kinfit - Routines for fitting kinetic models to chemical degradation data

Johannes Ranke
Product Safety
Harlan Laboratories Ltd.
Zelgliweg 1, CH–4452 Itingen, Switzerland

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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 regression. The R add-on package **kinfit** implements fitting the models recommended in this guidance from within R and calculates the recommended statistical measures for data series within one compartment without metabolite data.

Contents

Key words: Kinetics, FOCUS, nonlinear fitting

1 Introduction

Many approaches are possible regarding the evaluation of chemical degradation data. The **kinfit** package (kinfit, 2009) in R (R Development Core Team, 2009) 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 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("kinfit")
R> data("FOCUS_2006_C", package = "kinfit")
R> print(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 `t` 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 `t`.

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

```
R> kindata_example <- data.frame(
+   t = 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)
+ )
```

2.2 Fitting the kinetic models

The user can choose for which kinetic models the `kinfit` function will try to find optimised parameters. This is achieved by the argument `kinmodels` to the function, as shown below. The models currently implemented are abbreviated `SFO` (Single First-Order), `FOMC` (First-Order Multi-Compartment), `DFOP` (Double First-Order in Parallel) and `HS` (Hockey-Stick) as defined by the FOCUS Work Group on Degradation Kinetics (2006). From the DFOP model, corresponding parameters in the notation of the SFORB model (Single First-Order Reversible Binding) are additionally calculated.

```
R> kinfits.C <- kinfit(FOCUS_2006_C, kinmodels = c("SFO", "FOMC", "DFOP", "HS"))
```

The results of the fitting procedure are returned by the function, and can then be inspected by the function `kinresults`.

```
R> kinresults(kinfits.C)
```

```
$parms
$parms$SFO
```

```
$parms$SFO$parent.0
[1] 82.49215

$parms$SFO$k
[1] 0.3060631


$parms$FOMC
$parms$FOMC$parent.0
[1] 85.87489

$parms$FOMC$alpha
[1] 1.053294

$parms$FOMC$beta
[1] 1.917394


$parms$DFOP
$parms$DFOP$parent.0
[1] 85.00274

$parms$DFOP$k1
[1] 0.4595574

$parms$DFOP$k2
[1] 0.01784880

$parms$DFOP$g
[1] 0.8539454


$parms$SFORB
$parms$SFORB$parent.0
[1] 85.00274

$parms$SFORB$k1out
[1] 0.3950439

$parms$SFORB$k21
[1] 0.02076364

$parms$SFORB$k12
[1] 0.06159872


$parms$HS
$parms$HS$parent.0
[1] 84.50157
```

```
$parms$HS$k1
[1] 0.3561582

$parms$HS$k2
[1] 0.02266093

$parms$HS$tb
[1] 5.152759



$stats
     n.times df mean.means        RSS    err.min
SFO        9  7   23.58889 196.533408 0.15843954
FOMC       9  6   23.58889  31.050882 0.06656760
DFOP       9  5   23.58889   4.362714 0.02662111
HS         9  5   23.58889  13.585774 0.04695151

$results
         DT50      DT90
SFO  2.264720  7.523236
FOMC 1.785233 15.147899
DFOP 1.886916 21.250728
HS   1.946184 25.778033
```

The higher level functions `kinplot` and `kinreport` work on lists called `kinobject`. They contain the fitted models, optionally the data used for fitting the models, and the name of the parent compound as well as the test system type used for generating the data, as well as some more optional entries. The construction of such an object is shown below.

```
R> kinobject.C <- kinobject <- list(
+         parent = "Compound XY",
+         type = "Degradation in the environment",
+         system = "System 1",
+         source = "Synthetic example data from FOCUS kinetics",
+         data = FOCUS_2006_C,
+         fits = kinfits.C,
+         results = kinresults(kinfits.C))
```

The plotting and reporting functions then work on this object. The example below outputs the report to the console, because no `file` argument is specified. If a filename is specified, the report will be written to a text file.

```
R> kinreport(kinobject.C)
```

```
Parent compound:  Compound XY
Study type:       Degradation in the environment
```

```
System:           System 1
Source:           Synthetic example data from FOCUS kinetics


---
Nonlinear least squares fit of the SFO model

Parameter estimation:
         Estimate Std. Error t value   Pr(>t)
parent.0   82.492     4.7402   17.40 2.54e-07
k           0.306     0.0459    6.67 1.43e-04

Chi2 error estimation:        15.84 %



---
Nonlinear least squares fit of the FOMC model

Parameter estimation:
         Estimate Std. Error t value   Pr(>t)
parent.0    85.87      2.246   38.23 1.07e-08
alpha        1.05      0.169    6.23 3.95e-04
beta         1.92      0.537    3.57 5.89e-03

Chi2 error estimation:        6.66 %



---
Nonlinear least squares fit of the DFOP model

Parameter estimation:
         Estimate Std. Error t value   Pr(>t)
parent.0  85.0027    0.89067   95.44 1.20e-09
k1         0.4596    0.02036   22.57 1.59e-06
k2         0.0178    0.00304    5.87 1.02e-03
g          0.8539    0.01344   63.54 9.14e-09

Chi2 error estimation:        2.66 %



---
Nonlinear least squares fit of the HS model

Parameter estimation:
         Estimate Std. Error t value   Pr(>t)
```

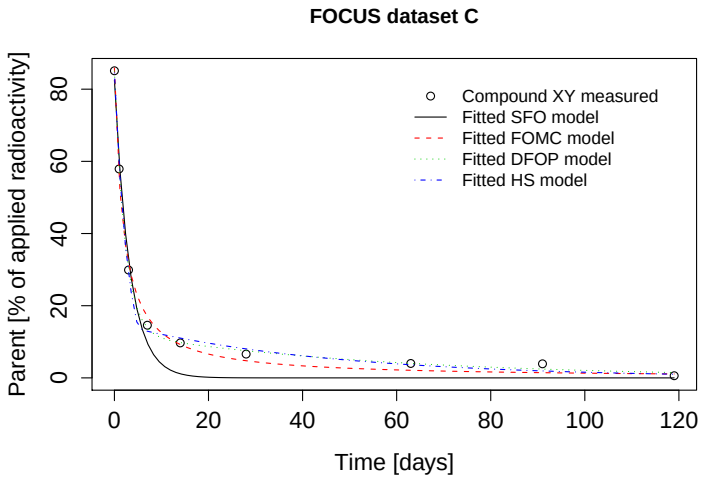

Figure 1: Fits of standard models to FOCUS dataset C.

```
parent.0  84.5016    1.53770    55.0 1.89e-08
k1         0.3562    0.01852    19.2 3.51e-06
k2         0.0227    0.00567     4.0 5.18e-03
tb         5.1528    0.41051    12.6 2.85e-05

Chi2 error estimation:        4.7 %


---
Endpoint estimates

     DT50 DT90
SFO   2.3  7.5
FOMC  1.8 15.1
DFOP  1.9 21.3
HS    1.9 25.8
```

Plotting is done on an on-screen device. Graphics files in vector based formats can be obtained using the R devices `pdf`, `eps`, or, subject to platform restrictions, `windows.metafile`.

A residual plot can be obtained with the function `kinresplot` as shown in Figure 2.

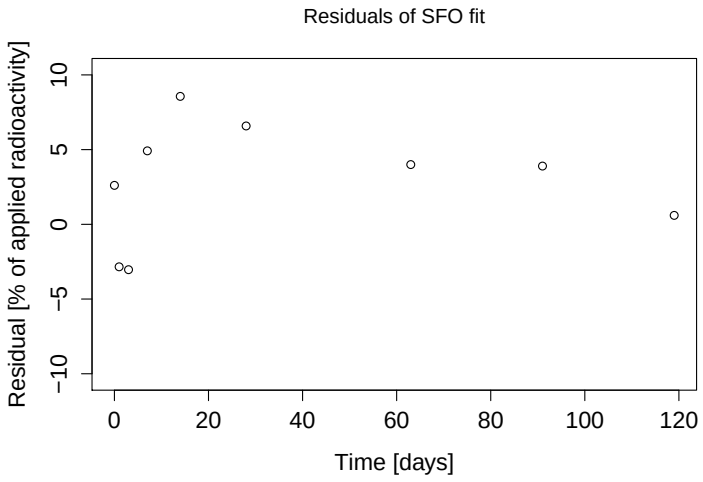

Figure 2: Residual plot for fitting the SFO model to FOCUS dataset C.

3 Validation

In the following comparisons, the results for fitting the four recommended kinetic models to FOCUS datasets A to F with **kinfit** were obtained.

3.1 Single First Order Model

In Tables 1 to 6, the results from fitting the SFO model to FOCUS example datasets with various software packages as given in the report by the FOCUS Work Group on Degradation Kinetics (2006) are compared with the results obtained with **kinfit**.

The comparisons show that all packages evaluated in the FOCUS report give very similar results for the SFO model. The results obtained with **kinfit** are very close to the median of the results reported for the other packages.

3.2 First Order Multi Compartment Model

The comparison of the results obtained for the FOMC model show much more variability between software packages. For dataset A, results for the `alpha` and `beta` parameters differ over several orders of magnitude between the different packages. The method used by the `kinfit` routine does not converge for this dataset. The same applies to the total system and water phase only data for example dataset F and the FOMC model.

For datasets B and C, the **kinfit** function produces results which are very close to the median of the results obtained by the other packages.

Table 1: Results of fitting the SFO model to the example dataset A (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	k	DT_{50}	DT_{90}
ACSL	109.20	0.0372	18.63	61.90
Excel	109.15	0.0372	18.62	61.87
Kinetica	109.11	0.0371	18.66	62.00
Madonna	109.20	0.0372	18.63	61.90
Mathematica	109.15	0.0372	18.62	61.87
MatLab	109.15	0.0372	18.63	61.87
ModelMaker	109.10	0.0371	18.68	62.06
ModelManager	109.15	0.0372	18.62	61.86
PRISM	109.20	0.0372	18.63	61.90
Statistica	109.15	0.0372	18.63	61.90
Tablecurve	109.15	0.0372	18.62	61.87
Median	109.15	0.0372	18.63	61.90
kinfit	109.15	0.0372	18.62	61.87

Table 2: Results of fitting the SFO model to the example dataset B (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	k	DT_{50}	DT_{90}
ACSL	99.20	0.0782	8.86	29.44
Excel	99.17	0.0782	8.87	29.46
Kinetica	99.17	0.0781	8.87	29.47
Madonna	99.18	0.0782	8.87	29.46
Mathematica	99.17	0.0782	8.87	29.46
MatLab	99.17	0.0782	8.89	29.46
ModelMaker	99.20	0.0780	8.89	29.52
ModelManager	99.17	0.0782	8.87	29.46
PRISM	99.17	0.0782	8.87	29.46
Statistica	99.17	0.0782	8.87	29.46
Tablecurve 2D	99.17	0.0782	8.87	29.46
Median	99.17	0.0782	8.87	29.46
kinfit	99.17	0.0782	8.87	29.46

Table 3: Results of fitting the SFO model to the example dataset C (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	k	DT_{50}	DT_{90}
ACSL	82.50	0.3062	2.26	7.52
Kinetica	82.40	0.3043	2.28	7.57
Madonna	82.49	0.3060	2.27	7.52
Mathematica	82.49	0.3060	2.26	7.52
MatLab	82.49	0.3060	2.27	7.52
ModelMaker	82.49	0.3054	2.27	7.54
PRISM	82.49	0.3061	2.26	7.52
Tablecurve 2D	82.49	0.3061	2.26	7.52
Median	82.49	0.3060	2.265	7.52
kinfit	82.49	0.3061	2.26	7.52

Table 4: Results of fitting the SFO model to the example dataset D (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	k	DT_{50}	DT_{90}
ACSL	99.64	0.0989	7.01	23.29
Madonna	99.45	0.0979	7.08	23.52
MatLab	98.31	0.0989	7.00	23.28
PRISM	99.44	0.0979	7.08	23.51
Tablecurve 2D	99.44	0.0979	7.08	23.51
Median	99.44	0.0979	7.08	23.51
kinfit	99.44	0.0979	7.08	23.51

Table 5: Results of fitting the SFO model to the total system data from example dataset F (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	k	DT_{50}	DT_{90}
Kinetica	104.42	0.0398	17.40	57.80
Madonna	104.49	0.0399	17.35	57.64
Mathematica	104.48	0.0399	17.35	57.64
MatLab	104.48	0.0400	17.35	57.63
ModelMaker	104.50	0.0398	17.42	57.85
ModelManager	104.47	0.0399	17.35	57.64
PRISM	104.50	0.0400	17.35	57.64
Median	104.48	0.0399	17.35	57.64
kinfit	104.47	0.0399	17.35	57.64

Table 6: Results of fitting the SFO model to the water phase data from example dataset F (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	k	DT_{50}	DT_{90}
ACSL	100.54	0.0551	12.58	41.80
Kinetica	100.88	0.0554	12.51	41.57
Madonna	100.54	0.0550	12.59	41.83
Mathematica	100.55	0.0551	12.58	41.80
MatLab	100.55	0.0551	12.58	41.80
ModelMaker	100.50	0.0549	12.63	41.94
ModelManager	100.55	0.0551	12.58	41.80
PRISM	100.50	0.0551	12.58	41.80
Median	100.545	0.0551	12.58	41.80
kinfit	100.55	0.0551	12.58	41.80

Table 7: Results of fitting the FOMC model to the example dataset A (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	α	β	DT_{50}	DT_{90}
ACSL	109.34	2.93e+03	780000	18.43	61.32
Excel	109.20	2.36e+06	63300000	18.62	61.87
Kinetica	107.29	4.26e+05	9640000	15.68	52.09
Madonna	109.18	2.08e+06	55900000	18.60	61.79
Mathematica	109.15	1.07e+06	28700000	18.62	61.87
MatLab	109.45	2.74e+01	718	18.39	62.93
ModelMaker	109.20	2.54e+04	682000	18.62	61.87
Modelmaker[a]	109.16	2.99e+02	8040	18.66	62.15
ModelManager	109.17	5.15e+02	13800	18.61	61.93
PRISM	109.20	5.50e+05	14800000	18.62	61.86
Statistica	109.20	1.25e+04	337000	18.62	61.87
Tablecurve 2D	109.14	-3.43e-04	-922	18.62	61.90
Median	109.19	1.895e+04	731000	18.62	61.87
kinfit	no fit				

3.3 Dual First Order in Parallel Model

Regarding fitting the DFOP model to FOCUS example dataset A, it is already indicated in the report that it is not a good example dataset for fitting this particular model, as the two kinetic constants postulated by the DFOP model are hardly distinguishable. As a consequence, the software packages strongly disagree especially on the model parameter f specifying the distribution between the kinetic domains that are characterised by the two kinetic constants. Again, the **kinfit** routine does not show conversion for this model and this dataset (Table 12).

Fitting the DFOP model with **kinfit** to dataset B yields results that are very close to the median of the results obtained by other packages, as illustrated in Table 13.

3.4 Hockey Stick Model

Analysis of dataset A shows basically two different parameter sets generated by the 8 packages reported in the FOCUS report (FOCUS Work Group on Degradation Kinetics, 2006). The **kinfit** package does not show conversion with the standard paramater defaults, but can reproduce the two parameter sets when given the respective paramter values as

Table 8: Results of fitting the FOMC model to the example dataset B (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	α	β	DT_{50}	DT_{90}
ACSL	99.60	1.32e-03	161	8.69	30.71
Excel	99.20	4.94e+06	63200000	8.87	29.46
Kinetica	99.66	1.27e+01	155	8.67	30.72
Madonna	99.66	1.28e+01	13.8	8.69	30.76
Mathematica	99.67	1.28e+01	156	8.68	30.75
MatLab	99.75	1.10e+01	133	8.65	30.98
ModelMaker	99.70	1.28e+01	156	8.69	30.76
ModelMaker[a]	99.67	1.25e+01	153	8.72	30.95
ModelManager	99.67	1.28e+01	156	8.68	30.75
PRISM	99.67	1.28e+01	156	8.68	30.74
Statistica	99.66	1.28e+01	156	8.68	30.76
Tablecurve	99.66	1.28e+01	156	8.68	30.76
Median	99.66	1.28e+01	156	8.68	30.76
kinfit	99.67	12.805	156.1122	8.68	30.75

Table 9: Results of fitting the FOMC model to the example dataset C (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	α	β	DT_{50}	DT_{90}
Kinetica	85.87	1.06	1.92	1.79	15.12
Madonna	85.88	1.05	1.92	1.79	15.14
Mathematica	85.87	1.05	1.92	1.79	15.15
MatLab	85.88	1.05	1.92	1.79	15.15
ModelMaker	85.88	1.04	1.89	1.79	15.39
PRISM	85.88	1.05	1.92	1.79	15.16
Tablecurve 2D	85.87	1.05	1.92	1.79	15.15
Median	85.88	1.05	1.92	1.79	15.15
kinfit	85.87	1.0533	1.9174	1.79	15.15

Table 10: Results of fitting the FOMC model to the total system data from example dataset F (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	α	β	DT_{50}	DT_{90}
Kinetica	103.94	2.21e+03	52200	16.41	54.55
Madonna	104.49	2.51e+06	62700000	17.34	57.59
Mathematica	104.47	1.28e+06	31900000	17.35	57.64
MatLab	104.68	3.84e+01	942	17.17	58.26
ModelMaker	104.50	1.05e+02	2630	17.39	58.21
ModelManager	104.48	2.13e+03	53200	17.35	57.65
PRISM	104.50	8.38e+04	2.1e+07	17.35	57.65
Median	104.49	2210.0000	52200	17.35	57.65
kinfit	no fit				

Table 11: Results of fitting the FOMC model to the water phase data from example dataset F (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	α	β	DT_{50}	DT_{90}
Kinetica	100.51	1.26e+03	2.27E+04	12.51	41.58
Madonna	100.55	3.76e+06	6.83E+07	12.59	41.81
Mathematica	100.55	1.86e+06	3.39E+07	12.58	41.80
MatLab	100.73	4.79e+01	8.55E +02	12.47	42.13
MMaker	100.60	1.20e+02	2.18E+03	12.60	42.15
ModelManager	100.55	2.14e+03	3.89E+04	12.58	41.81
PRISM	100.50	9.78e+04	1.77E+06	12.55	41.68
Median	100.55	2140.0000	3.39E+07	12.58	41.81
kinfit	no fit				

Table 12: Results of fitting the DFOP model to the example dataset A (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	f	k_1	k_2	DT_{50}	DT_{90}
ACSL	109.30	1.00	0.0376	0.0000	18.43	61.24
Madonna	109.15	0.54	0.0372	0.0372	18.62	61.87
Mathematica	109.15	0.58	0.0372	0.0372	18.62	61.87
MatLab	109.15	0.50	0.0372	0.0372	18.62	61.86
ModelMaker	109.10	0.07	0.0369	0.0371	18.70	62.10
PRISM	109.16	0.50	0.0372	0.0372	18.65	61.88
Tablecurve	109.14	0.79	0.0372	0.0373	18.63	61.86
Median	109.15	0.54	0.0372	0.0372	18.62	61.87
kinfit	no fit					

Table 13: Results of fitting the DFOP model to the example dataset B (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	f	k_1	k_2	DT_{50}	DT_{90}
ACSL	99.59	0.82	0.0890	0.0439	8.70	30.60
Madonna	99.65	0.67	0.0959	0.0526	8.64	30.34
Mathematica	99.65	0.67	0.0958	0.0525	8.68	30.79
MatLab	99.61	0.80	0.0903	0.0452	8.69	30.71
ModelMaker	99.70	0.68	0.0955	0.0517	8.70	30.90
PRISM	99.65	0.67	0.0958	0.0525	8.68	30.79
Statistica	99.65	0.67	0.0958	0.0526	8.64	30.74
Tablecurve 2D	99.65	0.67	0.0958	0.0526	8.68	30.79
Median	99.65	0.67	0.0958	0.0525	8.68	30.77
kinfit	99.65	0.67	0.0958	0.0525	8.68	30.79

Table 14: Results of fitting the HS model to the example dataset A (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	t_b	k_1	k_2	DT_{50}	DT_{90}
Excel[a]	102.31	10.92	0.0167	0.0544	20.29	49.86
Excel[a]	100.75	5.11	0.0006	0.0456	20.22	55.49
Kinetica	101.24	5.96	0.0066	0.0462	20.13	54.99
Madonna	102.31	10.91	0.0167	0.0544	20.29	49.86
Mathematica	100.26	5.33	0.0462	0	20.33	49.56
ModelMaker	102.30	10.90	0.0167	0.0543	20.31	49.95
ModelManager	102.31	10.91	0.0167	0.0545	20.29	49.85
PRISM	102.30	10.91	0.0167	0.0545	20.29	49.85
Statistica	102.31	10.92	0.0167	0.0544	20.31	49.89
Median	102.30	10.91	0.0167	0.0544	20.29	49.86
kinfit	no fit					
kinfit	101.24	5.97	0.0066	0.0462	20.12	54.95
kinfit	102.31	10.91	0.0167	0.0544	20.29	49.85

starting values, as shown in the last two lines in Table 14.

The HS fit did not converge for dataset B with **kinfit**. Again, this should be viewed in the light of the vastly differing results produced by the other software packages as listed in Table 15.

The results from fitting the HS model to dataset C with **kinfit** agree nicely with the median of the results obtained with the other packages, as shown in Table 16.

3.5 χ^2 statistics

As no values for the minimum error rate that has to be assumed for the model to agree with the data (χ^2 statistics) are reported for the FOCUS datasets A to F, the respective values calculated by **kinfit** are compared to the χ^2 values calculated by the KinGUI package (Schäfer et al., 2007) as shown in Table 17.

For this, the possibility to write KinGUI input files using the function `kinwrite.KinGUI` from **kinfit** was used.

The comparison shows that whenever a minimum error level χ^2 was calculated using the **kinfit** package, it was very close to the value generated by KinGUI.

Table 15: Results of fitting the HS model to the example dataset B (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	t_b	k_1	k_2	DT_{50}	DT_{90}
Excel[a]	99.33	26.00	0.0788	0.0592	8.79	30.27
Excel[a]	100.42	7.00	0.0848	0.0702	8.42	31.36
Kinetica	100.14	7.00	0.0833	0.071	8.55	31.23
Madonna	100.19	7.00	0.0839	0.0704	8.50	31.37
Mathematica	98.62	26.26	0.0744	NA	8.93	29.05
ModelManager	99.34	26.01	0.0789	0.0592	8.79	30.26
PRISM	99.20	35.03	0.0783	0.0538	8.86	29.42
Statistica	99.33	26.00	0.0789	0.0592	8.79	30.26
Median	99.335	26.00	0.0789	NA	8.79	30.27
kinfit	no fit					

Table 16: Results of fitting the HS model to the example dataset C (FOCUS Work Group on Degradation Kinetics, 2006), as given in the report, in comparison to the results obtained by **kinfit**.

Package	M_0	t_b	k_1	k_2	DT_{50}	DT_{90}
ACSL	84.50	5.10	0.3562	0.0247	1.95	24.76
Kinetica	84.50	5.16	0.3562	0.0225	1.95	25.84
Madonna	84.50	5.15	0.3562	0.0227	1.95	25.78
Mathematica	91.45	-0.33	0.3060	0	1.93	7.10
ModelMaker	84.51	5.15	0.3555	0.0225	1.95	26.12
PRISM	84.50	5.15	0.3562	0.0227	1.95	25.77
Median	84.50	5.15	0.3562	0.0226	1.95	25.77
kinfit	84.5	5.15	0.3562	0.0227	1.95	25.78

Table 17: Comparison of χ^2 error levels in percent calculated for model fits by the KinGUI and **kinfit** packages.

	SFO		FOMC		DFOP		HS	
Dataset	KinGUI	**kinfit**	KinGUI	**kinfit**	KinGUI	**kinfit**	KinGUI	**kinfit**
A	8.3852	8.3848	9.3116		9.66		4.1106	1.6766
B	4.4562	4.4555	4.6641	4.5886	4.9562	4.9527	4.4535	
C	15.8456	15.844	6.6574	6.6568	2.6613	2.6621	4.6963	4.6952
D	6.4539	6.4524	6.808	6.7802	7.2751	6.5652	5.8196	
F system	12.5386	12.5379	13.4533		14.1524		3.2178	3.2188
F water	10.8069	10.8055	11.6682		12.1821		1.6558	

4 Conclusion

The **kinfit** package for R gives access to the possibility to fit the kinetic models recommended by the FOCUS group (FOCUS Work Group on Degradation Kinetics, 2006) from within R. Comparison with the results obtained with other software packages shows that **kinfit** produces kinetic endpoints that are within the variability and even very close to the median of results obtained with other packages, except for some cases where **kinfit** does not produce results and the results obtained with other software packages are strongly divergent.

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.

kinfit. *kinfit: Routines for fitting kinetic models to chemical degradation data*, 2009. URL http://CRAN.R-project.org. R package version 1.0-0.

R Development Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2009. URL http://www.R-project.org. ISBN 3-900051-07-0.

D. Schäfer, M. Mikolasch, P. Rainbird, and B. Harvey. KinGUI: a new kinetic software tool for evaluations according to FOCUS degradation kinetics. In Del Re A. A. M., Capri E., Fragoulis G., and Trevisan M., editors, *Proceedings of the XIII Symposium Pesticide Chemistry*, pages 916–923, Piacenza, 2007.