Manual for gmkin

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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.

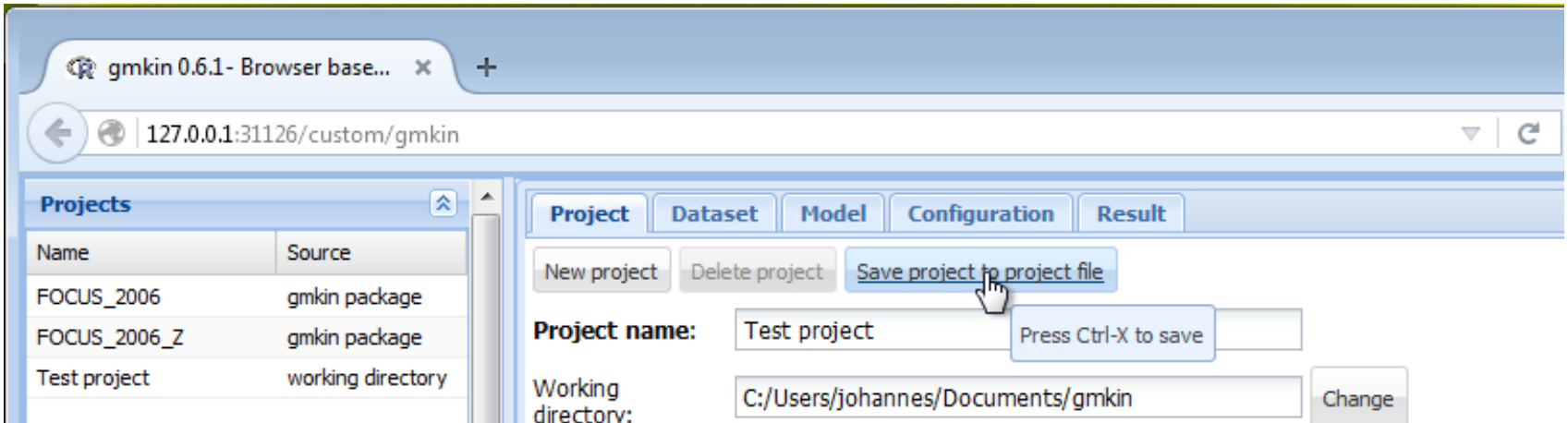
In the central, tabbed area, the projects, datasets, models and fits are defined. The area to the right is mainly for showing information intended to support the user, and results. However, it also contains a tab 'Data' for editing kinetic data.

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 manangement area in the center gives the possibility to save these projects under a new name, or to start a new, empty project.

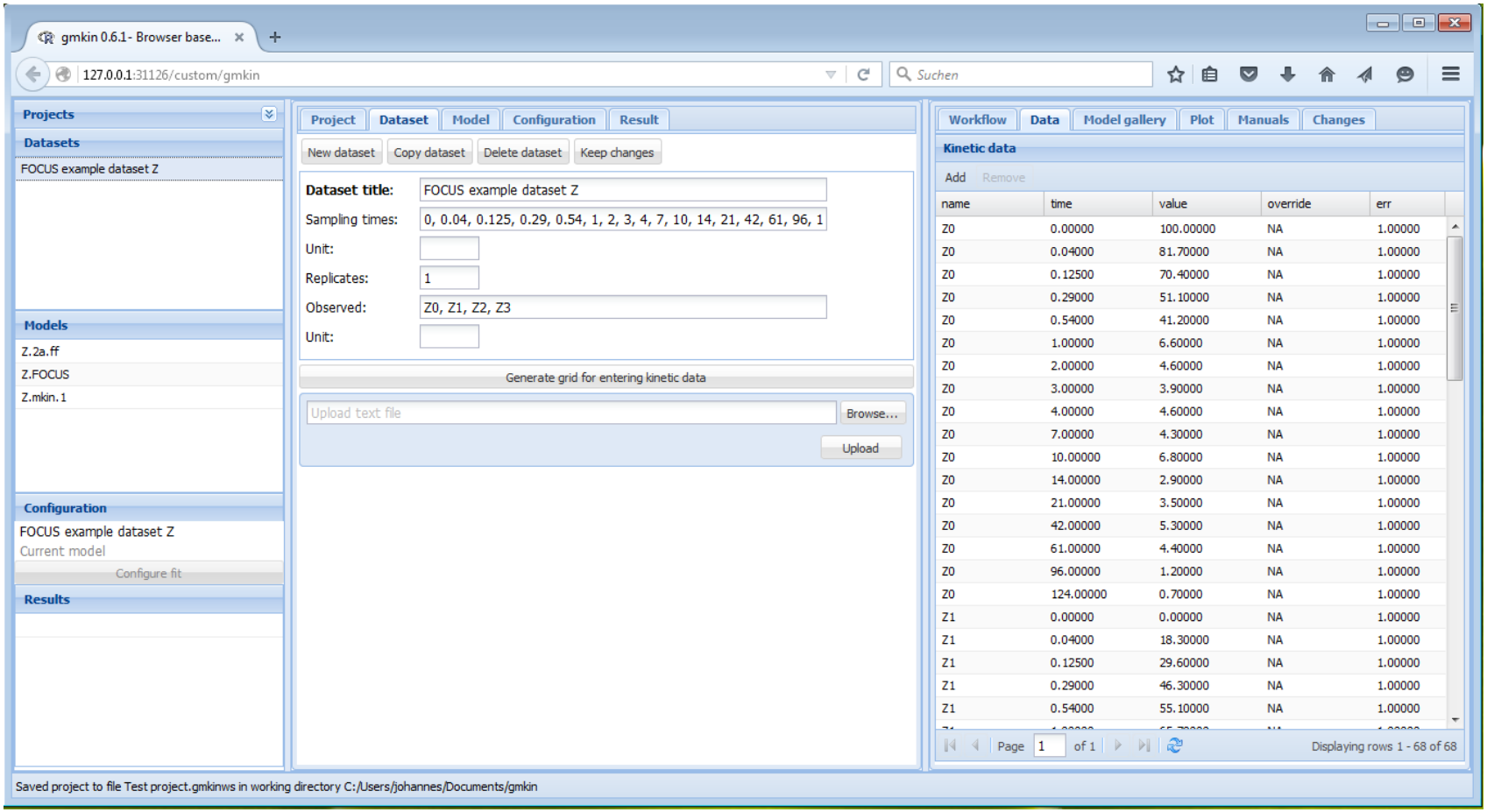
A gmkin project workspace contains datasets, kinetic models for fitting, and so-called fits, i.e. the results of fitting models to data. The project area also shows the current working directory, where project workspace files are saved using the file extension `.gmkinws`.

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



Dataset editor

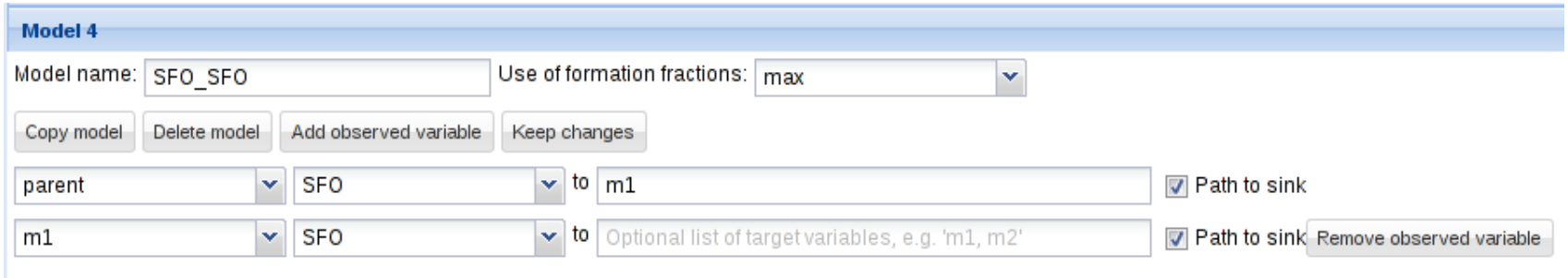
When you select one of the datasets in the dataset explorer to the left, some summary information about the dataset is shown in the center, and the data itself is loaded into the data editor to the right.



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.



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.