	1.00000
Z0	0.29000	51.10000	NA	1.00000
Z0	0.54000	41.20000	NA	1.00000
Z0	1.00000	6.60000	NA	1.00000
Z0	2.00000	4.60000	NA	1.00000
Z0	3.00000	3.90000	NA	1.00000
Z0	4.00000	4.60000	NA	1.00000
Z0	7.00000	4.30000	NA	1.00000
Z0	10.00000	6.80000	NA	1.00000
Z0	14.00000	2.90000	NA	1.00000
Z0	21.00000	3.50000	NA	1.00000
Z0	42.00000	5.30000	NA	1.00000
Z0	61.00000	4.40000	NA	1.00000
Z0	96.00000	1.20000	NA	1.00000
Z0	124.00000	0.70000	NA	1.00000
Z1	0.00000	0.00000	NA	1.00000
Z1	0.04000	18.30000	NA	1.00000
Z1	0.12500	29.60000	NA	1.00000
Z1	0.29000	46.30000	NA	1.00000
Z1	0.54000	55.10000	NA	1.00000

The bottom status bar indicates 'Page 1 of 1' and 'Displaying rows 1 - 68 of 68'.

When you have added information about the units, or edited the data to the right, you should hit the button 'Keep changes'. This

## Model editor

The following screenshot shows the model editor for the model number 4 in the list of models that are in the initial workspace.

The screenshot shows the 'Model 4' editor. At the top, the 'Model name' is 'SFO\_SFO' and 'Use of formation fractions' is set to 'max'. Below this are four buttons: 'Copy model', 'Delete model', 'Add observed variable', and 'Keep changes'. The main area contains two rows of state variable specifications. The first row shows 'parent' as the parent, 'SFO' as the state variable, and 'm1' as the target, with a checked 'Path to sink' box. The second row shows 'm1' as the parent, 'SFO' as the state variable, and a text box for 'Optional list of target variables, e.g. 'm1, m2'' as the target, also with a checked 'Path to sink' box and a 'Remove observed variable' button.

In the first line the name of the model can be edited. You can also specify “min” or “max” for minimum or maximum use of formation fractions. Maximum use of formation fractions means that the differential equations in the degradation model are formulated using formation fractions. When you specify “min”, then formation fractions are only used for the parent compound when you use the FOMC, DFOP or the HS model for it.

Pressing “Copy model” keeps the model name, so you should change it for the newly generated copy. Pressing “Add observed variable” adds a line in the array of state variable specifications below. The observed variables to be added are usually transformation products

## Plotting and fitting

If the dataset(s) to be used in a project are created, and suitable kinetic models have been defined, kinetic evaluations can be configured by selecting one dataset and one model in the lists to the left, and the pressing the button “Configure fit for selected dataset and model” below these lists.

This opens the “Plotting and fitting” tab area to the right, consisting of a graphical window showing the data points in the selected dataset and the model, evaluated with the initial parameters defined by calling `mkinfit` without defining starting parameters. The value of the objective function to be minimized for these default parameters can be seen in the R console, e.g. as

```
Model cost at call 1: 15156.12
```

for the example shown below, where the FOCUS example dataset D and the model SFO\_SFO were selected.

The screenshot shows a software window titled "Dataset 2, Model SFO\_SFO". The main content area displays "FOCUS example dataset D". Above this area is a control bar with several buttons: "Run", "Keep fit", "Delete fit", "Show initial", and "Get initials from". To the right of these buttons is a dropdown menu currently showing "Fit 1". Below the control bar, there are four tabs: "Parameters", "Fit options", "Summary", and "Plot options". The "Parameters" tab is currently selected. In the bottom right corner of the window, there are three small circular icons: a refresh icon, a search icon, and a help icon.