

mkin -
Routines for fitting kinetic models with one or more
state variables to chemical degradation data

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Abstract

In the regulatory evaluation of chemical substances like plant protection products (pesticides), biocides and other chemicals, degradation data play an important role. For the evaluation of pesticide degradation experiments, detailed guidance has been developed, based on nonlinear optimisation. The R add-on package **mkin** implements fitting the models recommended in this guidance from within R and calculates the recommended statistical measures for data series within one or more compartments, for parent and metabolites.

Contents

1	Introduction	1
2	Example	1
2.1	Data format	1

Key words: Kinetics, FOCUS, nonlinear optimisation

1 Introduction

Many approaches are possible regarding the evaluation of chemical degradation data. The **mk**in package ([mk](#)in, 2010) in R ([R Development Core Team, 2010](#)) implements the approach recommended in the kinetics report provided by the FORum for Co-ordination of pesticide fate models and their USe ([FOCUS Work Group on Degradation Kinetics, 2006](#)) for simple data series for one parent compound in one compartment.

2 Example

In the following, requirements for data formatting are explained. Then the procedure for fitting the four kinetic models recommended by the FOCUS group to an example dataset for parent only given in the FOCUS kinetics report is illustrated. The explanations are kept rather verbose in order to lower the barrier for R newcomers.

2.1 Data format

The following listing shows example dataset C from the FOCUS kinetics report as distributed with the **kinfit** package

```
R> library("mk
```

```
R> FOCUS_2006_C
      t parent
1    0  85.1
2    1  57.9
3    3  29.9
4    7  14.6
5   14   9.7
6   28   6.6
7   63   4.0
8   91   3.9
9  119   0.6
```

Note that the data needs to be in the format of a data frame containing a variable `time` containing sampling times and a variable `parent` containing the measured data. Replicate measurements are not recorded in extra columns but simply appended, leading to multiple occurrences of the sampling times `time`.

Small to medium size dataset can be conveniently entered directly as R code as shown in the following listing

```
R> example_data <- data.frame(  
+   time = c(0, 1, 3, 7, 14, 28, 63, 91, 119),  
+   parent = c(85.1, 57.9, 29.9, 14.6, 9.7, 6.6, 4, 3.9, 0.6)  
+ )
```

References

FOCUS Work Group on Degradation Kinetics. *Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration. Report of the FOCUS Work Group on Degradation Kinetics*, 2006. URL <http://focus.jrc.ec.europa.eu/dk>. EC Document Reference Sanco/10058/2005 version 2.0.

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