

Renewal Assessment Report

beta-Cyfluthrin

Volume 3 – B.8 Environmental fate and behaviour

Appendix 2

Rapporteur Member State: Germany

Co-Rapporteur Member State: Hungary

Appendix 2:

KinGUI results from the study

Kinetic Evaluation of the Aerobic Aquatic Metabolism of Cyfluthrin and Beta-cyfluthrin and their Metabolites in Water / Sediment Systems According to FOCUS Kinetics

Cyfluthrin (FCR 1272)

Beta-Cyfluthrin (FCR 4545)

DCVA (AE0433590)

FPB-aldehyd (FCR 1260)

FPB-acid (AE F105561)

Klaus Hammel

Ruth Porschewski

Date: 26 November 2013

Report No. EnSa-13-0711

11 APPENDIX 2: KINGUI OUTPUT FILES

11.1 Cyfluthrin Degradation Total System

11.1.1 Barmen

11.1.1.1 SFO

```
# Trial      : Barmentotalsystmet
# File name  : Barmentotalsystmet IRLS SFO  Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_total-syst_met
# Created    : on 17 Jun 2013
#            : at 11:09
#            : by EZCIA on ADEMONC6031(4CPUs)
# KingUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See total system
# # Barmener See total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
```

		Initial Value	Lower Bound	Upper Bound	Fixed
M(0)	Par	92.43	0	Inf	False
k	Par	0.10	0	Inf	False
k	Met	0.10	0	Inf	False
FF	Par -> Met	0.10	0	1	False
M(0)	Met	0			True

```
# -----
# Chi2 error estimation
# -----
```

	Par	Met	All
Chi2Err%	15.92	33.10	23.97
Kinetic model	SFO	SFO	

```
# -----
# Parameter estimation
# -----
```

Degrees of Freedom : 42

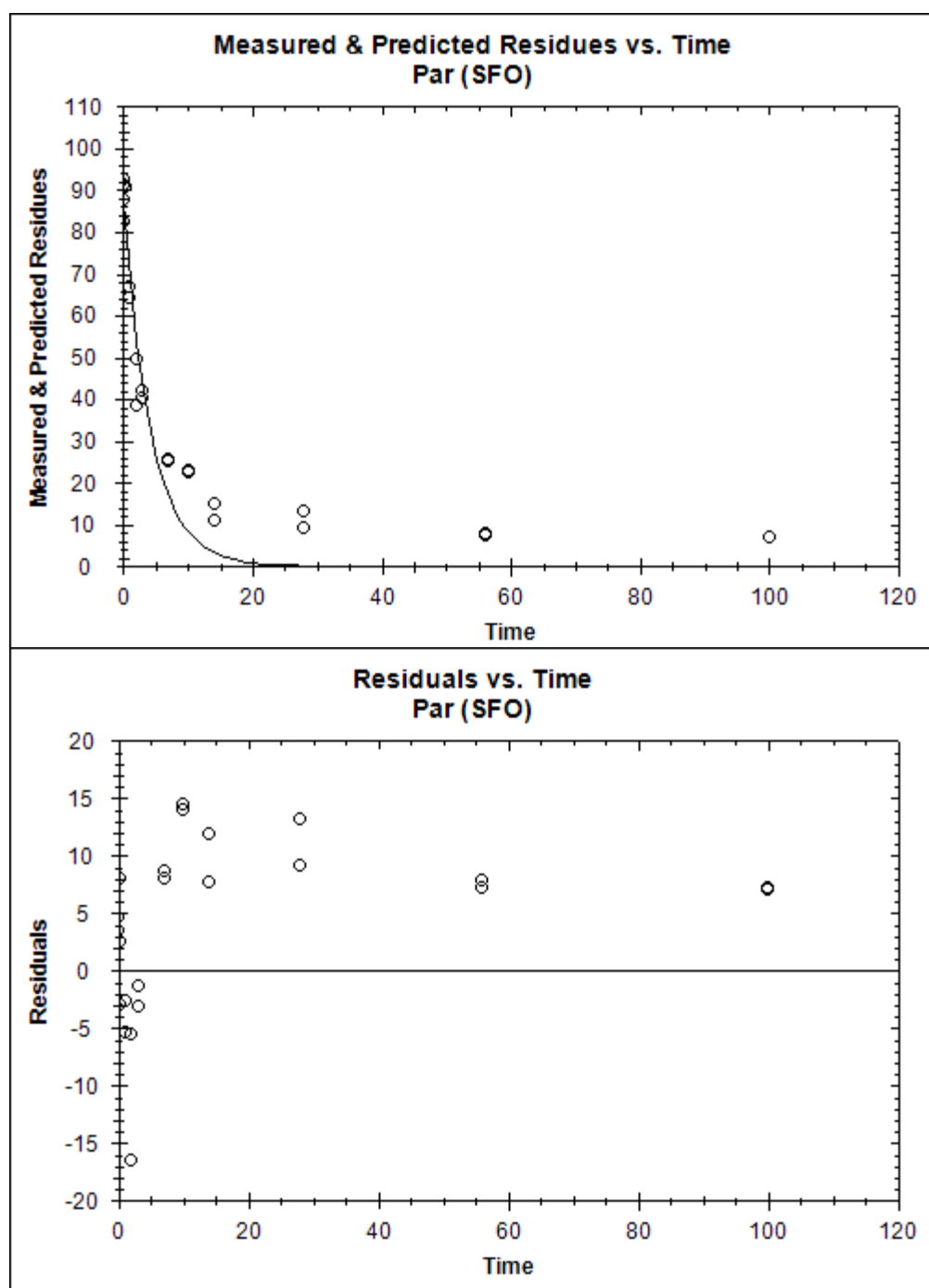
Parameter	Estimate	Lower CI	Upper CI	St.Dev	Prob > t
M(0) Par	87.845411	79.776178	95.915	4.117031	< 2e-16
k Par	0.234674	0.156659	0.313	0.039804	2.81e-07
k Met	0.001694	-0.004578	0.008	0.003200	0.300
FF Par -> Met	0.4276			0.064177	

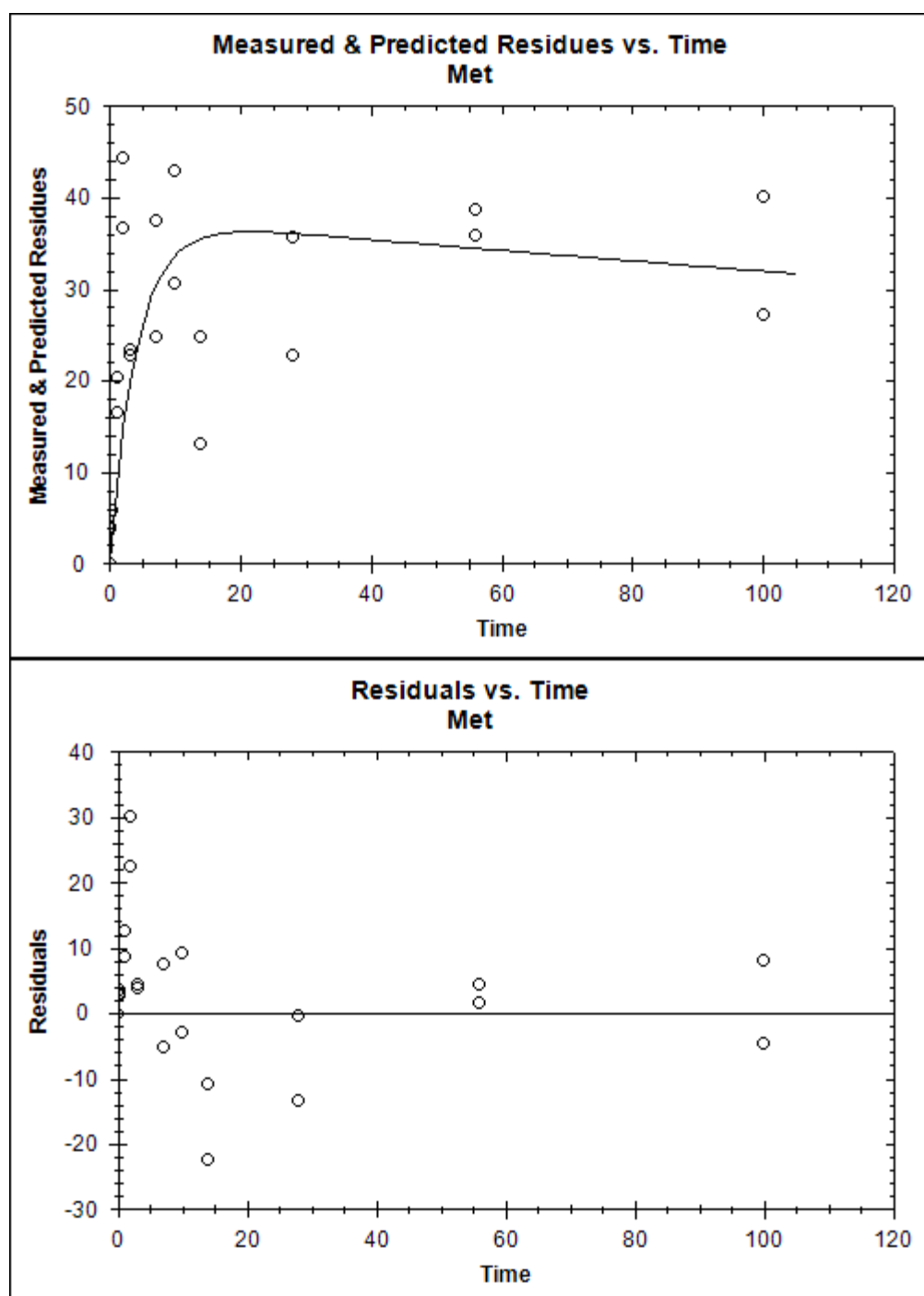
```
# -----
# DT50 and DT90 values
# -----
```

	Par	Met
DT50	2.9537	409.26
DT90	9.8118	1359.5
Kinetic model	SFO	SFO

```
# -----
# Measured vs. predicted values
# -----
```

Compartment Par					Compartment Met				
time	observed	err-std	predicted	residual	observed	err-std	predicted	residual	
0.0000	92.4300	8.5525	87.8454	4.5846	0.0000	11.0226	0.0000	0.0000	
0.0000	91.4500	8.5525	87.8454	3.6046	0.0000	11.0226	0.0000	0.0000	
0.1250	82.3200	8.5525	85.3060	-2.9860	4.0100	11.0226	1.0856	2.9244	
0.1250	87.9200	8.5525	85.3060	2.6140	3.8300	11.0226	1.0856	2.7444	
0.2500	90.9000	8.5525	82.8399	8.0601	5.7300	11.0226	2.1397	3.5903	
0.2500	NA	8.5525	82.8399	NA	NA	11.0226	2.1397	NA	
1.0000	64.0600	8.5525	69.4707	-5.4107	20.3900	11.0226	7.8493	12.5407	
1.0000	66.9400	8.5525	69.4707	-2.5307	16.5300	11.0226	7.8493	8.6807	
2.0000	38.5300	8.5525	54.9394	-16.4094	44.2600	11.0226	14.0435	30.2165	
2.0000	49.4200	8.5525	54.9394	-5.5194	36.5900	11.0226	14.0435	22.5465	
3.0000	40.3000	8.5525	43.4476	-3.1476	22.7300	11.0226	18.9288	3.8012	
3.0000	42.2100	8.5525	43.4476	-1.2376	23.3100	11.0226	18.9288	4.3812	
7.0000	25.1100	8.5525	16.9940	8.1160	37.5200	11.0226	30.0673	7.4527	
7.0000	25.6900	8.5525	16.9940	8.6960	24.8200	11.0226	30.0673	-5.2473	
10.0000	22.4100	8.5525	8.4051	14.0049	42.8600	11.0226	33.5768	9.2832	
10.0000	22.8200	8.5525	8.4051	14.4149	30.6700	11.0226	33.5768	-2.9068	
14.0000	15.1500	8.5525	3.2875	11.8625	24.7400	11.0226	35.5296	-10.7896	
14.0000	10.9800	8.5525	3.2875	7.6925	13.1800	11.0226	35.5296	-22.3496	
28.0000	9.3300	8.5525	0.1230	9.2070	22.7500	11.0226	36.0267	-13.2767	
28.0000	13.3200	8.5525	0.1230	13.1970	35.7200	11.0226	36.0267	-0.3067	
56.0000	7.3000	8.5525	0.0002	7.2998	38.7600	11.0226	34.4086	4.3514	
56.0000	7.8700	8.5525	0.0002	7.8698	35.9300	11.0226	34.4086	1.5214	
100.0000	7.0100	8.5525	0.0000	7.0100	27.2300	11.0226	31.9377	-4.7077	
100.0000	7.1700	8.5525	0.0000	7.1700	40.0400	11.0226	31.9377	8.1023	





11.1.1.2HS

```

# Trial      : Barmentotalsystmet
# File name  : Barmentotalsystmet IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_total-syst_met
# Created    : on 17 Jun 2013
#            : at 11:30
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See total system
# # Barmener See total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      92.43              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
tb    Par      :       3.00              0              Inf      False
k      Met      :       0.10              0              Inf      False
FF    Par -> Met :       0.10              0              1      False
M(0)  Met      :          0                      True

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      17.29      Par      Met      All
      Kinetic model :      HS      SFO      25.05

# -----
# Parameter estimation
# -----

Degrees of Freedom : 40
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      87.838646      79.576720      96.101      4.215345      < 2e-16
k1    Par      0.234568      0.154725      0.314      0.040737      5.17e-07
k2    Par      0.432464      NA      NA      NA      NA
tb    Par      46.202775      NA      NA      NA      NA
k      Met      0.001695      -0.004736      0.008      0.003281      0.304
FF    Par -> Met      0.4276      0.065804

# -----
# DT50 and DT90 values
# -----

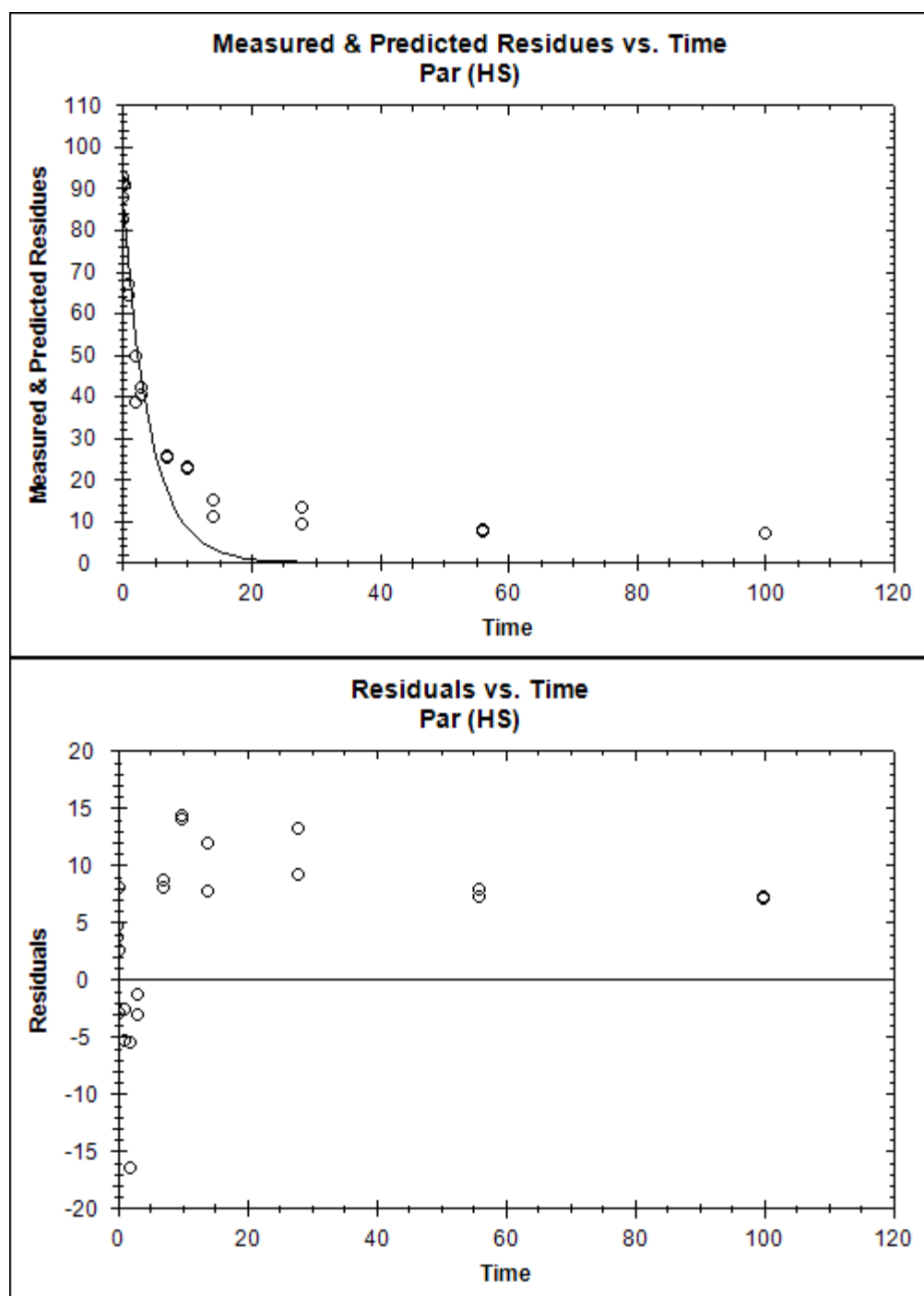
      DT50 :      2.9550      Par      Met
      DT90 :      9.8163      408.93
      Kinetic model :      HS      SFO

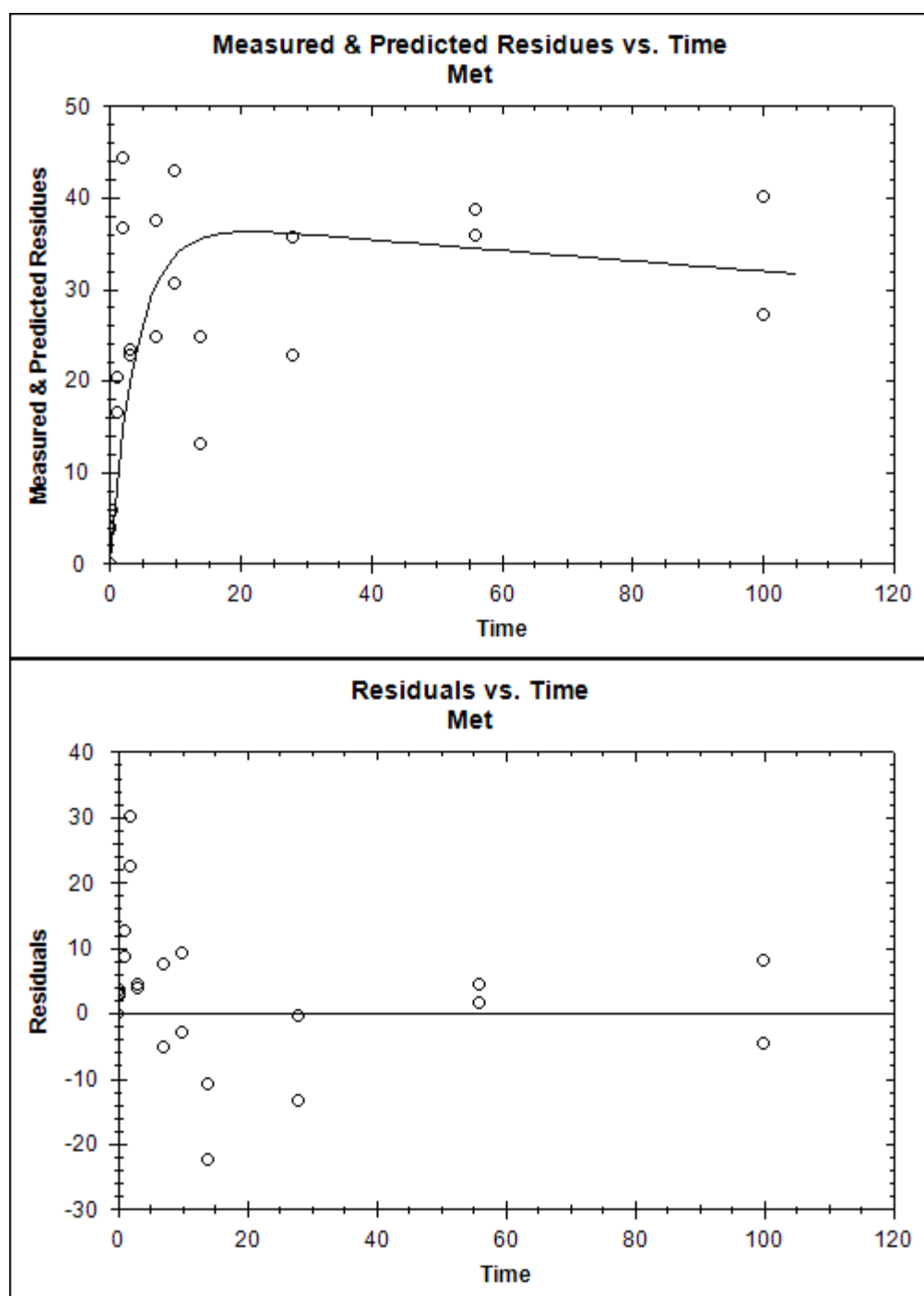
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000 92.4300 8.5461 87.8386 4.5914 0.0000 11.0308 0.0000 0.0000
0.0000 91.4500 8.5461 87.8386 3.6114 0.0000 11.0308 0.0000 0.0000

```

0.1250	82.3200	8.5461	85.3005	-2.9805	4.0100	11.0308	1.0853	2.9247
0.1250	87.9200	8.5461	85.3005	2.6195	3.8300	11.0308	1.0853	2.7447
0.2500	90.9000	8.5461	82.8357	8.0643	5.7300	11.0308	2.1389	3.5911
0.2500	NA	8.5461	82.8357	NA	NA	11.0308	2.1389	NA
1.0000	64.0600	8.5461	69.4727	-5.4127	20.3900	11.0308	7.8469	12.5431
1.0000	66.9400	8.5461	69.4727	-2.5327	16.5300	11.0308	7.8469	8.6831
2.0000	38.5300	8.5461	54.9468	-16.4168	44.2600	11.0308	14.0399	30.2201
2.0000	49.4200	8.5461	54.9468	-5.5268	36.5900	11.0308	14.0399	22.5501
3.0000	40.3000	8.5461	43.4582	-3.1582	22.7300	11.0308	18.9247	3.8053
3.0000	42.2100	8.5461	43.4582	-1.2482	23.3100	11.0308	18.9247	4.3853
7.0000	25.1100	8.5461	17.0053	8.1047	37.5200	11.0308	30.0647	7.4553
7.0000	25.6900	8.5461	17.0053	8.6847	24.8200	11.0308	30.0647	-5.2447
10.0000	22.4100	8.5461	8.4134	13.9966	42.8600	11.0308	33.5760	9.2840
10.0000	22.8200	8.5461	8.4134	14.4066	30.6700	11.0308	33.5760	-2.9060
14.0000	15.1500	8.5461	3.2922	11.8578	24.7400	11.0308	35.5305	-10.7905
14.0000	10.9800	8.5461	3.2922	7.6878	13.1800	11.0308	35.5305	-22.3505
28.0000	9.3300	8.5461	0.1234	9.2066	22.7500	11.0308	36.0290	-13.2790
28.0000	13.3200	8.5461	0.1234	13.1966	35.7200	11.0308	36.0290	-0.3090
56.0000	7.3000	8.5461	0.0000	7.3000	38.7600	11.0308	34.4097	4.3503
56.0000	7.8700	8.5461	0.0000	7.8700	35.9300	11.0308	34.4097	1.5203
100.0000	7.0100	8.5461	0.0000	7.0100	27.2300	11.0308	31.9368	-4.7068
100.0000	7.1700	8.5461	0.0000	7.1700	40.0400	11.0308	31.9368	8.1032





11.1.1.3 FOMC

```

# Trial      : Barmentotalsystmet
# File name  : Barmentotalsystmet IRLS FOMC Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_total-syst_met
# Created    : on 17 Jun 2013
#            : at 11:40
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See total system
# # Barmener See total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      92.43              0              Inf      False
alpha Par      :       0.10              0              Inf      False
beta  Par      :       0.10              0              Inf      False
k      Met      :       0.10              0              Inf      False
FF     Par -> Met :       0.10              0              1      False
M(0)  Met      :              0                      True

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      6.741      25.418      15.798
      Kinetic model :      FOMC      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 41
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :  93.813465  89.870497  97.756  2.011755  < 2e-16
alpha Par      :   0.671853  0.529200  0.815  0.072784  7.28e-12
beta  Par      :   1.178508  0.650056  1.707  0.269623  4.13e-05
k      Met      :   0.002574 -0.002609  0.008  0.002645  0.168
FF     Par -> Met :   0.4551          0.049656

# -----
# DT50 and DT90 values
# -----

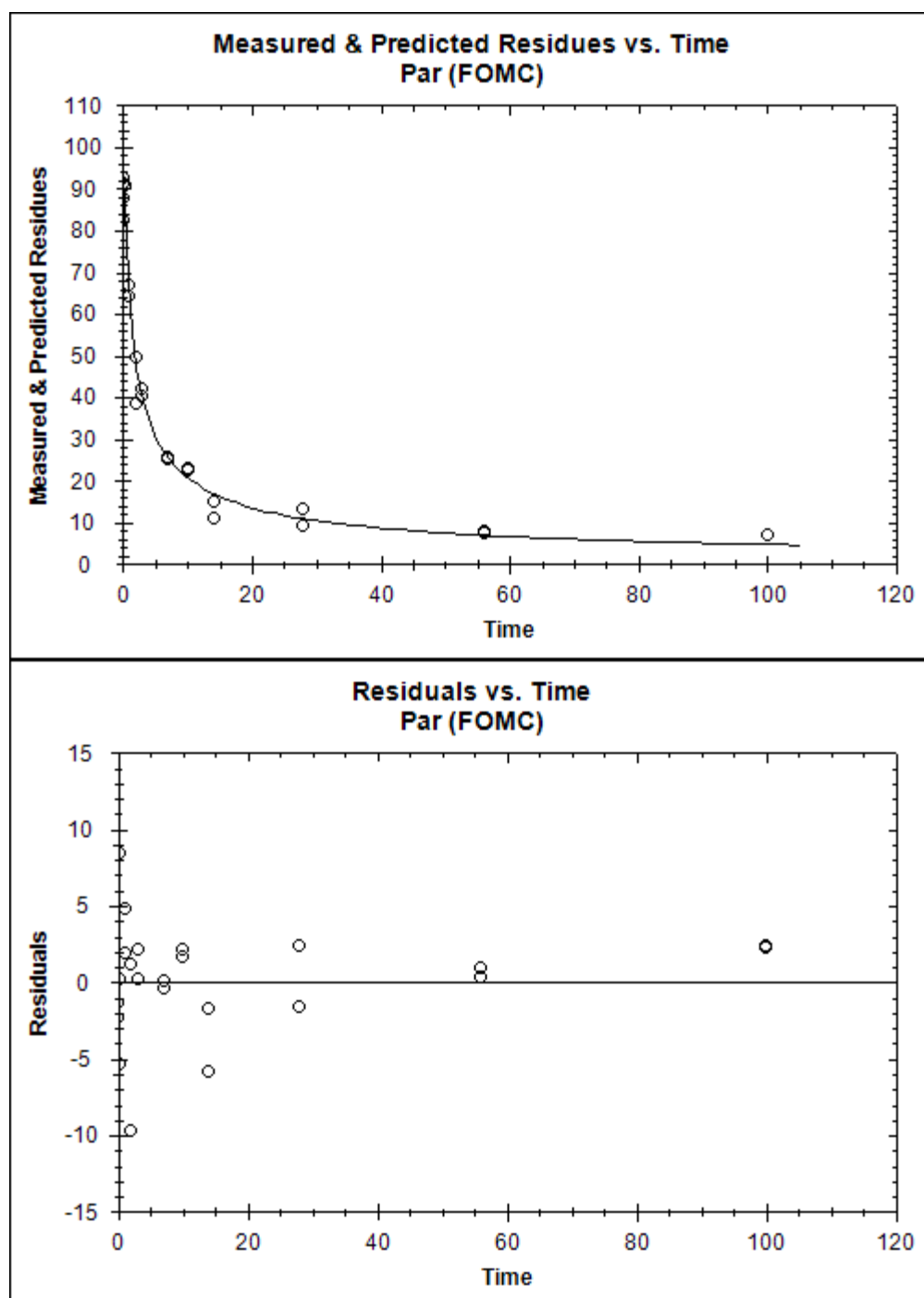
      DT50 :      2.1282      269.25
      DT90 :      35.109      894.41
      Kinetic model :      FOMC      SFO

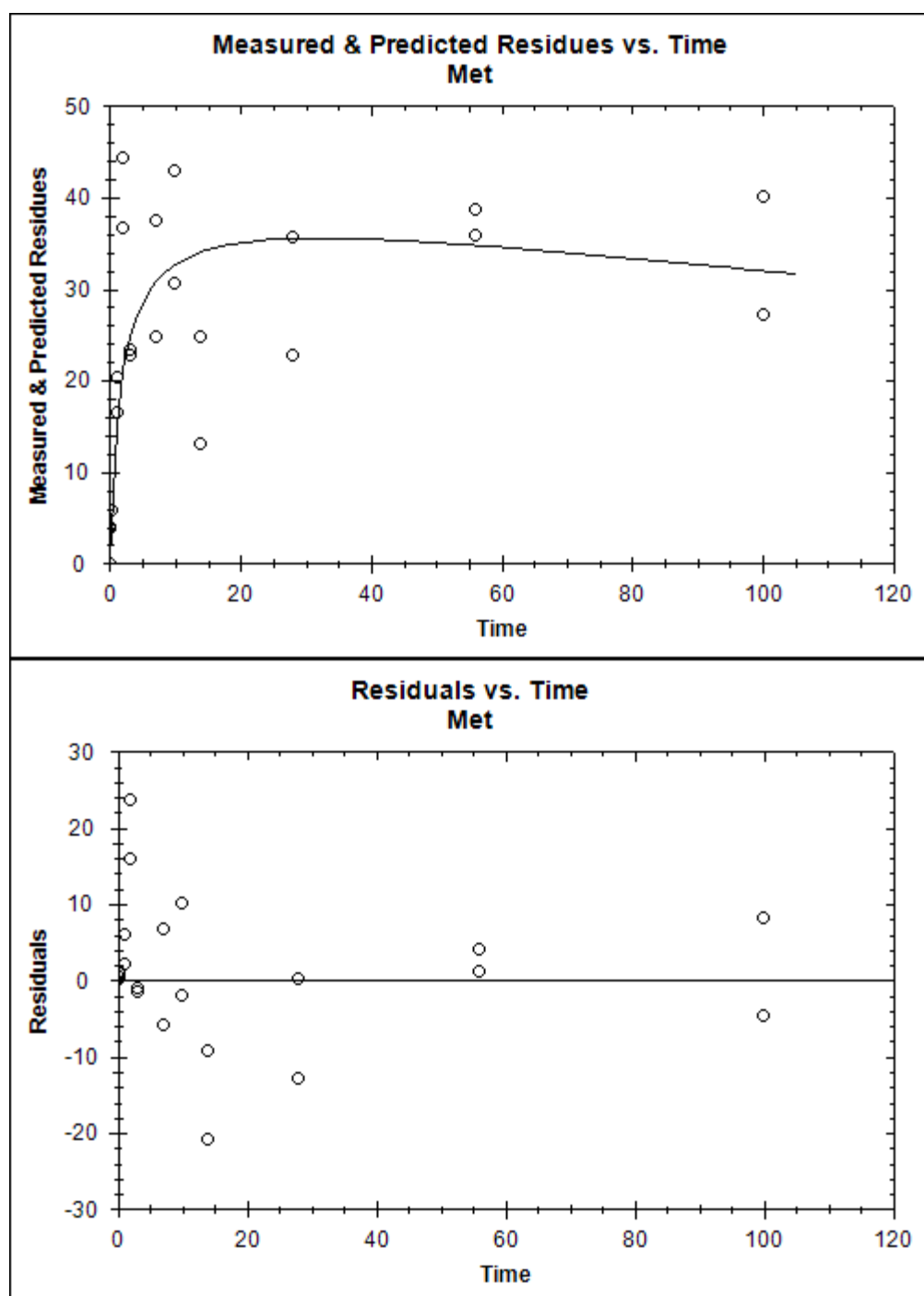
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000  92.4300  3.6121  93.8135 -1.3835  0.0000  8.9239  0.0000  0.0000
0.0000  91.4500  3.6121  93.8135 -2.3635  0.0000  8.9239  0.0000  0.0000
0.1250  82.3200  3.6121  87.6699 -5.3499  4.0100  8.9239  2.7954  1.2146
0.1250  87.9200  3.6121  87.6699  0.2501  3.8300  8.9239  2.7954  1.0346

```

0.2500	90.9000	3.6121	82.4388	8.4612	5.7300	8.9239	5.1748	0.5552
0.2500	NA	3.6121	82.4388	NA	NA	8.9239	5.1748	NA
1.0000	64.0600	3.6121	62.0865	1.9735	20.3900	8.9239	14.4171	5.9729
1.0000	66.9400	3.6121	62.0865	4.8535	16.5300	8.9239	14.4171	2.1129
2.0000	38.5300	3.6121	48.1693	-9.6393	44.2600	8.9239	20.7047	23.5553
2.0000	49.4200	3.6121	48.1693	1.2507	36.5900	8.9239	20.7047	15.8853
3.0000	40.3000	3.6121	40.0825	0.2175	22.7300	8.9239	24.3266	-1.5966
3.0000	42.2100	3.6121	40.0825	2.1275	23.3100	8.9239	24.3266	-1.0166
7.0000	25.1100	3.6121	25.5275	-0.4175	37.5200	8.9239	30.6611	6.8589
7.0000	25.6900	3.6121	25.5275	0.1625	24.8200	8.9239	30.6611	-5.8411
10.0000	22.4100	3.6121	20.6933	1.7167	42.8600	8.9239	32.6160	10.2440
10.0000	22.8200	3.6121	20.6933	2.1267	30.6700	8.9239	32.6160	-1.9460
14.0000	15.1500	3.6121	16.8492	-1.6992	24.7400	8.9239	34.0215	-9.2815
14.0000	10.9800	3.6121	16.8492	-5.8692	13.1800	8.9239	34.0215	-20.8415
28.0000	9.3300	3.6121	10.8613	-1.5313	22.7500	8.9239	35.4850	-12.7350
28.0000	13.3200	3.6121	10.8613	2.4587	35.7200	8.9239	35.4850	0.2350
56.0000	7.3000	3.6121	6.9118	0.3882	38.7600	8.9239	34.7398	4.0202
56.0000	7.8700	3.6121	6.9118	0.9582	35.9300	8.9239	34.7398	1.1902
100.0000	7.0100	3.6121	4.7105	2.2995	27.2300	8.9239	31.9580	-4.7280
100.0000	7.1700	3.6121	4.7105	2.4595	40.0400	8.9239	31.9580	8.0820





11.1.1.4DFOP

```

# Trial      : Barmentotalsystmet
# File name  : Barmentotalsystmet IRLS DFOP Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_total-syst_met
# Created    : on 17 Jun 2013
#            : at 11:21
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See total system
# # Barmener See total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      92.43              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
g     Par      :       0.50              0              1      False
k     Met      :       0.10              0              Inf      False
FF    Par -> Met :       0.10              0              1      False
M(0)  Met      :              0              0              1      True

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      7.29      25.16      16.12
      Kinetic model :      DFOP      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 40
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :  92.416068    88.424292    96.408      2.036657    < 2e-16
k1    Par      :   0.516427    0.382312    0.651      0.068427    1.64e-09
k2    Par      :   0.020282    0.005048    0.036      0.007772    0.00635
g     Par      :   0.736373    0.655569    0.817      0.041227    < 2e-16
k     Met      :   0.002820   -0.002549    0.008      0.002739    0.15473
FF    Par -> Met :   0.4676              0.051490

# -----
# DT50 and DT90 values
# -----

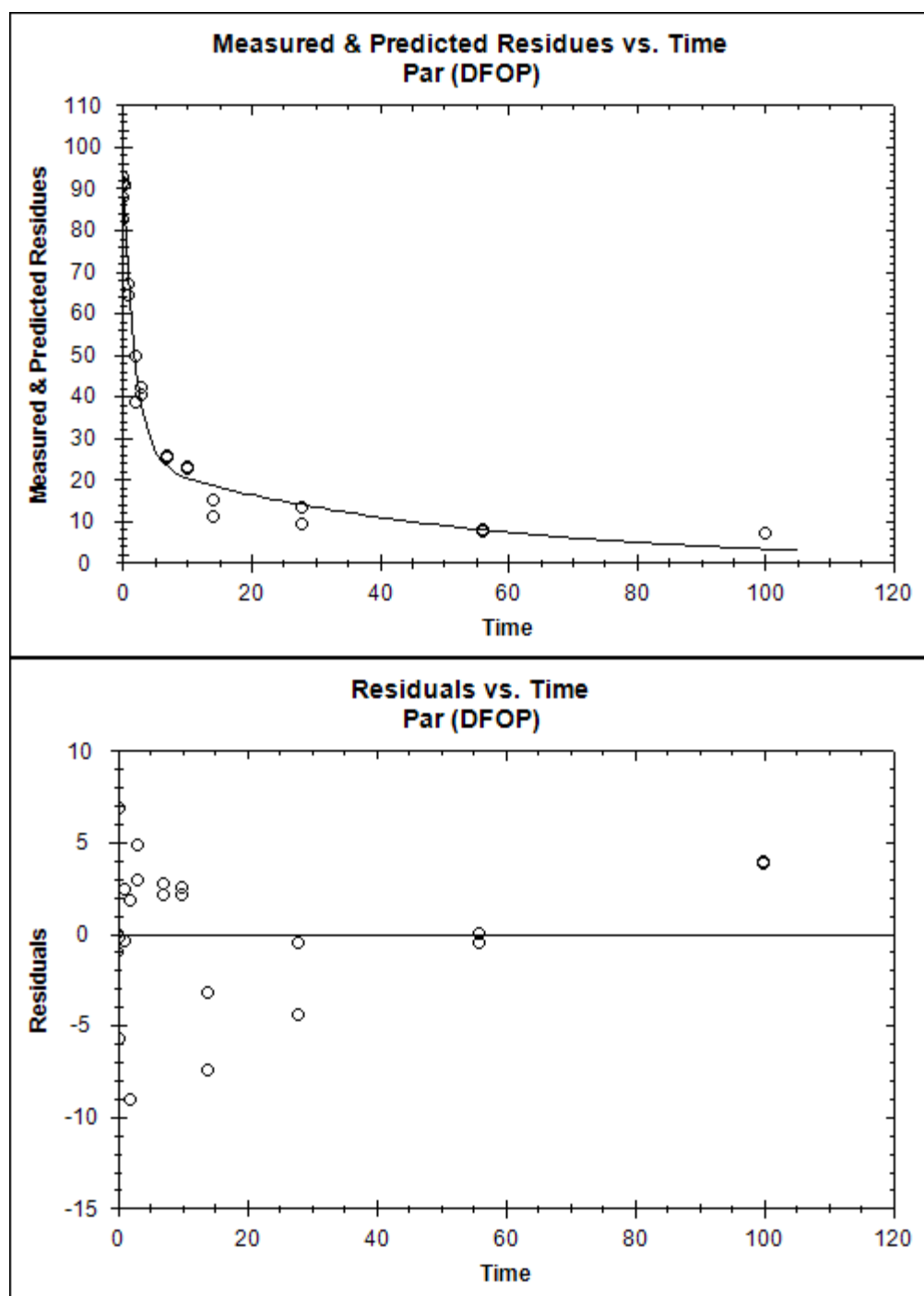
      DT50 :      2.1119      245.84
      DT90 :      47.795     816.65
      Kinetic model :      DFOP      SFO

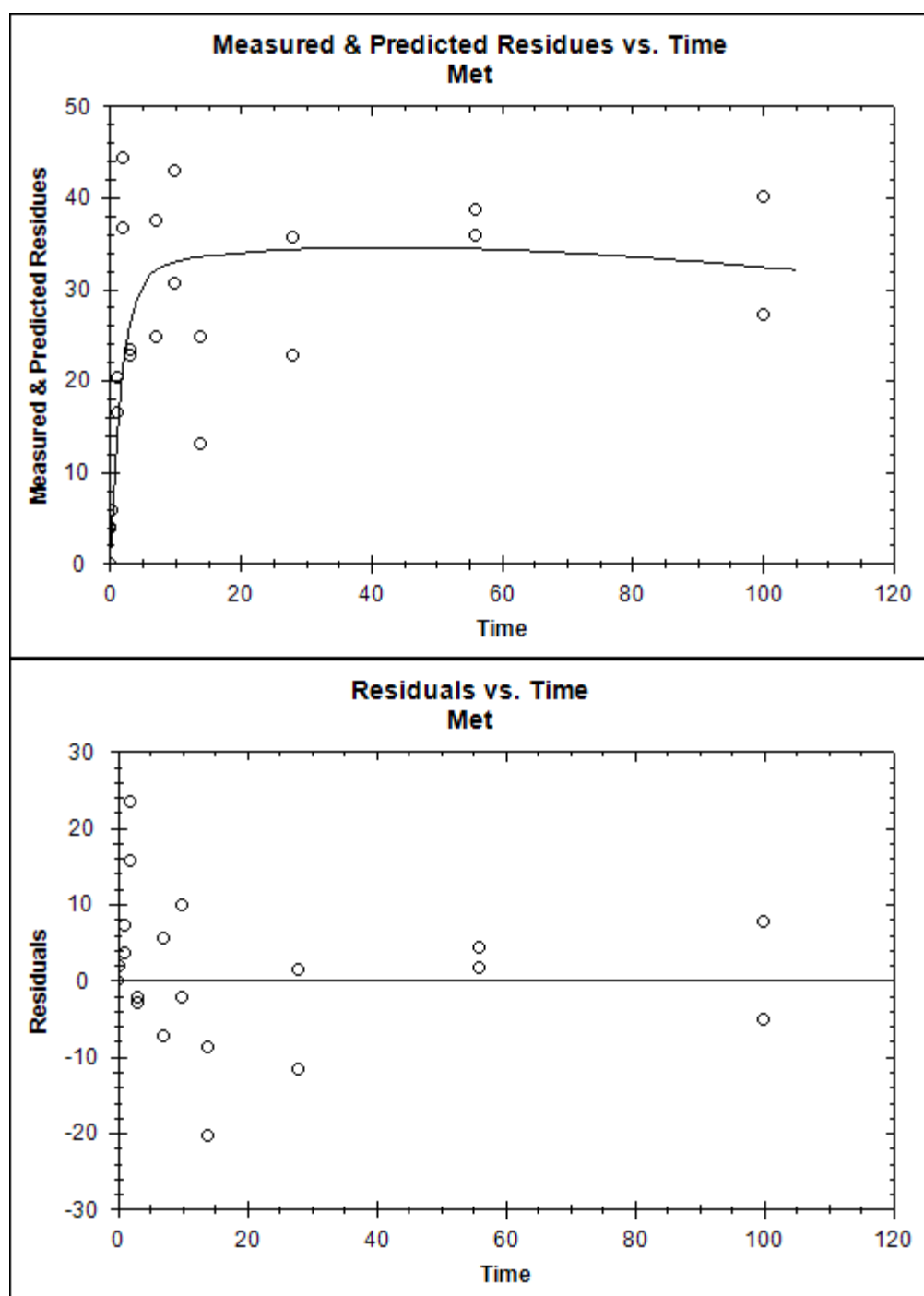
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000  92.4300  3.8698  92.4161  0.0139  0.0000  8.8464  0.0000  0.0000
0.0000  91.4500  3.8698  92.4161 -0.9661  0.0000  8.8464  0.0000  0.0000

```

0.1250	82.3200	3.8698	88.1001	-5.7801	4.0100	8.8464	2.0179	1.9921
0.1250	87.9200	3.8698	88.1001	-0.1801	3.8300	8.8464	2.0179	1.8121
0.2500	90.9000	3.8698	84.0503	6.8497	5.7300	8.8464	3.9107	1.8193
0.2500	NA	3.8698	84.0503	NA	NA	8.8464	3.9107	NA
1.0000	64.0600	3.8698	64.4778	-0.4178	20.3900	8.8464	13.0449	7.3451
1.0000	66.9400	3.8698	64.4778	2.4622	16.5300	8.8464	13.0449	3.4851
2.0000	38.5300	3.8698	47.6209	-9.0909	44.2600	8.8464	20.8790	23.3810
2.0000	49.4200	3.8698	47.6209	1.7991	36.5900	8.8464	20.8790	15.7110
3.0000	40.3000	3.8698	37.3796	2.9204	22.7300	8.8464	25.6021	-2.8721
3.0000	42.2100	3.8698	37.3796	4.8304	23.3100	8.8464	25.6021	-2.2921
7.0000	25.1100	3.8698	22.9706	2.1394	37.5200	8.8464	32.0045	5.5155
7.0000	25.6900	3.8698	22.9706	2.7194	24.8200	8.8464	32.0045	-7.1845
10.0000	22.4100	3.8698	20.2800	2.1300	42.8600	8.8464	32.9871	9.8729
10.0000	22.8200	3.8698	20.2800	2.5400	30.6700	8.8464	32.9871	-2.3171
14.0000	15.1500	3.8698	18.3903	-3.2403	24.7400	8.8464	33.4956	-8.7556
14.0000	10.9800	3.8698	18.3903	-7.4103	13.1800	8.8464	33.4956	-20.3156
28.0000	9.3300	3.8698	13.8073	-4.4773	22.7500	8.8464	34.2983	-11.5483
28.0000	13.3200	3.8698	13.8073	-0.4873	35.7200	8.8464	34.2983	1.4217
56.0000	7.3000	3.8698	7.8249	-0.5249	38.7600	8.8464	34.3746	4.3854
56.0000	7.8700	3.8698	7.8249	0.0451	35.9300	8.8464	34.3746	1.5554
100.0000	7.0100	3.8698	3.2057	3.8043	27.2300	8.8464	32.3770	-5.1470
100.0000	7.1700	3.8698	3.2057	3.9643	40.0400	8.8464	32.3770	7.6630





11.1.2 Genkel

11.1.2.1 SFO

```
# Trial      : Genkeltotalsystmet
# File name  : Genkeltotalsystmet IRLS SFO  Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_total-syst_met
# Created    : on 16 Jun 2013
#            : at 10:40
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      98.14              0              Inf      False
k      Par      :       0.10              0              Inf      False
k      Met      :       0.10              0              Inf      False
FF      Par -> Met :       0.10              0              1      False
M(0)  Met      :              0                      True

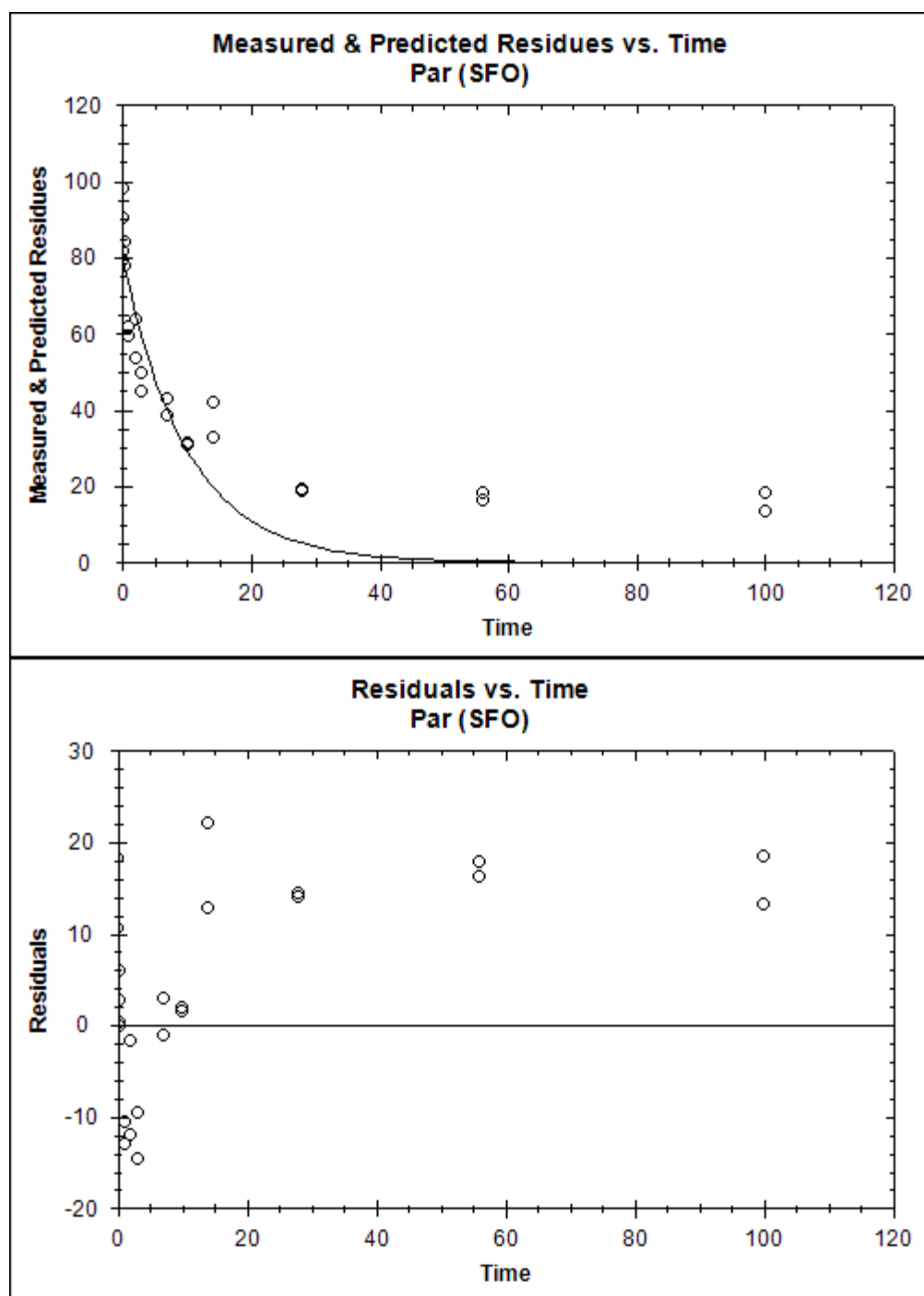
# -----
# Chi2 error estimation
# -----
# -----
#           Par      Met      All
Chi2Err% :      19.22      22.06      22.26
Kinetic model :      SFO      SFO

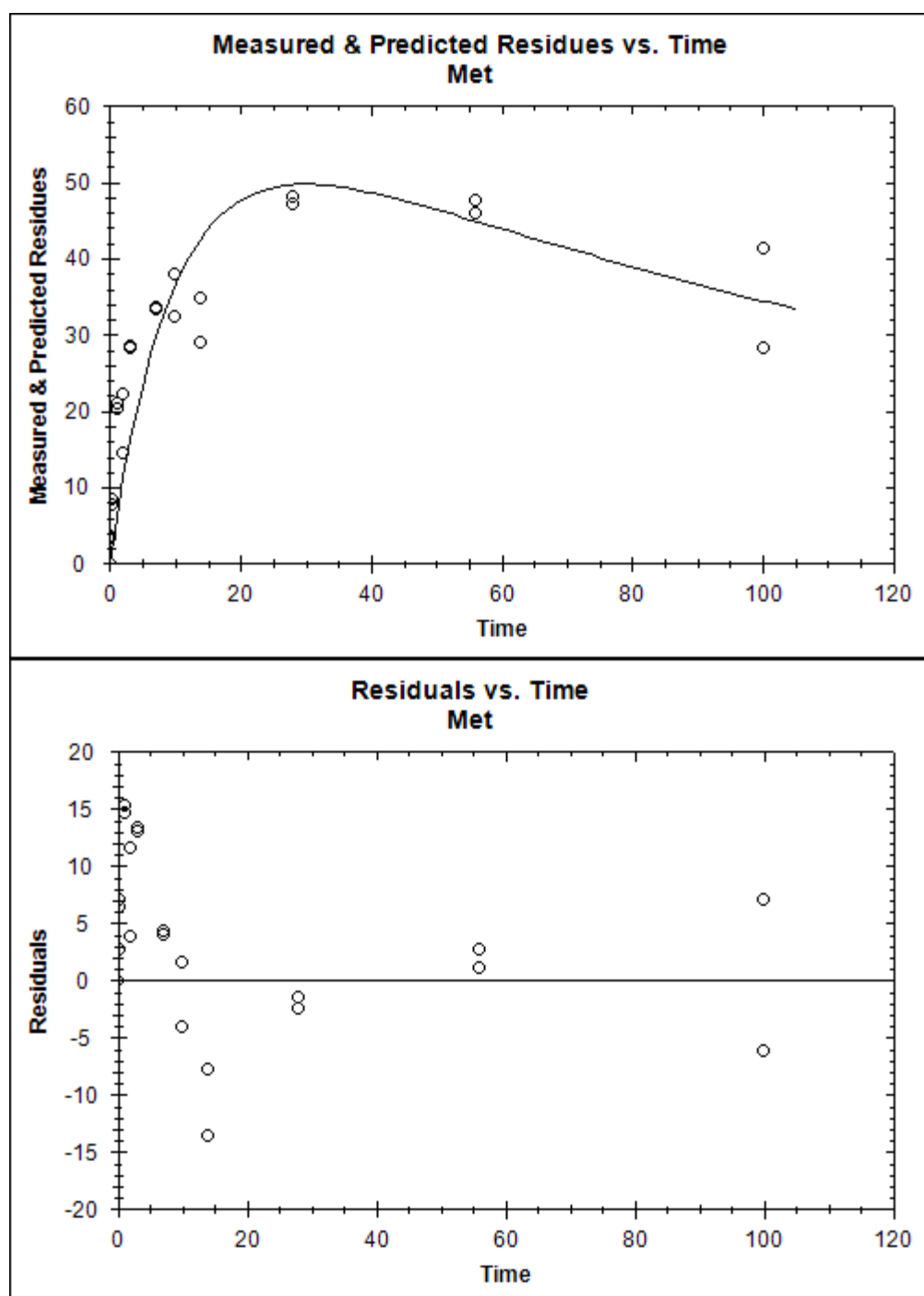
# -----
# Parameter estimation
# -----
# -----
# Degrees of Freedom : 44
# Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      7.996e+01      7.119e+01      88.728      4.474e+00      < 2e-16
k      Par      :      9.975e-02      5.758e-02      0.142      2.152e-02      1.59e-05
k      Met      :      6.155e-03      7.752e-04      0.012      2.745e-03      0.015
FF      Par -> Met :      0.7467      1.209e-01

# -----
# DT50 and DT90 values
# -----
# -----
#           Par      Met
DT50 :      6.9487      112.61
DT90 :      23.083      374.08
Kinetic model :      SFO      SFO

# -----
# Measured vs. predicted values
# -----
# -----
# Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000  98.1400 11.8696 79.9590 18.1810 0.0000 7.7747 0.0000 0.0000
0.0000  90.5800 11.8696 79.9590 10.6210 0.0000 7.7747 0.0000 0.0000
0.1250  79.3000 11.8696 78.9682 0.3318 3.4400 7.7747 0.7395 2.7005
0.1250  81.6700 11.8696 78.9682 2.7018 3.4900 7.7747 0.7395 2.7505
```

0.2500	83.9000	11.8696	77.9897	5.9103	7.8200	7.7747	1.4693	6.3507
0.2500	78.0000	11.8696	77.9897	0.0103	8.5500	7.7747	1.4693	7.0807
1.0000	59.3900	11.8696	72.3679	-12.9779	20.3100	7.7747	5.6504	14.6596
1.0000	61.8600	11.8696	72.3679	-10.5079	20.9300	7.7747	5.6504	15.2796
2.0000	53.6300	11.8696	65.4974	-11.8674	22.2900	7.7747	10.7297	11.5603
2.0000	63.8200	11.8696	65.4974	-1.6774	14.5300	7.7747	10.7297	3.8003
3.0000	49.7000	11.8696	59.2792	-9.5792	28.6100	7.7747	15.2924	13.3176
3.0000	44.7100	11.8696	59.2792	-14.5692	28.2700	7.7747	15.2924	12.9776
7.0000	42.7900	11.8696	39.7754	3.0146	33.6700	7.7747	29.2938	4.3762
7.0000	38.6100	11.8696	39.7754	-1.1654	33.2500	7.7747	29.2938	3.9562
10.0000	31.3700	11.8696	29.4883	1.8817	32.3100	7.7747	36.3650	-4.0550
10.0000	31.0800	11.8696	29.4883	1.5917	37.8800	7.7747	36.3650	1.5150
14.0000	41.8000	11.8696	19.7862	22.0138	29.0800	7.7747	42.6305	-13.5505
14.0000	32.6100	11.8696	19.7862	12.8238	34.8600	7.7747	42.6305	-7.7705
28.0000	19.2500	11.8696	4.8962	14.3538	48.1100	7.7747	49.6598	-1.5498
28.0000	19.0200	11.8696	4.8962	14.1238	47.1500	7.7747	49.6598	-2.5098
56.0000	16.4900	11.8696	0.2998	16.1902	45.8800	7.7747	44.8388	1.0412
56.0000	18.2100	11.8696	0.2998	17.9102	47.6100	7.7747	44.8388	2.7712
100.0000	13.3000	11.8696	0.0037	13.2963	28.2000	7.7747	34.3796	-6.1796
100.0000	18.4500	11.8696	0.0037	18.4463	41.3900	7.7747	34.3796	7.0104





11.1.2.2HS

```

# Trial      : Genkeltotalsystmet
# File name  : Genkeltotalsystmet IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Genkel_total-syst_met
# Created    : on 16 Jun 2013
#            : at 10:51
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      98.14              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
tb    Par      :       3.00              0              Inf      False
k      Met      :       0.10              0              Inf      False
FF    Par -> Met :       0.10              0              1      False
M(0)  Met      :              0              0              1      True

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      9.80      13.26      11.89
      Kinetic model :      HS      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 42
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      : 85.815486      80.454146      91.177      2.735428      < 2e-16
k1    Par      : 0.212772      0.164150      0.261      0.024807      4.45e-11
k2    Par      : 0.019352      0.007916      0.031      0.005835      0.000943
tb    Par      : 3.423033      2.402596      4.443      0.520641      2.96e-08
k      Met      : 0.005540      0.001809      0.009      0.001904      0.002878
FF    Par -> Met : 0.7639              0.074369

# -----
# DT50 and DT90 values
# -----

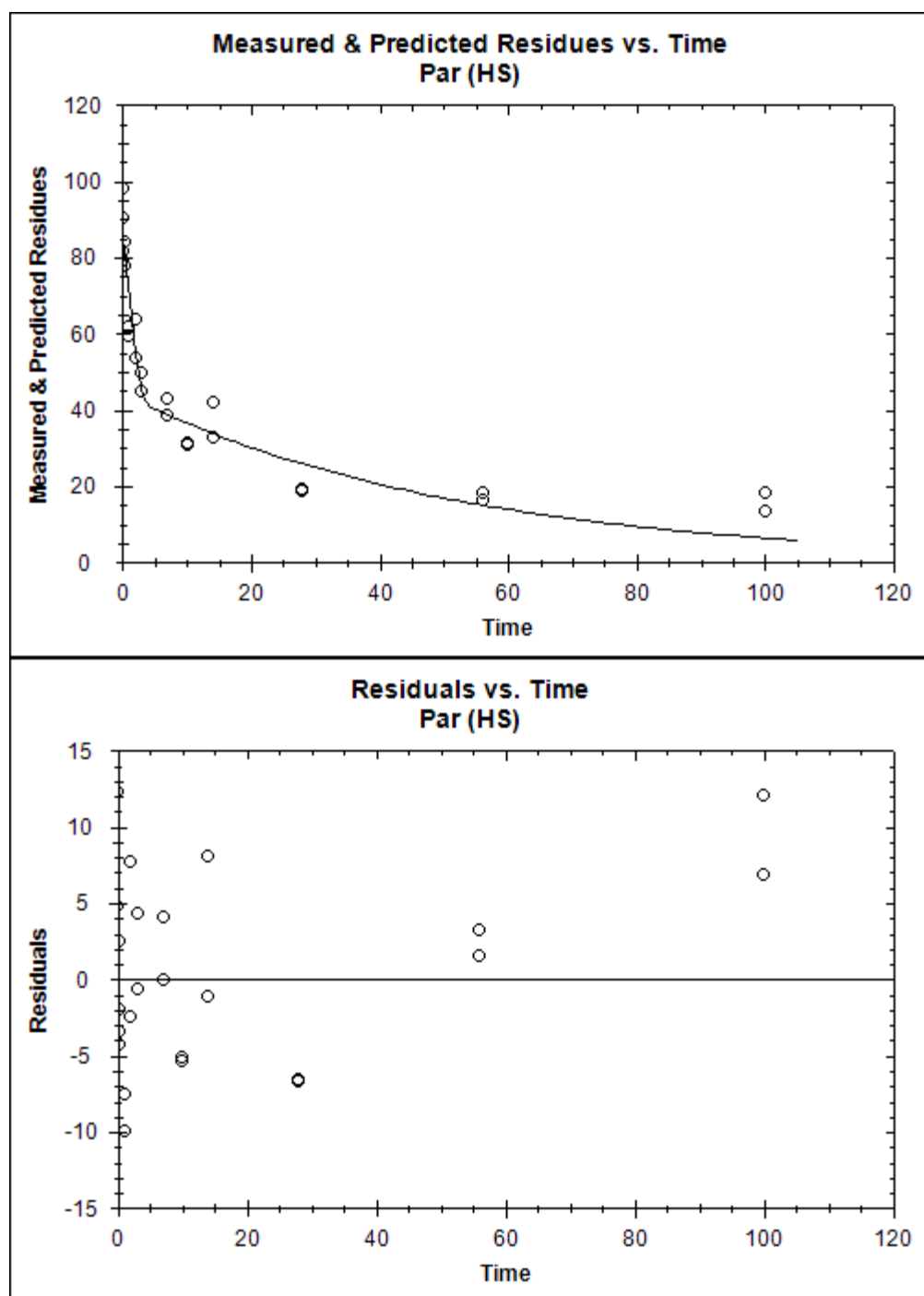
      DT50 :      3.2577      125.12
      DT90 :      84.772      415.63
      Kinetic model :      HS      SFO

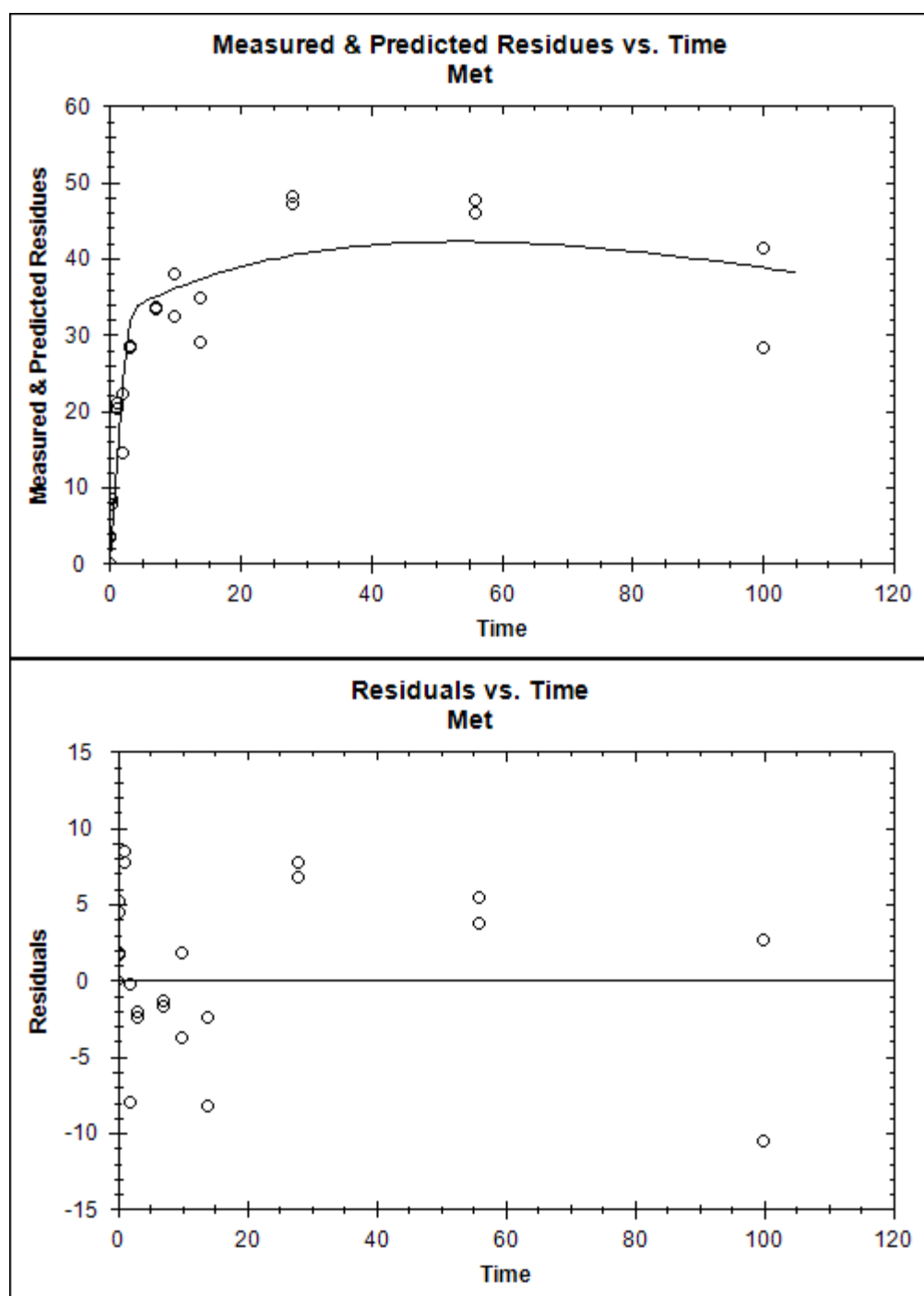
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000 98.1400 6.0872 85.8155 12.3245 0.0000 5.0797 0.0000 0.0000
0.0000 90.5800 6.0872 85.8155 4.7645 0.0000 5.0797 0.0000 0.0000

```

0.1250	79.3000	6.0872	83.5632	-4.2632	3.4400	5.0797	1.7199	1.7201
0.1250	81.6700	6.0872	83.5632	-1.8932	3.4900	5.0797	1.7199	1.7701
0.2500	83.9000	6.0872	81.3700	2.5300	7.8200	5.0797	3.3934	4.4266
0.2500	78.0000	6.0872	81.3700	-3.3700	8.5500	5.0797	3.3934	5.1566
1.0000	59.3900	6.0872	69.3681	-9.9781	20.3100	5.0797	12.5278	7.7822
1.0000	61.8600	6.0872	69.3681	-7.5081	20.9300	5.0797	12.5278	8.4022
2.0000	53.6300	6.0872	56.0731	-2.4431	22.2900	5.0797	22.5852	-0.2952
2.0000	63.8200	6.0872	56.0731	7.7469	14.5300	5.0797	22.5852	-8.0552
3.0000	49.7000	6.0872	45.3261	4.3739	28.6100	5.0797	30.6463	-2.0363
3.0000	44.7100	6.0872	45.3261	-0.6161	28.2700	5.0797	30.6463	-2.3763
7.0000	42.7900	6.0872	38.6541	4.1359	33.6700	5.0797	34.9882	-1.3182
7.0000	38.6100	6.0872	38.6541	-0.0441	33.2500	5.0797	34.9882	-1.7382
10.0000	31.3700	6.0872	36.4739	-5.1039	32.3100	5.0797	36.0630	-3.7530
10.0000	31.0800	6.0872	36.4739	-5.3939	37.8800	5.0797	36.0630	1.8170
14.0000	41.8000	6.0872	33.7571	8.0429	29.0800	5.0797	37.3249	-8.2449
14.0000	32.6100	6.0872	33.7571	-1.1471	34.8600	5.0797	37.3249	-2.4649
28.0000	19.2500	6.0872	25.7456	-6.4956	48.1100	5.0797	40.4175	7.6925
28.0000	19.0200	6.0872	25.7456	-6.7256	47.1500	5.0797	40.4175	6.7325
56.0000	16.4900	6.0872	14.9754	1.5146	45.8800	5.0797	42.1777	3.7023
56.0000	18.2100	6.0872	14.9754	3.2346	47.6100	5.0797	42.1777	5.4323
100.0000	13.3000	6.0872	6.3913	6.9087	28.2000	5.0797	38.7739	-10.5739
100.0000	18.4500	6.0872	6.3913	12.0587	41.3900	5.0797	38.7739	2.6161





11.1.2.3 FOMC

```

# Trial      : Genkeltotalsystmet
# File name  : Genkeltotalsystmet IRLS FOMC Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Genkel_total-syst_met
# Created    : on 16 Jun 2013
#            : at 10:57
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      98.14           0           Inf      False
alpha Par      :       0.10           0           Inf      False
beta  Par      :       0.10           0           Inf      False
k      Met      :       0.10           0           Inf      False
FF     Par -> Met :       0.10           0             1      False
M(0)  Met      :              0                      True

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      6.280      11.509      8.772
      Kinetic model :      FOMC      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 43
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      9.063e+01      8.560e+01      95.657      2.565e+00      < 2e-16
alpha Par      3.371e-01      2.700e-01      0.404      3.422e-02      6.84e-13
beta  Par      5.706e-01      2.173e-01      0.924      1.803e-01      0.00142
k      Met      2.589e-03      2.137e-04      0.005      1.212e-03      0.01919
FF     Par -> Met      0.6559                      5.011e-02

# -----
# DT50 and DT90 values
# -----

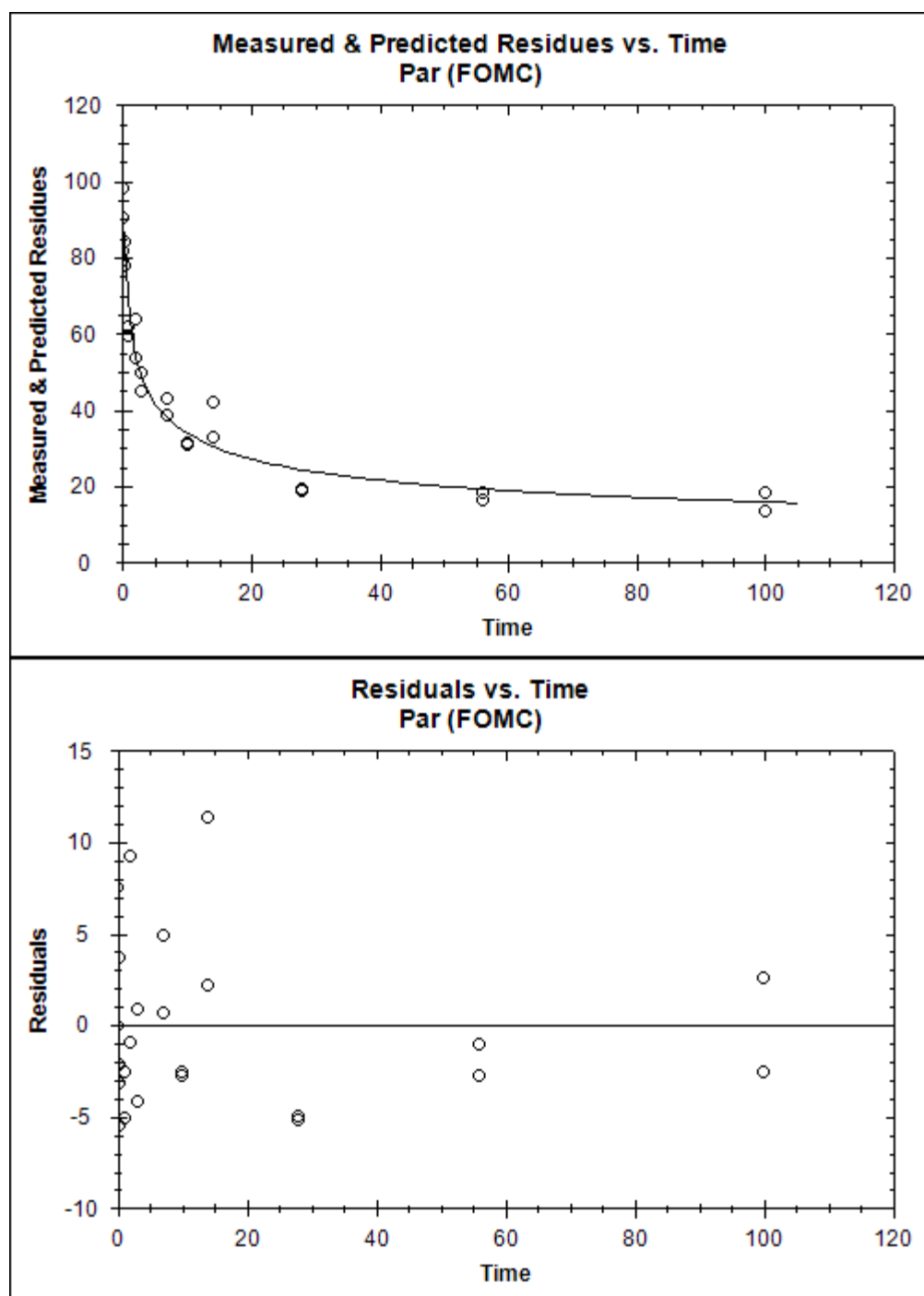
      DT50 :      3.8902      267.71
      DT90 :      527.94      889.32
      Kinetic model :      FOMC      SFO

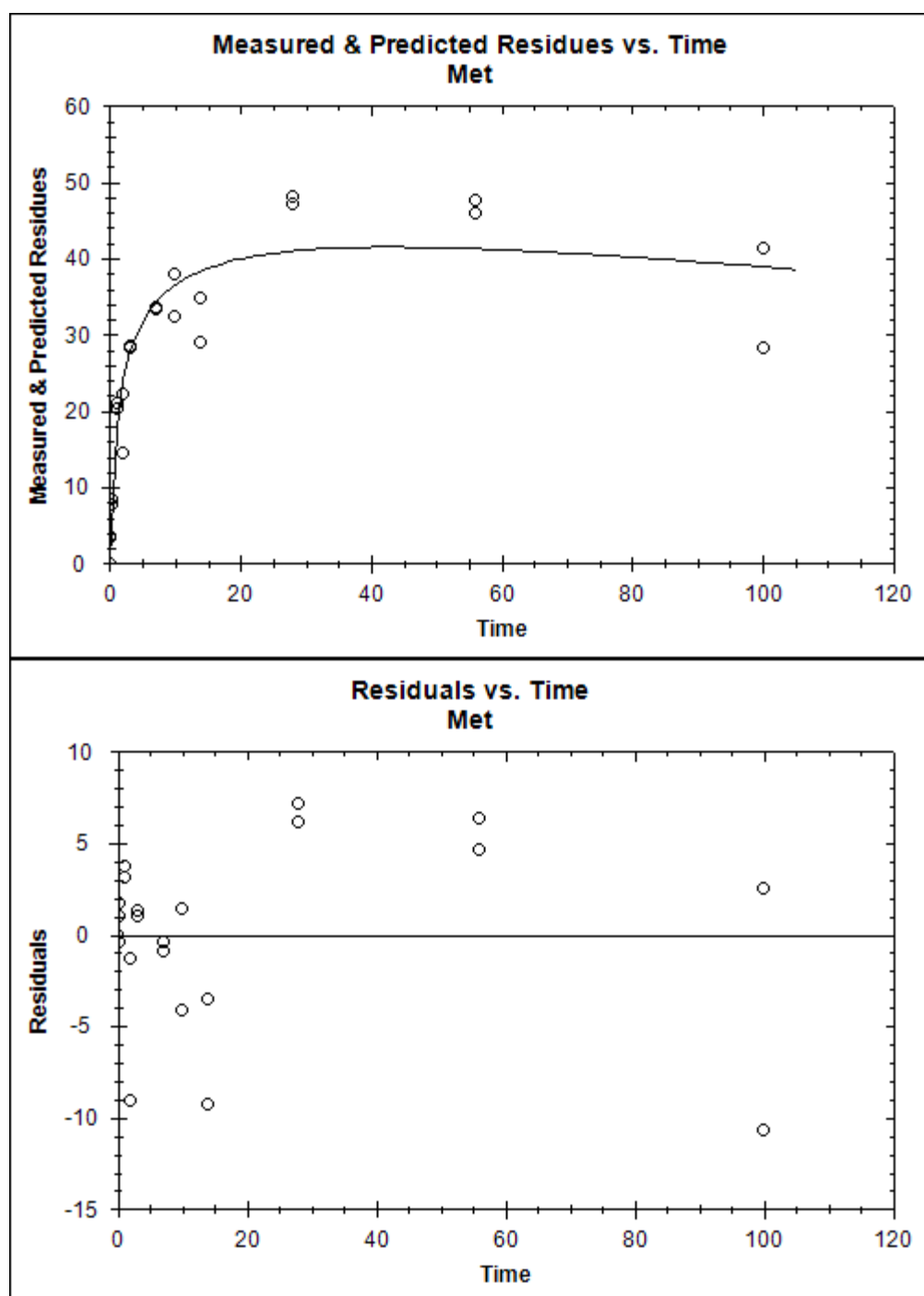
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000 98.1400 4.5547 90.6307 7.5093 0.0000 4.5878 0.0000 0.0000
0.0000 90.5800 4.5547 90.6307 -0.0507 0.0000 4.5878 0.0000 0.0000
0.1250 79.3000 4.5547 84.7771 -5.4771 3.4400 4.5878 3.8389 -0.3989
0.1250 81.6700 4.5547 84.7771 -3.1071 3.4900 4.5878 3.8389 -0.3489

```

0.2500	83.9000	4.5547	80.1838	3.7162	7.8200	4.5878	6.8499	0.9701
0.2500	78.0000	4.5547	80.1838	-2.1838	8.5500	4.5878	6.8499	1.7001
1.0000	59.3900	4.5547	64.4252	-5.0352	20.3100	4.5878	17.1616	3.1484
1.0000	61.8600	4.5547	64.4252	-2.5652	20.9300	4.5878	17.1616	3.7684
2.0000	53.6300	4.5547	54.5674	-0.9374	22.2900	4.5878	23.5739	-1.2839
2.0000	63.8200	4.5547	54.5674	9.2526	14.5300	4.5878	23.5739	-9.0439
3.0000	49.7000	4.5547	48.8462	0.8538	28.6100	4.5878	27.2604	1.3496
3.0000	44.7100	4.5547	48.8462	-4.1362	28.2700	4.5878	27.2604	1.0096
7.0000	42.7900	4.5547	37.9153	4.8747	33.6700	4.5878	34.1062	-0.4362
7.0000	38.6100	4.5547	37.9153	0.6947	33.2500	4.5878	34.1062	-0.8562
10.0000	31.3700	4.5547	33.8804	-2.5104	32.3100	4.5878	36.4779	-4.1679
10.0000	31.0800	4.5547	33.8804	-2.8004	37.8800	4.5878	36.4779	1.4021
14.0000	41.8000	4.5547	30.4066	11.3934	29.0800	4.5878	38.3680	-9.2880
14.0000	32.6100	4.5547	30.4066	2.2034	34.8600	4.5878	38.3680	-3.5080
28.0000	19.2500	4.5547	24.2323	-4.9823	48.1100	4.5878	40.9688	7.1412
28.0000	19.0200	4.5547	24.2323	-5.2123	47.1500	4.5878	40.9688	6.1812
56.0000	16.4900	4.5547	19.2484	-2.7584	45.8800	4.5878	41.2400	4.6400
56.0000	18.2100	4.5547	19.2484	-1.0384	47.6100	4.5878	41.2400	6.3700
100.0000	13.3000	4.5547	15.8550	-2.5550	28.2000	4.5878	38.8880	-10.6880
100.0000	18.4500	4.5547	15.8550	2.5950	41.3900	4.5878	38.8880	2.5020





11.1.2.4 DFOP

```

# Trial      : Genkeltotalsystmet
# File name  : Genkeltotalsystmet IRLS DFOP Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_total-syst_met
# Created    : on 16 Jun 2013
#            : at 10:43
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      98.14              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
g     Par      :       0.50              0              1      False
k     Met      :       0.10              0              Inf      False
FF    Par -> Met :       0.10              0              1      False
M(0)  Met      :       0                  0              1      True

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      9.841      10.538      11.009
      Kinetic model :      DFOP      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 42
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      88.109233      82.071678      94.147      3.080442      < 2e-16
k1    Par      0.860843      0.236539      1.485      0.318528      0.004943
k2    Par      0.025927      0.010337      0.042      0.007954      0.001108
g     Par      0.436566      0.307670      0.565      0.065765      2.40e-08
k     Met      0.006093      0.002923      0.009      0.001617      0.000254
FF    Par -> Met      0.7397      0.069977

# -----
# DT50 and DT90 values
# -----

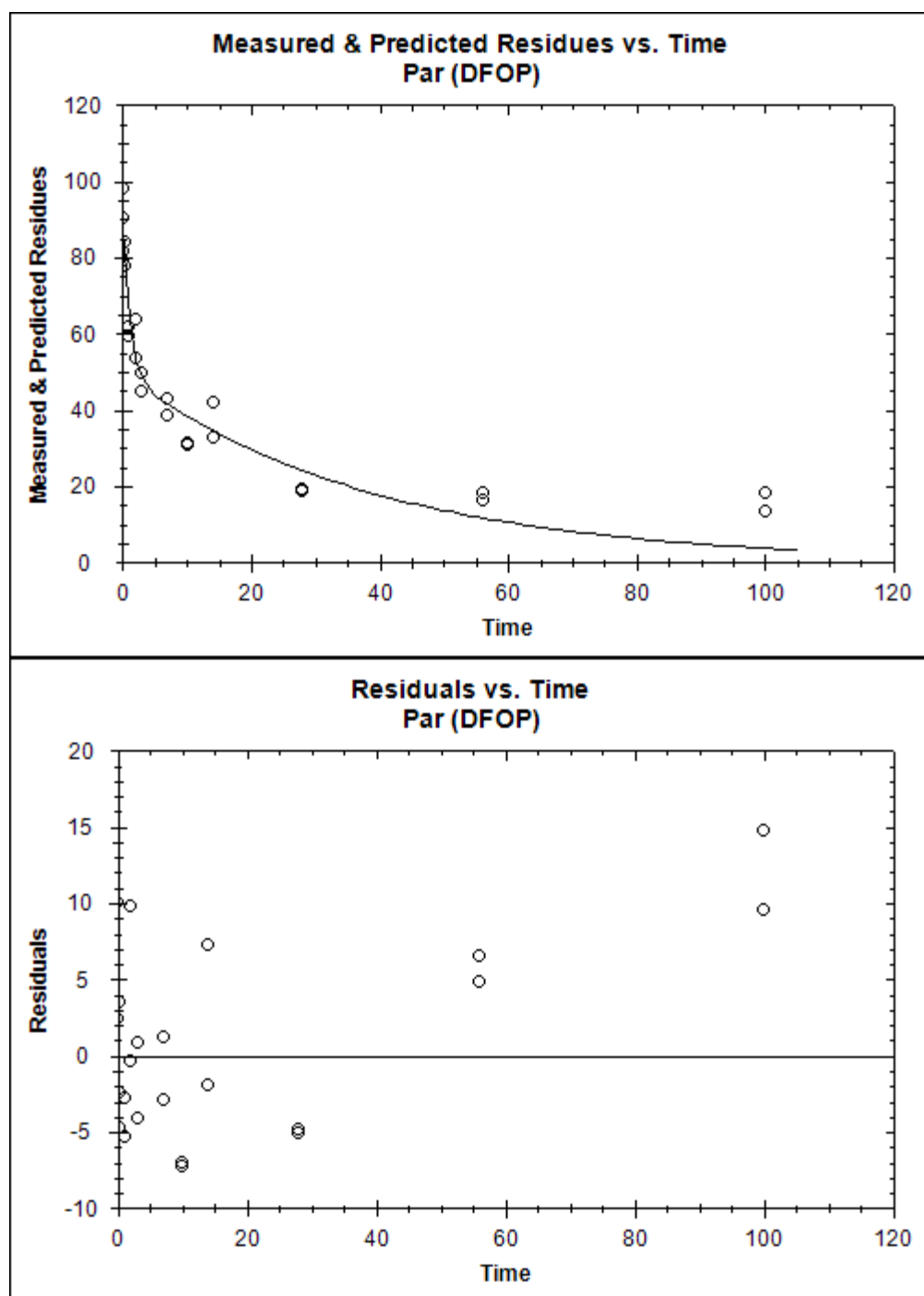
      DT50 :      5.0465      113.77
      DT90 :      66.683      377.94
      Kinetic model :      DFOP      SFO

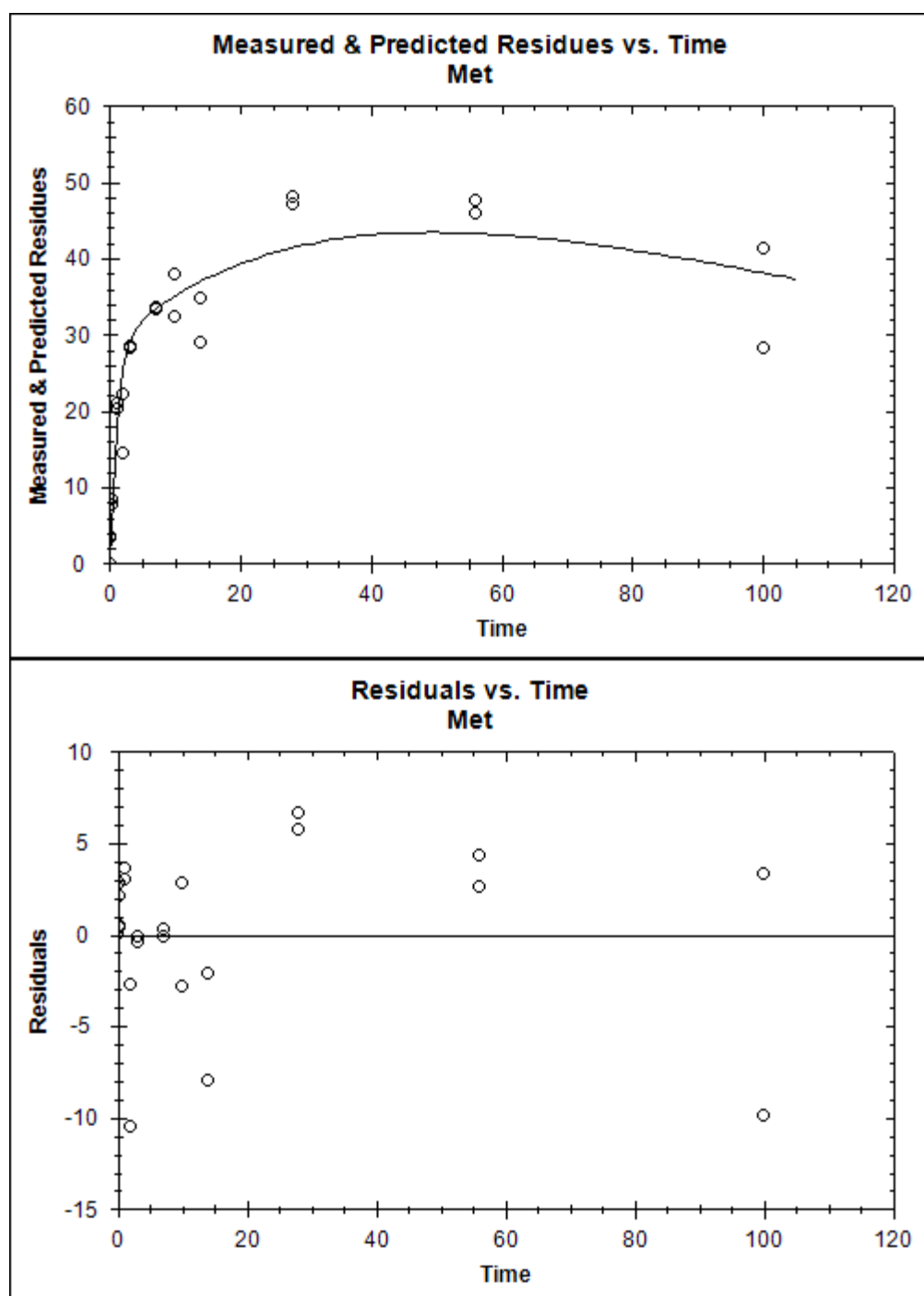
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000  98.1400  6.0809  88.1092  10.0308  0.0000  4.3344  0.0000  0.0000
0.0000  90.5800  6.0809  88.1092  2.4708  0.0000  4.3344  0.0000  0.0000

```

0.1250	79.3000	6.0809	84.0244	-4.7244	3.4400	4.3344	3.0204	0.4196
0.1250	81.6700	6.0809	84.0244	-2.3544	3.4900	4.3344	3.0204	0.4696
0.2500	83.9000	6.0809	80.3405	3.5595	7.8200	4.3344	5.7422	2.0778
0.2500	78.0000	6.0809	80.3405	-2.3405	8.5500	4.3344	5.7422	2.8078
1.0000	59.3900	6.0809	64.6366	-5.2466	20.3100	4.3344	17.3033	3.0067
1.0000	61.8600	6.0809	64.6366	-2.7766	20.9300	4.3344	17.3033	3.6267
2.0000	53.6300	6.0809	54.0114	-0.3814	22.2900	4.3344	25.0309	-2.7409
2.0000	63.8200	6.0809	54.0114	9.8086	14.5300	4.3344	25.0309	-10.5009
3.0000	49.7000	6.0809	48.8361	0.8639	28.6100	4.3344	28.6943	-0.0843
3.0000	44.7100	6.0809	48.8361	-4.1261	28.2700	4.3344	28.6943	-0.4243
7.0000	42.7900	6.0809	41.4972	1.2928	33.6700	4.3344	33.3537	0.3163
7.0000	38.6100	6.0809	41.4972	-2.8872	33.2500	4.3344	33.3537	-0.1037
10.0000	31.3700	6.0809	38.3129	-6.9429	32.3100	4.3344	35.0832	-2.7732
10.0000	31.0800	6.0809	38.3129	-7.2329	37.8800	4.3344	35.0832	2.7968
14.0000	41.8000	6.0809	34.5325	7.2675	29.0800	4.3344	37.0005	-7.9205
14.0000	32.6100	6.0809	34.5325	-1.9225	34.8600	4.3344	37.0005	-2.1405
28.0000	19.2500	6.0809	24.0208	-4.7708	48.1100	4.3344	41.4096	6.7004
28.0000	19.0200	6.0809	24.0208	-5.0008	47.1500	4.3344	41.4096	5.7404
56.0000	16.4900	6.0809	11.6228	4.8672	45.8800	4.3344	43.2606	2.6194
56.0000	18.2100	6.0809	11.6228	6.5872	47.6100	4.3344	43.2606	4.3494
100.0000	13.3000	6.0809	3.7143	9.5857	28.2000	4.3344	38.0923	-9.8923
100.0000	18.4500	6.0809	3.7143	14.7357	41.3900	4.3344	38.0923	3.2977





11.1.3 Ijzendoorn

11.1.3.1 SFO

```
# Trial      : Ijzendoorntotsystponly
# File name  : Ijzendoorntotsystponly IRLS SFO  Par.r
# Target path :
C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_tot_syst_ponly
# Created    : on 18 Oct 2013
#            : at 11:09
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil : Ijzendoorn total system
# # Ijzendoorn total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par           :      88.90          0          Inf      False
k      Par           :       0.01          0          Inf      False

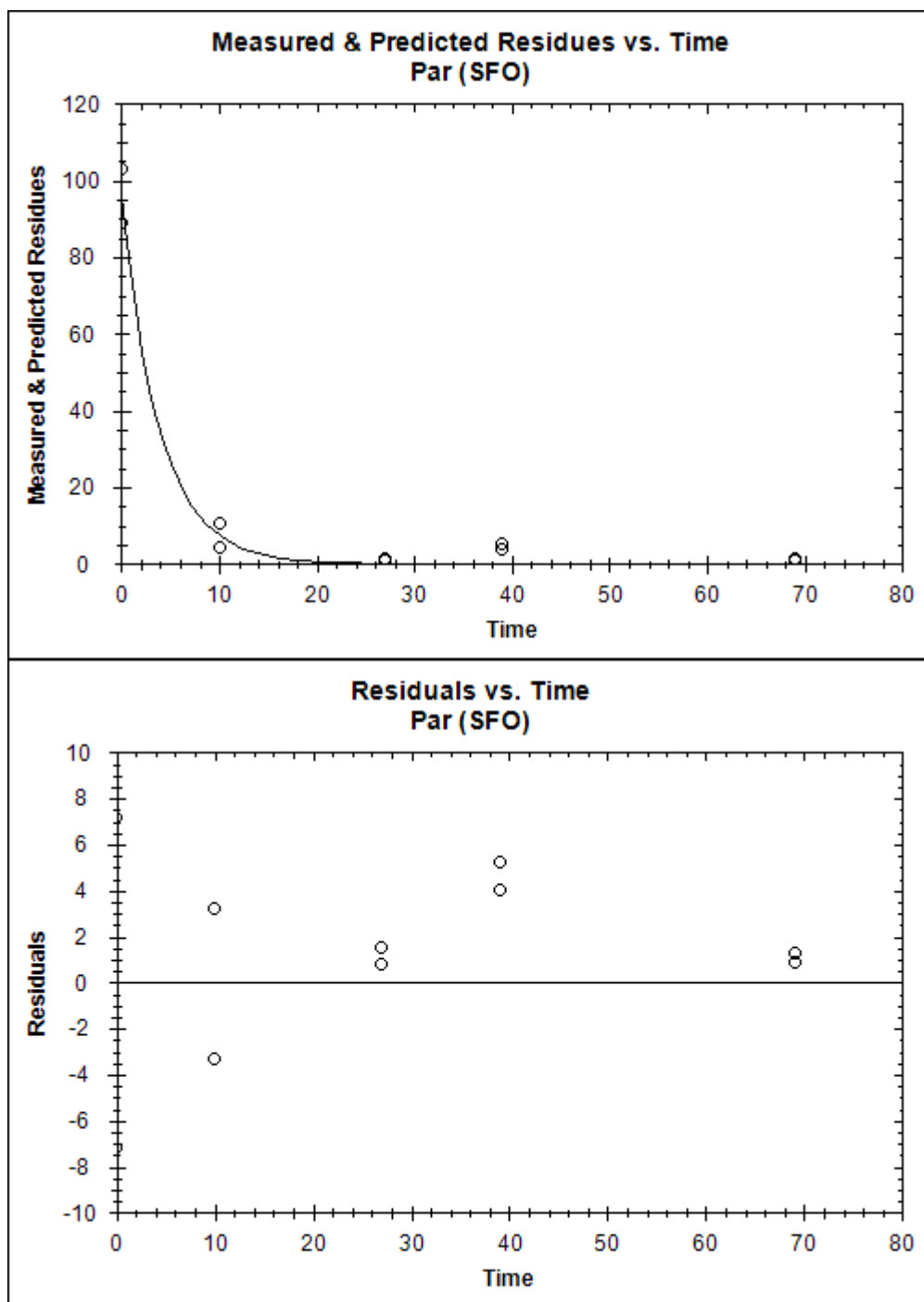
# -----
# Chi2 error estimation
# -----
# -----
# Par      All
Chi2Err% :      7.876      7.876
Kinetic model :      SFO

# -----
# Parameter estimation
# -----
# -----
Degrees of Freedom : 8
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      96.04735      89.26171      102.833      3.46212      1.54e-09
k      Par      :       0.25497       0.16888       0.341      0.04392      0.000201

# -----
# DT50 and DT90 values
# -----
# -----
# Par
DT50 :      2.7185
DT90 :      9.0308
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----
# -----
Compartment Par
time observed err-std predicted residual
0.0000 88.9000 4.1440 96.0474 -7.1474
0.0000 103.2000 4.1440 96.0474 7.1526
10.0000 4.2000 4.1440 7.5018 -3.3018
10.0000 10.7000 4.1440 7.5018 3.1982
27.0000 1.6000 4.1440 0.0983 1.5017
27.0000 0.9000 4.1440 0.0983 0.8017
39.0000 5.2000 4.1440 0.0046 5.1954
39.0000 4.0000 4.1440 0.0046 3.9954
```

69.0000	0.9000	4.1440	0.0000	0.9000
69.0000	1.3000	4.1440	0.0000	1.3000



11.1.3.2HS

```

# Trial      : Ijzendoorn_totsystponly
# File name  : Ijzendoorn_totsystponly IRLS HS   Par.r
# Target path :
C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_tot_syst_ponly
# Created    : on 18 Oct 2013
#            : at 10:33
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments     :
# # study ID: Anderson
# # label: 14C
# # soil : Ijzendoorn total system
# # Ijzendoorn total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
#
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      88.90              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
tb    Par      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----
#
# Par      All
Chi2Err% :      6.282      6.282
Kinetic model :      HS

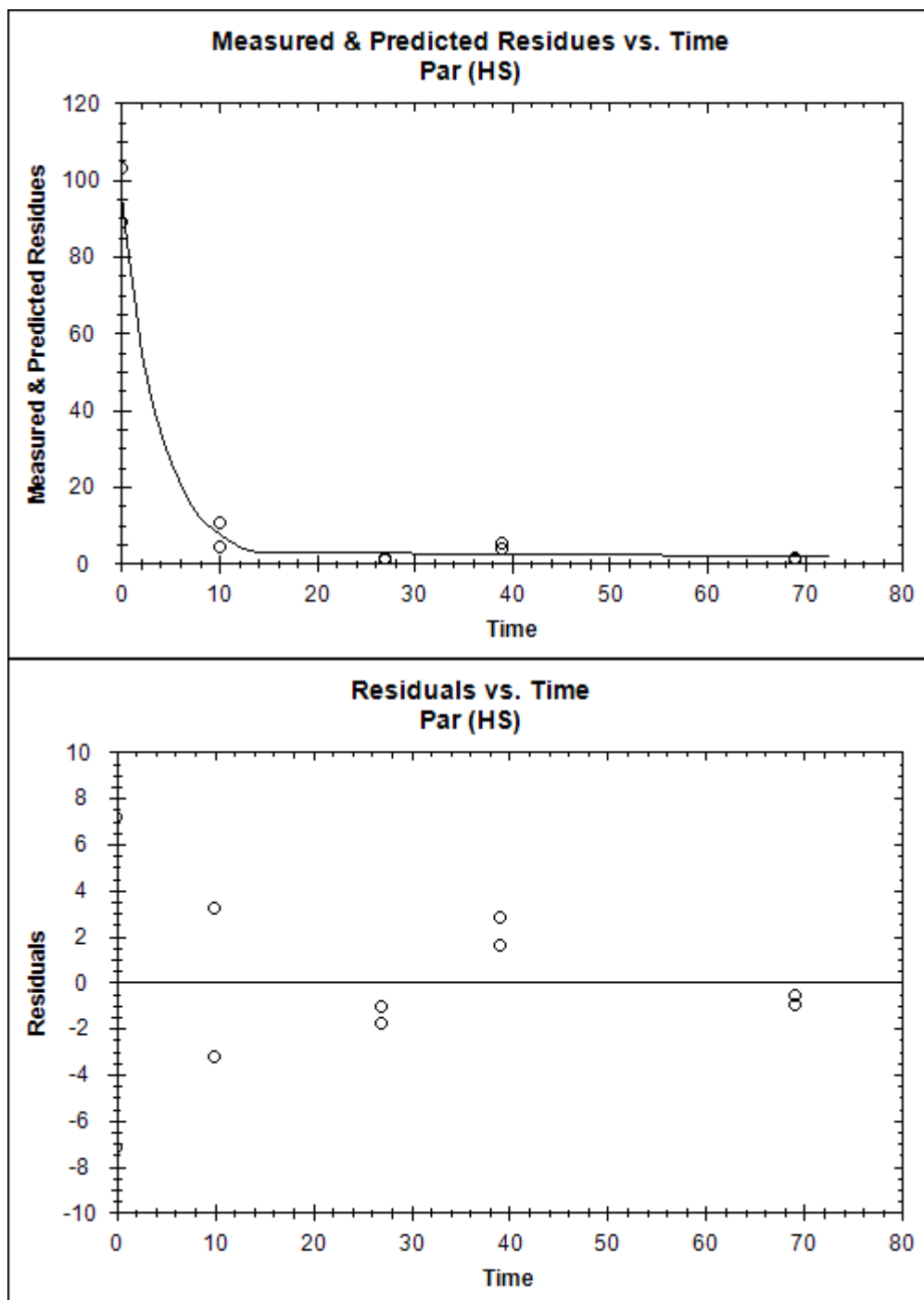
# -----
# Parameter estimation
# -----
#
# Degrees of Freedom : 6
#
# Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      96.049988      89.340609      102.759      3.423215      6.78e-08
k1    Par      :       0.255665      0.165381      0.346      0.046064      0.000723
k2    Par      :       0.008108      -0.077536      0.094      0.043696      0.429456
tb    Par      :      13.596792      1.181953      26.012      6.334218      0.037732

# -----
# DT50 and DT90 values
# -----
#
# Par
DT50 :      2.7112
DT90 :      9.0063
Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----
#
# Compartment Par
# time observed err-std predicted residual
0.0000 88.9000 3.7311 96.0500 -7.1500
0.0000 103.2000 3.7311 96.0500 7.1500
10.0000 4.2000 3.7311 7.4501 -3.2501
10.0000 10.7000 3.7311 7.4501 3.2499
27.0000 1.6000 3.7311 2.6644 -1.0644
27.0000 0.9000 3.7311 2.6644 -1.7644

```

39.0000	5.2000	3.7311	2.4174	2.7826
39.0000	4.0000	3.7311	2.4174	1.5826
69.0000	0.9000	3.7311	1.8954	-0.9954
69.0000	1.3000	3.7311	1.8954	-0.5954



11.1.3.3 FOMC

```

# Trial      : Ijzendoorn_totsystonly
# File name  : Ijzendoorn_totsystonly IRLS FOMC Par.r
# Target path :
C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_tot_syst_only
# Created    : on 18 Oct 2013
#            : at 10:33
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil : Ijzendoorn total system
# # Ijzendoorn total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      88.9              0              Inf      False
alpha Par      :       0.1              0              Inf      False
beta  Par      :       0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
Chi2Err% :      5.554      5.554
Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      96.0502      89.9005      102.200      3.1377      5.12e-09
alpha Par      :       0.8436      -0.7537       2.441      0.8150      0.168
beta  Par      :       0.4891      -2.7325       3.711      1.6437      0.387

# -----
# DT50 and DT90 values
# -----

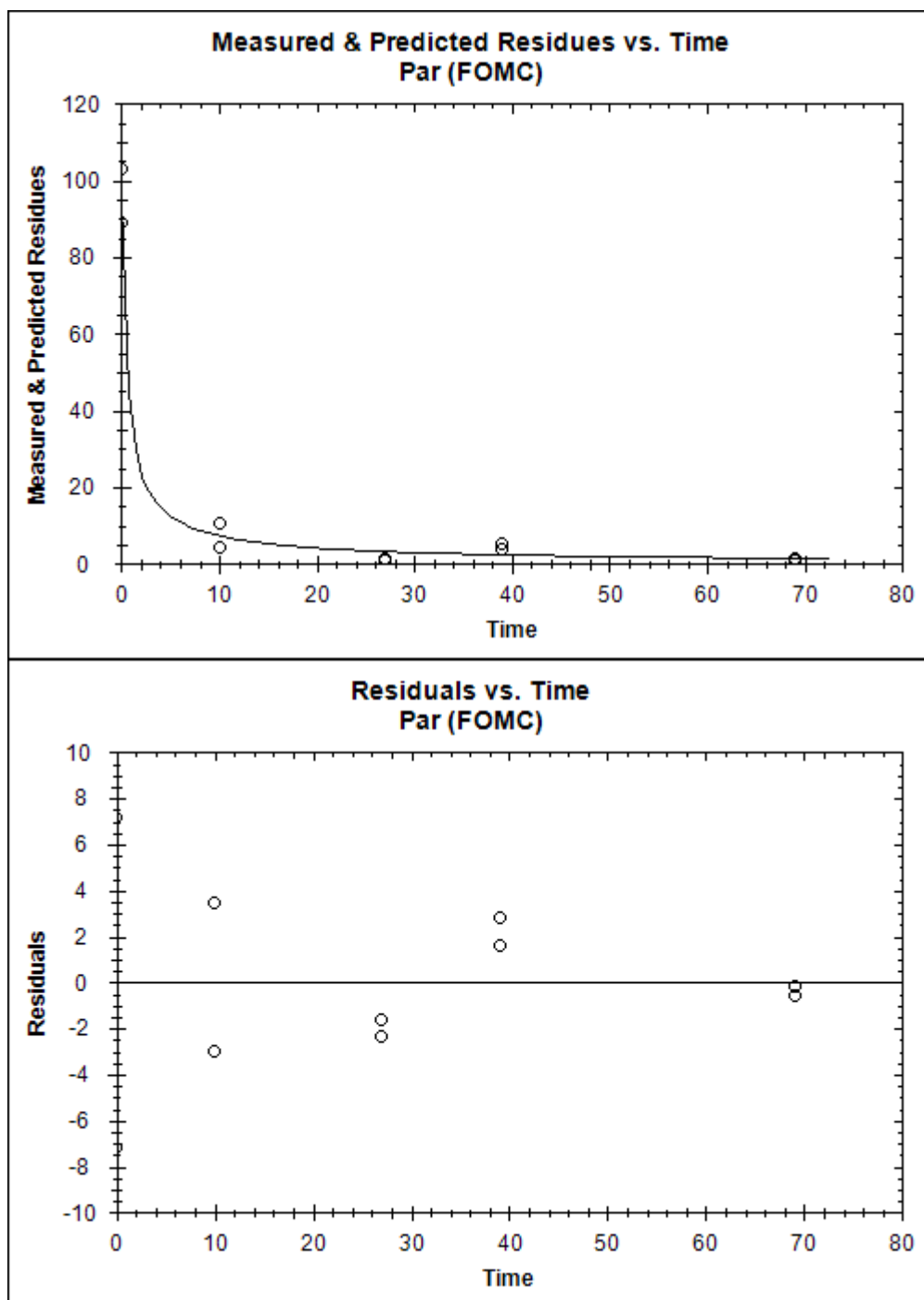
      Par
DT50 :      0.6232
DT90 :      7.0060
Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

Compartment Par
time observed err-std predicted residual
0.0000 88.9000 3.7743 96.0502 -7.1502
0.0000 103.2000 3.7743 96.0502 7.1498
10.0000 4.2000 3.7743 7.2338 -3.0338
10.0000 10.7000 3.7743 7.2338 3.4662
27.0000 1.6000 3.7743 3.2092 -1.6092
27.0000 0.9000 3.7743 3.2092 -2.3092
39.0000 5.2000 3.7743 2.3642 2.8358
39.0000 4.0000 3.7743 2.3642 1.6358

```

69.0000	0.9000	3.7743	1.4677	-0.5677
69.0000	1.3000	3.7743	1.4677	-0.1677



11.1.3.4DFOP

```

# Trial      : Ijzendoorntotsystonly
# File name  : Ijzendoorntotsystonly IRLS DFOP Par.r
# Target path :
C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_tot_syst_only
# Created    : on 18 Oct 2013
#            : at 10:33
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil : Ijzendoorn total system
# # Ijzendoorn total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      88.90              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
g     Par      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

      Par      All
Chi2Err% :      6.31      6.31
Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      96.050572      89.362953      102.738      3.412113      6.65e-08
k1    Par      :       0.305754       0.045638       0.566      0.132715      0.0304
k2    Par      :       0.008266      -0.079401       0.096      0.044729      0.4297
g     Par      :       0.965262       0.827327       1.103      0.070377      4.67e-06

# -----
# DT50 and DT90 values
# -----

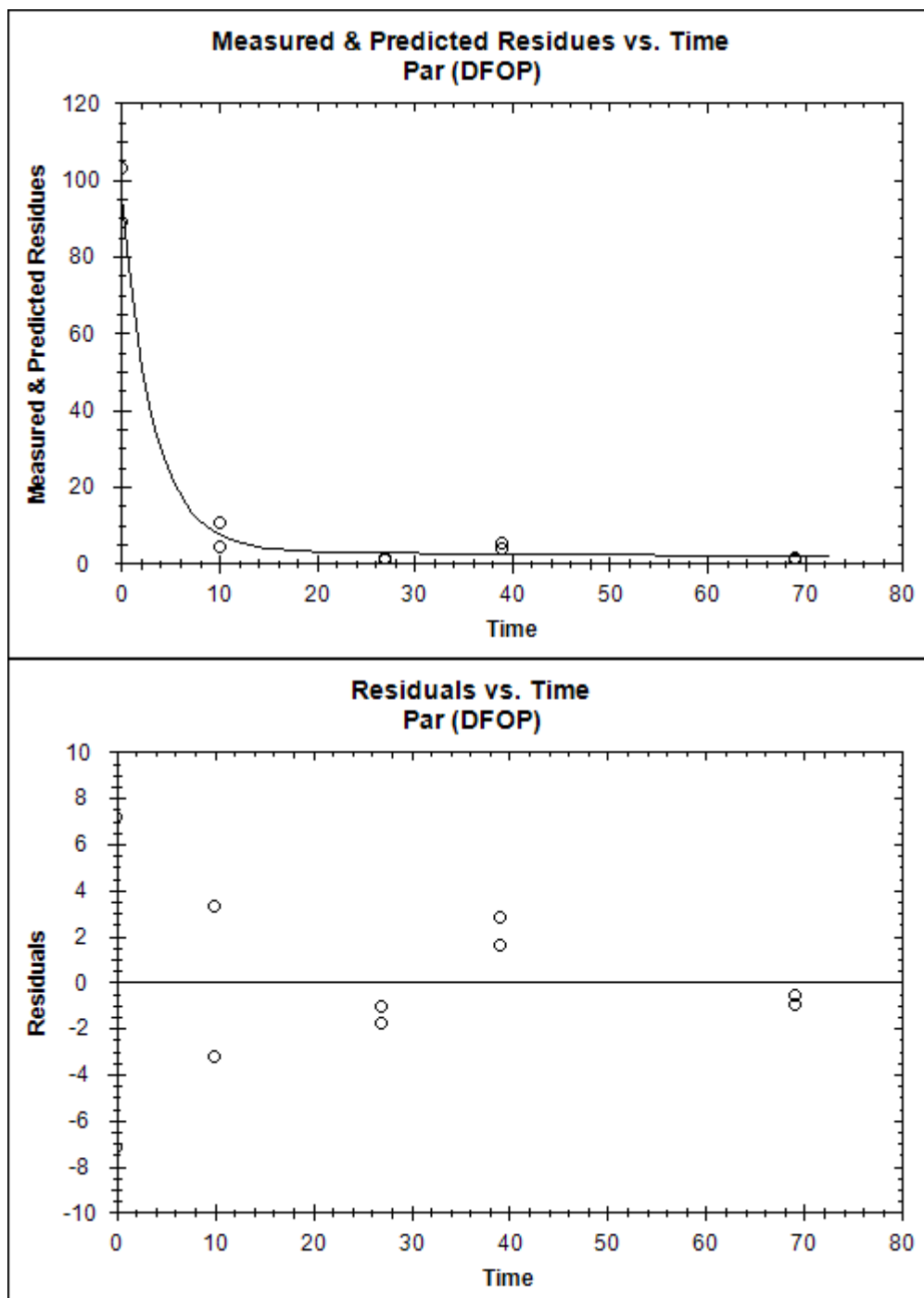
      Par
DT50 :      2.3821
DT90 :      8.6924
Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

Compartment Par
time observed err-std predicted residual
0.0000 88.9000 3.7329 96.0506 -7.1506
0.0000 103.2000 3.7329 96.0506 7.1494
10.0000 4.2000 3.7329 7.4297 -3.2297
10.0000 10.7000 3.7329 7.4297 3.2703
27.0000 1.6000 3.7329 2.6933 -1.0933
27.0000 0.9000 3.7329 2.6933 -1.7933

```

39.0000	5.2000	3.7329	2.4177	2.7823
39.0000	4.0000	3.7329	2.4177	1.5823
69.0000	0.9000	3.7329	1.8863	-0.9863
69.0000	1.3000	3.7329	1.8863	-0.5863



11.1.4 Lienden

11.1.4.1 SFO

```
# Trial      : Liendentotsystponly
# File name  : Liendentotsystponly IRLS SFO Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_tot_syst_ponly
# Created    : on 18 Oct 2013
#            : at 11:42
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil : Lienden total system
# # Lienden total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

M(0)  Par      :      100.10      Lower Bound      0      Upper Bound      Inf      Fixed      False
k      Par      :       0.01      Lower Bound      0      Upper Bound      Inf      Fixed      False

# -----
# Chi2 error estimation
# -----

Chi2Err% :      6.327      Par      All
Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 8
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      100.44641      97.21937      103.673      1.64648      2.90e-12
k      Par      :       0.33179      0.23564      0.428      0.04905      7.15e-05

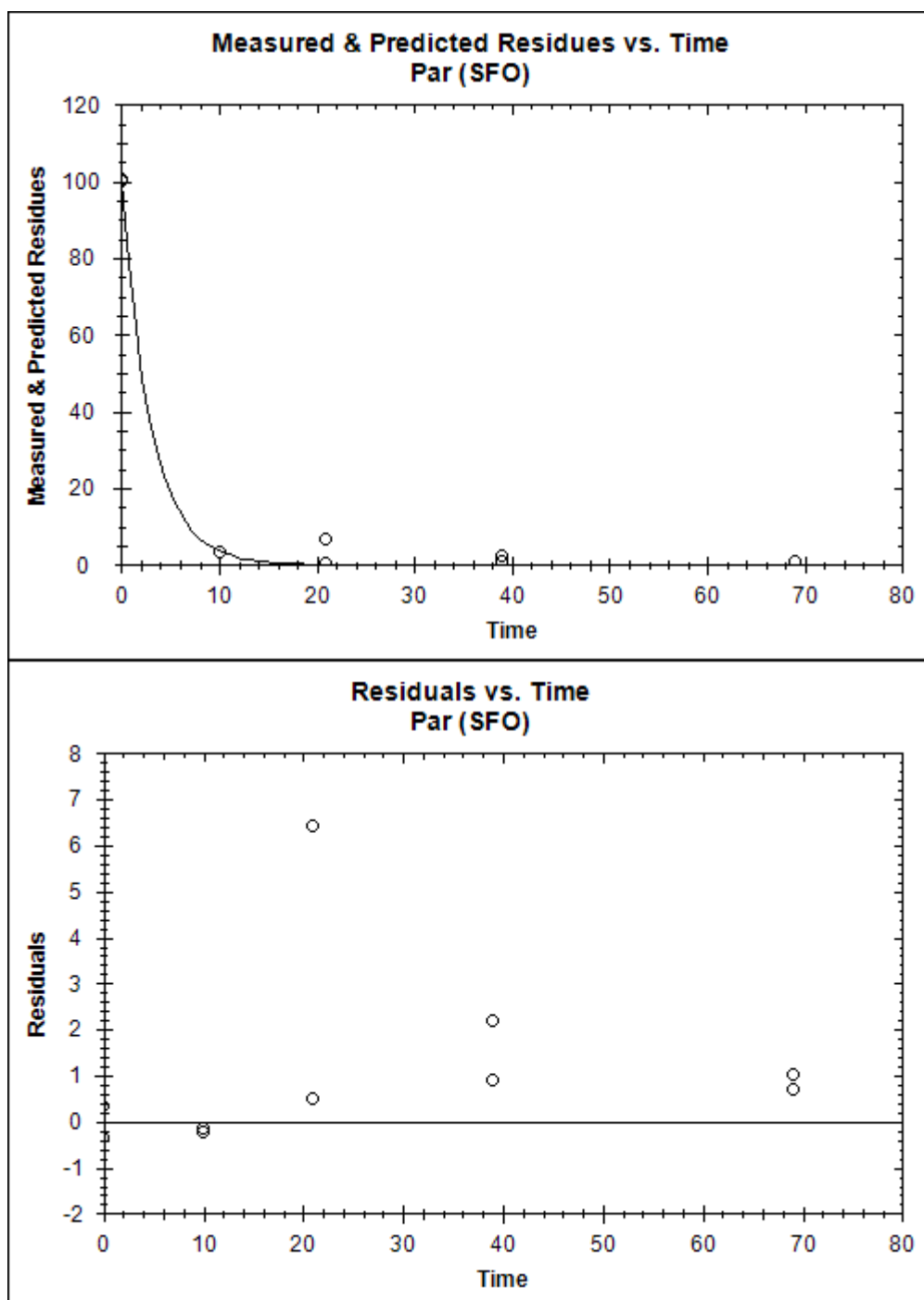
# -----
# DT50 and DT90 values
# -----

DT50 :      2.0891      Par
DT90 :      6.9399
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

Compartment Par
time observed err-std predicted residual
0.0000 100.1000 2.2078 100.4464 -0.3464
0.0000 100.8000 2.2078 100.4464 0.3536
10.0000 3.5000 2.2078 3.6391 -0.1391
10.0000 3.4000 2.2078 3.6391 -0.2391
21.0000 6.5000 2.2078 0.0946 6.4054
21.0000 0.6000 2.2078 0.0946 0.5054
39.0000 0.9000 2.2078 0.0002 0.8998
39.0000 2.2000 2.2078 0.0002 2.1998
69.0000 0.7000 2.2078 0.0000 0.7000
```

69.0000 1.0000 2.2078 0.0000 1.0000



11.1.4.2HS

```

# Trial      : Liendentotsystponly
# File name  : Liendentotsystponly IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_tot_syst_ponly
# Created    : on 18 Oct 2013
#            : at 11:42
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil : Lienden total system
# # Lienden total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      100.10           0           Inf      False
k1    Par      :           0.10           0           Inf      False
k2    Par      :           0.01           0           Inf      False
tb    Par      :           3.00           0           Inf      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :      1.863      1.863
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      100.44998      97.92210      102.978      1.28976      1.51e-10
k1    Par      :           0.40478           0.22902           0.581      0.08968           0.00202
k2    Par      :           0.02414          -0.01069           0.059      0.01777           0.11158
tb    Par      :           7.98533           3.28666          12.684      2.39732           0.00789

# -----
# DT50 and DT90 values
# -----

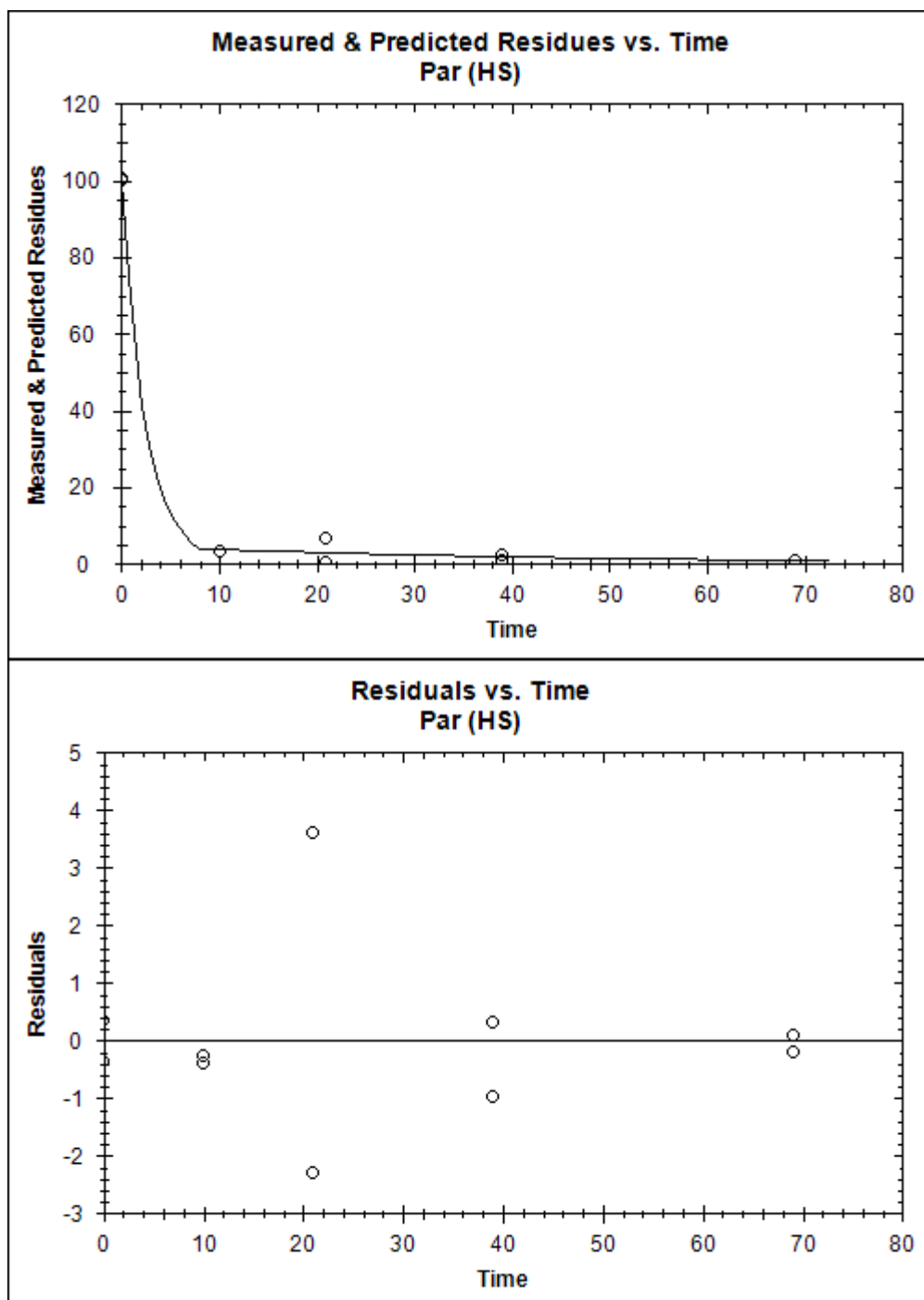
              Par
      DT50 :           1.7124
      DT90 :           5.6884
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 100.1000 1.4083 100.4500 -0.3500
0.0000 100.8000 1.4083 100.4500 0.3500
10.0000 3.5000 1.4083 3.7761 -0.2761
10.0000 3.4000 1.4083 3.7761 -0.3761
21.0000 6.5000 1.4083 2.8956 3.6044
21.0000 0.6000 1.4083 2.8956 -2.2956
39.0000 0.9000 1.4083 1.8752 -0.9752

```

39.0000	2.2000	1.4083	1.8752	0.3248
69.0000	0.7000	1.4083	0.9090	-0.2090
69.0000	1.0000	1.4083	0.9090	0.0910



11.1.4.3 FOMC

```

# Trial      : Liendentotsystponly
# File name  : Liendentotsystponly IRLS FOMC Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_tot_syst_ponly
# Created    : on 18 Oct 2013
#            : at 11:43
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil : Lienden total system
# # Lienden total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      100.1           0           Inf      False
alpha Par      :       0.1           0           Inf      False
beta  Par      :       0.1           0           Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      2.234      2.234
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      100.45000      98.07665      102.823      1.21091      4.87e-12
alpha Par      :       0.54788      -0.20043      1.296      0.38180      0.0972
beta  Par      :       0.02573      -0.19655      0.248      0.11341      0.4135

# -----
# DT50 and DT90 values
# -----

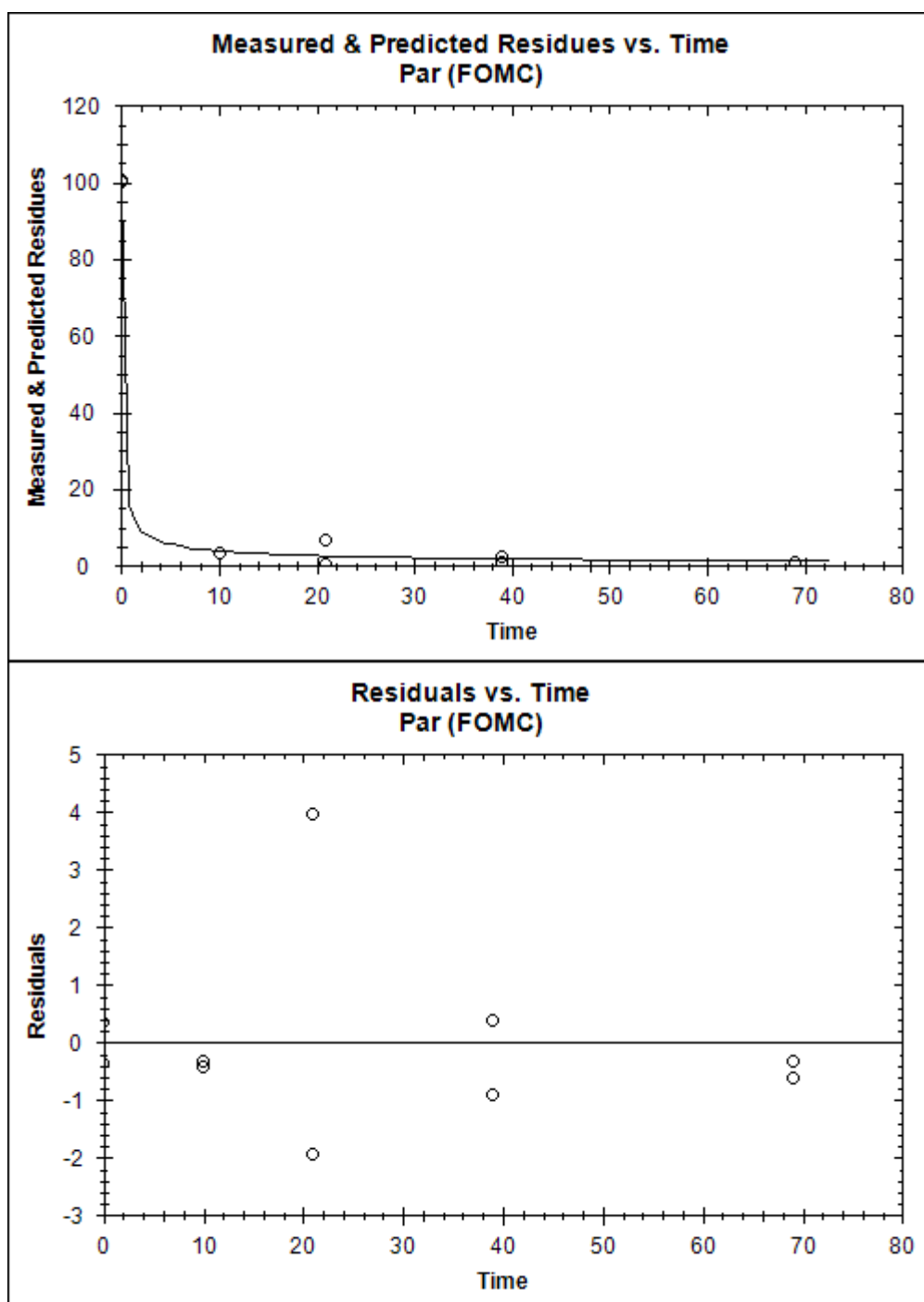
      Par
      DT50 :      0.0654
      DT90 :      1.6947
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 100.1000 1.4639 100.4500 -0.3500
0.0000 100.8000 1.4639 100.4500 0.3500
10.0000 3.5000 1.4639 3.8243 -0.3243
10.0000 3.4000 1.4639 3.8243 -0.4243
21.0000 6.5000 1.4639 2.5488 3.9512
21.0000 0.6000 1.4639 2.5488 -1.9488
39.0000 0.9000 1.4639 1.8163 -0.9163
39.0000 2.2000 1.4639 1.8163 0.3837
69.0000 0.7000 1.4639 1.3289 -0.6289

```

69.0000 1.0000 1.4639 1.3289 -0.3289



11.1.4.4DFOP

```

# Trial      : Liendentotsystponly
# File name  : Liendentotsystponly IRLS DFOP Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_tot_syst_ponly
# Created    : on 18 Oct 2013
#            : at 11:42
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Anderson
# # label: 14C
# # soil : Lienden total system
# # Lienden total system (water+sediment)
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0) Par :          100.10              0              Inf      False
k1  Par :           0.10              0              Inf      False
k2  Par :           0.01              0              Inf      False
g   Par :           0.50              0              1      False

# -----
# Chi2 error estimation
# -----
# -----
# Par      All
Chi2Err% :    1.863      1.863
Kinetic model :      DFOP

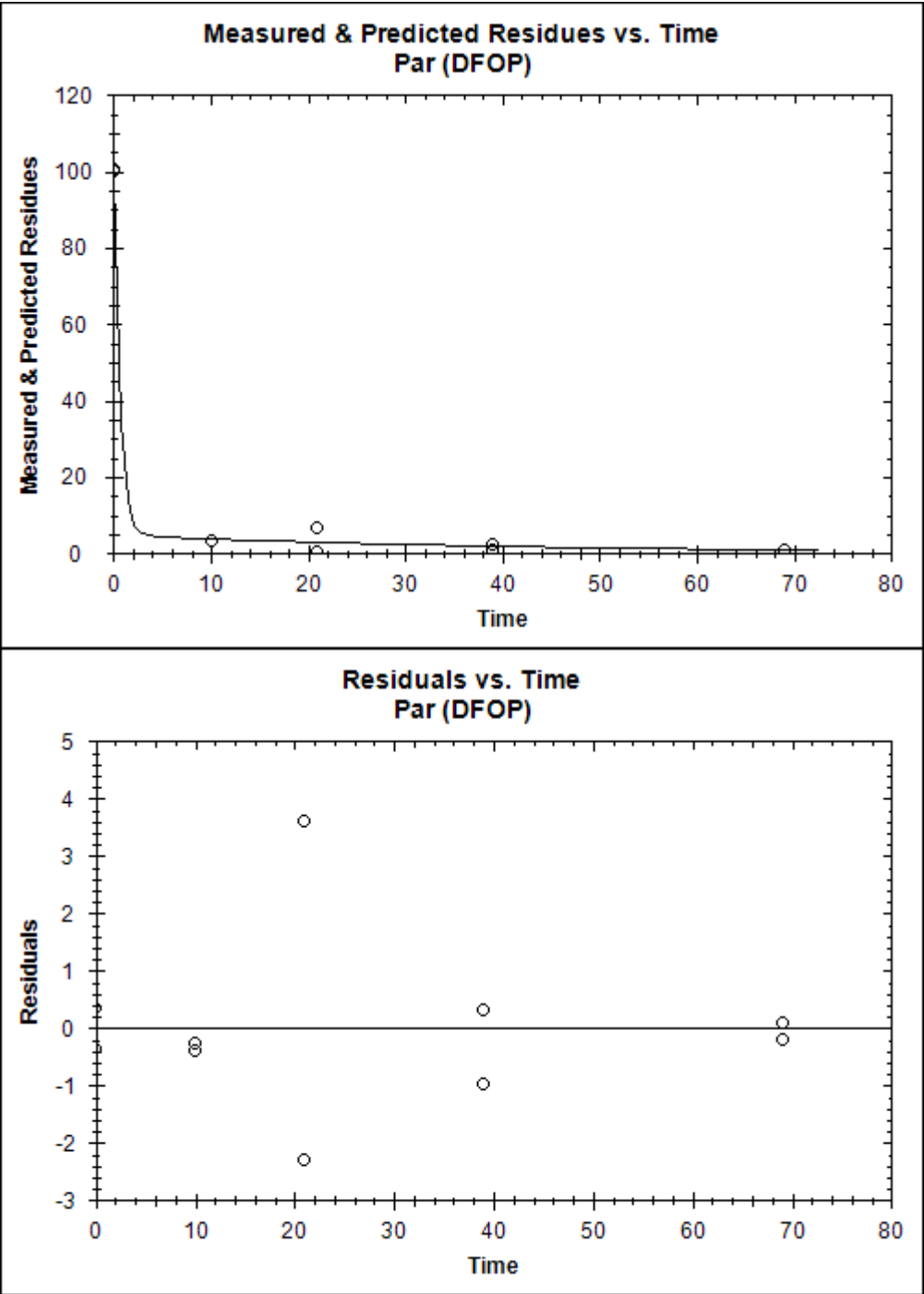
# -----
# Parameter estimation
# -----
# -----
Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0) Par :    100.449975    98.275482    102.624    1.109456    6.12e-11
k1  Par :     1.606950    -65.843730    69.058    34.414245    0.482
k2  Par :     0.024139    -0.008948    0.057    0.016882    0.101
g   Par :     0.952144     0.910190     0.994    0.021405    4.32e-09

# -----
# DT50 and DT90 values
# -----
# -----
# Par
DT50 :      0.4627
DT90 :      1.7840
Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----
# -----
Compartment Par
time observed err-std predicted residual
0.0000 100.1000 1.4083 100.4500 -0.3500
0.0000 100.8000 1.4083 100.4500 0.3500
10.0000 3.5000 1.4083 3.7762 -0.2762
10.0000 3.4000 1.4083 3.7762 -0.3762
21.0000 6.5000 1.4083 2.8955 3.6045
21.0000 0.6000 1.4083 2.8955 -2.2955

```

39.0000	0.9000	1.4083	1.8751	-0.9751
39.0000	2.2000	1.4083	1.8751	0.3249
69.0000	0.7000	1.4083	0.9089	-0.2089
69.0000	1.0000	1.4083	0.9089	0.0911



11.2 Beta-Cyfluthrin (Isomers II +IV) Degradation Total System

11.2.1 Barmen

11.2.1.1 SFO

```

# Trial      : Barmentsbeta
# File name  : Barmentsbeta IRLS SFO Beta.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:32
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See ts beta
# # Barmener See total system mit Isomeren Verhl. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
#
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0) Beta          :      39.01          0          Inf      False
k      Beta          :      0.10          0          Inf      False

# -----
# Chi2 error estimation
# -----
#
# Chi2Err% :      13.06      13.06
# Kinetic model :      SFO

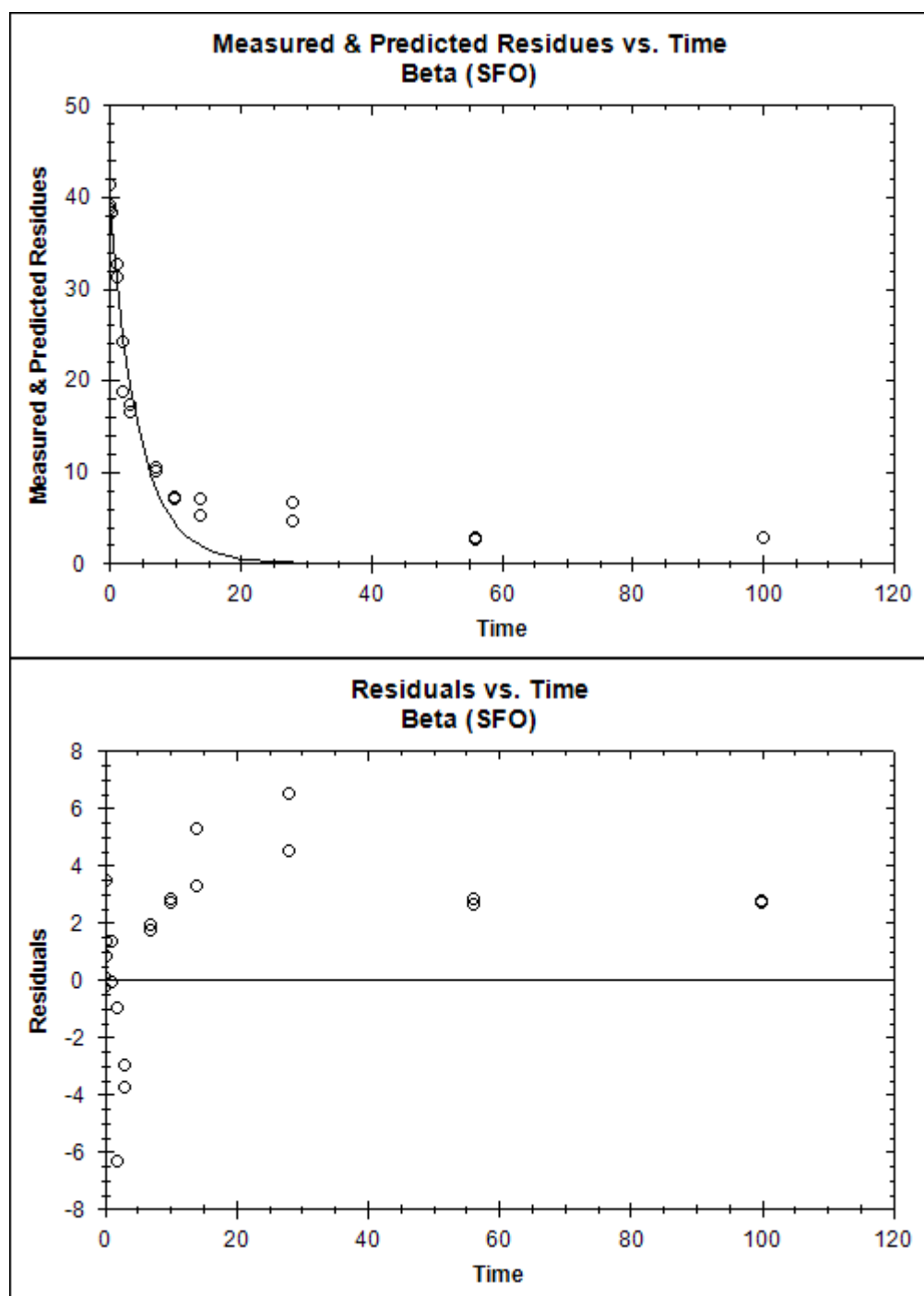
# -----
# Parameter estimation
# -----
#
# Degrees of Freedom : 21
# Parameter          Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0) Beta          :      38.87850      36.00774      41.749      1.46470      < 2e-16
k      Beta          :      0.21824      0.16237      0.274      0.02851      8.27e-08

# -----
# DT50 and DT90 values
# -----
#
# DT50 :      3.1760
# DT90 :      10.550
# Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----
#
# Compartment Beta
# time observed err-std predicted residual
0.0000 39.0100 3.1920 38.8785 0.1315
0.0000 38.5900 3.1920 38.8785 -0.2885
0.1250 38.6900 3.1920 37.8322 0.8578
0.1250 41.3200 3.1920 37.8322 3.4878
0.2500 38.1800 3.1920 36.8141 1.3659
0.2500 NA 3.1920 36.8141 NA
1.0000 31.2000 3.1920 31.2556 -0.0556
1.0000 32.6000 3.1920 31.2556 1.3444

```

2.0000	18.8000	3.1920	25.1273	-6.3273
2.0000	24.1200	3.1920	25.1273	-1.0073
3.0000	16.4400	3.1920	20.2005	-3.7605
3.0000	17.2200	3.1920	20.2005	-2.9805
7.0000	10.1400	3.1920	8.4379	1.7021
7.0000	10.3800	3.1920	8.4379	1.9421
10.0000	7.0800	3.1920	4.3842	2.6958
10.0000	7.2100	3.1920	4.3842	2.8258
14.0000	7.0900	3.1920	1.8313	5.2587
14.0000	5.1400	3.1920	1.8313	3.3087
28.0000	4.6200	3.1920	0.0863	4.5337
28.0000	6.5900	3.1920	0.0863	6.5037
56.0000	2.6400	3.1920	0.0002	2.6398
56.0000	2.8500	3.1920	0.0002	2.8498
100.0000	2.7200	3.1920	0.0000	2.7200
100.0000	2.7800	3.1920	0.0000	2.7800



11.2.1.2HS

```

# Trial      : Barmentsbeta
# File name  : Barmentsbeta IRLS HS   Beta.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:32
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See ts beta
# # Barmener See total system mit Isomeren Verhl. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Beta      :      39.01              0              Inf      False
k1    Beta      :       0.10              0              Inf      False
k2    Beta      :       0.01              0              Inf      False
tb    Beta      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      5.454      5.454
      Kinetic model :      HS      All

# -----
# Parameter estimation
# -----

Degrees of Freedom : 19
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Beta      :  40.499896  38.978629      42.021      0.776171      < 2e-16
k1    Beta      :   0.291185   0.253929      0.328      0.019009      1.90e-12
k2    Beta      :   0.019099   0.006258      0.032      0.006552      0.00444
tb    Beta      :   5.285730   4.295330      6.276      0.505315      1.27e-09

# -----
# DT50 and DT90 values
# -----

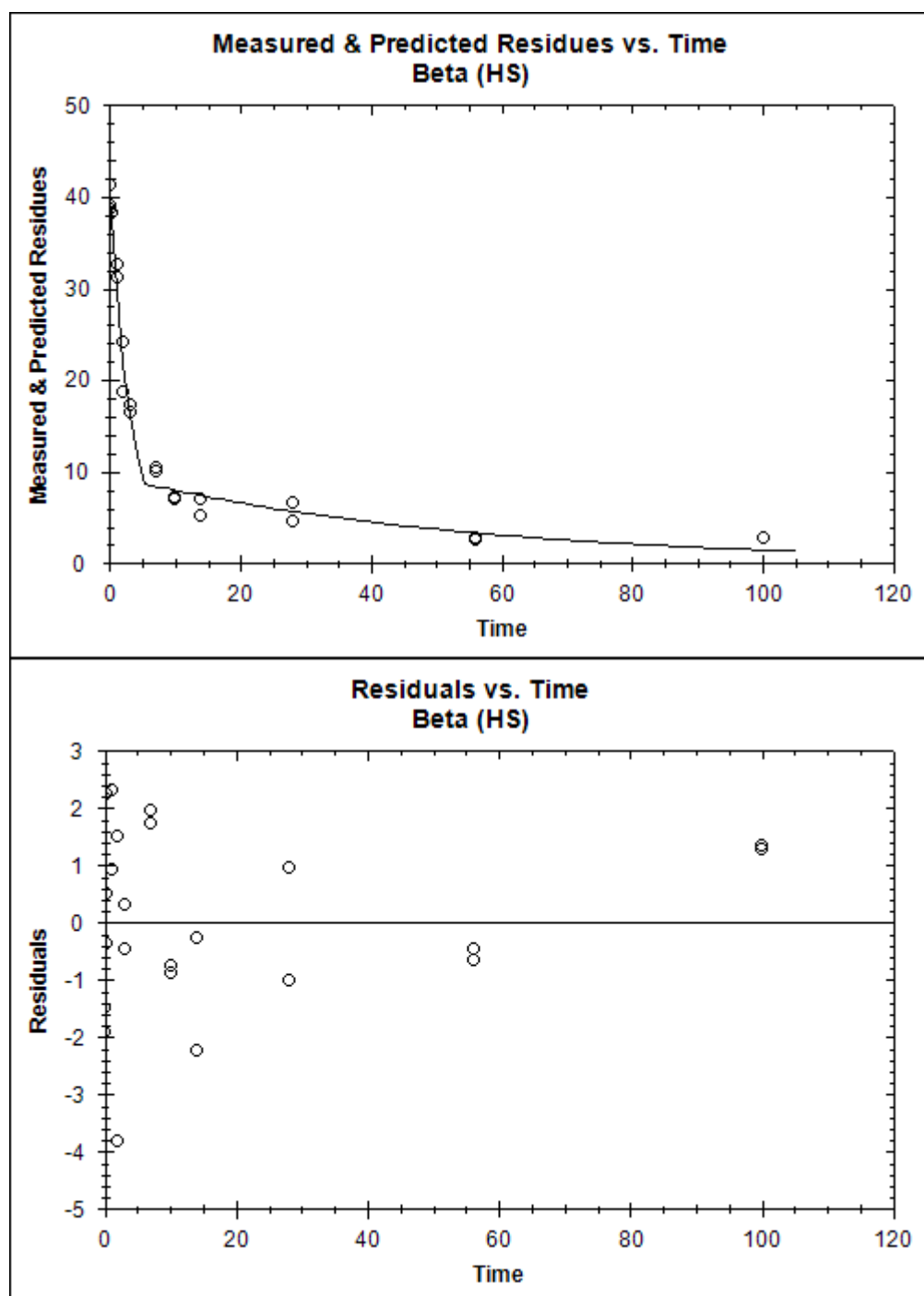
      DT50 :      2.3804
      DT90 :      45.260
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Beta
      time observed err-std predicted residual
0.0000  39.0100  1.5340  40.4999  -1.4899
0.0000  38.5900  1.5340  40.4999  -1.9099
0.1250  38.6900  1.5340  39.0523  -0.3623
0.1250  41.3200  1.5340  39.0523  2.2677
0.2500  38.1800  1.5340  37.6564  0.5236
0.2500      NA   1.5340  37.6564      NA
1.0000  31.2000  1.5340  30.2687  0.9313

```

1.0000	32.6000	1.5340	30.2687	2.3313
2.0000	18.8000	1.5340	22.6221	-3.8221
2.0000	24.1200	1.5340	22.6221	1.4979
3.0000	16.4400	1.5340	16.9073	-0.4673
3.0000	17.2200	1.5340	16.9073	0.3127
7.0000	10.1400	1.5340	8.4101	1.7299
7.0000	10.3800	1.5340	8.4101	1.9699
10.0000	7.0800	1.5340	7.9418	-0.8618
10.0000	7.2100	1.5340	7.9418	-0.7318
14.0000	7.0900	1.5340	7.3576	-0.2676
14.0000	5.1400	1.5340	7.3576	-2.2176
28.0000	4.6200	1.5340	5.6314	-1.0114
28.0000	6.5900	1.5340	5.6314	0.9586
56.0000	2.6400	1.5340	3.2989	-0.6589
56.0000	2.8500	1.5340	3.2989	-0.4489
100.0000	2.7200	1.5340	1.4237	1.2963
100.0000	2.7800	1.5340	1.4237	1.3563



11.2.1.3 FOMC

```

# Trial      : Barmentsbeta
# File name  : Barmentsbeta IRLS FOMC Beta.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:34
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See ts beta
# # Barmener See total system mit Isomeren Verhl. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Beta      :      39.01              0              Inf      False
alpha Beta      :       0.10              0              Inf      False
beta  Beta      :       0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Beta      All
Chi2Err% :      7.03      7.03
Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 20
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Beta      :      40.9979      38.8122      43.184      1.1152      < 2e-16
alpha Beta      :       0.9307       0.6573       1.204      0.1395      8.5e-07
beta  Beta      :       2.1972       1.0861       3.308      0.5669      0.00047

# -----
# DT50 and DT90 values
# -----

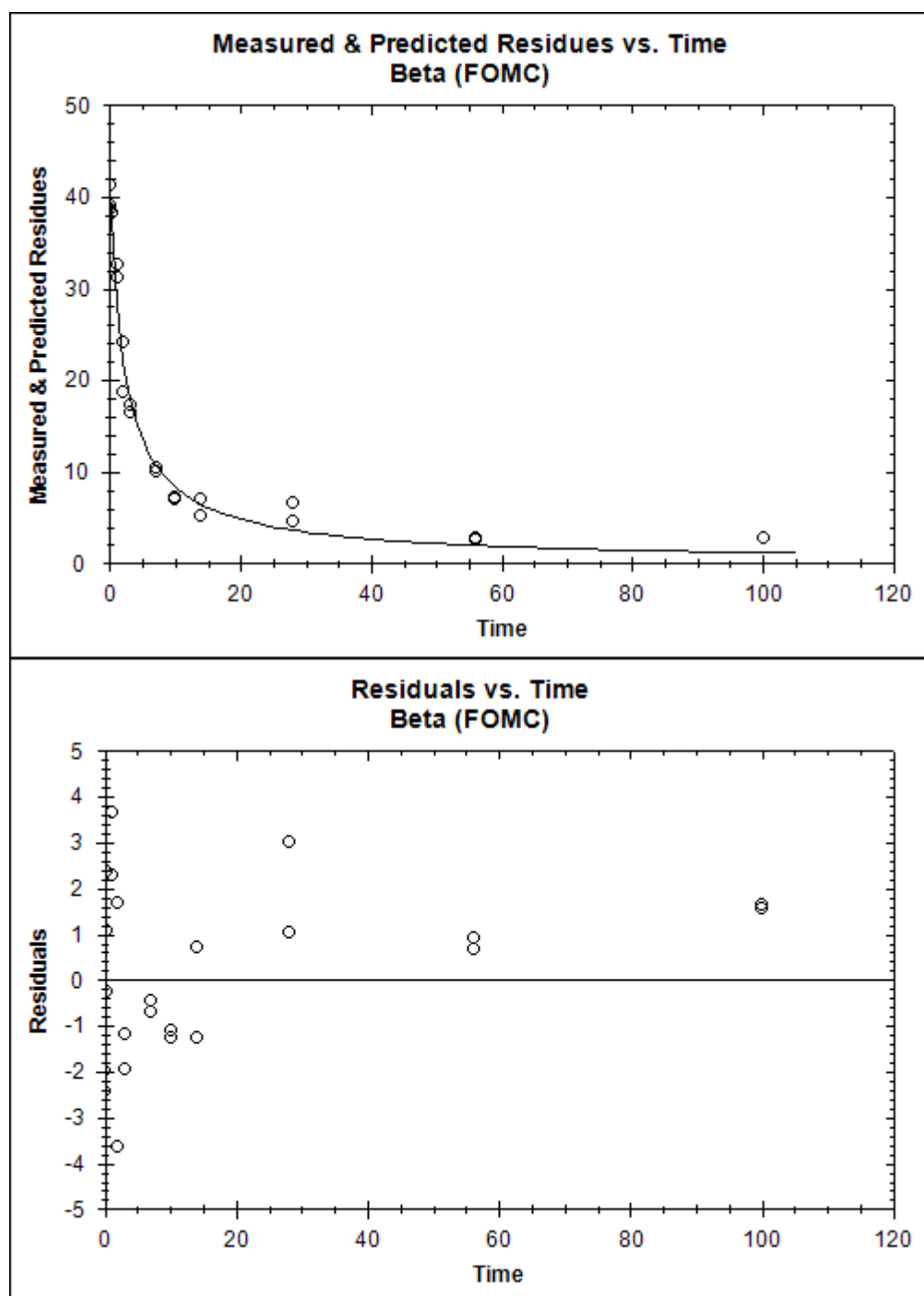
      Beta
DT50 :      2.4301
DT90 :      23.887
Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Beta
      time observed err-std predicted residual
0.0000 39.0100 1.8512 40.9979 -1.9879
0.0000 38.5900 1.8512 40.9979 -2.4079
0.1250 38.6900 1.8512 38.9402 -0.2502
0.1250 41.3200 1.8512 38.9402 2.3798
0.2500 38.1800 1.8512 37.0858 1.0942
0.2500      NA 1.8512 37.0858      NA
1.0000 31.2000 1.8512 28.9174 2.2826
1.0000 32.6000 1.8512 28.9174 3.6826
2.0000 18.8000 1.8512 22.4473 -3.6473

```

2.0000	24.1200	1.8512	22.4473	1.6727
3.0000	16.4400	1.8512	18.3989	-1.9589
3.0000	17.2200	1.8512	18.3989	-1.1789
7.0000	10.1400	1.8512	10.8167	-0.6767
7.0000	10.3800	1.8512	10.8167	-0.4367
10.0000	7.0800	1.8512	8.3175	-1.2375
10.0000	7.2100	1.8512	8.3175	-1.1075
14.0000	7.0900	1.8512	6.3878	0.7022
14.0000	5.1400	1.8512	6.3878	-1.2478
28.0000	4.6200	1.8512	3.5775	1.0425
28.0000	6.5900	1.8512	3.5775	3.0125
56.0000	2.6400	1.8512	1.9427	0.6973
56.0000	2.8500	1.8512	1.9427	0.9073
100.0000	2.7200	1.8512	1.1503	1.5697
100.0000	2.7800	1.8512	1.1503	1.6297



11.2.1.4 DFOP

```

# Trial      : Barmentsbeta
# File name  : Barmentsbeta IRLS DFOP Beta.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:32
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See ts beta
# # Barmener See total system mit Isomeren Verhl. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Beta      :      39.01              0              Inf      False
k1    Beta      :       0.10              0              Inf      False
k2    Beta      :       0.01              0              Inf      False
g     Beta      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              Beta      All
      Chi2Err% :      5.034      5.034
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 19
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Beta      :      40.572540      39.077649      42.067      0.762713      < 2e-16
k1    Beta      :       0.382638      0.312285      0.453      0.035895      9.3e-10
k2    Beta      :       0.012843      0.003065      0.023      0.004989      0.00929
g     Beta      :       0.814973      0.758733      0.871      0.028694      < 2e-16

# -----
# DT50 and DT90 values
# -----

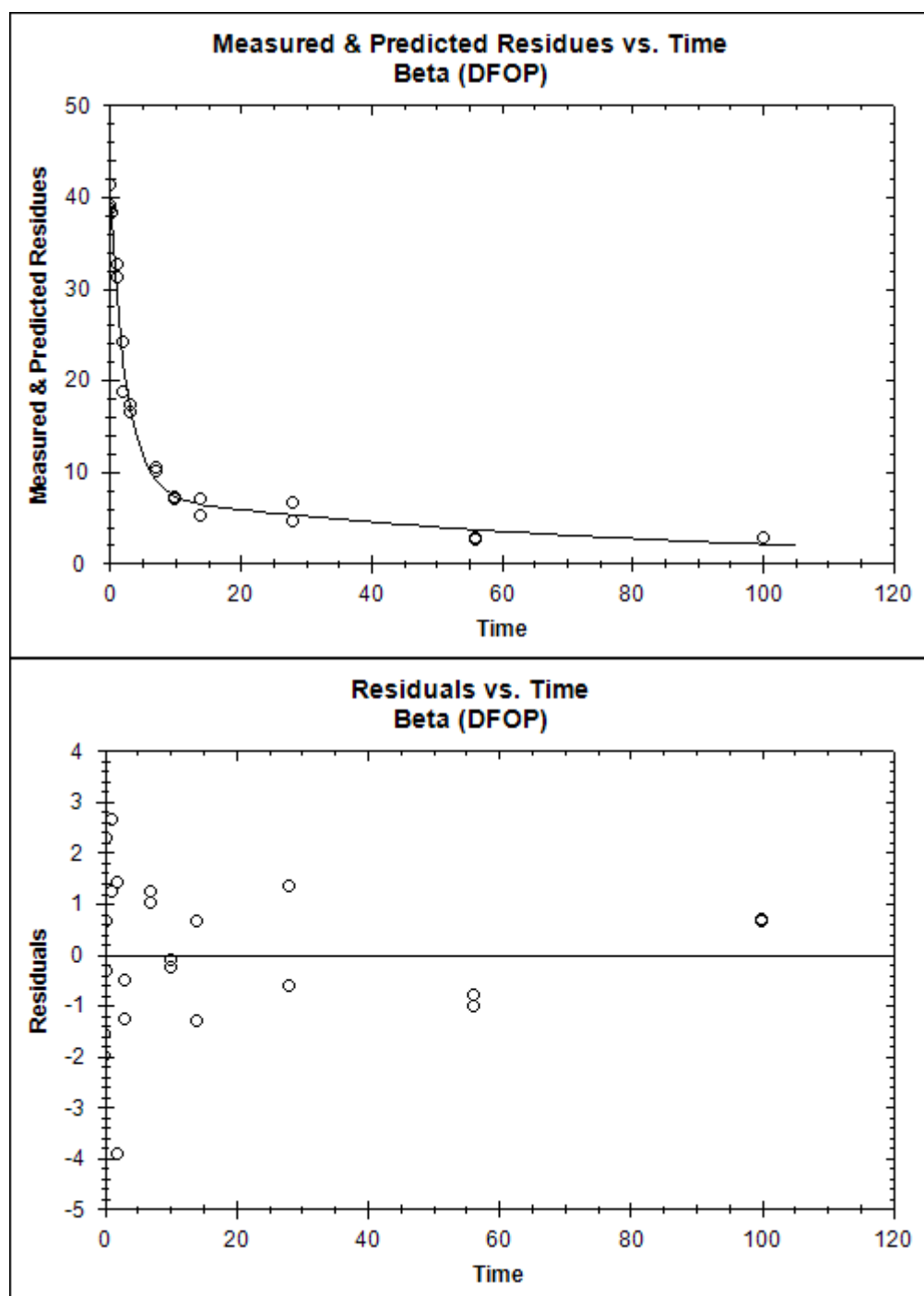
              Beta
      DT50 :       2.4376
      DT90 :       47.911
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Beta
      time observed err-std predicted residual
0.0000  39.0100  1.4642  40.5725  -1.5625
0.0000  38.5900  1.4642  40.5725  -1.9825
0.1250  38.6900  1.4642  39.0162  -0.3262
0.1250  41.3200  1.4642  39.0162  2.3038
0.2500  38.1800  1.4642  37.5320  0.6480
0.2500      NA  1.4642  37.5320      NA
1.0000  31.2000  1.4642  29.9639  1.2361

```

1.0000	32.6000	1.4642	29.9639	2.6361
2.0000	18.8000	1.4642	22.6989	-3.8989
2.0000	24.1200	1.4642	22.6989	1.4211
3.0000	16.4400	1.4642	17.7149	-1.2749
3.0000	17.2200	1.4642	17.7149	-0.4949
7.0000	10.1400	1.4642	9.1321	1.0079
7.0000	10.3800	1.4642	9.1321	1.2479
10.0000	7.0800	1.4642	7.3227	-0.2427
10.0000	7.2100	1.4642	7.3227	-0.1127
14.0000	7.0900	1.4642	6.4275	0.6625
14.0000	5.1400	1.4642	6.4275	-1.2875
28.0000	4.6200	1.4642	5.2402	-0.6202
28.0000	6.5900	1.4642	5.2402	1.3498
56.0000	2.6400	1.4642	3.6569	-1.0169
56.0000	2.8500	1.4642	3.6569	-0.8069
100.0000	2.7200	1.4642	2.0782	0.6418
100.0000	2.7800	1.4642	2.0782	0.7018



11.2.2 Genkel

11.2.2.1 SFO

```
# Trial      : Genkeltsbeta
# File name  : Genkeltsbeta IRLS SFO Beta.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:35
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system mit Isomeren Verh1. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Beta      :      41.42              0              Inf      False
k      Beta      :      0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Beta      All
Chi2Err% :      21.08      21.08
Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 22
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Beta      :      32.4994      -842.7151      907.71      446.5462      0.471
k      Beta      :      0.1039      -12.1868      12.39      6.2709      0.493

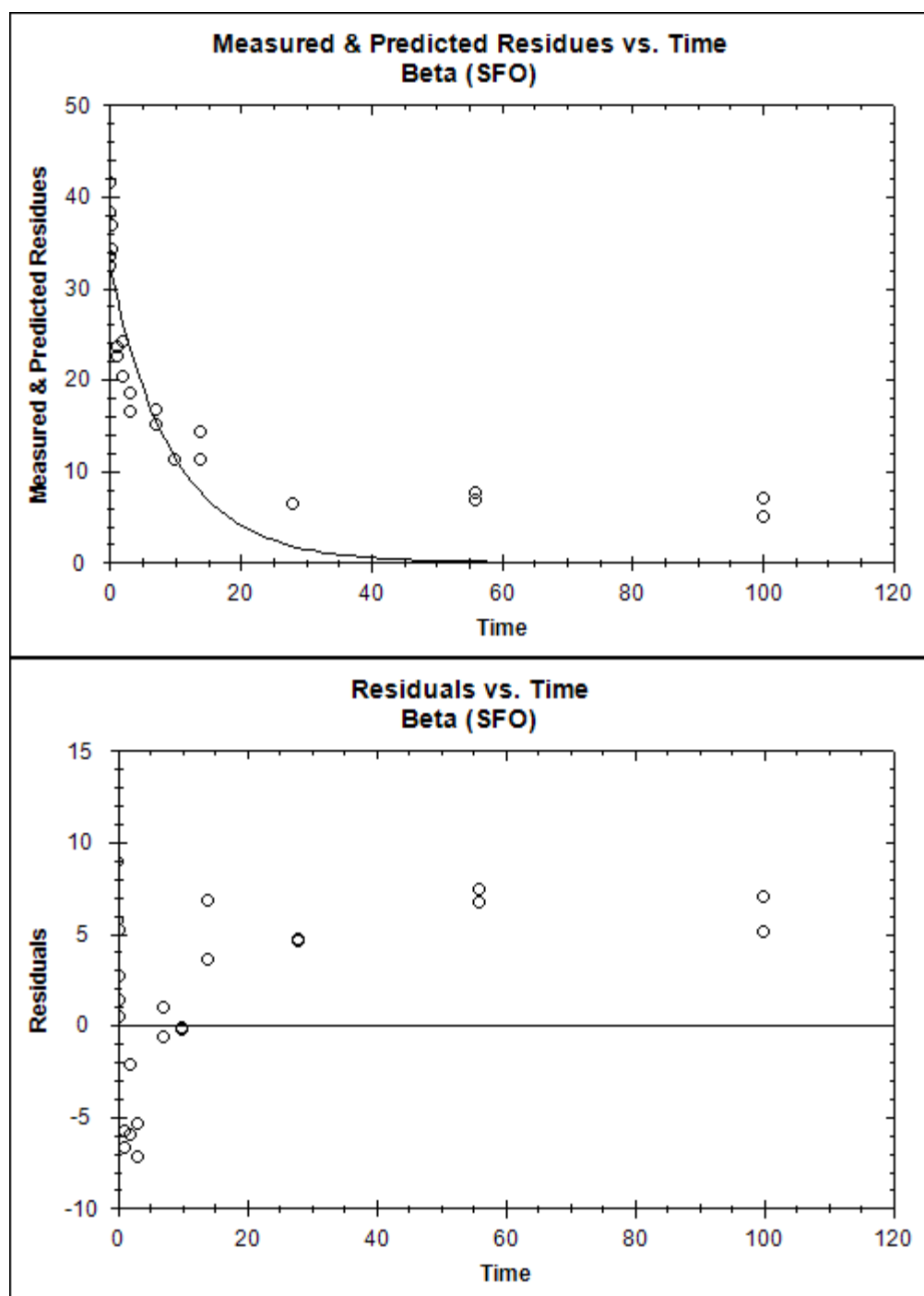
# -----
# DT50 and DT90 values
# -----

      Beta
DT50 :      6.6701
DT90 :      22.158
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment Beta
time observed err-std predicted residual
0.0000 41.4200 5.1204 32.4994 8.9206
0.0000 38.2200 5.1204 32.4994 5.7206
0.1250 32.5100 5.1204 32.0800 0.4300
0.1250 33.4800 5.1204 32.0800 1.4000
0.2500 36.9200 5.1204 31.6659 5.2541
0.2500 34.3200 5.1204 31.6659 2.6541
1.0000 22.5700 5.1204 29.2917 -6.7217
1.0000 23.5100 5.1204 29.2917 -5.7817
2.0000 20.3800 5.1204 26.4006 -6.0206
```

2.0000	24.2500	5.1204	26.4006	-2.1506
3.0000	18.4400	5.1204	23.7948	-5.3548
3.0000	16.5900	5.1204	23.7948	-7.2048
7.0000	16.6500	5.1204	15.7021	0.9479
7.0000	15.0200	5.1204	15.7021	-0.6821
10.0000	11.3200	5.1204	11.4965	-0.1765
10.0000	11.2200	5.1204	11.4965	-0.2765
14.0000	14.3800	5.1204	7.5865	6.7935
14.0000	11.2200	5.1204	7.5865	3.6335
28.0000	6.4700	5.1204	1.7709	4.6991
28.0000	6.3900	5.1204	1.7709	4.6191
56.0000	6.8300	5.1204	0.0965	6.7335
56.0000	7.5400	5.1204	0.0965	7.4435
100.0000	5.0700	5.1204	0.0010	5.0690
100.0000	7.0300	5.1204	0.0010	7.0290



11.2.2.2HS

```

# Trial      : Genkeltsbeta
# File name  : Genkeltsbeta IRLS HS   Beta.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:35
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system mit Isomeren Verh1. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Beta      :      41.42              0              Inf      False
k1    Beta      :       0.10              0              Inf      False
k2    Beta      :       0.01              0              Inf      False
tb    Beta      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Beta      All
Chi2Err% :      11.15      11.15
Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 20
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Beta      :      36.659569      34.172847      39.146      1.268759      < 2e-16
k1    Beta      :       0.277836      0.207750      0.348      0.035759      9.12e-08
k2    Beta      :       0.012412      0.002878      0.022      0.004865      0.0095
tb    Beta      :       3.552063      2.390528      4.714      0.592631      3.67e-06

# -----
# DT50 and DT90 values
# -----

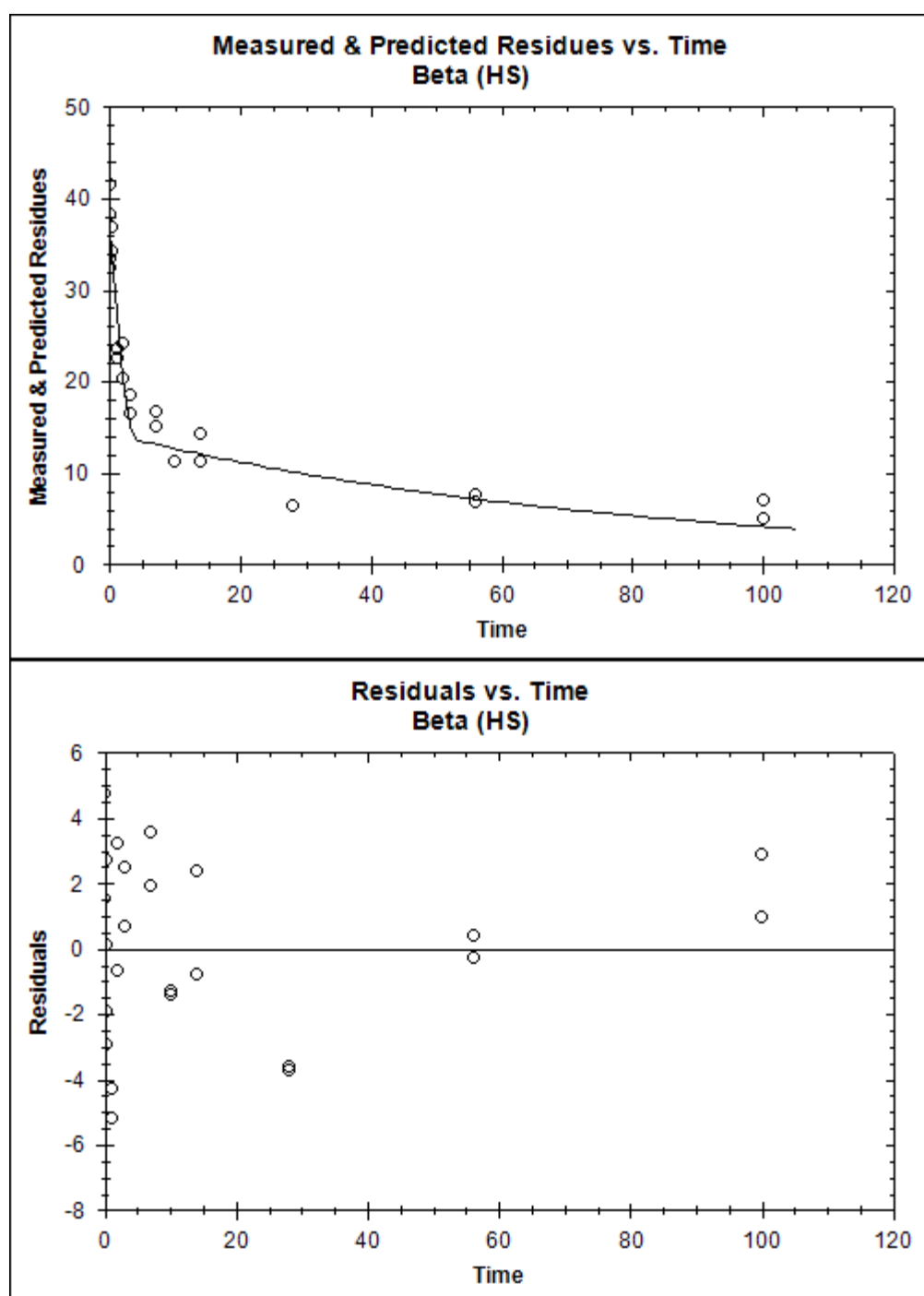
      Beta
DT50 :      2.4948
DT90 :      109.55
Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

Compartment Beta
time observed err-std predicted residual
0.0000 41.4200 2.6605 36.6596 4.7604
0.0000 38.2200 2.6605 36.6596 1.5604
0.1250 32.5100 2.6605 35.4083 -2.8983
0.1250 33.4800 2.6605 35.4083 -1.9283
0.2500 36.9200 2.6605 34.1997 2.7203
0.2500 34.3200 2.6605 34.1997 0.1203
1.0000 22.5700 2.6605 27.7667 -5.1967

```

1.0000	23.5100	2.6605	27.7667	-4.2567
2.0000	20.3800	2.6605	21.0311	-0.6511
2.0000	24.2500	2.6605	21.0311	3.2189
3.0000	18.4400	2.6605	15.9294	2.5106
3.0000	16.5900	2.6605	15.9294	0.6606
7.0000	16.6500	2.6605	13.0918	3.5582
7.0000	15.0200	2.6605	13.0918	1.9282
10.0000	11.3200	2.6605	12.6133	-1.2933
10.0000	11.2200	2.6605	12.6133	-1.3933
14.0000	14.3800	2.6605	12.0023	2.3777
14.0000	11.2200	2.6605	12.0023	-0.7823
28.0000	6.4700	2.6605	10.0878	-3.6178
28.0000	6.3900	2.6605	10.0878	-3.6978
56.0000	6.8300	2.6605	7.1262	-0.2962
56.0000	7.5400	2.6605	7.1262	0.4138
100.0000	5.0700	2.6605	4.1273	0.9427
100.0000	7.0300	2.6605	4.1273	2.9027



11.2.2.3 FOMC

```

# Trial      : Genkeltsbeta
# File name  : Genkeltsbeta IRLS FOMC Beta.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:35
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system mit Isomeren Verh1. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Beta      :      41.42              0              Inf      False
alpha Beta      :       0.10              0              Inf      False
beta  Beta      :       0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Beta      All
      Chi2Err% :      7.448      7.448
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 21
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Beta      :      39.22903      36.61789      41.840      1.33224      < 2e-16
alpha Beta      :       0.34531       0.27519       0.415      0.03578      1.79e-09
beta  Beta      :       0.37586       0.10426       0.647      0.13857      0.00652

# -----
# DT50 and DT90 values
# -----

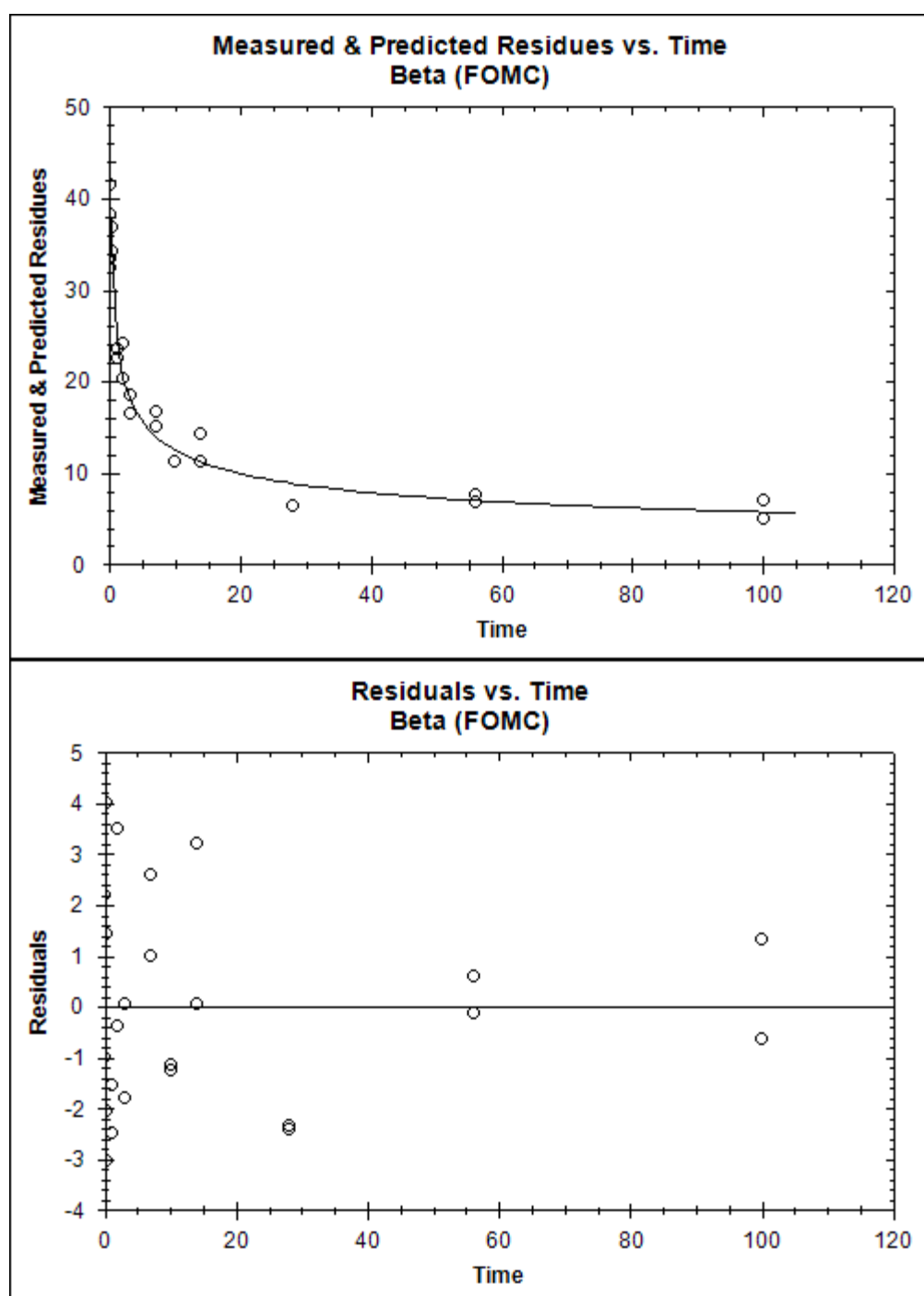
      Beta
      DT50 :      2.4217
      DT90 :      295.38
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Beta
      time observed err-std predicted residual
0.0000 41.4200 2.0063 39.2290 2.1910
0.0000 38.2200 2.0063 39.2290 -1.0090
0.1250 32.5100 2.0063 35.5263 -3.0163
0.1250 33.4800 2.0063 35.5263 -2.0463
0.2500 36.9200 2.0063 32.8955 4.0245
0.2500 34.3200 2.0063 32.8955 1.4245
1.0000 22.5700 2.0063 25.0614 -2.4914
1.0000 23.5100 2.0063 25.0614 -1.5514
2.0000 20.3800 2.0063 20.7530 -0.3730

```

2.0000	24.2500	2.0063	20.7530	3.4970
3.0000	18.4400	2.0063	18.3822	0.0578
3.0000	16.5900	2.0063	18.3822	-1.7922
7.0000	16.6500	2.0063	14.0342	2.6158
7.0000	15.0200	2.0063	14.0342	0.9858
10.0000	11.3200	2.0063	12.4741	-1.1541
10.0000	11.2200	2.0063	12.4741	-1.2541
14.0000	14.3800	2.0063	11.1457	3.2343
14.0000	11.2200	2.0063	11.1457	0.0743
28.0000	6.4700	2.0063	8.8132	-2.3432
28.0000	6.3900	2.0063	8.8132	-2.4232
56.0000	6.8300	2.0063	6.9531	-0.1231
56.0000	7.5400	2.0063	6.9531	0.5869
100.0000	5.0700	2.0063	5.6972	-0.6272
100.0000	7.0300	2.0063	5.6972	1.3328



11.2.2.4 DFOP

```

# Trial      : Genkeltsbeta
# File name  : Genkeltsbeta IRLS DFOP Beta.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Genkel_ts_beta
# Created    : on 20 Sep 2013
#            : at 06:35
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel total system
# # Genkel total system mit Isomeren Verh1. aus Wasser+sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Beta      :      41.42              0              Inf      False
k1    Beta      :       0.10              0              Inf      False
k2    Beta      :       0.01              0              Inf      False
g     Beta      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

      Beta      All
      Chi2Err% :      9.828      9.828
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 20
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Beta      :      37.755357      35.174893      40.336      1.316588      < 2e-16
k1    Beta      :       0.692851      0.334047      1.052      0.183066      0.000582
k2    Beta      :       0.013058      0.003023      0.023      0.005120      0.009532
g     Beta      :       0.612868      0.519837      0.706      0.047466      1.84e-11

# -----
# DT50 and DT90 values
# -----

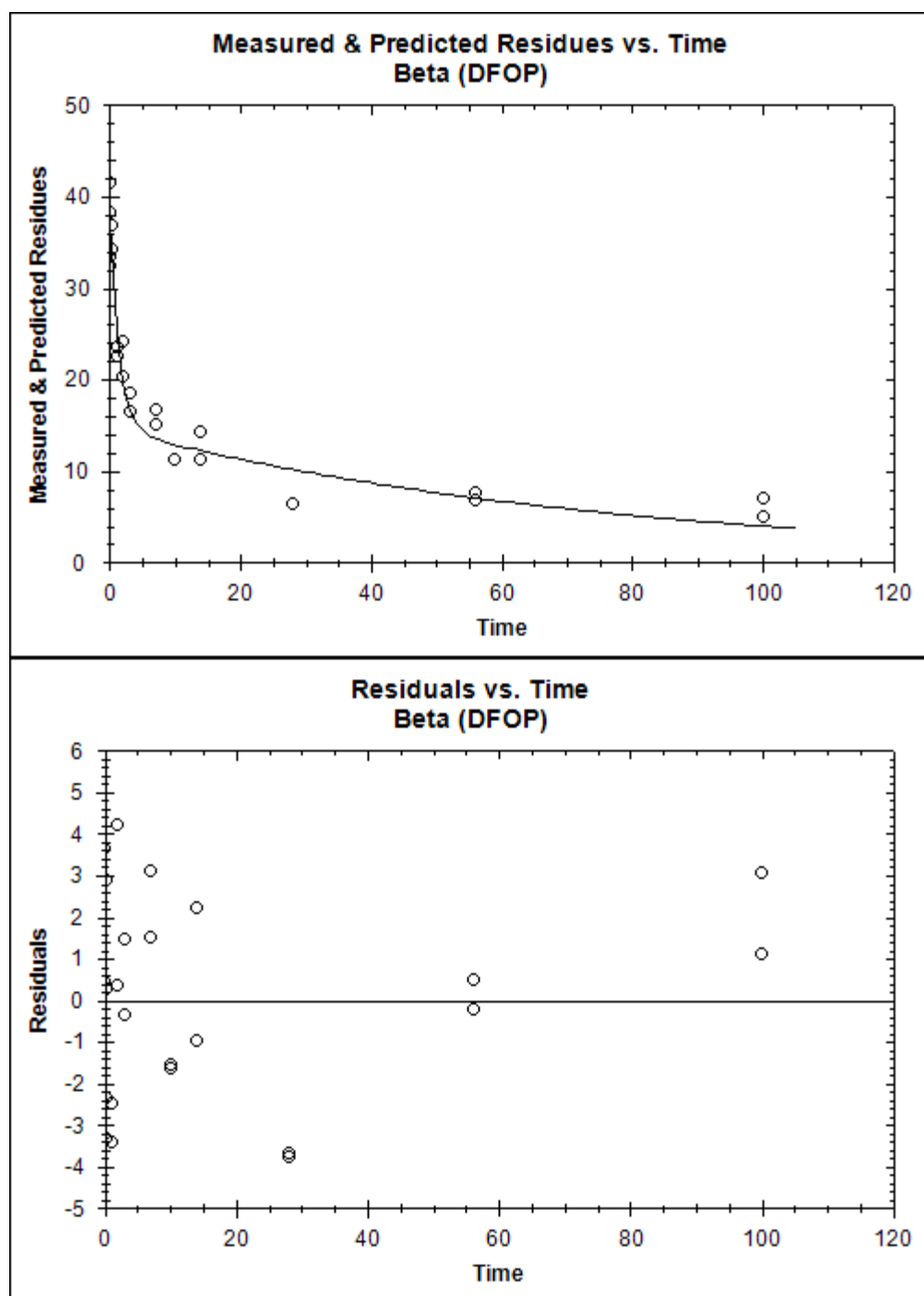
      Beta
      DT50 :       2.3024
      DT90 :      103.66
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Beta
      time observed err-std predicted residual
0.0000  41.4200  2.3979  37.7554  3.6646
0.0000  38.2200  2.3979  37.7554  0.4646
0.1250  32.5100  2.3979  35.8119 -3.3019
0.1250  33.4800  2.3979  35.8119 -2.3319
0.2500  36.9200  2.3979  34.0277  2.8923
0.2500  34.3200  2.3979  34.0277  0.2923
1.0000  22.5700  2.3979  25.9997 -3.4297

```


1.0000	23.5100	2.3979	25.9997	-2.4897
2.0000	20.3800	2.3979	20.0277	0.3523
2.0000	24.2500	2.3979	20.0277	4.2223
3.0000	18.4400	2.3979	16.9498	1.4902
3.0000	16.5900	2.3979	16.9498	-0.3598
7.0000	16.6500	2.3979	13.5207	3.1293
7.0000	15.0200	2.3979	13.5207	1.4993
10.0000	11.3200	2.3979	12.8498	-1.5298
10.0000	11.2200	2.3979	12.8498	-1.6298
14.0000	14.3800	2.3979	12.1758	2.2042
14.0000	11.2200	2.3979	12.1758	-0.9558
28.0000	6.4700	2.3979	10.1404	-3.6704
28.0000	6.3900	2.3979	10.1404	-3.7504
56.0000	6.8300	2.3979	7.0351	-0.2051
56.0000	7.5400	2.3979	7.0351	0.5049
100.0000	5.0700	2.3979	3.9605	1.1095
100.0000	7.0300	2.3979	3.9605	3.0695



11.3 FPB-Aldehyd (FCR 1260) Degradation Total System (Decline Fit)

11.3.1 Ijzendoorn

11.3.1.1 SFO

```

# Trial      : IjzendoornntsFCR1260
# File name  : IjzendoornntsFCR1260 IRLS SFO  FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:16
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      15.70              0              Inf      False
k      FCR1260      :       0.01              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      15.08      15.08
Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 8
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FCR1260      :      15.64111      14.00483      17.277      0.83485
3.4e-08
k      FCR1260      :       0.21008      0.11754      0.303      0.04721
0.00107

# -----
# DT50 and DT90 values
# -----

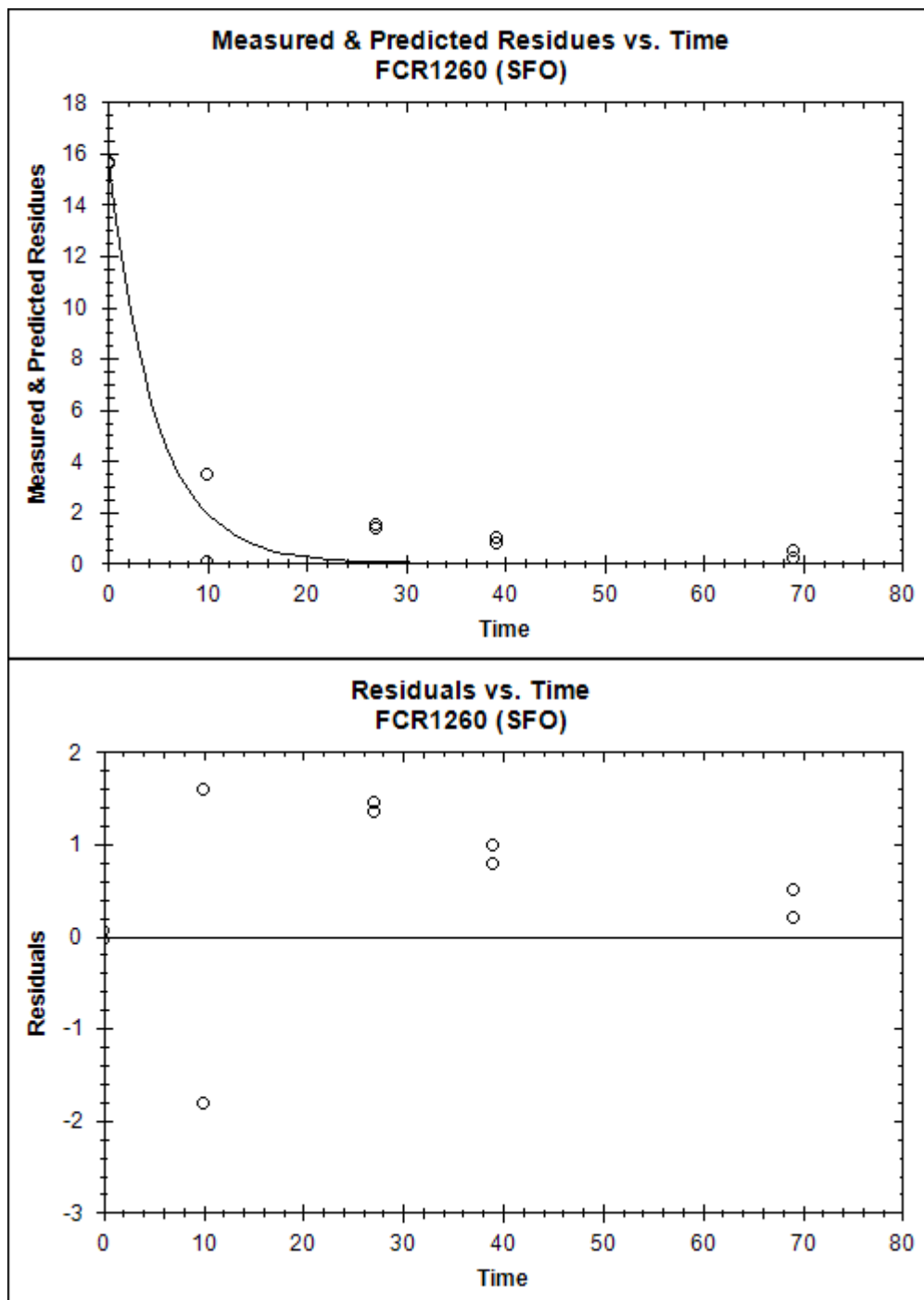
      FCR1260
DT50 :      3.2995
DT90 :      10.961
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  15.7000  1.0784  15.6411  0.0589
0.0000  15.6000  1.0784  15.6411 -0.0411
10.0000  0.1000  1.0784   1.9139 -1.8139

```

10.0000	3.5000	1.0784	1.9139	1.5861
27.0000	1.5000	1.0784	0.0538	1.4462
27.0000	1.4000	1.0784	0.0538	1.3462
39.0000	0.8000	1.0784	0.0043	0.7957
39.0000	1.0000	1.0784	0.0043	0.9957
69.0000	0.2000	1.0784	0.0000	0.2000
69.0000	0.5000	1.0784	0.0000	0.5000



11.3.1.2HS

```

# Trial      : IjzendoornntsFCR1260
# File name  : IjzendoornntsFCR1260 IRLS HS   FCR1260.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 10:36
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      15.70              0              Inf      False
k1    FCR1260      :       0.10              0              Inf      False
k2    FCR1260      :       0.01              0              Inf      False
tb    FCR1260      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
      Chi2Err% :      3.074      3.074
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260      :      15.64999      14.27506      17.025      0.70151      2.65e-07
k1    FCR1260      :       0.26920       0.01661       0.522      0.12887      0.0409
k2    FCR1260      :       0.02385      -0.01163       0.059      0.01810      0.1179
tb    FCR1260      :       7.66101      -0.87909      16.201      4.35727      0.0646

# -----
# DT50 and DT90 values
# -----

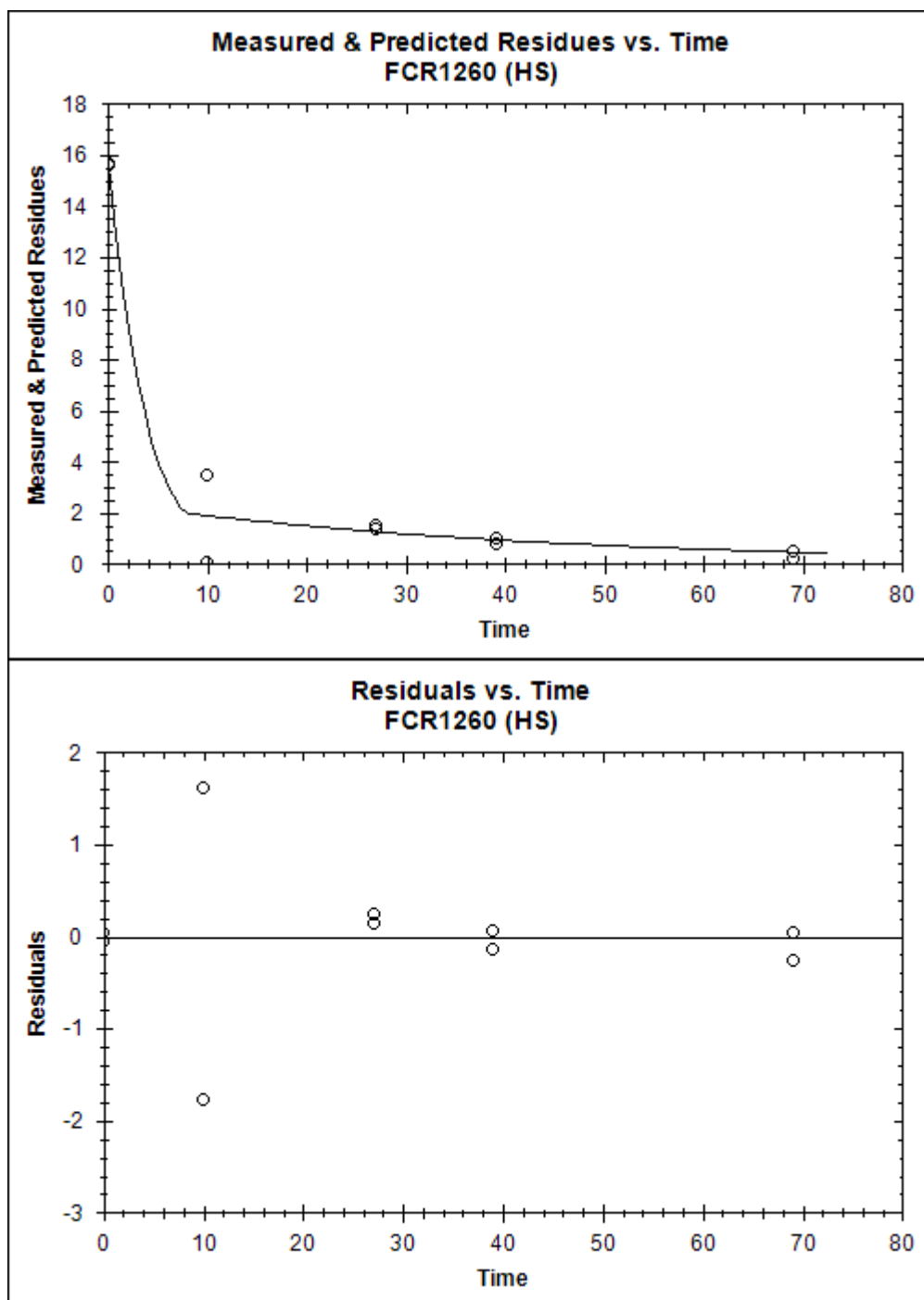
      FCR1260
      DT50 :       2.5748
      DT90 :       17.732
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  15.7000  0.7728  15.6500  0.0500
0.0000  15.6000  0.7728  15.6500 -0.0500
10.0000  0.1000  0.7728   1.8819 -1.7819
10.0000  3.5000  0.7728   1.8819  1.6181
27.0000  1.5000  0.7728   1.2546  0.2454
27.0000  1.4000  0.7728   1.2546  0.1454
39.0000  0.8000  0.7728   0.9424 -0.1424

```

39.0000	1.0000	0.7728	0.9424	0.0576
69.0000	0.2000	0.7728	0.4607	-0.2607
69.0000	0.5000	0.7728	0.4607	0.0393



11.3.1.3FOMC

```

# Trial      : IjzendoornntsFCR1260
# File name  : IjzendoornntsFCR1260 IRLS FOMC FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 10:36
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      15.7              0              Inf      False
alpha FCR1260      :       0.1              0              Inf      False
beta  FCR1260      :       0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      4.803      4.803
Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260      :      15.6499      14.3439      16.956      0.6663      3.22e-08
alpha FCR1260      :       0.5605      -0.2703      1.391      0.4239      0.114
beta  FCR1260      :       0.2385      -1.2879      1.765      0.7788      0.384

# -----
# DT50 and DT90 values
# -----

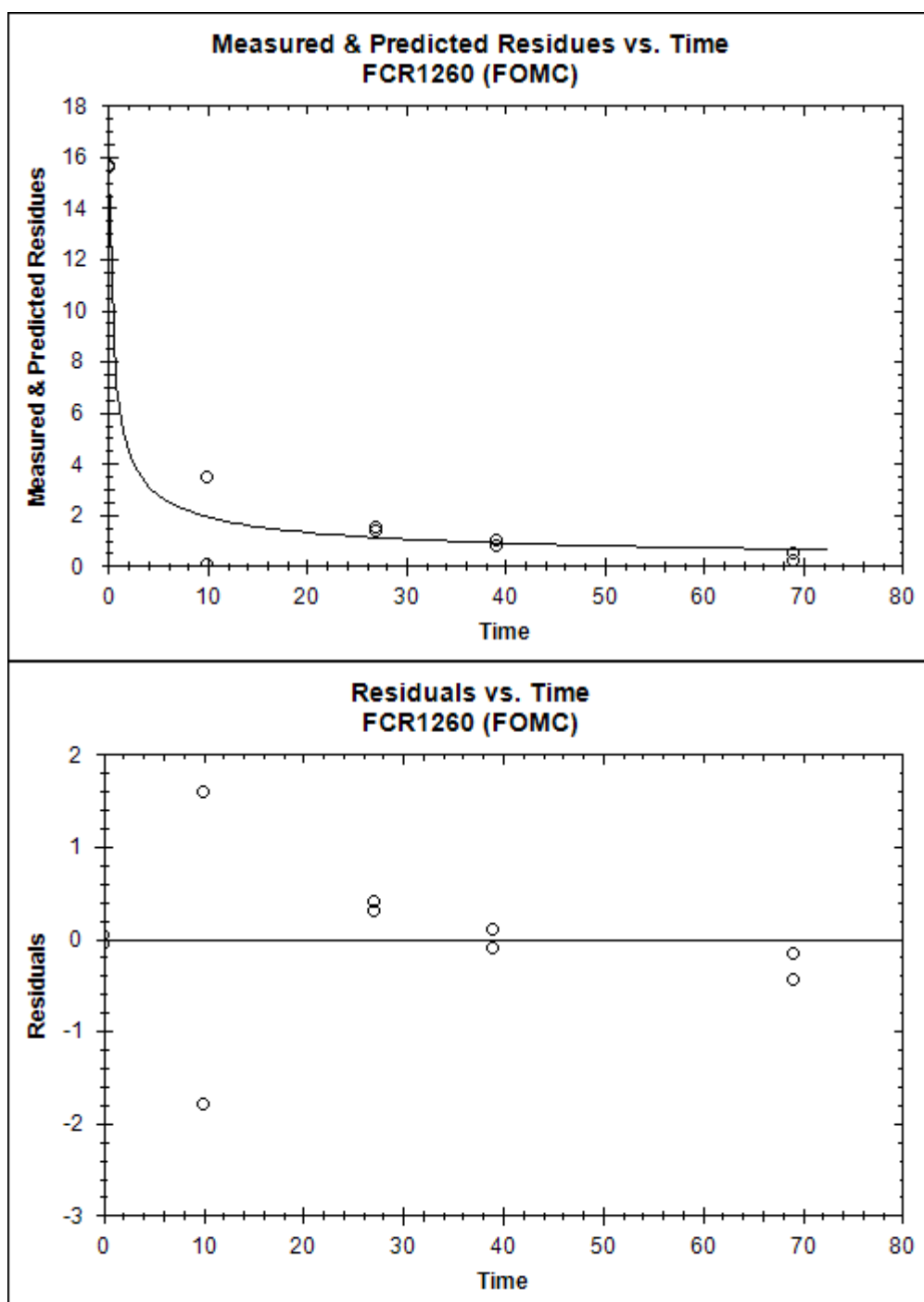
      FCR1260
DT50 :       0.5828
DT90 :      14.265
Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  15.7000  0.7940  15.6499  0.0501
0.0000  15.6000  0.7940  15.6499 -0.0499
10.0000  0.1000  0.7940  1.9023 -1.8023
10.0000  3.5000  0.7940  1.9023  1.5977
27.0000  1.5000  0.7940  1.0992  0.4008
27.0000  1.4000  0.7940  1.0992  0.3008
39.0000  0.8000  0.7940  0.8958 -0.0958
39.0000  1.0000  0.7940  0.8958  0.1042
69.0000  0.2000  0.7940  0.6516 -0.4516

```

69.0000 0.5000 0.7940 0.6516 -0.1516



11.3.1.4DFOP

```

# Trial      : IjzendoornntsFCR1260
# File name  : IjzendoornntsFCR1260 IRLS DFOP FCR1260.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 10:36
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      15.70              0              Inf      False
k1    FCR1260      :       0.10              0              Inf      False
k2    FCR1260      :       0.01              0              Inf      False
g     FCR1260      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      3.074      3.074
Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260      :      15.64997      14.49203      16.808      0.59080      9.55e-08
k1    FCR1260      :       1.39916     -70.32223      73.121      36.59322      0.485
k2    FCR1260      :       0.02385     -0.01131       0.059      0.01794      0.116
g     FCR1260      :       0.84736       0.70443       0.990      0.07293      1.22e-05

# -----
# DT50 and DT90 values
# -----

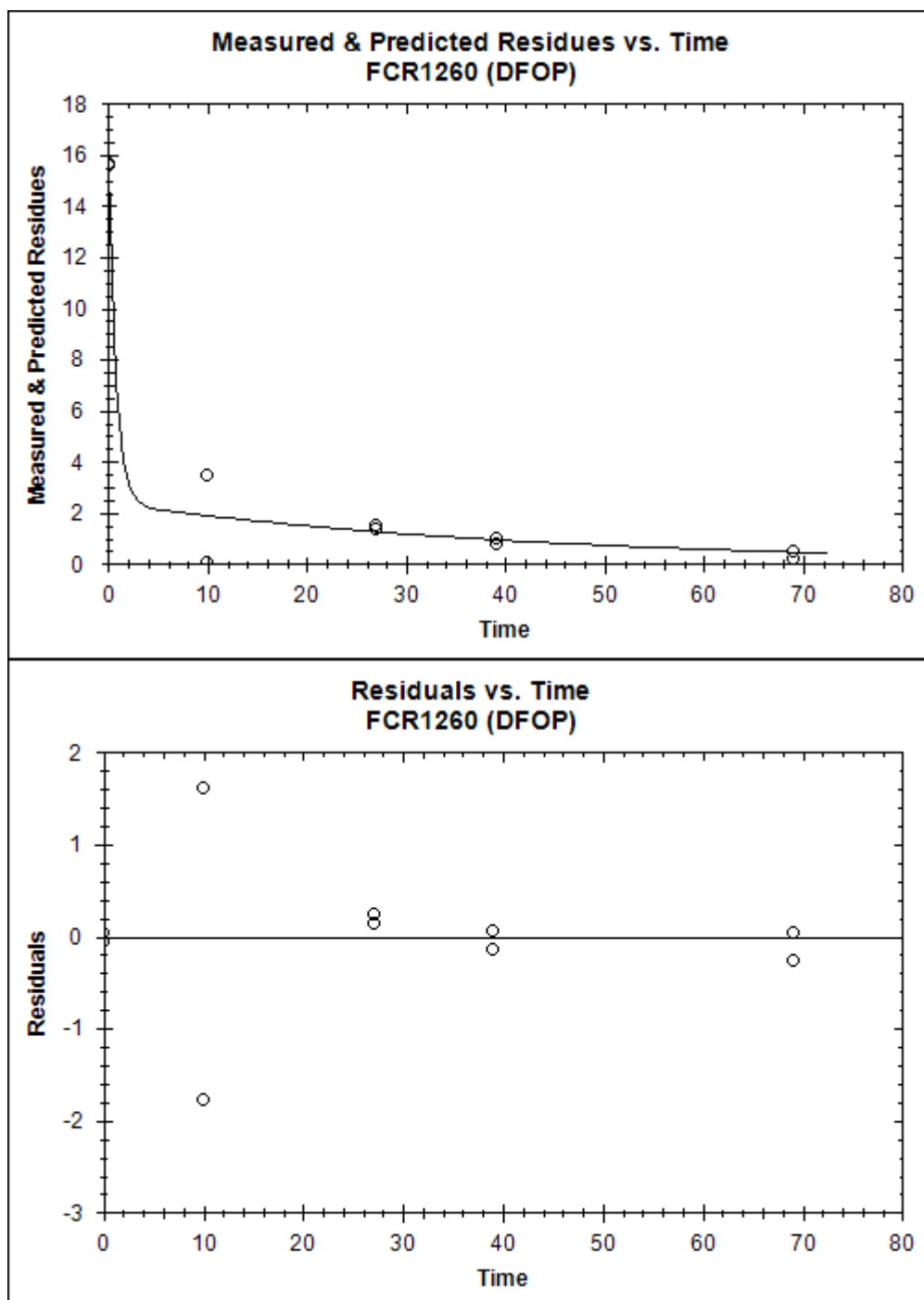
      FCR1260
DT50 :       0.6327
DT90 :       17.732
Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  15.7000  0.7728  15.6500  0.0500
0.0000  15.6000  0.7728  15.6500 -0.0500
10.0000  0.1000  0.7728   1.8819 -1.7819
10.0000  3.5000  0.7728   1.8819  1.6181
27.0000  1.5000  0.7728   1.2546  0.2454
27.0000  1.4000  0.7728   1.2546  0.1454
39.0000  0.8000  0.7728   0.9424 -0.1424

```

39.0000	1.0000	0.7728	0.9424	0.0576
69.0000	0.2000	0.7728	0.4608	-0.2608
69.0000	0.5000	0.7728	0.4608	0.0392



11.3.2 Lienden

11.3.2.1 SFO

```
# Trial      : LiendentsFCR1260
# File name  : LiendentsFCR1260 IRLS SFO  FCR1260.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:43
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      13.0              0              Inf      False
k      FCR1260      :       0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
      Chi2Err% :      23.09      23.09
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

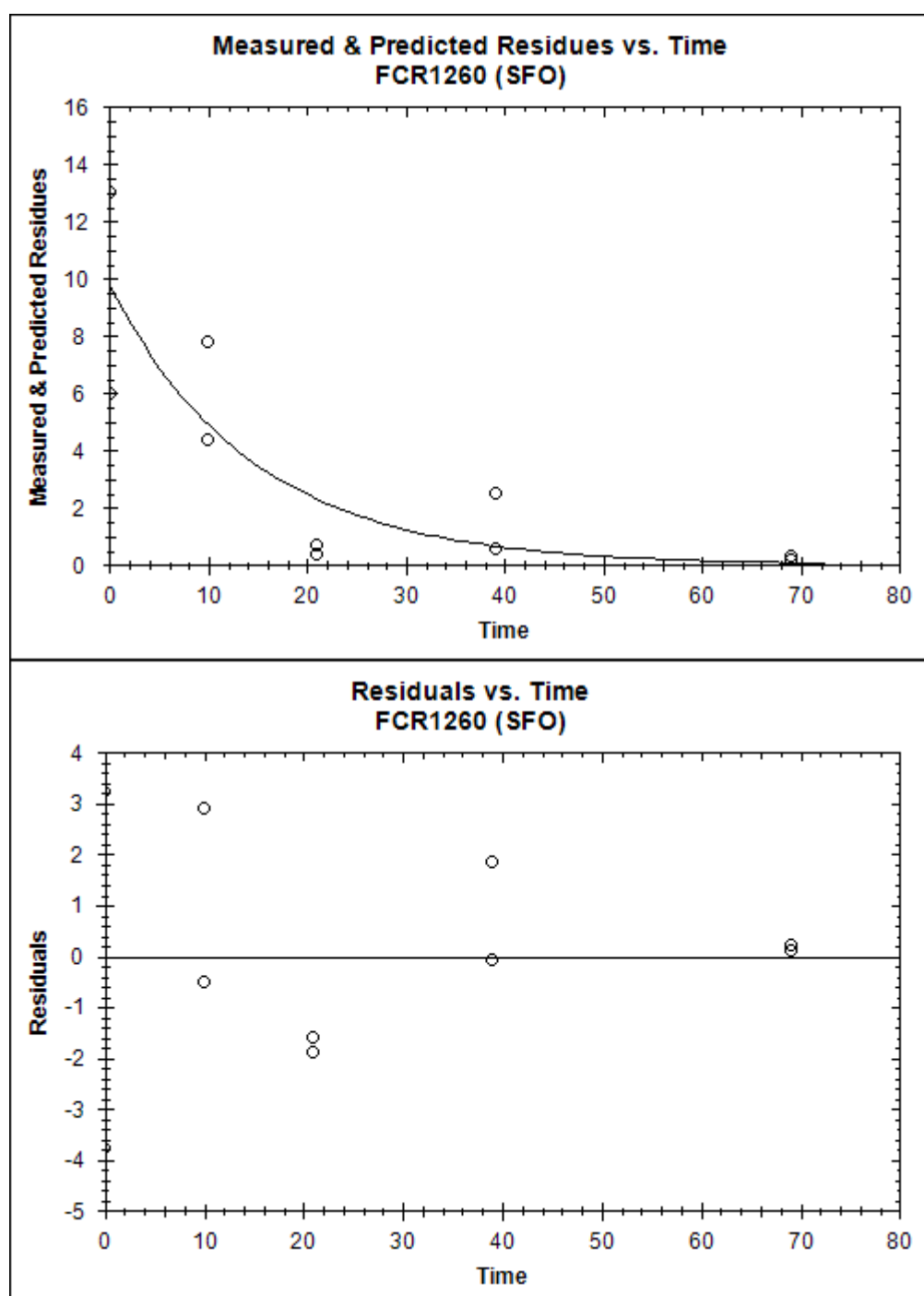
Degrees of Freedom : 8
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260      :      9.76320      6.59919      12.927      1.61432      0.000153
k      FCR1260      :      0.06919      0.02155      0.117      0.02431      0.010796

# -----
# DT50 and DT90 values
# -----

      FCR1260
      DT50 :      10.018
      DT90 :      33.278
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  13.0000  2.0706  9.7632  3.2368
0.0000  6.0000  2.0706  9.7632 -3.7632
10.0000  7.8000  2.0706  4.8875  2.9125
10.0000  4.4000  2.0706  4.8875 -0.4875
21.0000  0.7000  2.0706  2.2832 -1.5832
21.0000  0.4000  2.0706  2.2832 -1.8832
39.0000  2.5000  2.0706  0.6571  1.8429
39.0000  0.6000  2.0706  0.6571 -0.0571
69.0000  0.3000  2.0706  0.0824  0.2176
69.0000  0.2000  2.0706  0.0824  0.1176
```



11.3.2.2HS

```

# Trial      : LiendentsFCR1260
# File name  : LiendentsFCR1260 IRLS HS   FCR1260.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:44
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      13.00           0           Inf      False
k1    FCR1260      :       0.10           0           Inf      False
k2    FCR1260      :       0.01           0           Inf      False
tb    FCR1260      :       3.00           0           Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      22.12      22.12
Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FCR1260      :      9.50013      6.66092      12.339      1.44861
0.000301
k1    FCR1260      :      0.04413     -0.01446      0.103      0.02989
0.095177
k2    FCR1260      :      0.20272     -0.36870      0.774      0.29154
0.256432
tb    FCR1260      :      9.98190      4.85178     15.112      2.61746
0.004413

# -----
# DT50 and DT90 values
# -----

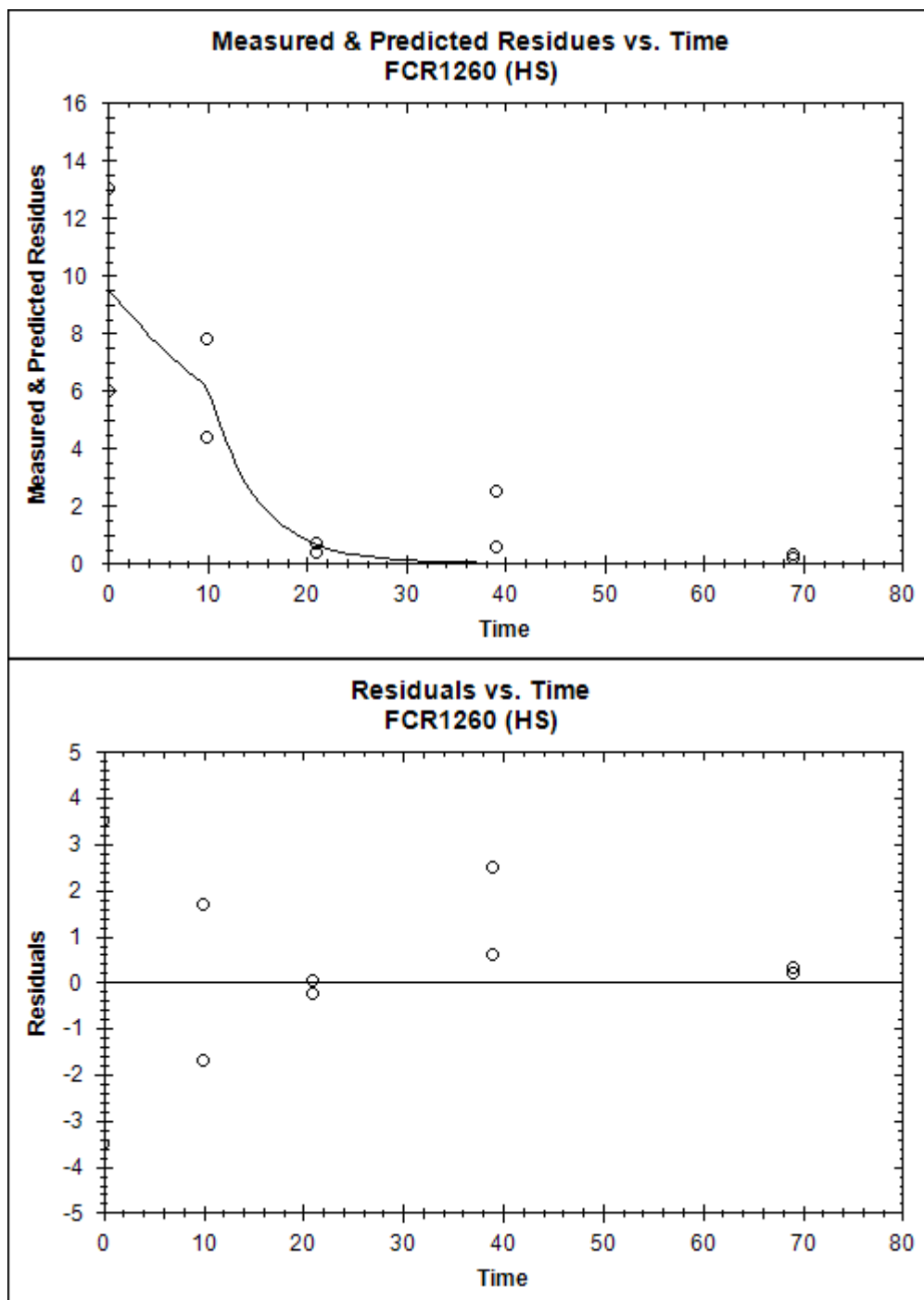
      FCR1260
DT50 :      11.228
DT90 :      19.167
Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  13.0000  1.9231   9.5001  3.4999
0.0000   6.0000  1.9231   9.5001 -3.5001

```

10.0000	7.8000	1.9231	6.0930	1.7070
10.0000	4.4000	1.9231	6.0930	-1.6930
21.0000	0.7000	1.9231	0.6552	0.0448
21.0000	0.4000	1.9231	0.6552	-0.2552
39.0000	2.5000	1.9231	0.0170	2.4830
39.0000	0.6000	1.9231	0.0170	0.5830
69.0000	0.3000	1.9231	0.0000	0.3000
69.0000	0.2000	1.9231	0.0000	0.2000



11.3.2.3 FOMC

```

# Trial      : LiendentsFCR1260
# File name  : LiendentsFCR1260 IRLS FOMC FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:44
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      13.0           0           Inf      False
alpha FCR1260      :       0.1           0           Inf      False
beta  FCR1260      :       0.1           0           Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      26.77      26.77
Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260 :       9.924       6.961      12.89       1.512      0.000157
alpha FCR1260 :      734.419     -7014.732     8483.57     3953.721     0.428953
beta  FCR1260 :     9728.101    -93013.462    112469.66    52420.128     0.429019

# -----
# DT50 and DT90 values
# -----

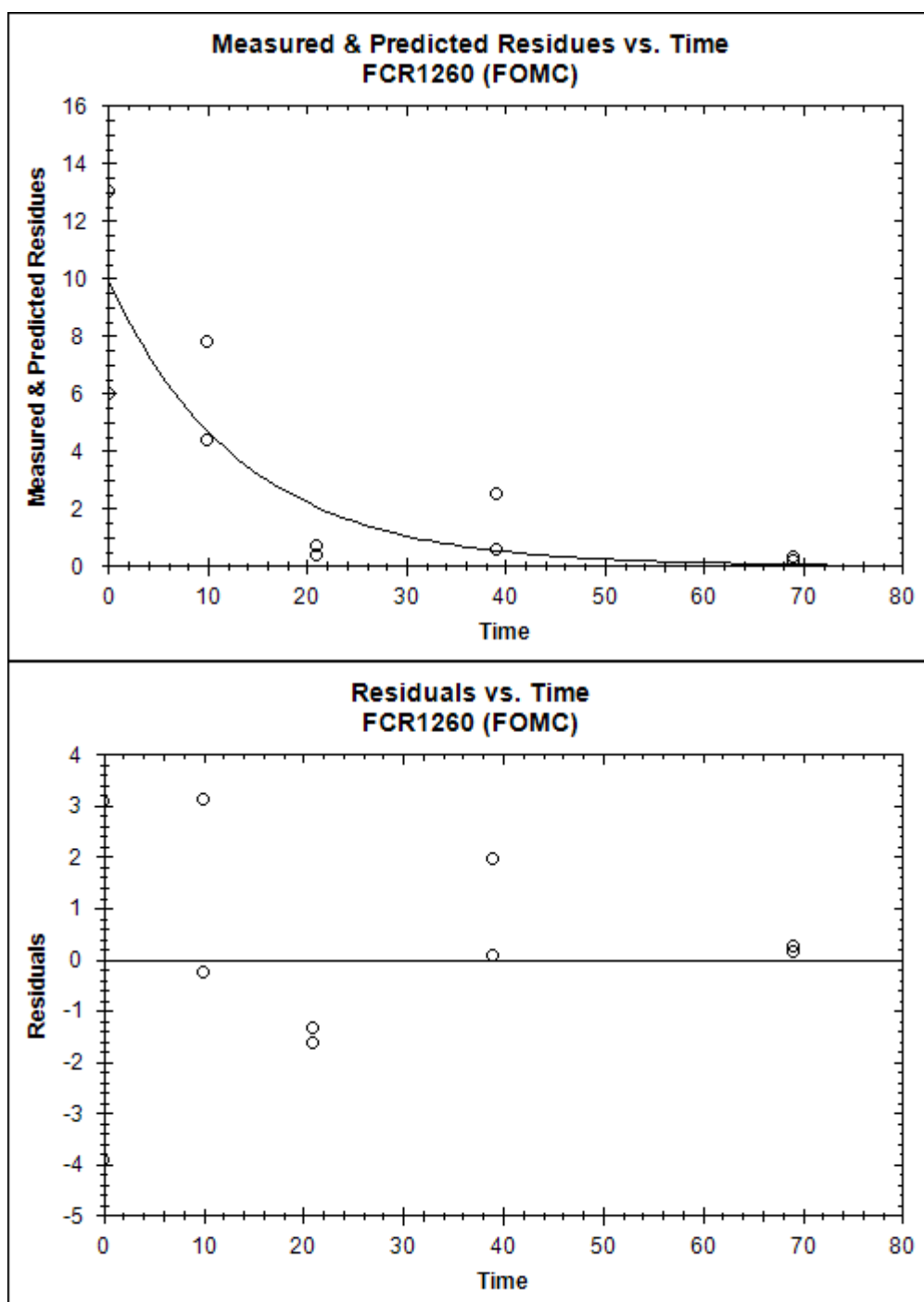
      FCR1260
DT50 :       9.1857
DT90 :      30.548
Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  13.0000  2.0785     9.9242     3.0758
0.0000   6.0000  2.0785     9.9242    -3.9242
10.0000  7.8000  2.0785     4.6666     3.1334
10.0000  4.4000  2.0785     4.6666    -0.2666
21.0000  0.7000  2.0785     2.0366    -1.3366
21.0000  0.4000  2.0785     2.0366    -1.6366
39.0000  2.5000  2.0785     0.5255     1.9745
39.0000  0.6000  2.0785     0.5255     0.0745
69.0000  0.3000  2.0785     0.0553     0.2447

```

69.0000 0.2000 2.0785 0.0553 0.1447



11.3.2.4DFOP

```

# Trial      : LiendentsFCR1260
# File name  : LiendentsFCR1260 IRLS DFOP FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_ts_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:44
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      13.00           0           Inf      False
k1    FCR1260      :       0.10           0           Inf      False
k2    FCR1260      :       0.01           0           Inf      False
g     FCR1260      :       0.50           0            1      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      32.74      32.74
Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FCR1260      :  9.783e+00  3.448e+00  16.117  3.232e+00
0.0116
k1    FCR1260      :  7.294e-02 -4.188e-02  0.188  5.859e-02
0.1298
k2    FCR1260      :  8.943e-07 -2.689e+00  2.689  1.372e+00
0.5000
g     FCR1260      :  9.778e-01 -1.173e+00  3.129  1.097e+00
0.2036

# -----
# DT50 and DT90 values
# -----

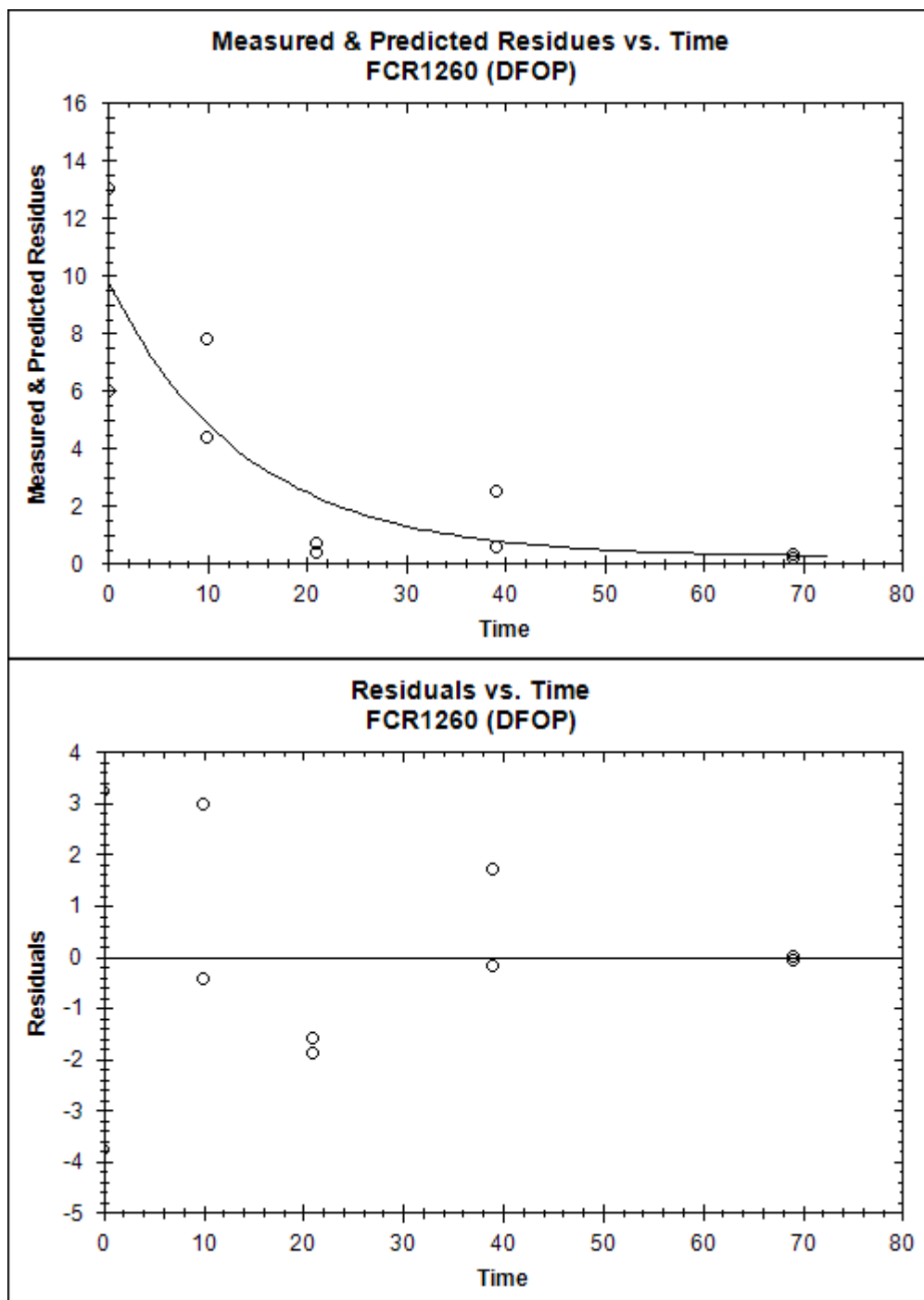
      FCR1260
DT50 :      9.8175
DT90 :      34.702
Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  13.0000  2.0676  9.7826  3.2174
0.0000   6.0000  2.0676  9.7826 -3.7826

```

10.0000	7.8000	2.0676	4.8295	2.9705
10.0000	4.4000	2.0676	4.8295	-0.4295
21.0000	0.7000	2.0676	2.2848	-1.5848
21.0000	0.4000	2.0676	2.2848	-1.8848
39.0000	2.5000	2.0676	0.7735	1.7265
39.0000	0.6000	2.0676	0.7735	-0.1735
69.0000	0.3000	2.0676	0.2797	0.0203
69.0000	0.2000	2.0676	0.2797	-0.0797



11.4 FPB-acid (FCR 3191) Degradation Total System (Decline Fit)

11.4.1 Ijzendoorn

11.4.1.1 SFO

```

# Trial      : IjzendoorntsFPB
# File name  : IjzendoorntsFPB IRLS SFO  FPB.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FPB
# Created    : on 18 Oct 2013
#            : at 11:21
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB           :      48.00           0             Inf          False
k      FPB           :       0.01           0             Inf          False

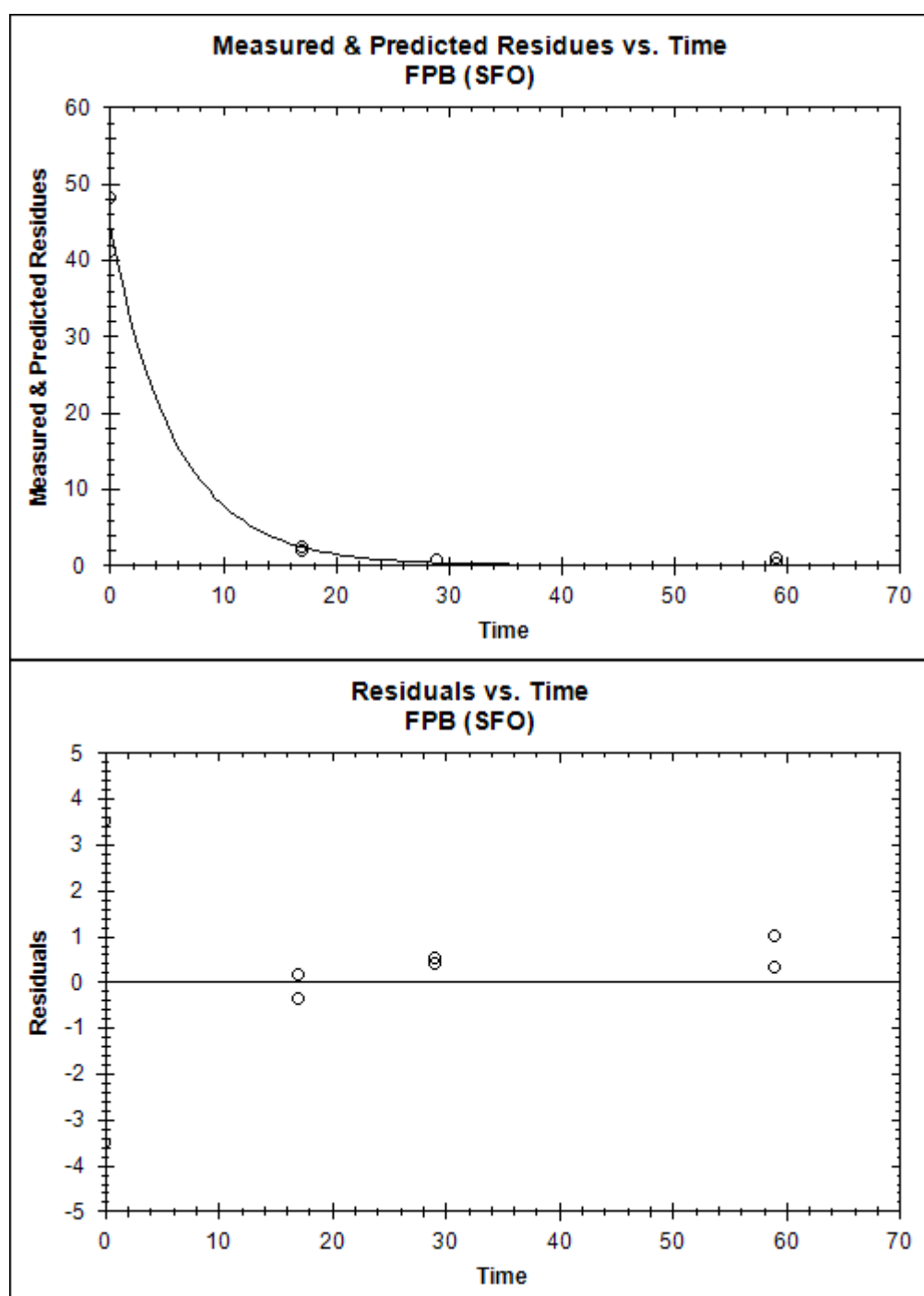
# -----
# Chi2 error estimation
# -----
# -----
# Chi2Err% :      2.71      2.71
# Kinetic model :      SFO

# -----
# Parameter estimation
# -----
# -----
# Degrees of Freedom : 6
# Parameter          Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB           :      44.49780    41.99481     47.001     1.27706     1.86e-08
k      FPB           :       0.17303     0.10263      0.243     0.03592     0.00147

# -----
# DT50 and DT90 values
# -----
# -----
# DT50 :      4.0060
# DT90 :      13.308
# Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----
# -----
# Compartment FPB
# time observed err-std predicted residual
0.0000  48.0000  1.8080  44.4978  3.5022
0.0000  41.0000  1.8080  44.4978 -3.4978
17.0000  2.0000  1.8080  2.3490 -0.3490
17.0000  2.5000  1.8080  2.3490  0.1510
29.0000  0.7000  1.8080  0.2945  0.4055
29.0000  0.8000  1.8080  0.2945  0.5055
59.0000  0.3000  1.8080  0.0016  0.2984
59.0000  1.0000  1.8080  0.0016  0.9984

```



11.4.1.2HS

```

# Trial      : IjzendoorntsFPB
# File name  : IjzendoorntsFPB IRLS HS   FPB.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FPB
# Created    : on 18 Oct 2013
#            : at 10:37
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
#
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB           :      48.00          0          Inf      False
k1    FPB           :       0.10          0          Inf      False
k2    FPB           :       0.01          0          Inf      False
tb    FPB           :       3.00          0          Inf      False

# -----
# Chi2 error estimation
# -----
#
# Chi2Err% :      Inf      All
# Kinetic model :      HS      Inf

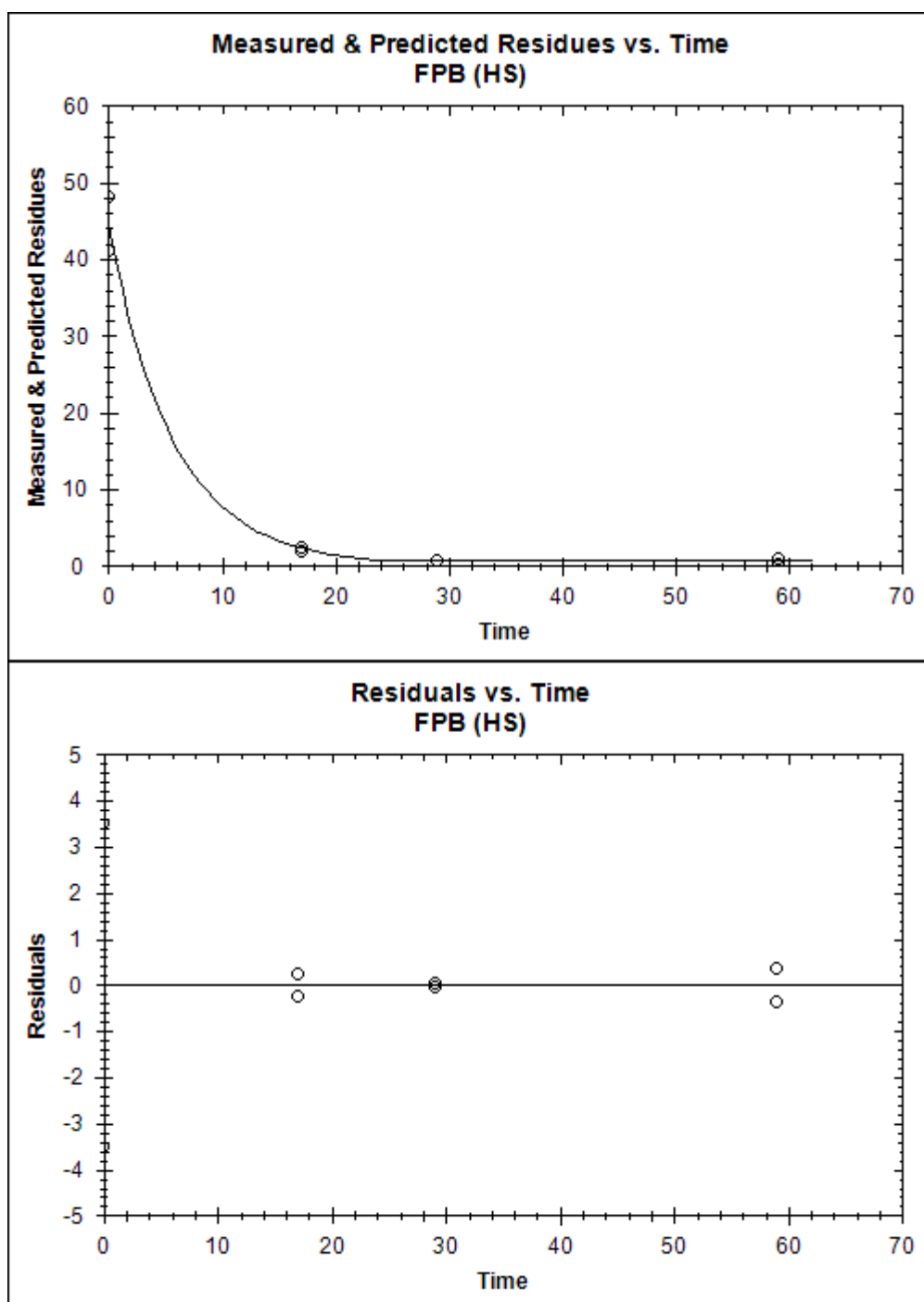
# -----
# Parameter estimation
# -----
#
# Degrees of Freedom : 4
#
# Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB       :      44.500010      41.338153      47.662      1.613222      5.14e-06
k1    FPB       :       0.175561       0.089179       0.262      0.044073      0.00818
k2    FPB       :       0.004772      -0.246403       0.256      0.128153      0.48604
tb    FPB       :      23.097331     -12.398133      58.593      18.110263      0.13561

# -----
# DT50 and DT90 values
# -----
#
# DT50 :      3.9482
# DT90 :      13.116
# Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----
#
# Compartment FPB
# time observed err-std predicted residual
0.0000 48.0000 1.7633 44.5000 3.5000
0.0000 41.0000 1.7633 44.5000 -3.5000
17.0000 2.0000 1.7633 2.2501 -0.2501
17.0000 2.5000 1.7633 2.2501 0.2499
29.0000 0.7000 1.7633 0.7500 -0.0500
29.0000 0.8000 1.7633 0.7500 0.0500
59.0000 0.3000 1.7633 0.6500 -0.3500

```

59.0000 1.0000 1.7633 0.6500 0.3500



11.4.1.3 FOMC

```

# Trial      : IjzendoorntsFPB
# File name  : IjzendoorntsFPB IRLS FOMC FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FPB
# Created    : on 18 Oct 2013
#            : at 10:38
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      48.0          0          Inf      False
alpha FPB      :      0.1          0          Inf      False
beta  FPB      :      0.1          0          Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      1.738      1.738
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 5
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      44.500      41.400      47.600      1.582      5.31e-07
alpha FPB      :      1.608      -6.518      9.734      4.146      0.357
beta  FPB      :      3.064      -32.619      38.748      18.206      0.436

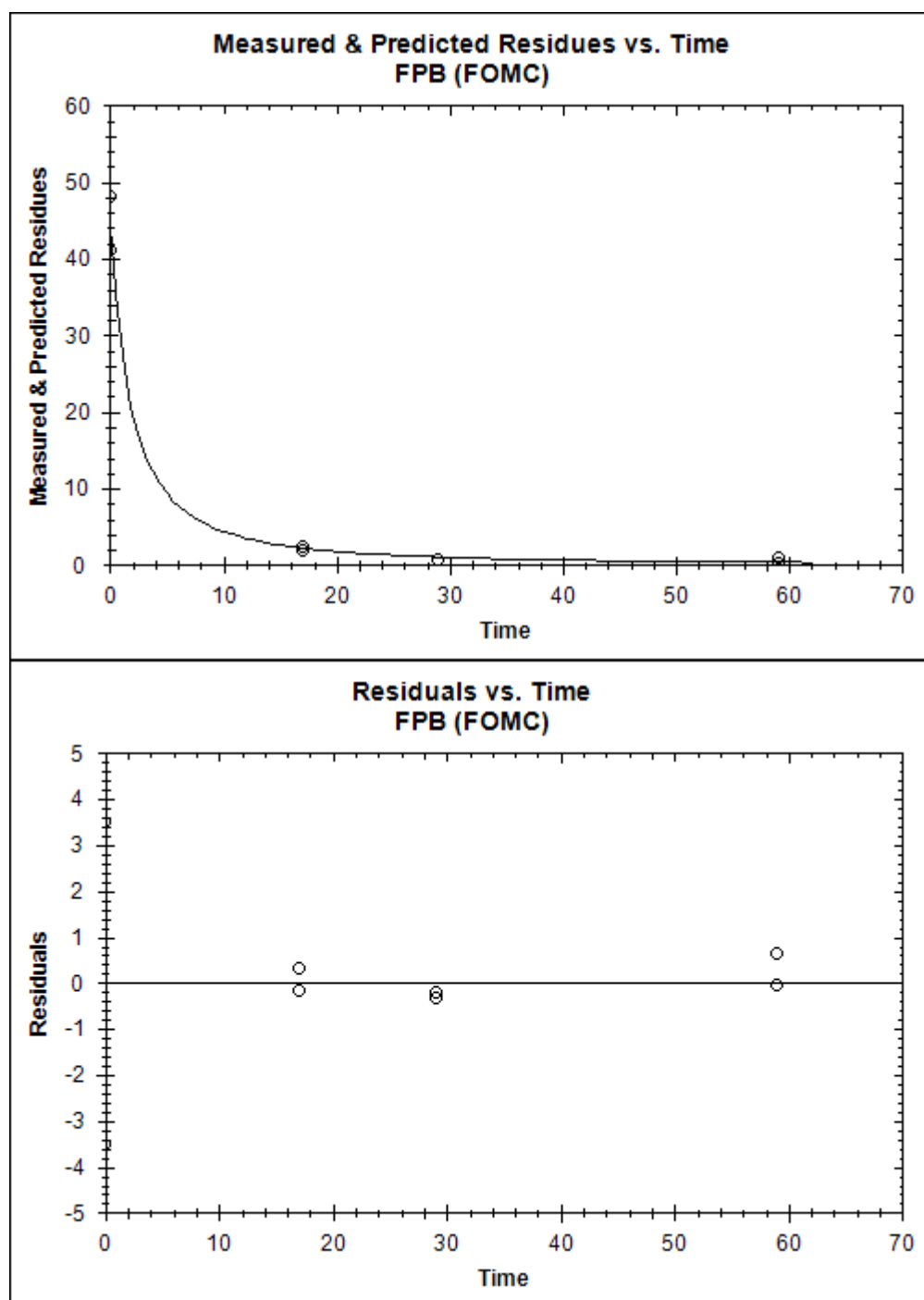
# -----
# DT50 and DT90 values
# -----

      DT50 :      1.6514
      DT90 :      9.7663
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 48.0000 1.7752 44.5001 3.4999
0.0000 41.0000 1.7752 44.5001 -3.5001
17.0000 2.0000 1.7752 2.1684 -0.1684
17.0000 2.5000 1.7752 2.1684 0.3316
29.0000 0.7000 1.7752 1.0204 -0.3204
29.0000 0.8000 1.7752 1.0204 -0.2204
59.0000 0.3000 1.7752 0.3528 -0.0528
59.0000 1.0000 1.7752 0.3528 0.6472

```



11.4.1.4DFOP

```

# Trial      : IjzendoornFPB
# File name  : IjzendoornFPB IRLS DFOP FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_ts_FPB
# Created    : on 18 Oct 2013
#            : at 10:37
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn ts
# # Ijzendoorn total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      48.00      0      Inf      False
k1    FPB      :      0.10      0      Inf      False
k2    FPB      :      0.01      0      Inf      False
g     FPB      :      0.50      0      1      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      Inf      All
      Kinetic model :      DFOP      Inf

# -----
# Parameter estimation
# -----

Degrees of Freedom : 4
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      4.450e+01      4.105e+01      47.955      1.763e+00      7.3e-06
k1    FPB      :      1.940e-01      -8.097e-02      0.469      1.403e-01      0.119449
k2    FPB      :      7.091e-07      -3.114e-01      0.311      1.589e-01      0.499998
g     FPB      :      9.860e-01      7.712e-01      1.201      1.096e-01      0.000423

# -----
# DT50 and DT90 values
# -----

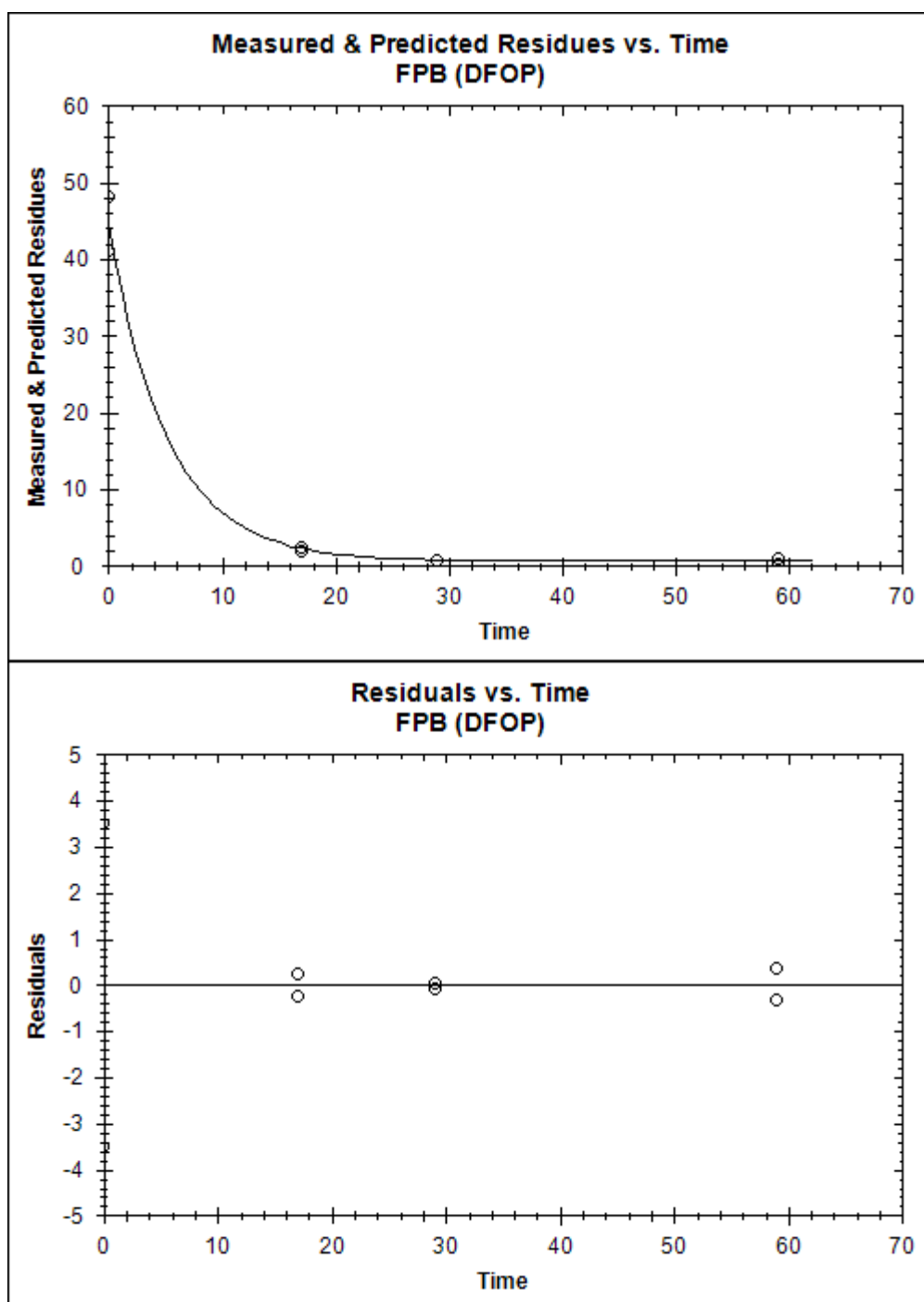
      DT50 :      3.6466
      DT90 :      12.574
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 48.0000 1.7635 44.5001 3.4999
0.0000 41.0000 1.7635 44.5001 -3.5001
17.0000 2.0000 1.7635 2.2448 -0.2448
17.0000 2.5000 1.7635 2.2448 0.2552
29.0000 0.7000 1.7635 0.7814 -0.0814
29.0000 0.8000 1.7635 0.7814 0.0186
59.0000 0.3000 1.7635 0.6238 -0.3238

```

59.0000 1.0000 1.7635 0.6238 0.3762



11.4.2 Lienden

11.4.2.1 SFO

```
# Trial : LiendentsFPB
# File name : LiendentsFPB IRLS SFO FPB.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_ts_FPB
# Created : on 18 Oct 2013
# at 11:45
# by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
# -----
# Initial Value Lower Bound Upper Bound Fixed
M(0) FPB : 30.5 0 Inf False
k FPB : 0.1 0 Inf False

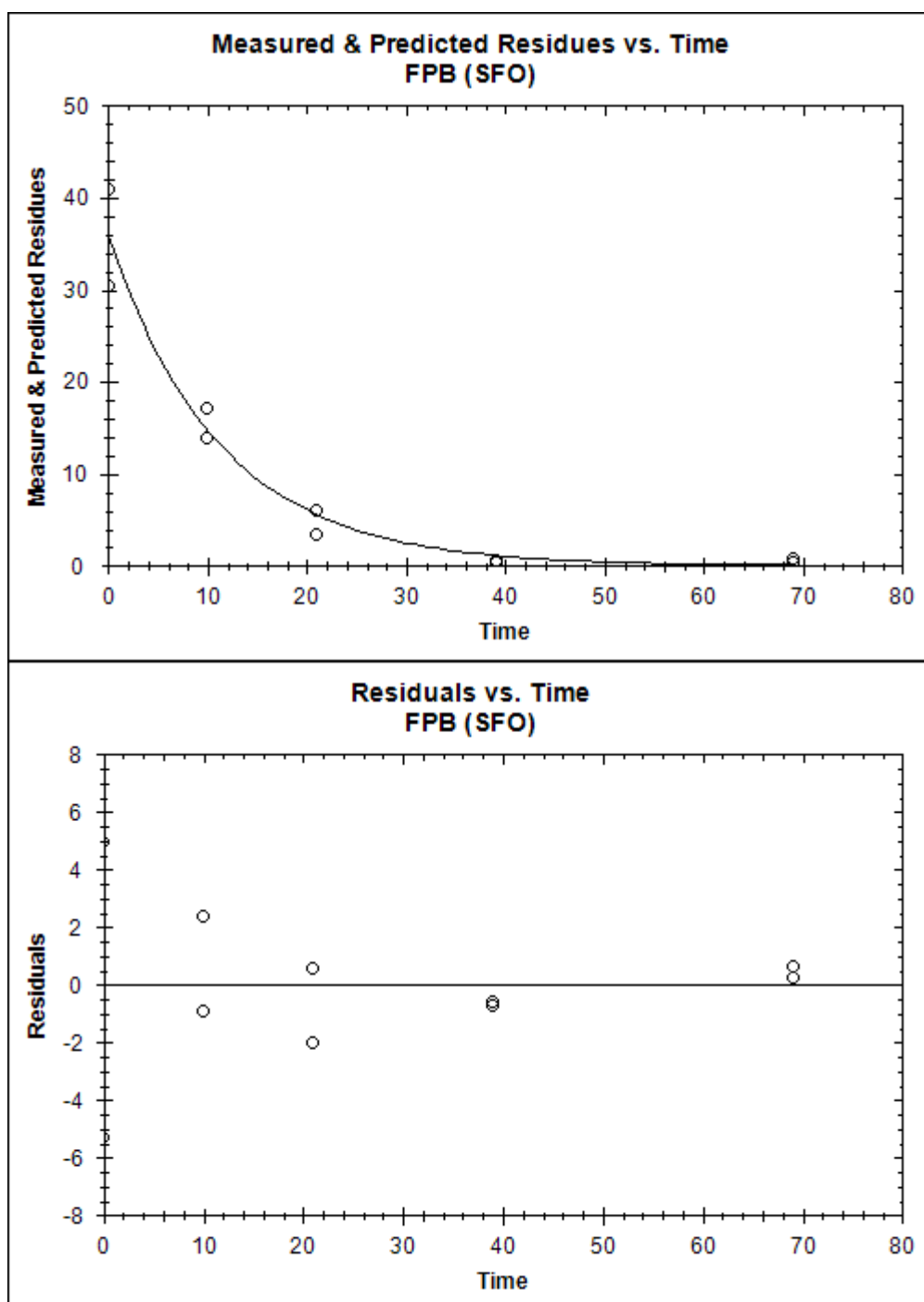
# -----
# Chi2 error estimation
# -----
# -----
# Chi2Err% : 4.13 4.13
# Kinetic model : SFO

# -----
# Parameter estimation
# -----
# -----
# Degrees of Freedom : 8
# Parameter Estimate Lower CI Upper CI St.Dev Prob > t
M(0) FPB : 35.82605 31.91590 39.736 1.99502 4.74e-08
k FPB : 0.08906 0.06722 0.111 0.01114 2.20e-05

# -----
# DT50 and DT90 values
# -----
# -----
# DT50 : 7.7827
# DT90 : 25.854
# Kinetic model : SFO

# -----
# Measured vs. predicted values
# -----
# -----
# Compartment FPB
# time observed err-std predicted residual
0.0000 30.5000 2.5574 35.8261 -5.3261
0.0000 40.8000 2.5574 35.8261 4.9739
10.0000 17.1000 2.5574 14.7030 2.3970
10.0000 13.8000 2.5574 14.7030 -0.9030
21.0000 3.5000 2.5574 5.5199 -2.0199
21.0000 6.1000 2.5574 5.5199 0.5801
39.0000 0.4000 2.5574 1.1110 -0.7110
39.0000 0.5000 2.5574 1.1110 -0.6110
69.0000 0.7000 2.5574 0.0768 0.6232
```

69.0000 0.3000 2.5574 0.0768 0.2232



11.4.2.2HS

```

# Trial      : LiendentsFPB
# File name  : LiendentsFPB IRLS HS   FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_ts_FPB
# Created    : on 18 Oct 2013
#            : at 11:45
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      30.50              0              Inf      False
k1    FPB      :       0.10              0              Inf      False
k2    FPB      :       0.01              0              Inf      False
tb    FPB      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

              Chi2Err% :      2.384      2.384
              Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      35.64995      31.29922      40.001      2.21980      1.85e-06
k1    FPB      :       0.05511      -0.08205      0.192      0.06998      0.2305
k2    FPB      :       0.10773       0.02714      0.188      0.04112      0.0198
tb    FPB      :       4.59976       0.45532      8.744      2.11455      0.0363

# -----
# DT50 and DT90 values
# -----

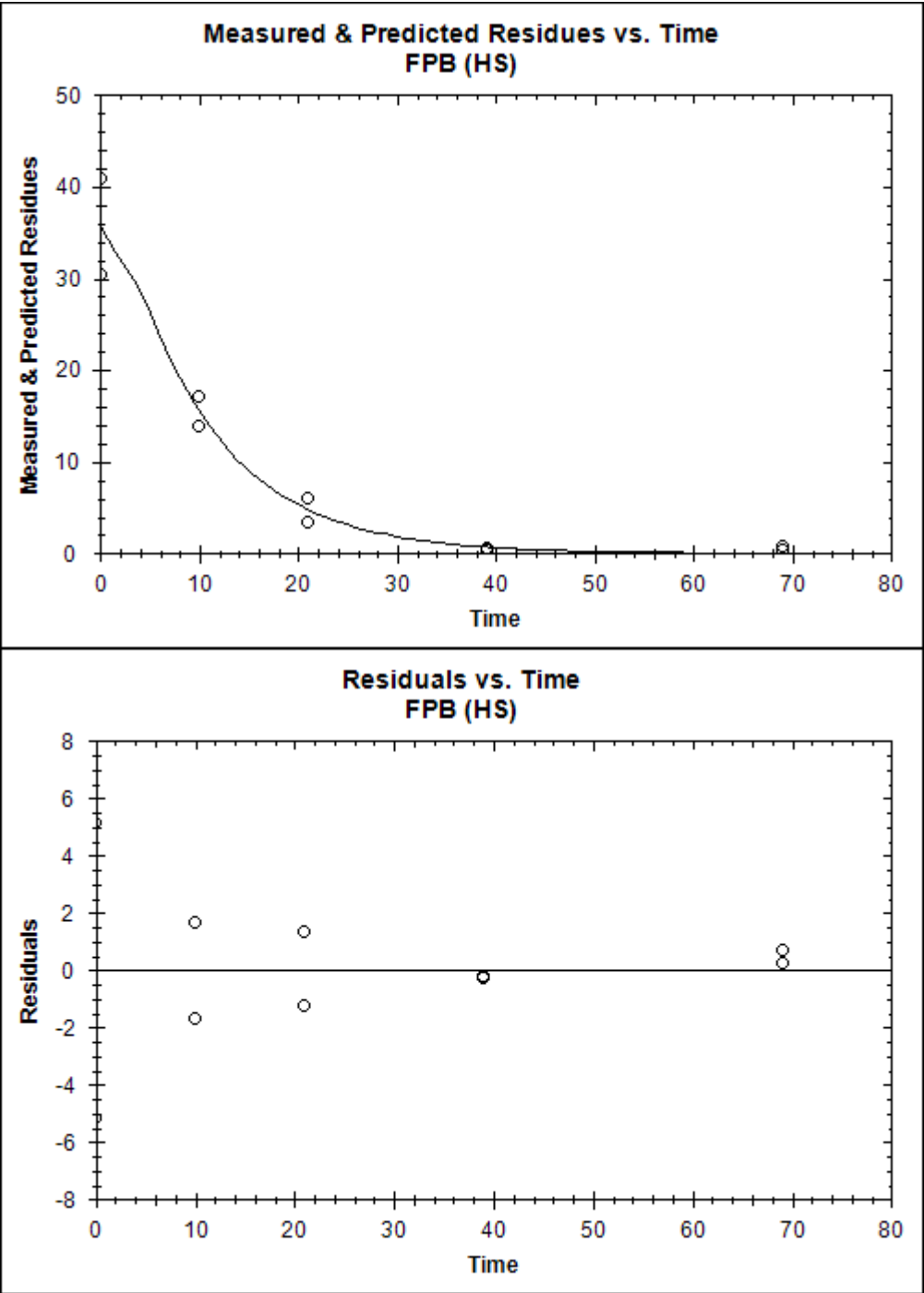
              DT50 :       8.6805
              DT90 :      23.619
              Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 30.5000 2.5004 35.6500 -5.1500
0.0000 40.8000 2.5004 35.6500 5.1500
10.0000 17.1000 2.5004 15.4629 1.6371
10.0000 13.8000 2.5004 15.4629 -1.6629
21.0000 3.5000 2.5004 4.7273 -1.2273
21.0000 6.1000 2.5004 4.7273 1.3727
39.0000 0.4000 2.5004 0.6799 -0.2799

```

39.0000	0.5000	2.5004	0.6799	-0.1799
69.0000	0.7000	2.5004	0.0268	0.6732
69.0000	0.3000	2.5004	0.0268	0.2732



11.4.2.3 FOMC

```

# Trial      : LiendentsFPB
# File name  : LiendentsFPB IRLS FOMC FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_ts_FPB
# Created    : on 18 Oct 2013
#            : at 11:45
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      30.5           0           Inf      False
alpha FPB      :       0.1           0           Inf      False
beta  FPB      :       0.1           0           Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      5.99      5.99
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      3.618e+01      3.298e+01      39.38      1.632e+00      4.81e-08
alpha FPB      :      1.022e+03      -1.119e+04      13237.36      6.233e+03      0.437
beta  FPB      :      1.076e+04      -1.180e+05      139551.25      6.571e+04      0.437

# -----
# DT50 and DT90 values
# -----

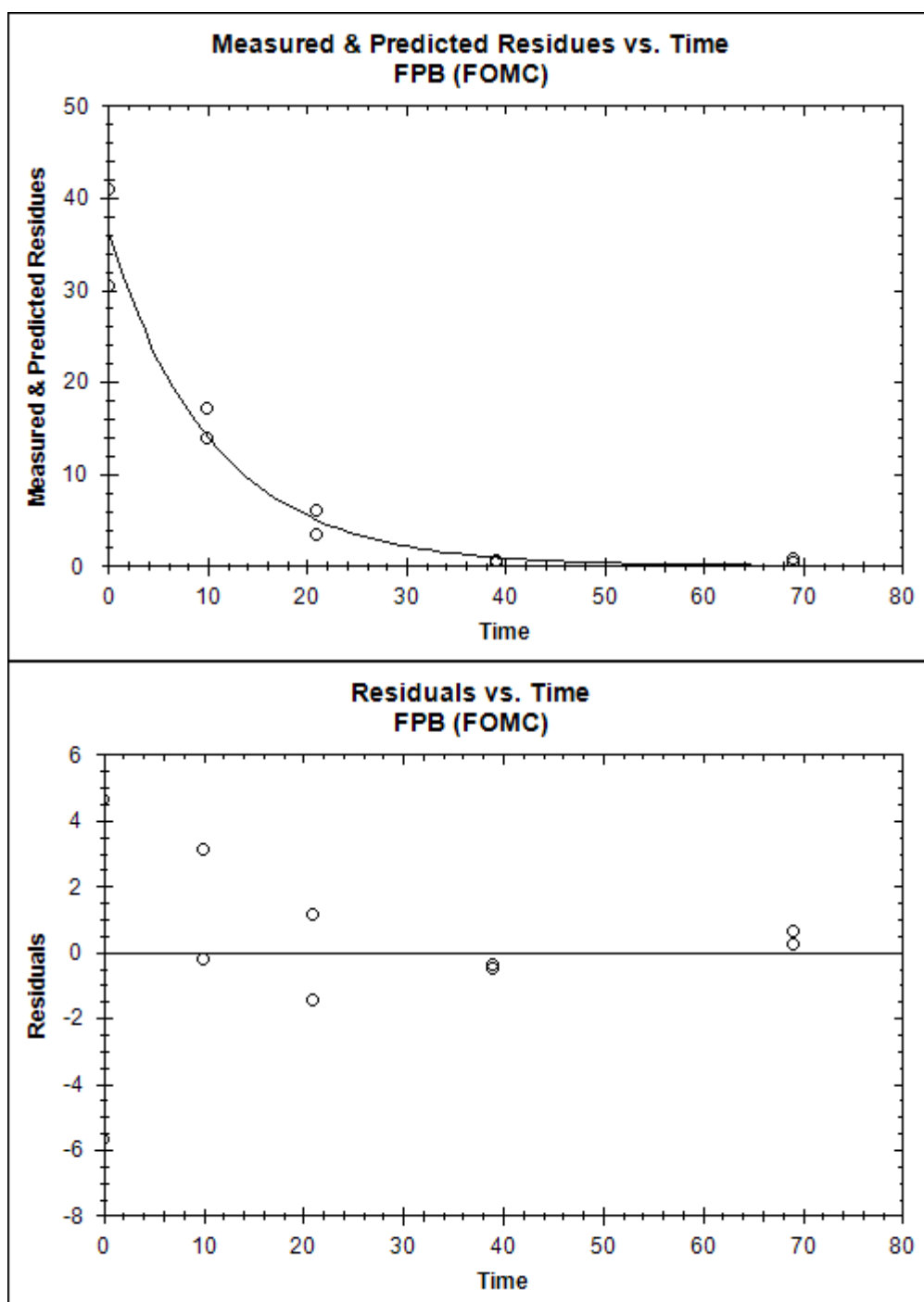
      DT50 :      7.3043
      DT90 :      24.284
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 30.5000 2.5983 36.1781 -5.6781
0.0000 40.8000 2.5983 36.1781 4.6219
10.0000 17.1000 2.5983 14.0079 3.0921
10.0000 13.8000 2.5983 14.0079 -0.2079
21.0000 3.5000 2.5983 4.9378 -1.4378
21.0000 6.1000 2.5983 4.9378 1.1622
39.0000 0.4000 2.5983 0.8985 -0.4985
39.0000 0.5000 2.5983 0.8985 -0.3985
69.0000 0.7000 2.5983 0.0528 0.6472

```

69.0000 0.3000 2.5983 0.0528 0.2472



11.4.2.4DFOP

```

# Trial      : LiendentsFPB
# File name  : LiendentsFPB IRLS DFOP FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_ts_FPB
# Created    : on 18 Oct 2013
#            : at 11:45
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden ts
# # Lienden total system FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      30.50              0              Inf      False
k1    FPB      :       0.10              0              Inf      False
k2    FPB      :       0.01              0              Inf      False
g     FPB      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              Chi2Err% :       5.891      5.891
              Kinetic model :      DFOP      All

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      35.82605      30.61812      41.034      2.65716      5.16e-06
k1    FPB      :       0.08906      -0.05955      0.238      0.07583      0.142
k2    FPB      :       0.01796      -0.41352      0.449      0.22015      0.469
g     FPB      :       1.00000      -0.40012      2.400      0.71436      0.106

# -----
# DT50 and DT90 values
# -----

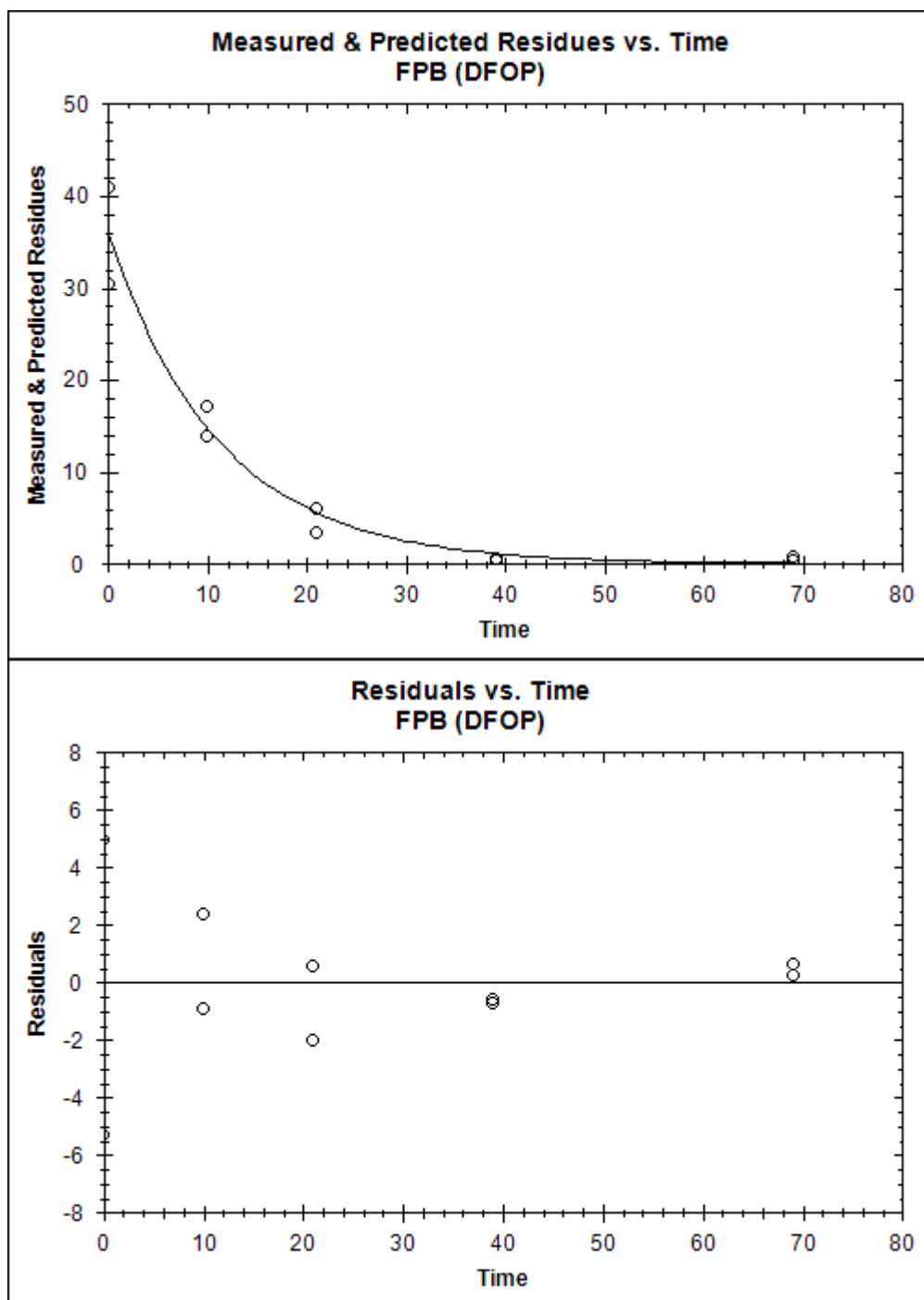
              DT50 :       7.7827
              DT90 :      25.854
              Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000  30.5000  2.5574  35.8261  -5.3261
0.0000  40.8000  2.5574  35.8261  4.9739
10.0000  17.1000  2.5574  14.7030  2.3970
10.0000  13.8000  2.5574  14.7030  -0.9030
21.0000   3.5000  2.5574   5.5199  -2.0199
21.0000   6.1000  2.5574   5.5199   0.5801
39.0000   0.4000  2.5574   1.1110  -0.7110

```

39.0000	0.5000	2.5574	1.1110	-0.6110
69.0000	0.7000	2.5574	0.0768	0.6232
69.0000	0.3000	2.5574	0.0768	0.2232



11.5 Cyfluthrin Dissipation Water Phase

11.5.1 Barmen

11.5.1.1 SFO

```
# Trial      : BarmenWponly
# File name  : BarmenWponly IRLS SFO  Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_w_ponly
# Created    : on 14 Jun 2013
#            : at 10:33
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See water
# # Barmener See water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      46.94              0              Inf      False
k      Par      :      0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      26.27      26.27
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 11
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      38.598      31.677      45.520      3.531      1.51e-07
k      Par      :      1.182      0.457      1.907      0.370      0.00426

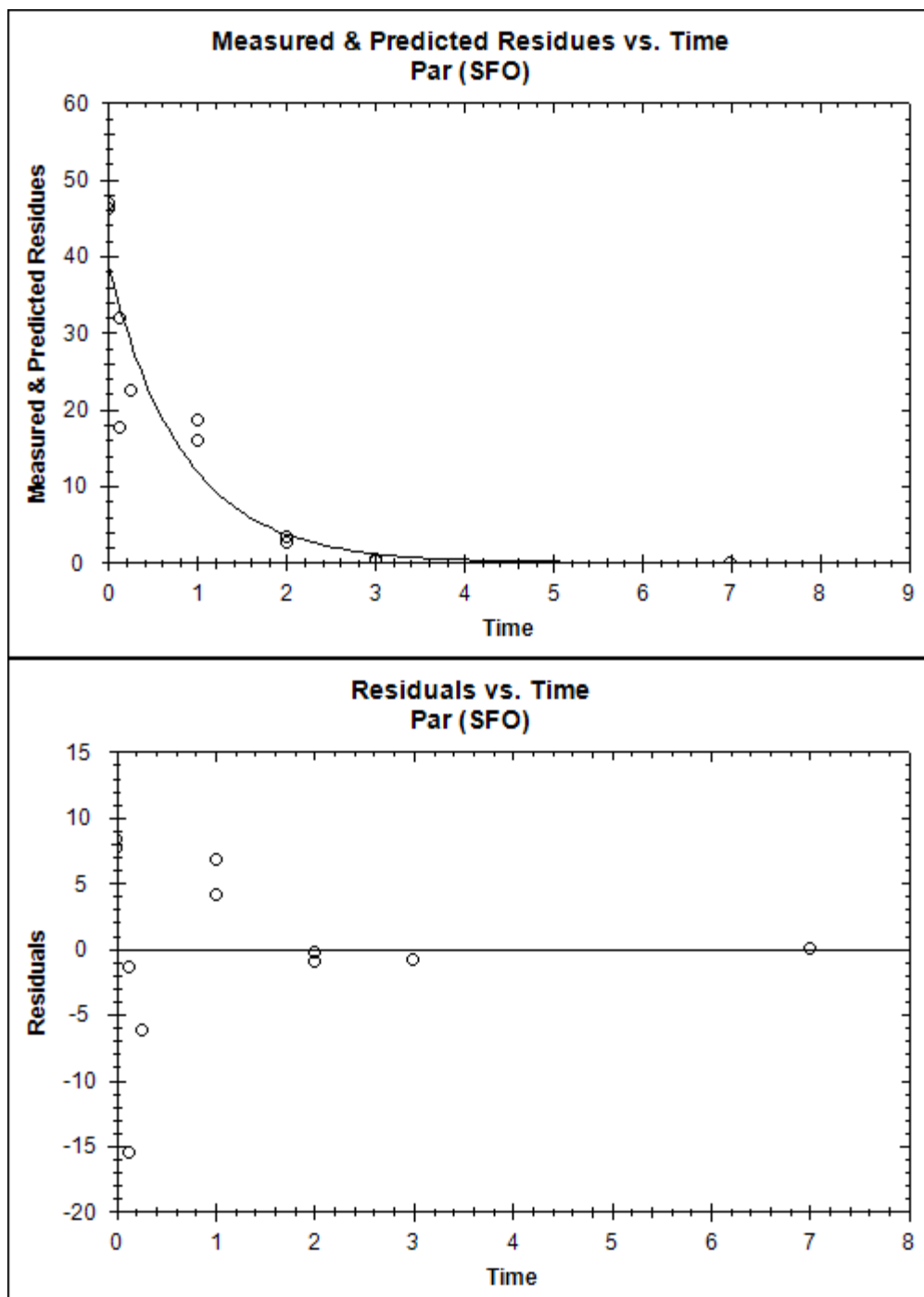
# -----
# DT50 and DT90 values
# -----

      Par
      DT50 :      0.5863
      DT90 :      1.9478
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 46.9400 6.0540 38.5983 8.3417
0.0000 46.2900 6.0540 38.5983 7.6917
0.1250 17.7400 6.0540 33.2961 -15.5561
0.1250 31.9100 6.0540 33.2961 -1.3861
0.2500 22.5400 6.0540 28.7222 -6.1822
0.2500 NA 6.0540 28.7222 NA
```

1.0000	15.8800	6.0540	11.8350	4.0450
1.0000	18.6900	6.0540	11.8350	6.8550
2.0000	3.3800	6.0540	3.6288	-0.2488
2.0000	2.6500	6.0540	3.6288	-0.9788
3.0000	0.3200	6.0540	1.1127	-0.7927
3.0000	0.3500	6.0540	1.1127	-0.7627
7.0000	0.0500	6.0540	0.0098	0.0402
7.0000	0.0500	6.0540	0.0098	0.0402



11.5.1.2_{HS}

```

# Trial      : BarmenWponly
# File name  : BarmenWponly IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_w_ponly
# Created    : on 14 Jun 2013
#            : at 10:33
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See water
# # Barmener See water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      46.94              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
tb    Par      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      31.26      31.26
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 9
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      38.59827      30.14763      47.049      4.31163      4.46e-06
k1    Par      1.18215      0.26200      2.102      0.46947      0.0164
k2    Par      0.01059      -19.97871      20.000      10.19881      0.4996
tb    Par      5.55893      -105.23536      116.353      56.52874      0.4619

# -----
# DT50 and DT90 values
# -----

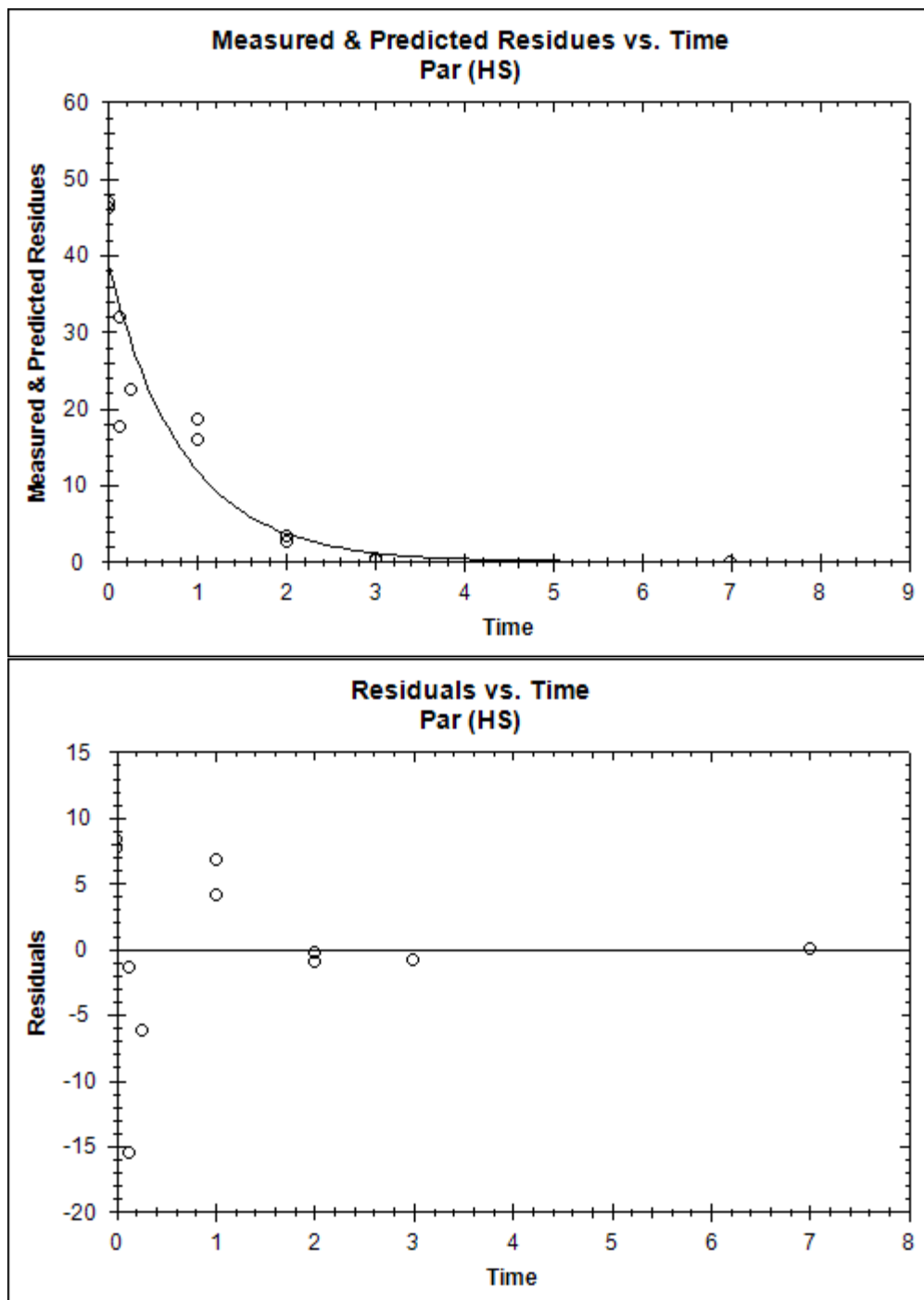
      Par
      DT50 :      0.5863
      DT90 :      1.9478
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000  46.9400  6.0540  38.5983  8.3417
0.0000  46.2900  6.0540  38.5983  7.6917
0.1250  17.7400  6.0540  33.2960 -15.5560
0.1250  31.9100  6.0540  33.2960 -1.3860
0.2500  22.5400  6.0540  28.7222 -6.1822
0.2500      NA  6.0540  28.7222      NA
1.0000  15.8800  6.0540  11.8350  4.0450

```

1.0000	18.6900	6.0540	11.8350	6.8550
2.0000	3.3800	6.0540	3.6288	-0.2488
2.0000	2.6500	6.0540	3.6288	-0.9788
3.0000	0.3200	6.0540	1.1127	-0.7927
3.0000	0.3500	6.0540	1.1127	-0.7627
7.0000	0.0500	6.0540	0.0532	-0.0032
7.0000	0.0500	6.0540	0.0532	-0.0032



11.5.1.3 FOMC

```

# Trial      : BarmenWponly
# File name  : BarmenWponly IRLS FOMC Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_w_ponly
# Created    : on 14 Jun 2013
#            : at 10:34
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See water
# # Barmener See water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      46.94      0      Inf      False
alpha Par      :      0.10      0      Inf      False
beta  Par      :      0.10      0      Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      20.49      20.49
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 10
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      46.0274      39.0693      52.985      3.5501      7.03e-08
alpha Par      :      0.7244      0.1856      1.263      0.2749      0.0125
beta  Par      :      0.1234      -0.0871      0.334      0.1074      0.1387

# -----
# DT50 and DT90 values
# -----

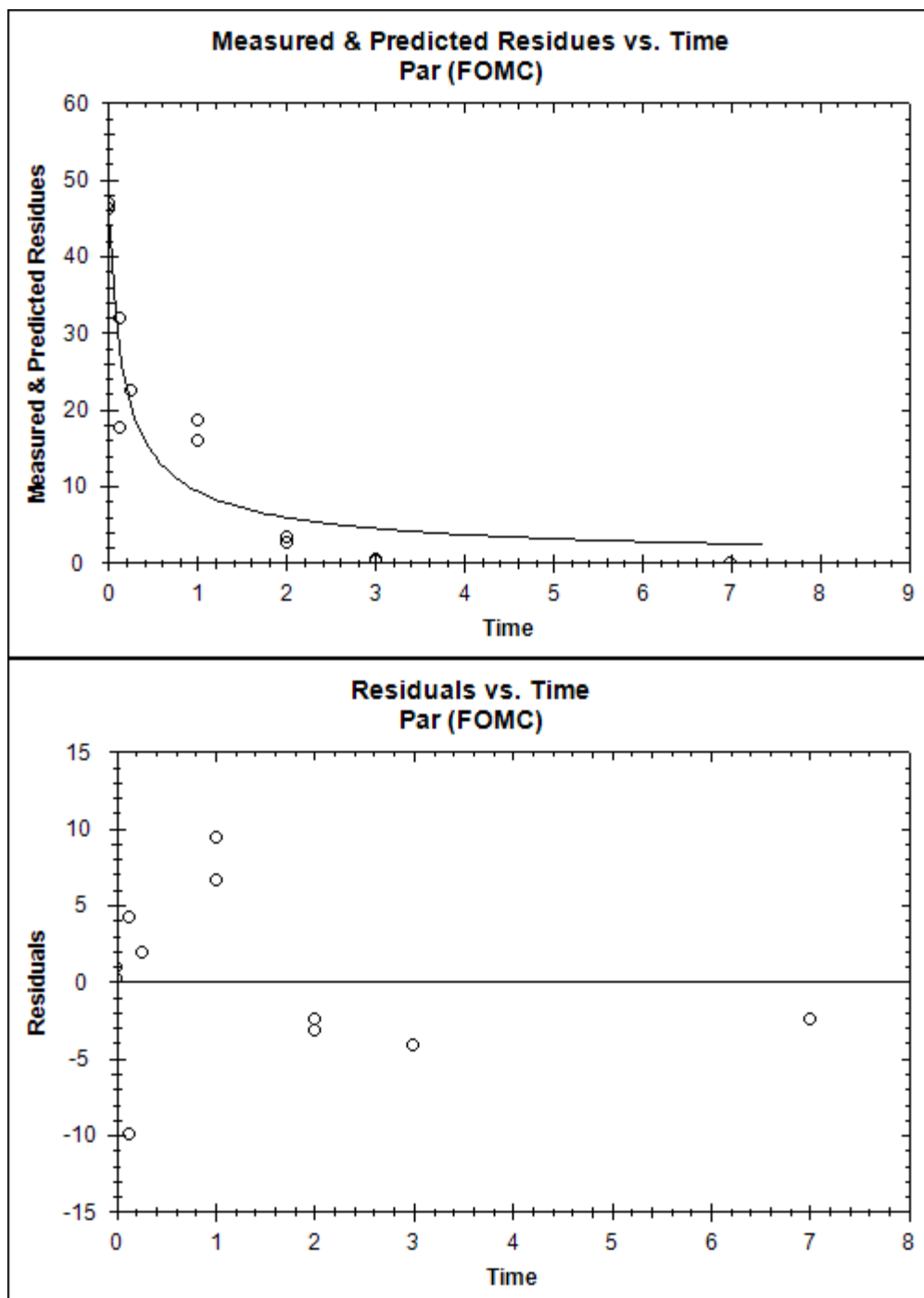
      Par
      DT50 :      0.1978
      DT90 :      2.8386
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 46.9400 4.9214 46.0274 0.9126
0.0000 46.2900 4.9214 46.0274 0.2626
0.1250 17.7400 4.9214 27.7245 -9.9845
0.1250 31.9100 4.9214 27.7245 4.1855
0.2500 22.5400 4.9214 20.6352 1.9048
0.2500 NA 4.9214 20.6352 NA
1.0000 15.8800 4.9214 9.2906 6.5894
1.0000 18.6900 4.9214 9.2906 9.3994
2.0000 3.3800 4.9214 5.8578 -2.4778

```

2.0000	2.6500	4.9214	5.8578	-3.2078
3.0000	0.3200	4.9214	4.4291	-4.1091
3.0000	0.3500	4.9214	4.4291	-4.0791
7.0000	0.0500	4.9214	2.4374	-2.3874
7.0000	0.0500	4.9214	2.4374	-2.3874



11.5.1.4 DFOP

```

# Trial      : BarmenWponly
# File name  : BarmenWponly IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_w_ponly
# Created    : on 14 Jun 2013
#            : at 10:33
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See water
# # Barmener See water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      46.94              0              Inf      False
k1    Par      :      0.10              0              Inf      False
k2    Par      :      0.01              0              Inf      False
g      Par      :      0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :      12.77      12.77
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 9
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      4.661e+01      4.071e+01      52.519      3.012e+00      4.3e-08
k1    Par      :      1.074e+02      -4.630e+03      4845.015      2.417e+03      0.482769
k2    Par      :      7.925e-01      4.553e-01      1.130      1.720e-01      0.000640
g      Par      :      3.893e-01      2.372e-01      0.542      7.764e-02      0.000362

# -----
# DT50 and DT90 values
# -----

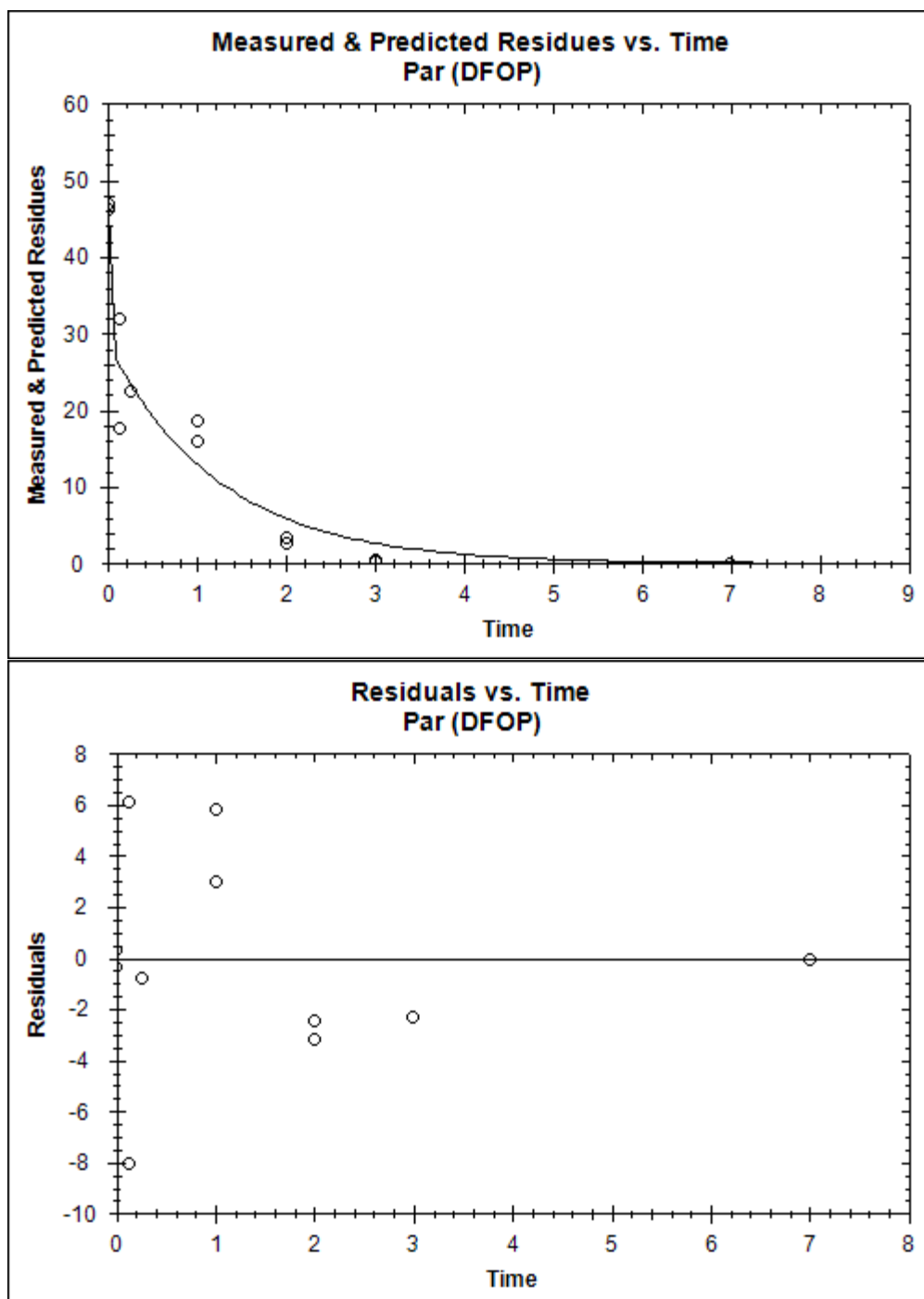
              Par
      DT50 :      0.2523
      DT90 :      2.2832
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000  46.9400  3.6430  46.6150  0.3250
0.0000  46.2900  3.6430  46.6150 -0.3250
0.1250  17.7400  3.6430  25.7817 -8.0417
0.1250  31.9100  3.6430  25.7817  6.1283
0.2500  22.5400  3.6430  23.3502 -0.8102
0.2500      NA  3.6430  23.3502      NA
1.0000  15.8800  3.6430  12.8875  2.9925

```

1.0000	18.6900	3.6430	12.8875	5.8025
2.0000	3.3800	3.6430	5.8345	-2.4545
2.0000	2.6500	3.6430	5.8345	-3.1845
3.0000	0.3200	3.6430	2.6414	-2.3214
3.0000	0.3500	3.6430	2.6414	-2.2914
7.0000	0.0500	3.6430	0.1110	-0.0610
7.0000	0.0500	3.6430	0.1110	-0.0610



11.5.2 Genkel

11.5.2.1 SFO

```
# Trial      : Genkelwponly
# File name  : Genkelwponly IRLS SFO  Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Water\Genkel_w_ponly
# Created    : on 05 Oct 2013
#            : at 10:19
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel water
# # Genkel water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.71              0              Inf      False
k      Par      :       0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :      19.56      19.56
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 14
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      31.942      27.893      35.99      2.066      1.71e-10
k      Par      :       1.791      1.152      2.43      0.326      3.95e-05

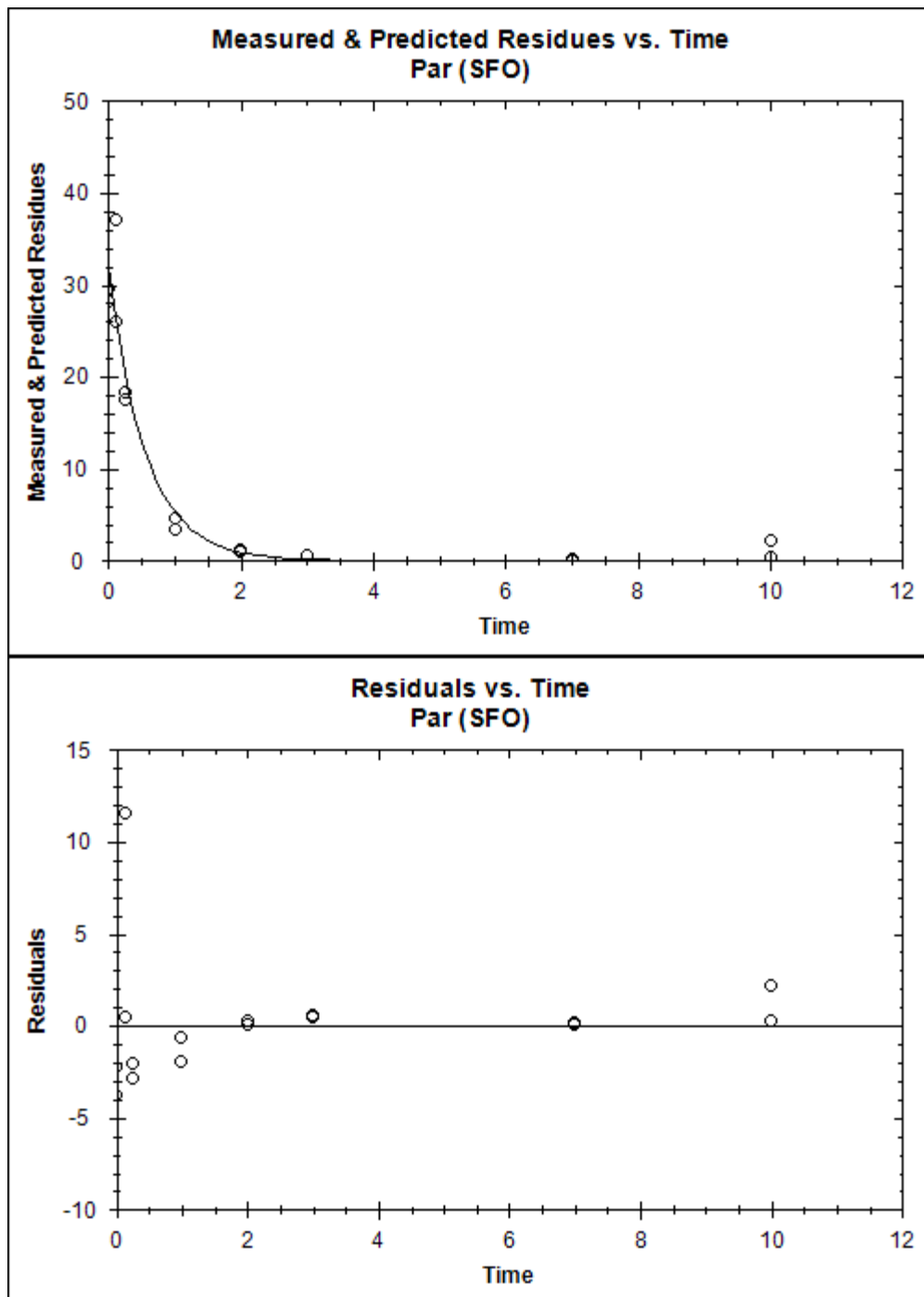
# -----
# DT50 and DT90 values
# -----

              Par
      DT50 :       0.3870
      DT90 :       1.2856
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 29.7100 3.3174 31.9425 -2.2325
0.0000 28.1500 3.3174 31.9425 -3.7925
0.1250 37.1200 3.3174 25.5350 11.5850
0.1250 25.9800 3.3174 25.5350 0.4450
0.2500 17.5300 3.3174 20.4128 -2.8828
0.2500 18.3500 3.3174 20.4128 -2.0628
1.0000 3.3400 3.3174 5.3272 -1.9872
1.0000 4.6400 3.3174 5.3272 -0.6872
2.0000 1.1400 3.3174 0.8884 0.2516
2.0000 1.0000 3.3174 0.8884 0.1116
```

3.0000	0.6100	3.3174	0.1482	0.4618
3.0000	0.6800	3.3174	0.1482	0.5318
7.0000	0.0500	3.3174	0.0001	0.0499
7.0000	0.1600	3.3174	0.0001	0.1599
10.0000	0.3100	3.3174	0.0000	0.3100
10.0000	2.1500	3.3174	0.0000	2.1500



11.5.2.2HS

```

# Trial      : Genkelwponly
# File name  : Genkelwponly IRLS HS   Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Water\Genkel_w_ponly
# Created    : on 05 Oct 2013
#            : at 10:20
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel water
# # Genkel water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.71              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
tb    Par      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      22.53      22.53
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 12
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      3.194e+01      2.358e+01      40.310      4.269e+00      3.7e-06
k1    Par      :      1.791e+00      4.034e-01      3.179      7.080e-01      0.0132
k2    Par      :      5.995e-03      -1.053e+01      10.540      5.374e+00      0.4996
tb    Par      :      1.918e+01      -1.157e+02      154.110      6.884e+01      0.3926

# -----
# DT50 and DT90 values
# -----

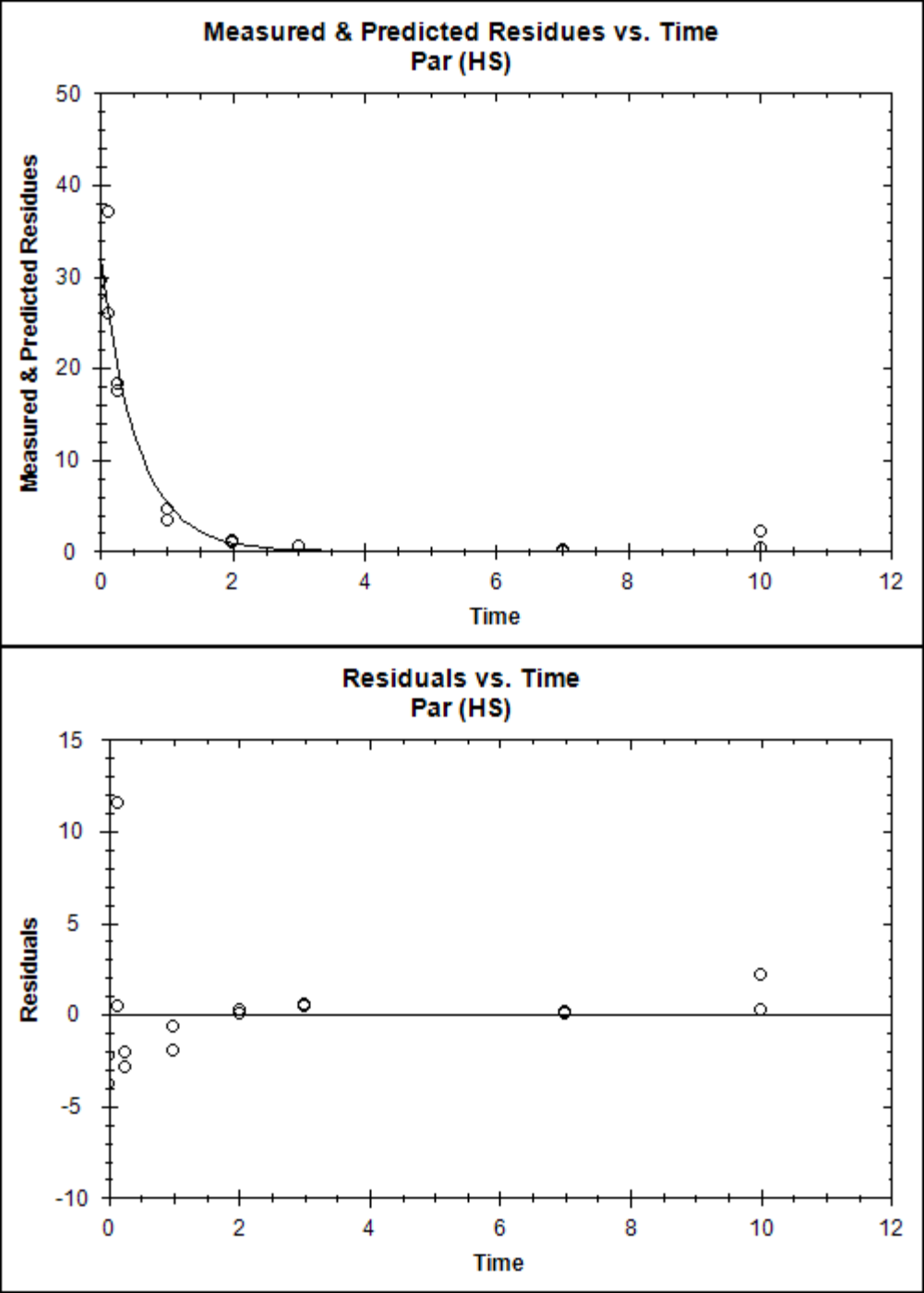
      Par
      DT50 :      0.3870
      DT90 :      1.2856
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 29.7100 3.3174 31.9426 -2.2326
0.0000 28.1500 3.3174 31.9426 -3.7926
0.1250 37.1200 3.3174 25.5350 11.5850
0.1250 25.9800 3.3174 25.5350 0.4450
0.2500 17.5300 3.3174 20.4128 -2.8828
0.2500 18.3500 3.3174 20.4128 -2.0628
1.0000 3.3400 3.3174 5.3272 -1.9872

```

1.0000	4.6400	3.3174	5.3272	-0.6872
2.0000	1.1400	3.3174	0.8884	0.2516
2.0000	1.0000	3.3174	0.8884	0.1116
3.0000	0.6100	3.3174	0.1482	0.4618
3.0000	0.6800	3.3174	0.1482	0.5318
7.0000	0.0500	3.3174	0.0001	0.0499
7.0000	0.1600	3.3174	0.0001	0.1599
10.0000	0.3100	3.3174	0.0000	0.3100
10.0000	2.1500	3.3174	0.0000	2.1500



11.5.2.3 FOMC

```

# Trial      : Genkelwponly
# File name  : Genkelwponly IRLS FOMC Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Water\Genkel_w_ponly
# Created    : on 05 Oct 2013
#            : at 10:20
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel water
# # Genkel water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.71              0              Inf      False
alpha Par      :       0.10              0              Inf      False
beta  Par      :       0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      22.62      22.62
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 13
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      33.322      28.922      37.72      2.244      7.84e-10
alpha Par      :      7423.428     -23939.628     38786.49     16001.853      0.325
beta  Par      :      3269.245     -10543.731     17082.22     7047.566      0.325

# -----
# DT50 and DT90 values
# -----

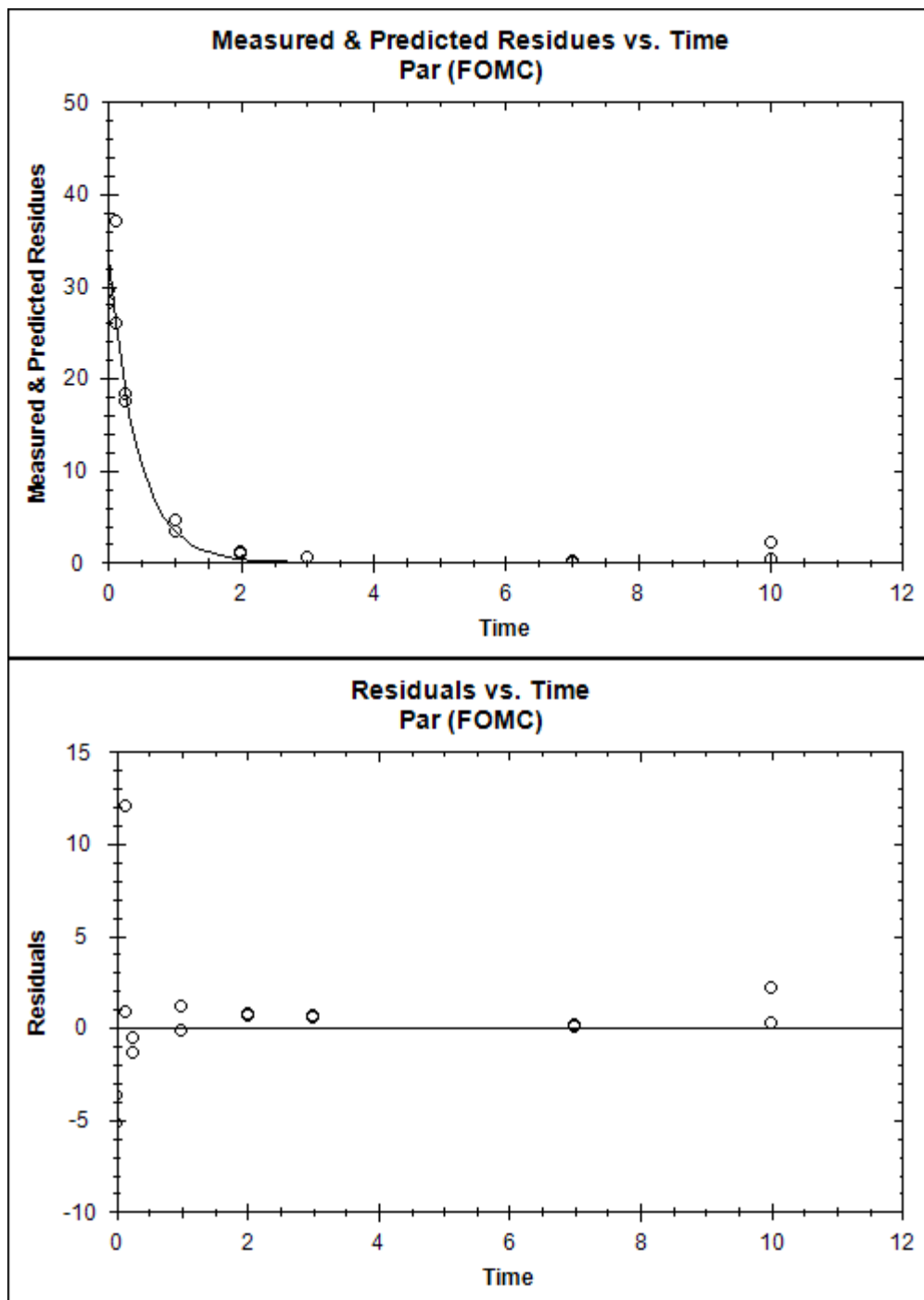
      Par
      DT50 :      0.3053
      DT90 :      1.0142
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000  29.7100  3.4952  33.3216  -3.6116
0.0000  28.1500  3.4952  33.3216  -5.1716
0.1250  37.1200  3.4952  25.0876  12.0324
0.1250  25.9800  3.4952  25.0876   0.8924
0.2500  17.5300  3.4952  18.8885  -1.3585
0.2500  18.3500  3.4952  18.8885  -0.5385
1.0000   3.3400  3.4952   3.4414  -0.1014
1.0000   4.6400  3.4952   3.4414   1.1986
2.0000   1.1400  3.4952   0.3557   0.7843

```

2.0000	1.0000	3.4952	0.3557	0.6443
3.0000	0.6100	3.4952	0.0368	0.5732
3.0000	0.6800	3.4952	0.0368	0.6432
7.0000	0.0500	3.4952	0.0000	0.0500
7.0000	0.1600	3.4952	0.0000	0.1600
10.0000	0.3100	3.4952	0.0000	0.3100
10.0000	2.1500	3.4952	0.0000	2.1500



11.5.2.4 DFOP

```

# Trial          : Genkelwponly
# File name     : Genkelwponly IRLS DFOP Par.r
# Target path   : C:\Emod\KinGUIII\WorkingDirectory\Water\Genkel_w_ponly
# Created      : on 05 Oct 2013
#              : at 10:20
#              : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel water
# # Genkel water
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.71              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
g     Par      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :      22.45      22.45
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 12
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      31.9986733      -9.0682132      73.066      20.9528782      0.0763
k1    Par      :       1.8362667      -7.6162263      11.289      4.8227891      0.3550
k2    Par      :       0.0001934      -7.4078546       7.408      3.7796858      0.5000
g     Par      :       0.9897719      -0.4393822       2.419      0.7291737      0.0998

# -----
# DT50 and DT90 values
# -----

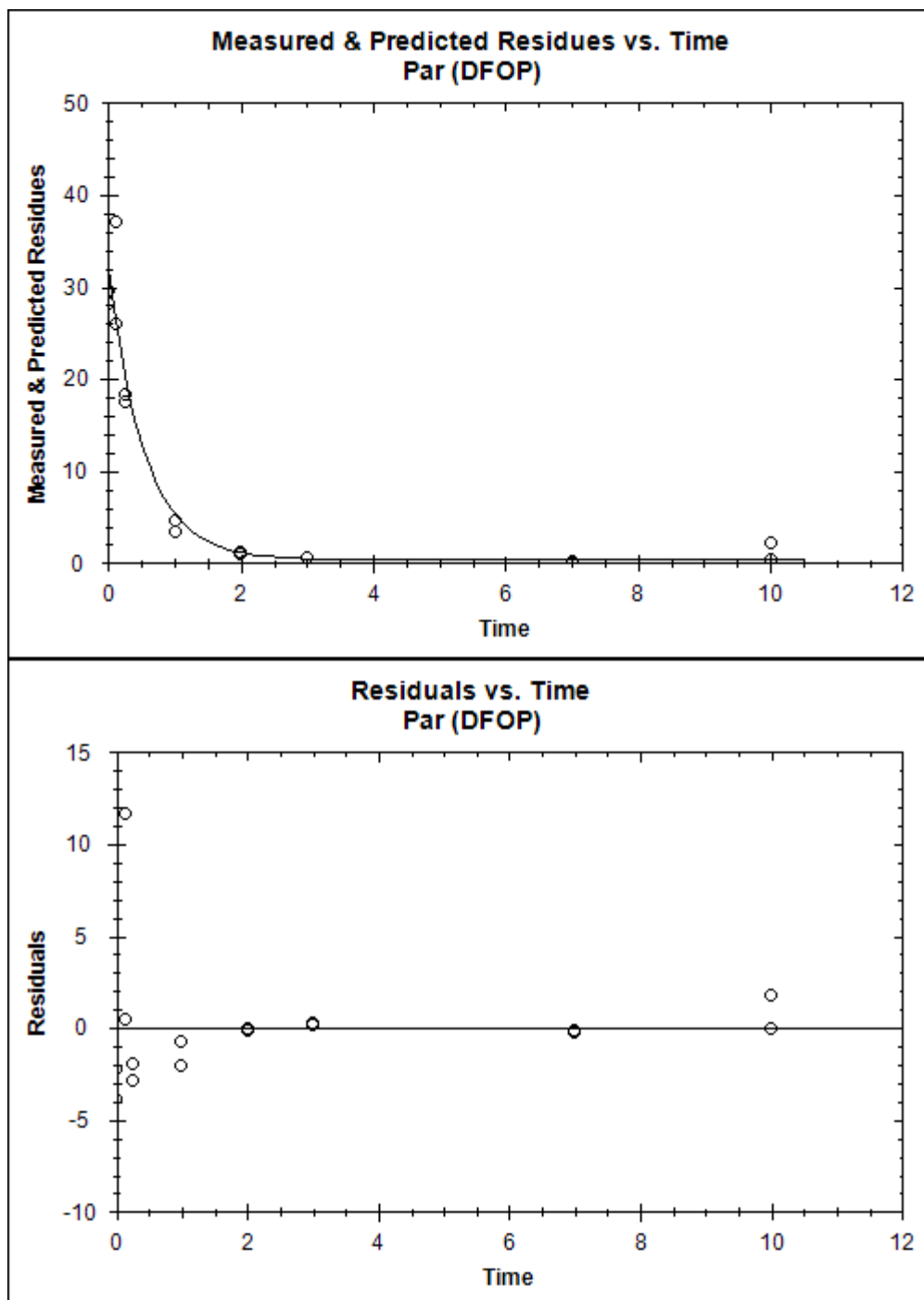
              Par
      DT50 :       0.3831
      DT90 :       1.3071
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 29.7100 3.3100 31.9987 -2.2887
0.0000 28.1500 3.3100 31.9987 -3.8487
0.1250 37.1200 3.3100 25.5030 11.6170
0.1250 25.9800 3.3100 25.5030 0.4770
0.2500 17.5300 3.3100 20.3396 -2.8096
0.2500 18.3500 3.3100 20.3396 -1.9896

```

1.0000	3.3400	3.3100	5.3760	-2.0360
1.0000	4.6400	3.3100	5.3760	-0.7360
2.0000	1.1400	3.3100	1.1320	0.0080
2.0000	1.0000	3.3100	1.1320	-0.1320
3.0000	0.6100	3.3100	0.4554	0.1546
3.0000	0.6800	3.3100	0.4554	0.2246
7.0000	0.0500	3.3100	0.3269	-0.2769
7.0000	0.1600	3.3100	0.3269	-0.1669
10.0000	0.3100	3.3100	0.3267	-0.0167
10.0000	2.1500	3.3100	0.3267	1.8233



11.6 Cyfluthrin Dissipation Sediment Phase

11.6.1 Barmen

11.6.1.1 SFO

```

# Trial      : Barmensponly
# File name  : Barmensponly IRLS SFO Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_s_ponly
# Created    : on 17 Sep 2013
#            : at 10:20
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See sediment
# # Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0) Par      :      68.36      0      Inf      False
k      Par      :      0.10      0      Inf      False

# -----
# Chi2 error estimation
# -----
# -----
# Par      All
Chi2Err% :      17.75      17.75
Kinetic model :      SFO

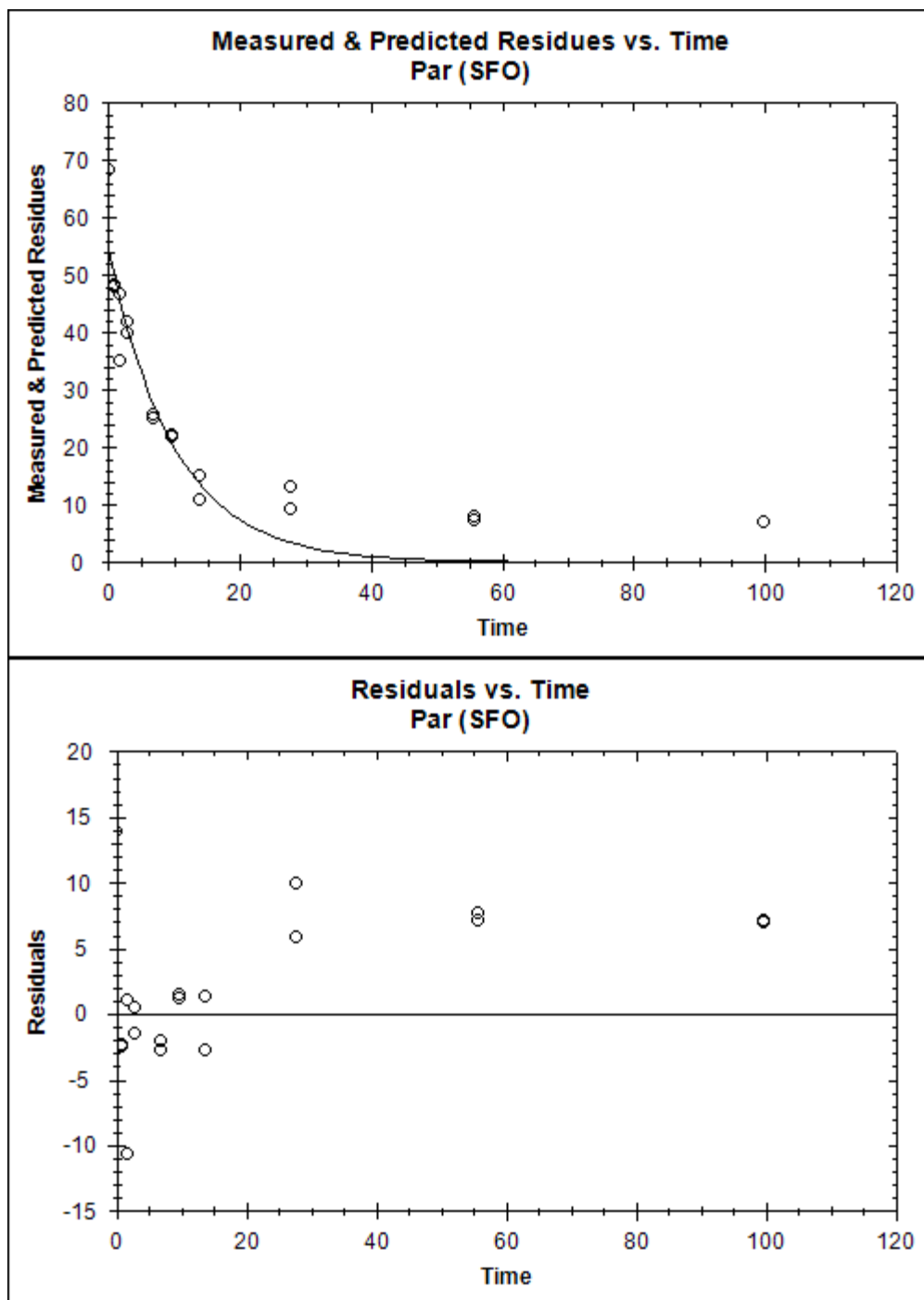
# -----
# Parameter estimation
# -----
# -----
Degrees of Freedom : 17
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0) Par      54.50527      47.67682      61.334      3.48397      7.93e-12
k      Par      0.09998      0.06497      0.135      0.01786      1.60e-05

# -----
# DT50 and DT90 values
# -----
# -----
# Par
DT50 :      6.9329
DT90 :      23.030
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----
# -----
Compartment Par
time observed err-std predicted residual
0.0000 68.3600 6.0127 54.5053 13.8547
0.0000 NA 6.0127 54.5053 NA
0.7500 48.1800 6.0127 50.5677 -2.3877
0.7500 48.2500 6.0127 50.5677 -2.3177
1.7500 35.1500 6.0127 45.7564 -10.6064
1.7500 46.7700 6.0127 45.7564 1.0136
2.7500 39.9800 6.0127 41.4030 -1.4230
2.7500 41.8600 6.0127 41.4030 0.4570

```

6.7500	25.0700	6.0127	27.7555	-2.6855
6.7500	25.6900	6.0127	27.7555	-2.0655
9.7500	21.7500	6.0127	20.5630	1.1870
9.7500	22.1200	6.0127	20.5630	1.5570
13.7500	15.1500	6.0127	13.7849	1.3651
13.7500	10.9800	6.0127	13.7849	-2.8049
27.7500	9.3300	6.0127	3.4003	5.9297
27.7500	13.3200	6.0127	3.4003	9.9197
55.7500	7.3000	6.0127	0.2069	7.0931
55.7500	7.8700	6.0127	0.2069	7.6631
99.7500	7.0100	6.0127	0.0025	7.0075
99.7500	7.1700	6.0127	0.0025	7.1675



11.6.1.2 HS

```

# Trial      : Barmensponly
# File name  : Barmensponly IRLS HS   Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_s_ponly
# Created    : on 17 Sep 2013
#            : at 10:20
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See sediment
# # Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      68.36      0      Inf      False
k1    Par      :      0.10      0      Inf      False
k2    Par      :      0.01      0      Inf      False
tb    Par      :      3.00      0      Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      13.22      13.22
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 15
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      60.736329      53.320205      68.152      3.783806      3.72e-11
k1    Par      :      0.183315      0.101504      0.265      0.041741      0.000263
k2    Par      :      0.022319      0.002562      0.042      0.010080      0.021363
tb    Par      :      5.479564      2.771744      8.187      1.381566      0.000621

# -----
# DT50 and DT90 values
# -----

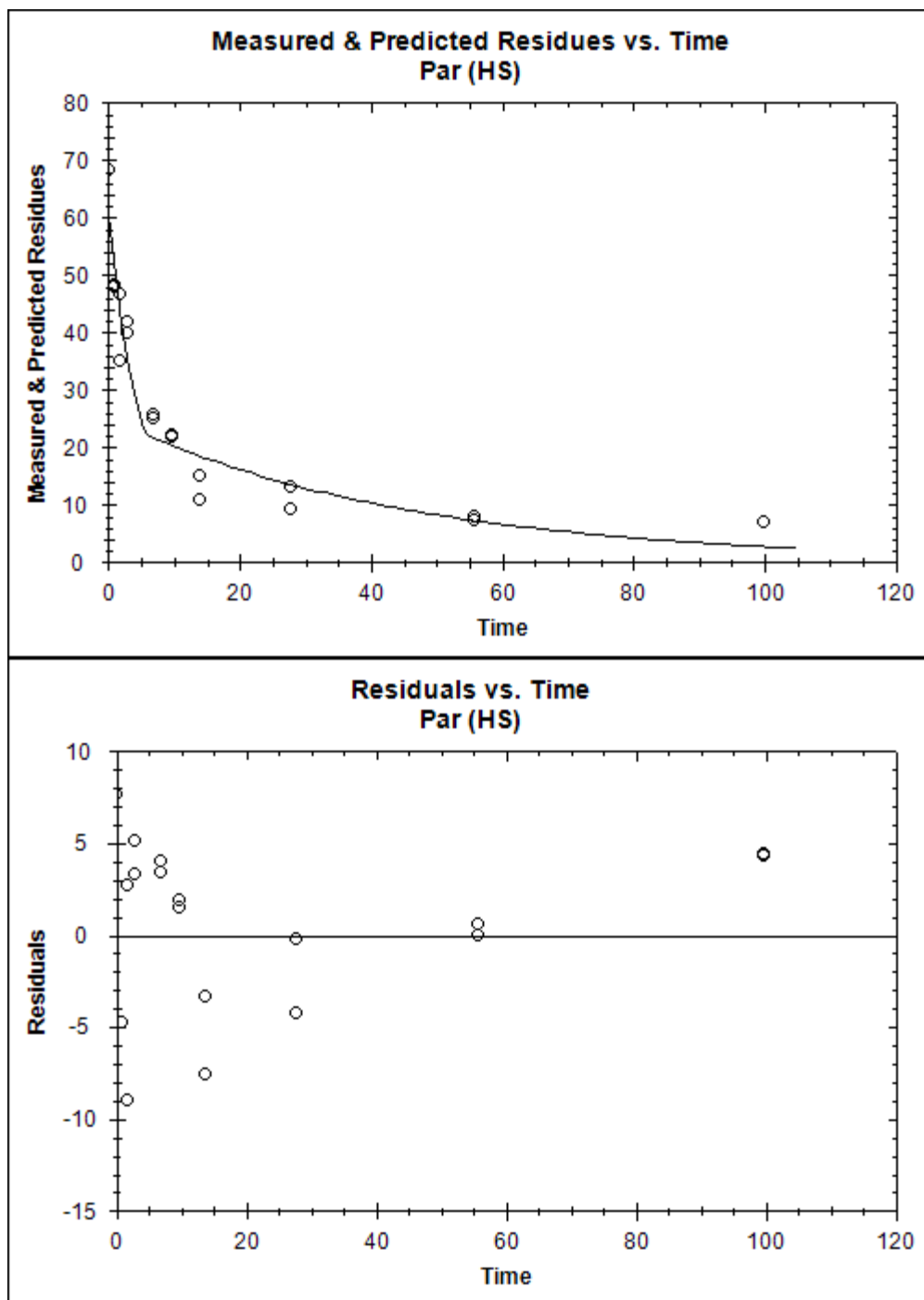
      Par
      DT50 :      3.7812
      DT90 :      63.640
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 68.3600 4.5047 60.7363 7.6237
0.0000 NA 4.5047 60.7363 NA
0.7500 48.1800 4.5047 52.9345 -4.7545
0.7500 48.2500 4.5047 52.9345 -4.6845
1.7500 35.1500 4.5047 44.0683 -8.9183
1.7500 46.7700 4.5047 44.0683 2.7017
2.7500 39.9800 4.5047 36.6871 3.2929
2.7500 41.8600 4.5047 36.6871 5.1729

```

6.7500	25.0700	4.5047	21.6217	3.4483
6.7500	25.6900	4.5047	21.6217	4.0683
9.7500	21.7500	4.5047	20.2214	1.5286
9.7500	22.1200	4.5047	20.2214	1.8986
13.7500	15.1500	4.5047	18.4943	-3.3443
13.7500	10.9800	4.5047	18.4943	-7.5143
27.7500	9.3300	4.5047	13.5311	-4.2011
27.7500	13.3200	4.5047	13.5311	-0.2111
55.7500	7.3000	4.5047	7.2431	0.0569
55.7500	7.8700	4.5047	7.2431	0.6269
99.7500	7.0100	4.5047	2.7129	4.2971
99.7500	7.1700	4.5047	2.7129	4.4571



11.6.1.3 FOMC

```

# Trial      : Barmensponly
# File name  : Barmensponly IRLS FOMC Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_s_ponly
# Created    : on 17 Sep 2013
#            : at 10:21
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See sediment
# # Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      68.36      0      Inf      False
alpha Par      :      0.10      0      Inf      False
beta  Par      :      0.10      0      Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      7.775      7.775
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 16
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      65.58888      58.64403      72.534      3.54336      1.57e-12
alpha Par      :      0.58122      0.42262      0.740      0.08092      1.09e-06
beta  Par      :      1.52717      0.31241      2.742      0.61979      0.0127

# -----
# DT50 and DT90 values
# -----

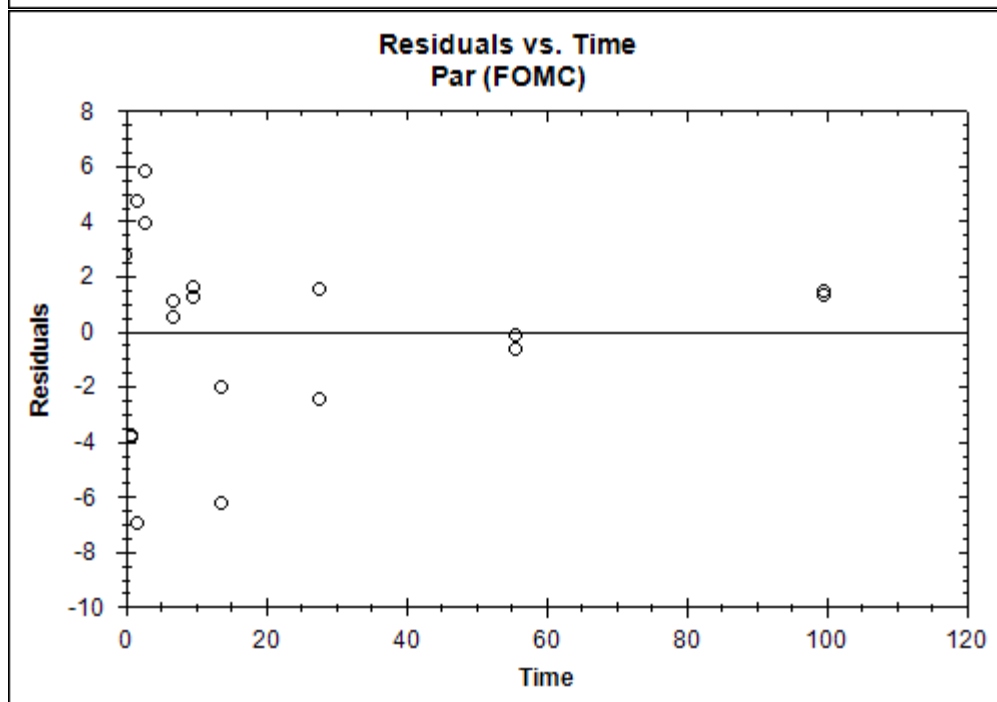
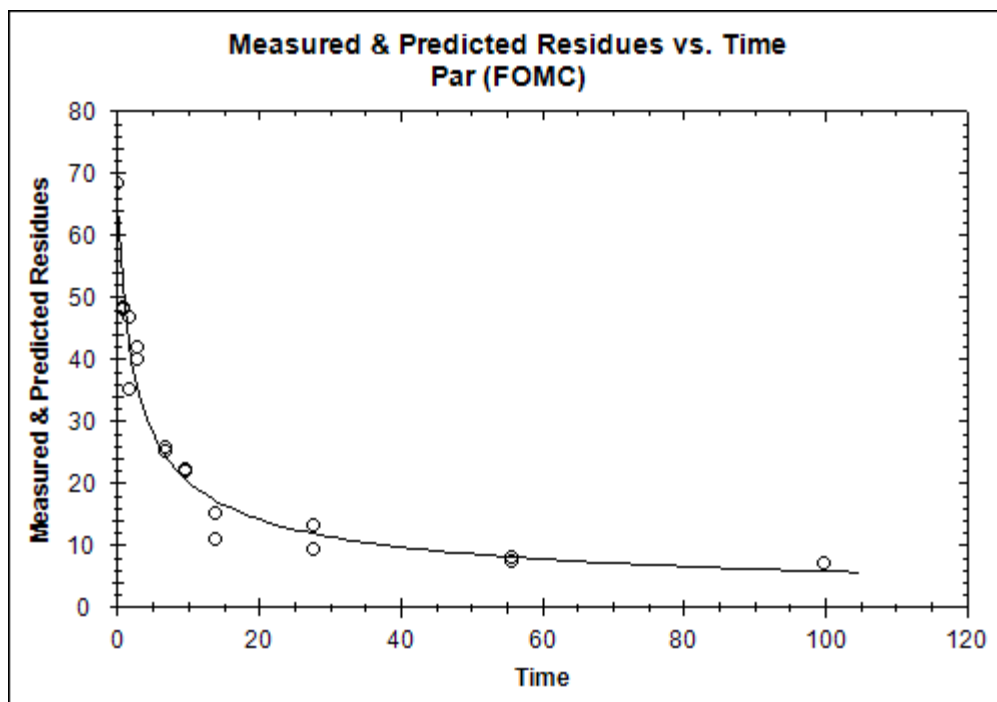
      Par
      DT50 :      3.5057
      DT90 :      78.715
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 68.3600 3.3769 65.5889 2.7711
0.0000 NA 3.3769 65.5889 NA
0.7500 48.1800 3.3769 51.9976 -3.8176
0.7500 48.2500 3.3769 51.9976 -3.7476
1.7500 35.1500 3.3769 42.0814 -6.9314
1.7500 46.7700 3.3769 42.0814 4.6886
2.7500 39.9800 3.3769 36.0469 3.9331
2.7500 41.8600 3.3769 36.0469 5.8131
6.7500 25.0700 3.3769 24.5593 0.5107
6.7500 25.6900 3.3769 24.5593 1.1307

```

9.7500	21.7500	3.3769	20.5186	1.2314
9.7500	22.1200	3.3769	20.5186	1.6014
13.7500	15.1500	3.3769	17.1996	-2.0496
13.7500	10.9800	3.3769	17.1996	-6.2196
27.7500	9.3300	3.3769	11.7851	-2.4551
27.7500	13.3200	3.3769	11.7851	1.5349
55.7500	7.3000	3.3769	7.9787	-0.6787
55.7500	7.8700	3.3769	7.9787	-0.1087
99.7500	7.0100	3.3769	5.7288	1.2812
99.7500	7.1700	3.3769	5.7288	1.4412



11.6.1.4 DFOP

```

# Trial      : Barmensponly
# File name  : Barmensponly IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_s_ponly
# Created    : on 17 Sep 2013
#            : at 10:20
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Sneikus
# # label: 14C
# # soil : Barmener See sediment
# # Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      68.36           0           Inf      False
k1    Par      :       0.10           0           Inf      False
k2    Par      :       0.01           0           Inf      False
g     Par      :       0.50           0            1      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      11.6      11.6
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 15
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :  59.514873  52.529222    66.501    3.564173    2.12e-11
k1    Par      :   0.227609   0.062458     0.393    0.084262     0.00821
k2    Par      :   0.009955  -0.006502     0.026    0.008397     0.12712
g     Par      :   0.739299   0.548155     0.930    0.097524     8.30e-07

# -----
# DT50 and DT90 values
# -----

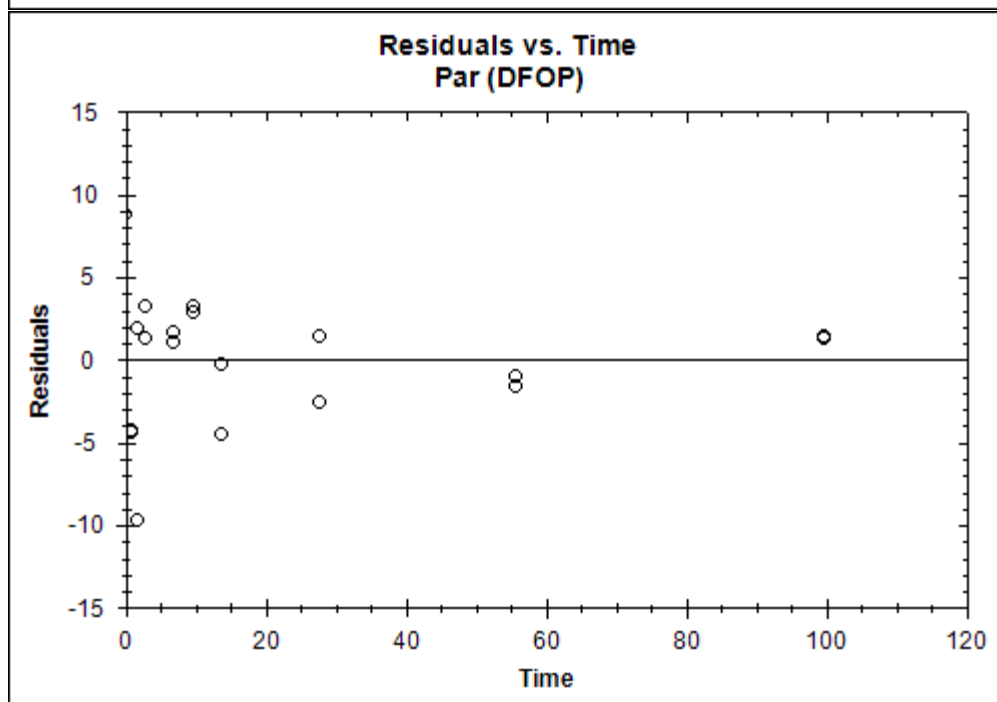
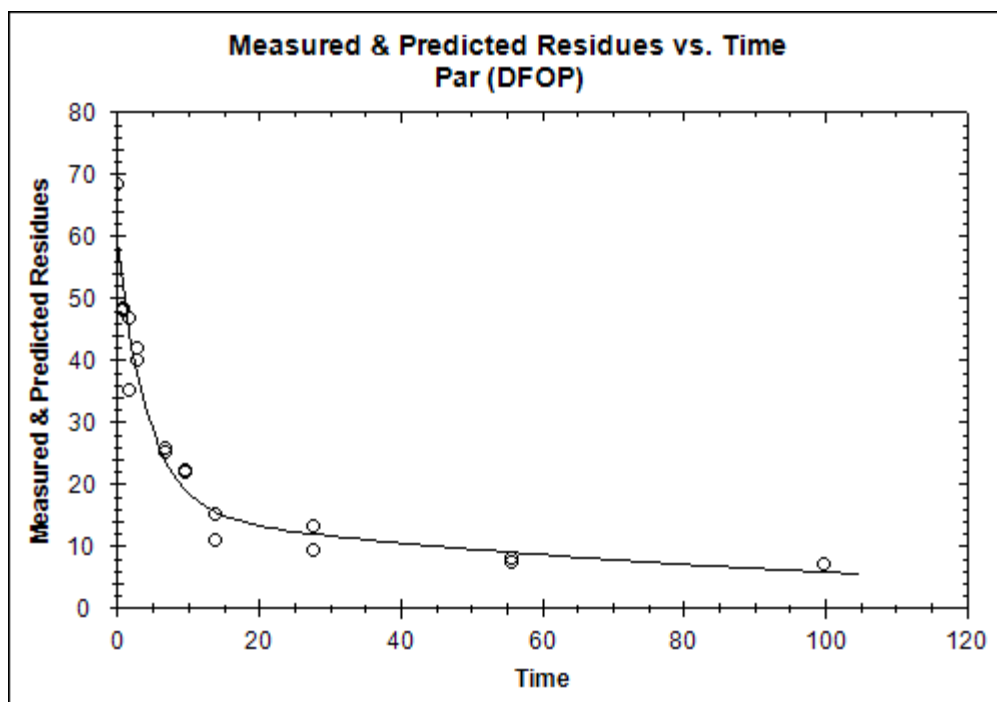
      Par
      DT50 :      4.7405
      DT90 :     96.255
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000  68.3600  3.8595  59.5149  8.8451
0.0000      NA  3.8595  59.5149      NA
0.7500  48.1800  3.8595  52.4946 -4.3146
0.7500  48.2500  3.8595  52.4946 -4.2446
1.7500  35.1500  3.8595  44.7909 -9.6409
1.7500  46.7700  3.8595  44.7909  1.9791
2.7500  39.9800  3.8595  38.6259  1.3541

```

2.7500	41.8600	3.8595	38.6259	3.2341
6.7500	25.0700	3.8595	23.9742	1.0958
6.7500	25.6900	3.8595	23.9742	1.7158
9.7500	21.7500	3.8595	18.8630	2.8870
9.7500	22.1200	3.8595	18.8630	3.2570
13.7500	15.1500	3.8595	15.4550	-0.3050
13.7500	10.9800	3.8595	15.4550	-4.4750
27.7500	9.3300	3.8595	11.8500	-2.5200
27.7500	13.3200	3.8595	11.8500	1.4700
55.7500	7.3000	3.8595	8.9074	-1.6074
55.7500	7.8700	3.8595	8.9074	-1.0374
99.7500	7.0100	3.8595	5.7480	1.2620
99.7500	7.1700	3.8595	5.7480	1.4220



11.6.2 Genkel

11.6.2.1 SFO

```
# Trial          : Genkelsponly
# File name     : Genkelsponly IRLS SFO  Par.r
# Target path   : C:\Emod\KinGUIII\WorkingDirectory\Genkel_s_ponly
# Created      : on 17 Sep 2013
#              : at 10:22
#              : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel sediment
# # Genkel sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par           :          66.37          0          Inf      False
k      Par           :           0.10          0          Inf      False

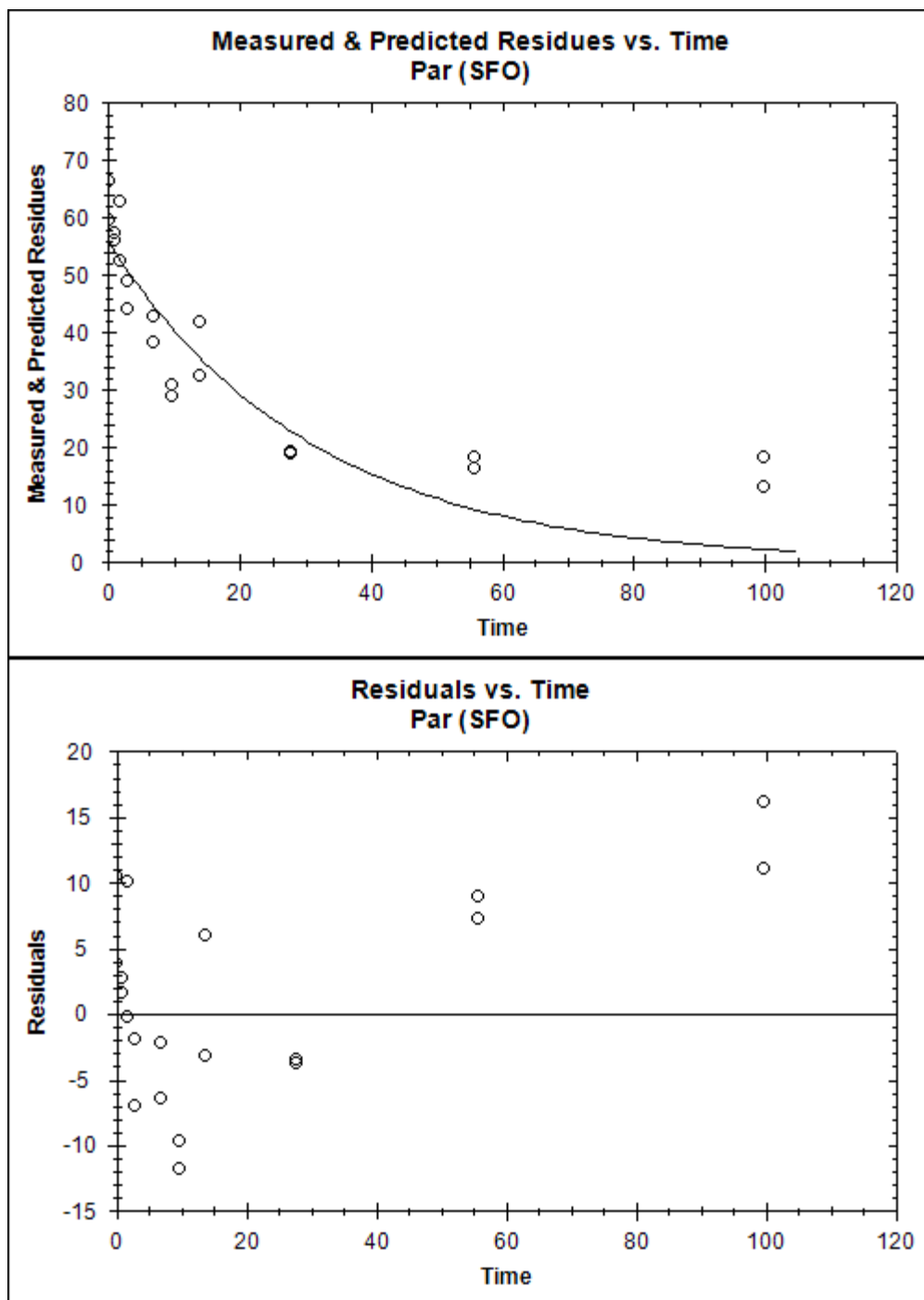
# -----
# Chi2 error estimation
# -----
# -----
# Par      All
Chi2Err% :      14.82      14.82
Kinetic model :      SFO

# -----
# Parameter estimation
# -----
# -----
Degrees of Freedom : 18
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      55.790009      49.125892      62.45      3.400123      1.42e-12
k      Par      :       0.032325       0.015007       0.05      0.008836      0.000899

# -----
# DT50 and DT90 values
# -----
# -----
# Par
DT50 :      21.443
DT90 :      71.232
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----
# -----
Compartment Par
time observed err-std predicted residual
0.0000 66.3700 7.6235 55.7900 10.5800
0.0000 59.6500 7.6235 55.7900 3.8600
0.7500 56.0500 7.6235 54.4537 1.5963
0.7500 57.2200 7.6235 54.4537 2.7663
1.7500 52.4900 7.6235 52.7216 -0.2316
1.7500 62.8200 7.6235 52.7216 10.0984
2.7500 49.0900 7.6235 51.0446 -1.9546
2.7500 44.0300 7.6235 51.0446 -7.0146
```

6.7500	42.7400	7.6235	44.8534	-2.1134
6.7500	38.4500	7.6235	44.8534	-6.4034
9.7500	31.0600	7.6235	40.7080	-9.6480
9.7500	28.9300	7.6235	40.7080	-11.7780
13.7500	41.8000	7.6235	35.7705	6.0295
13.7500	32.6100	7.6235	35.7705	-3.1605
27.7500	19.2500	7.6235	22.7502	-3.5002
27.7500	19.0200	7.6235	22.7502	-3.7302
55.7500	16.4900	7.6235	9.2024	7.2876
55.7500	18.2100	7.6235	9.2024	9.0076
99.7500	13.3000	7.6235	2.2192	11.0808
99.7500	18.4500	7.6235	2.2192	16.2308



11.6.2.2 HS

```

# Trial      : Genkelsponly
# File name  : Genkelsponly IRLS HS   Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_s_ponly
# Created    : on 17 Sep 2013
#            : at 10:23
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel sediment
# # Genkel sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      66.37      0      Inf      False
k1    Par      :      0.10      0      Inf      False
k2    Par      :      0.01      0      Inf      False
tb    Par      :      3.00      0      Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      9.969      9.969
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 16
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      62.899954      56.263094      69.537      3.386215      1.49e-12
k1    Par      :      0.092425      0.021732      0.163      0.036068      0.010435
k2    Par      :      0.013035      0.006323      0.020      0.003424      0.000776
tb    Par      :      6.062745      1.339777      10.786      2.409722      0.011463

# -----
# DT50 and DT90 values
# -----

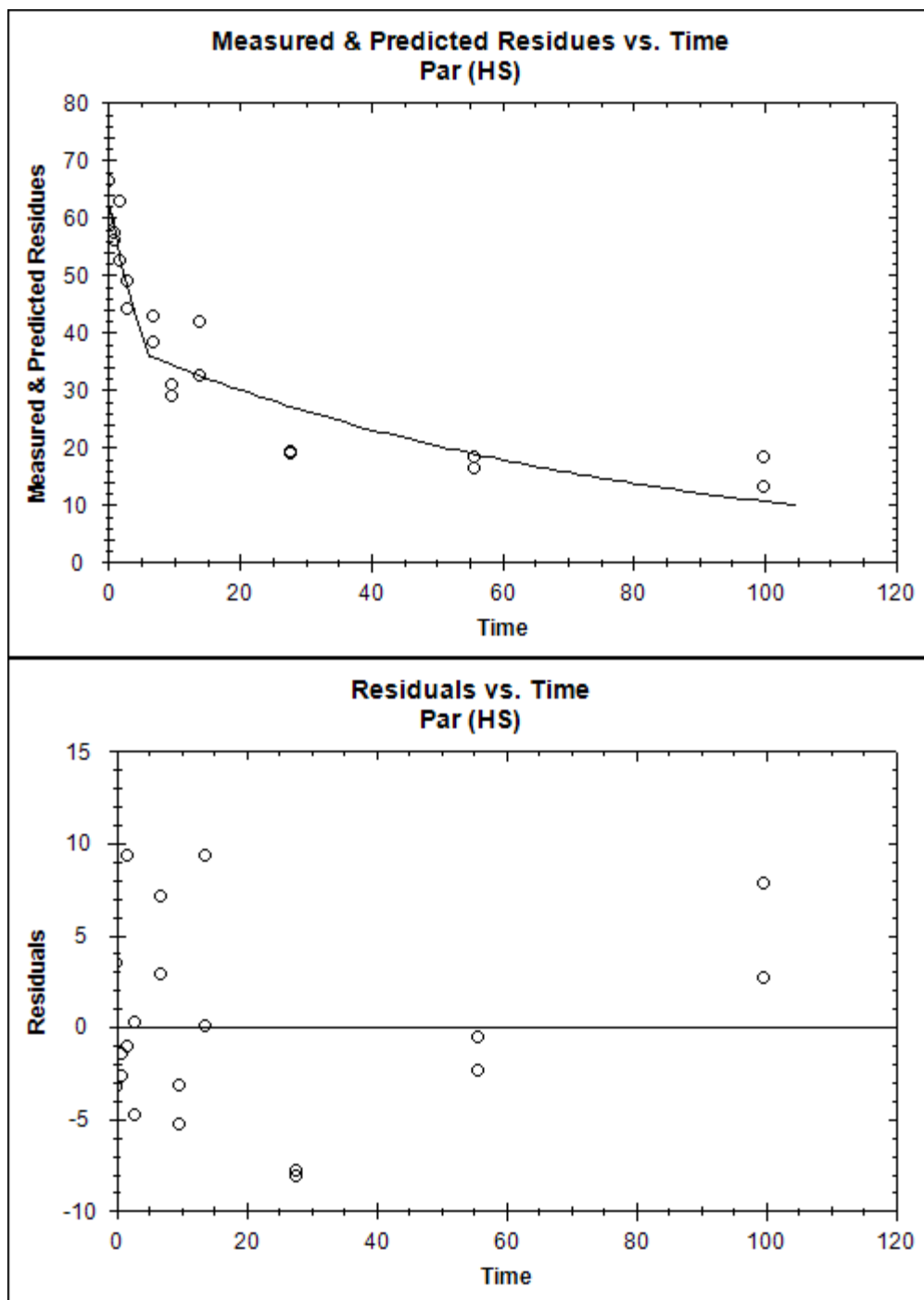
      Par
      DT50 :      16.251
      DT90 :      139.73
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 66.3700 5.1329 62.9000 3.4700
0.0000 59.6500 5.1329 62.9000 -3.2500
0.7500 56.0500 5.1329 58.6875 -2.6375
0.7500 57.2200 5.1329 58.6875 -1.4675
1.7500 52.4900 5.1329 53.5065 -1.0165
1.7500 62.8200 5.1329 53.5065 9.3135
2.7500 49.0900 5.1329 48.7828 0.3072
2.7500 44.0300 5.1329 48.7828 -4.7528

```

6.7500	42.7400	5.1329	35.5962	7.1438
6.7500	38.4500	5.1329	35.5962	2.8538
9.7500	31.0600	5.1329	34.2312	-3.1712
9.7500	28.9300	5.1329	34.2312	-5.3012
13.7500	41.8000	5.1329	32.4921	9.3079
13.7500	32.6100	5.1329	32.4921	0.1179
27.7500	19.2500	5.1329	27.0724	-7.8224
27.7500	19.0200	5.1329	27.0724	-8.0524
55.7500	16.4900	5.1329	18.7942	-2.3042
55.7500	18.2100	5.1329	18.7942	-0.5842
99.7500	13.3000	5.1329	10.5912	2.7088
99.7500	18.4500	5.1329	10.5912	7.8588



11.6.2.3 FOMC

```

# Trial      : Genkelsponly
# File name  : Genkelsponly IRLS FOMC Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_s_ponly
# Created    : on 17 Sep 2013
#            : at 10:23
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel sediment
# # Genkel sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      66.37              0              Inf      False
alpha Par      :      0.10              0              Inf      False
beta  Par      :      0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      7.619      Par      All
      Kinetic model :      FOMC              7.619

# -----
# Parameter estimation
# -----

Degrees of Freedom : 17
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      63.29576      57.94518      68.646      2.72994      1.32e-14
alpha Par      :      0.46541      0.25842      0.672      0.10561      0.000193
beta  Par      :      3.78930      -0.05059      7.629      1.95916      0.034960

# -----
# DT50 and DT90 values
# -----

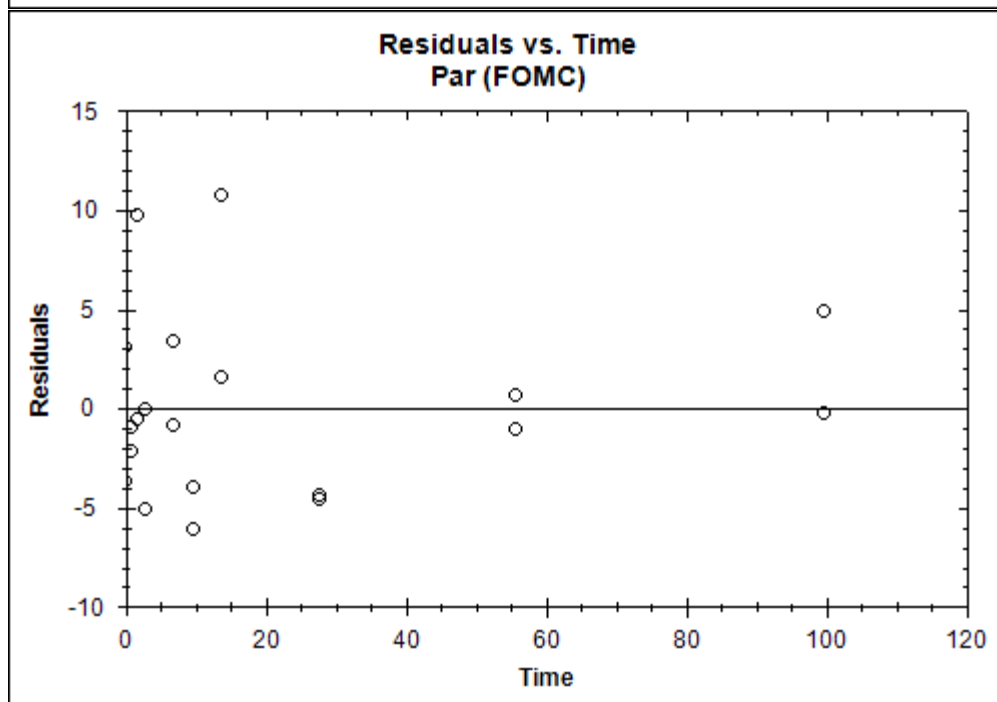
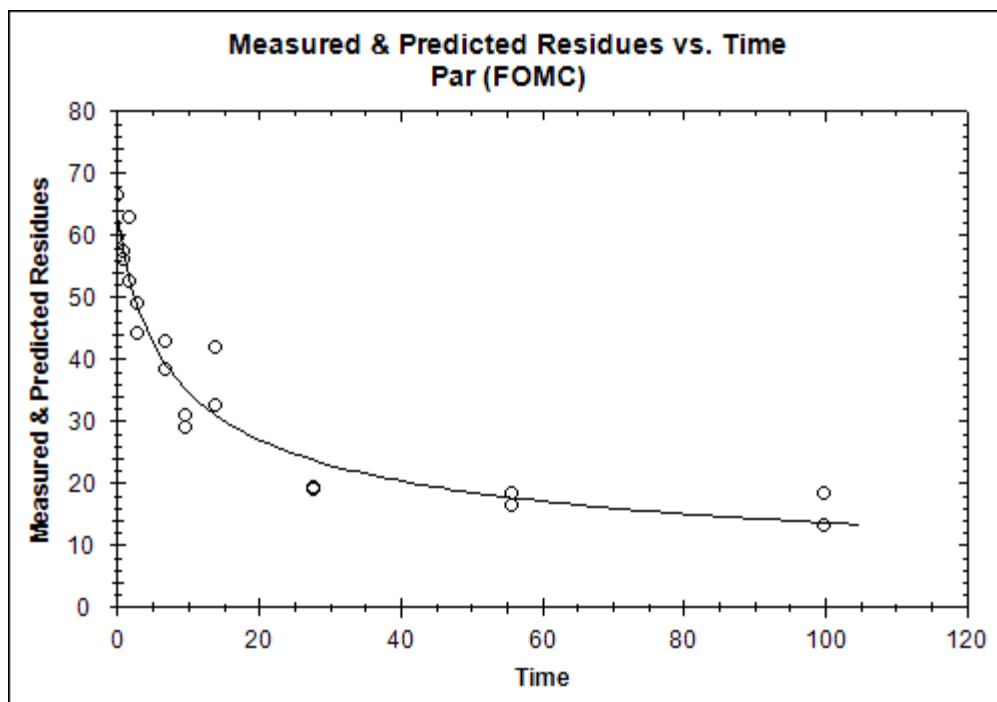
      Par
      DT50 :      13.013
      DT90 :      529.79
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 66.3700 4.4649 63.2958 3.0742
0.0000 59.6500 4.4649 63.2958 -3.6458
0.7500 56.0500 4.4649 58.1932 -2.1432
0.7500 57.2200 4.4649 58.1932 -0.9732
1.7500 52.4900 4.4649 53.0433 -0.5533
1.7500 62.8200 4.4649 53.0433 9.7767
2.7500 49.0900 4.4649 49.1004 -0.0104
2.7500 44.0300 4.4649 49.1004 -5.0704
6.7500 42.7400 4.4649 39.3201 3.4199
6.7500 38.4500 4.4649 39.3201 -0.8701

```

9.7500	31.0600	4.4649	34.9933	-3.9333
9.7500	28.9300	4.4649	34.9933	-6.0633
13.7500	41.8000	4.4649	31.0217	10.7783
13.7500	32.6100	4.4649	31.0217	1.5883
27.7500	19.2500	4.4649	23.6081	-4.3581
27.7500	19.0200	4.4649	23.6081	-4.5881
55.7500	16.4900	4.4649	17.5642	-1.0742
55.7500	18.2100	4.4649	17.5642	0.6458
99.7500	13.3000	4.4649	13.5766	-0.2766
99.7500	18.4500	4.4649	13.5766	4.8734



11.6.2.4 DFOP

```

# Trial      : Genkelsponly
# File name  : Genkelsponly IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Genkel_s_ponly
# Created    : on 17 Sep 2013
#            : at 10:23
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Sneikus
# # label: 14C
# # soil : Genkel sediment
# # Genkel sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      66.37              0              Inf      False
k1    Par      :      0.10              0              Inf      False
k2    Par      :      0.01              0              Inf      False
g     Par      :      0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :      8.117      8.117
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 16
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      61.204670      56.294726      66.115      2.505119      2.14e-14
k1    Par      :      0.105004      0.021262      0.189      0.042726      0.012889
k2    Par      :      0.003044      -0.008483      0.015      0.005881      0.305915
g     Par      :      0.657711      0.376816      0.939      0.143316      0.000151

# -----
# DT50 and DT90 values
# -----

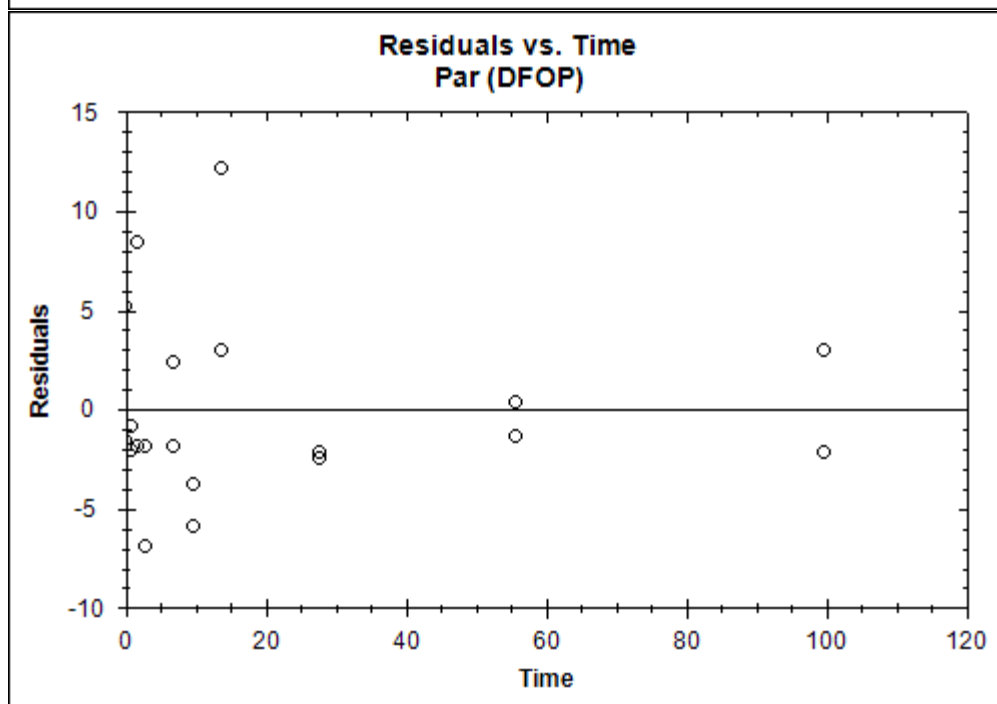
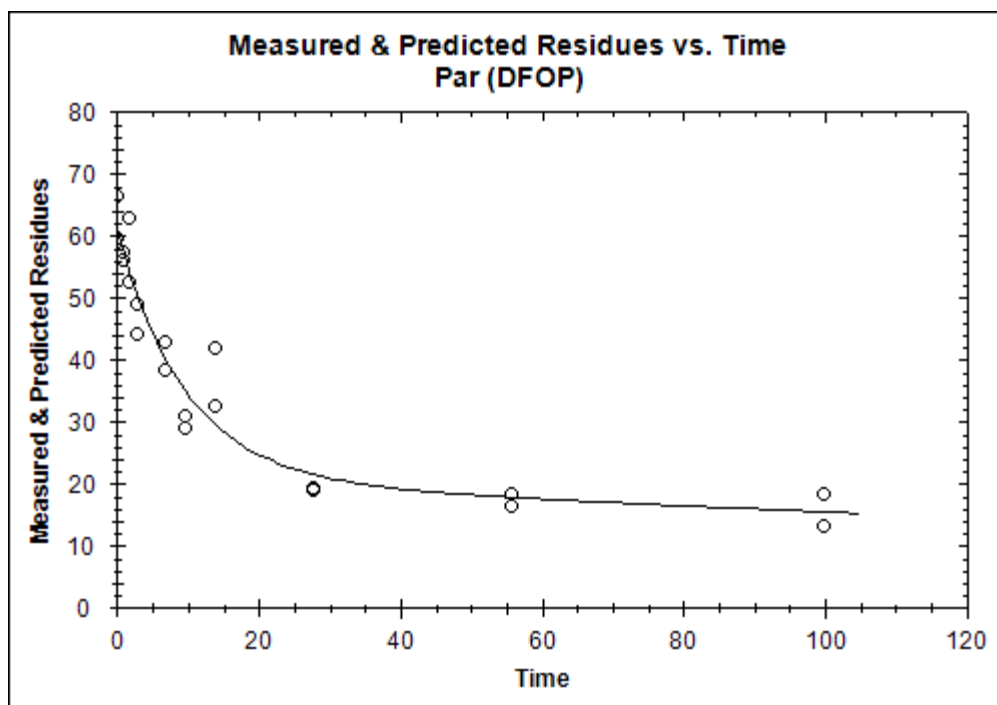
              Par
      DT50 :      12.838
      DT90 :      404.24
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 66.3700 4.4863 61.2047 5.1653
0.0000 59.6500 4.4863 61.2047 -1.5547
0.7500 56.0500 4.4863 58.1083 -2.0583
0.7500 57.2200 4.4863 58.1083 -0.8883
1.7500 52.4900 4.4863 54.3361 -1.8461
1.7500 62.8200 4.4863 54.3361 8.4839
2.7500 49.0900 4.4863 50.9337 -1.8437

```

2.7500	44.0300	4.4863	50.9337	-6.9037
6.7500	42.7400	4.4863	40.3389	2.4011
6.7500	38.4500	4.4863	40.3389	-1.8889
9.7500	31.0600	4.4863	34.7979	-3.7379
9.7500	28.9300	4.4863	34.7979	-5.8679
13.7500	41.8000	4.4863	29.5922	12.2078
13.7500	32.6100	4.4863	29.5922	3.0178
27.7500	19.2500	4.4863	21.4372	-2.1872
27.7500	19.0200	4.4863	21.4372	-2.4172
55.7500	16.4900	4.4863	17.7953	-1.3053
55.7500	18.2100	4.4863	17.7953	0.4147
99.7500	13.3000	4.4863	15.4648	-2.1648
99.7500	18.4500	4.4863	15.4648	2.9852



11.6.3 Ijzendoorn

11.6.3.1 SFO

```
# Trial : IjzendoornsCYF
# File name : IjzendoornsCYF IRLS SFO CYF.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_CYF
# Created : on 18 Oct 2013
# at 10:27
# by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      8.6              0              Inf      False
k      CYF      :      0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

CYF      All
Chi2Err% :      24.04      24.04
Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 8
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  CYF      :      19.83618      11.00216      28.670      4.50723      0.00114
k      CYF      :      0.10285      -0.03172      0.237      0.06866      0.08626

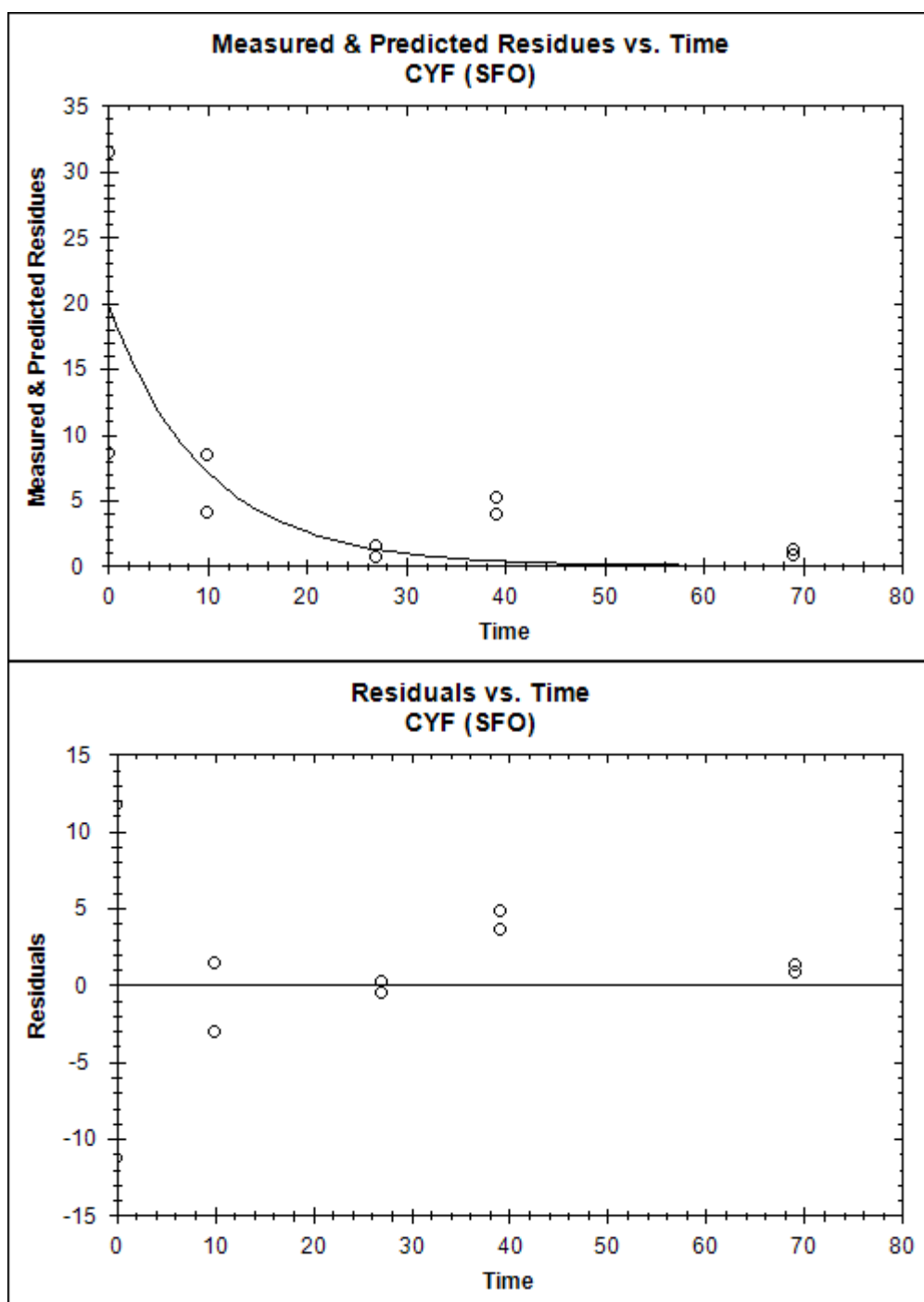
# -----
# DT50 and DT90 values
# -----

CYF
DT50 :      6.7391
DT90 :      22.387
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

Compartment CYF
time observed err-std predicted residual
0.0000  8.6000  5.5920  19.8362 -11.2362
0.0000  31.5000  5.5920  19.8362  11.6638
10.0000  4.1000  5.5920  7.0920 -2.9920
10.0000  8.5000  5.5920  7.0920  1.4080
27.0000  1.5000  5.5920  1.2342  0.2658
27.0000  0.7000  5.5920  1.2342 -0.5342
39.0000  5.2000  5.5920  0.3592  4.8408
39.0000  4.0000  5.5920  0.3592  3.6408
69.0000  0.9000  5.5920  0.0164  0.8836
```

69.0000 1.3000 5.5920 0.0164 1.2836



11.6.3.2HS

```

# Trial      : IjzendoornsCYF
# File name  : IjzendoornsCYF IRLS HS   CYF.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_CYF
# Created    : on 18 Oct 2013
#            : at 10:27
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      8.60              0              Inf      False
k1    CYF      :      0.10              0              Inf      False
k2    CYF      :      0.01              0              Inf      False
tb    CYF      :      3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      CYF      All
Chi2Err% :      61.21      61.21
Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  CYF      :      20.0500      8.7406      31.359      5.7702      0.00661
k1    CYF      :      2.7650     -92.9315      98.461     48.8256      0.47834
k2    CYF      :      0.3627     -7.8783      8.604      4.2046      0.46703
tb    CYF      :      6.0044     -72.0198     84.029     39.8090      0.44253

# -----
# DT50 and DT90 values
# -----

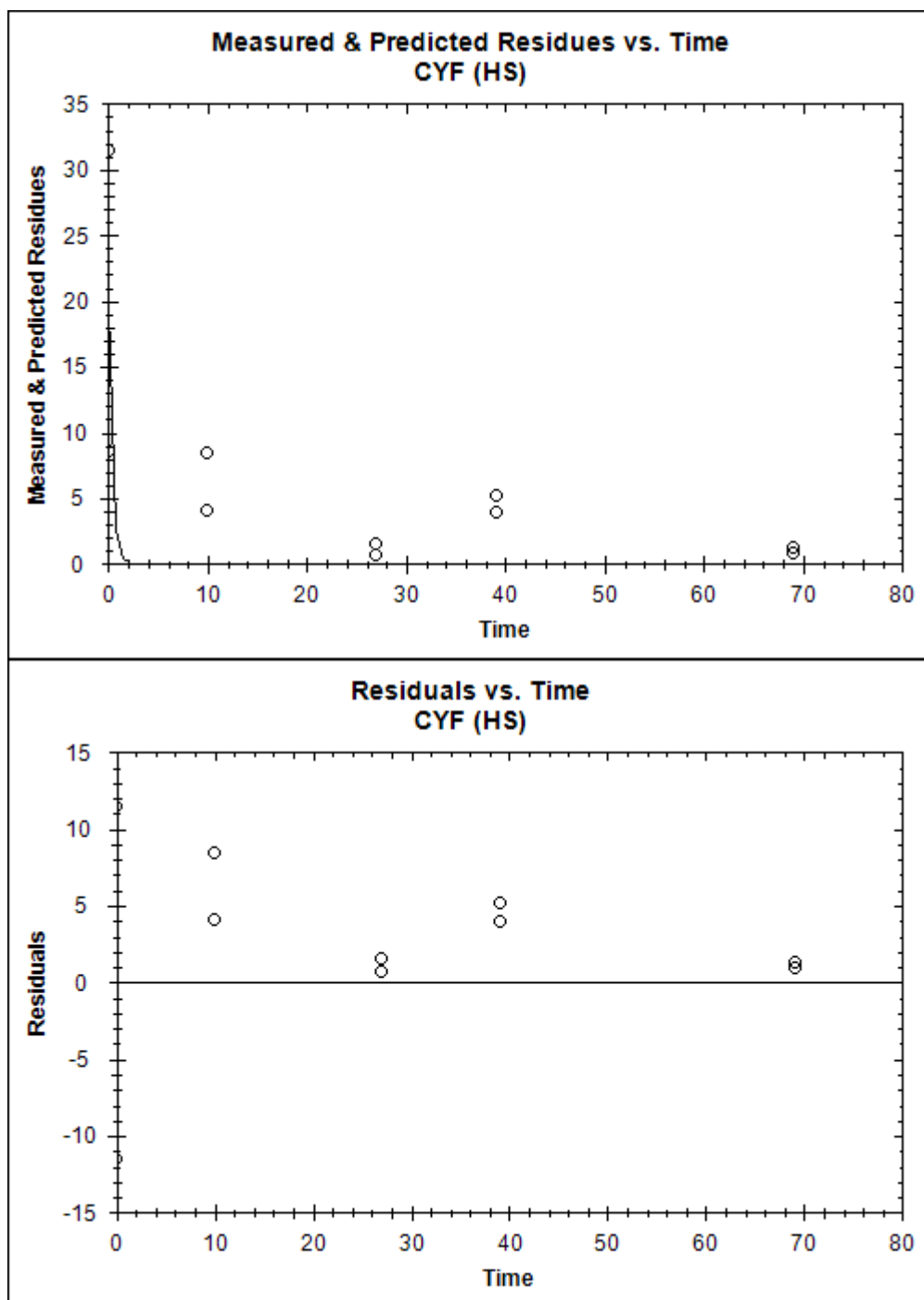
      CYF
DT50 :      0.2507
DT90 :      0.8328
Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment CYF
time observed err-std predicted residual
0.0000  8.6000  6.3210  20.0500 -11.4500
0.0000  31.5000  6.3210  20.0500  11.4500
10.0000  4.1000  6.3210   0.0000   4.1000
10.0000  8.5000  6.3210   0.0000   8.5000
27.0000  1.5000  6.3210   0.0000   1.5000
27.0000  0.7000  6.3210   0.0000   0.7000
39.0000  5.2000  6.3210   0.0000   5.2000

```

39.0000	4.0000	6.3210	0.0000	4.0000
69.0000	0.9000	6.3210	0.0000	0.9000
69.0000	1.3000	6.3210	0.0000	1.3000



11.6.3.3 FOMC

```

# Trial      : IjzendoornsCYF
# File name  : IjzendoornsCYF IRLS FOMC CYF.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_CYF
# Created    : on 18 Oct 2013
#            : at 10:27
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      8.6          0          Inf      False
alpha CYF      :      0.1          0          Inf      False
beta  CYF      :      0.1          0          Inf      False

# -----
# Chi2 error estimation
# -----

      CYF      All
Chi2Err% :      18.72      18.72
Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  CYF      :      20.056      10.964      29.148      4.639      0.00173
alpha CYF      :      0.783      -2.442      4.007      1.645      0.32431
beta  CYF      :      2.735      -23.278      28.748      13.272      0.42130

# -----
# DT50 and DT90 values
# -----

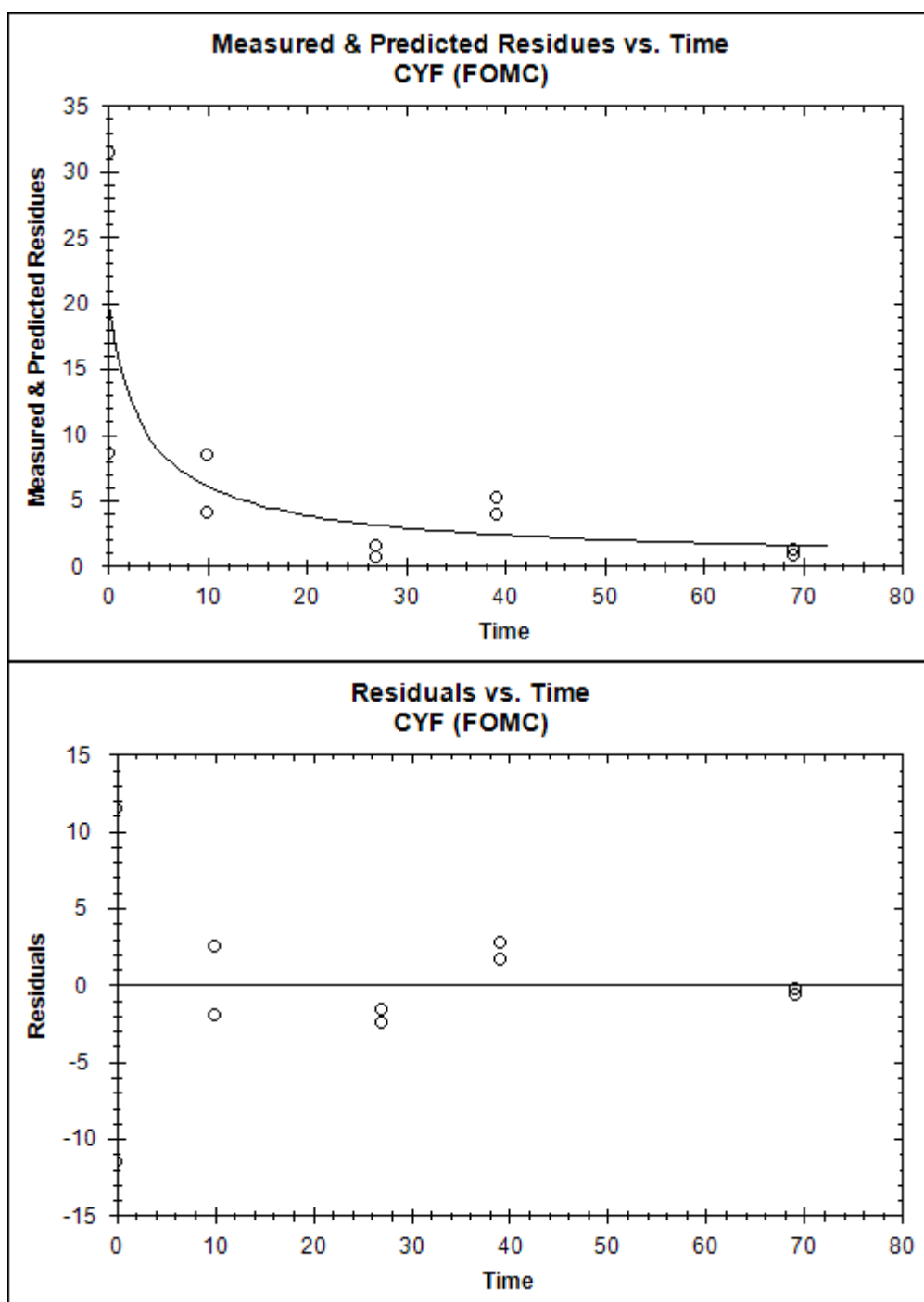
      CYF
DT50 :      3.8933
DT90 :      49.035
Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment CYF
time observed err-std predicted residual
0.0000  8.6000  5.3987  20.0560 -11.4560
0.0000  31.5000  5.3987  20.0560  11.4440
10.0000  4.1000  5.3987   6.0139  -1.9139
10.0000  8.5000  5.3987   6.0139   2.4861
27.0000  1.5000  5.3987   3.0960  -1.5960
27.0000  0.7000  5.3987   3.0960  -2.3960
39.0000  5.2000  5.3987   2.3742   2.8258
39.0000  4.0000  5.3987   2.3742   1.6258
69.0000  0.9000  5.3987   1.5536  -0.6536

```

69.0000 1.3000 5.3987 1.5536 -0.2536



11.6.3.4 DFOP

```

# Trial      : IjzendoornsCYF
# File name  : IjzendoornsCYF IRLS DFOP CYF.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_CYF
# Created    : on 18 Oct 2013
#            : at 10:27
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      8.60              0              Inf      False
k1    CYF      :      0.10              0              Inf      False
k2    CYF      :      0.01              0              Inf      False
g     CYF      :      0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              CYF      All
      Chi2Err% :      22.21      22.21
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  CYF      :      20.070937      10.254465      29.887      5.008496      0.00353
k1    CYF      :      0.169896      -0.353628      0.693      0.267109      0.27411
k2    CYF      :      0.008752      -0.128812      0.146      0.070187      0.45242
g     CYF      :      0.834404      -0.268107      1.937      0.562516      0.09425

# -----
# DT50 and DT90 values
# -----

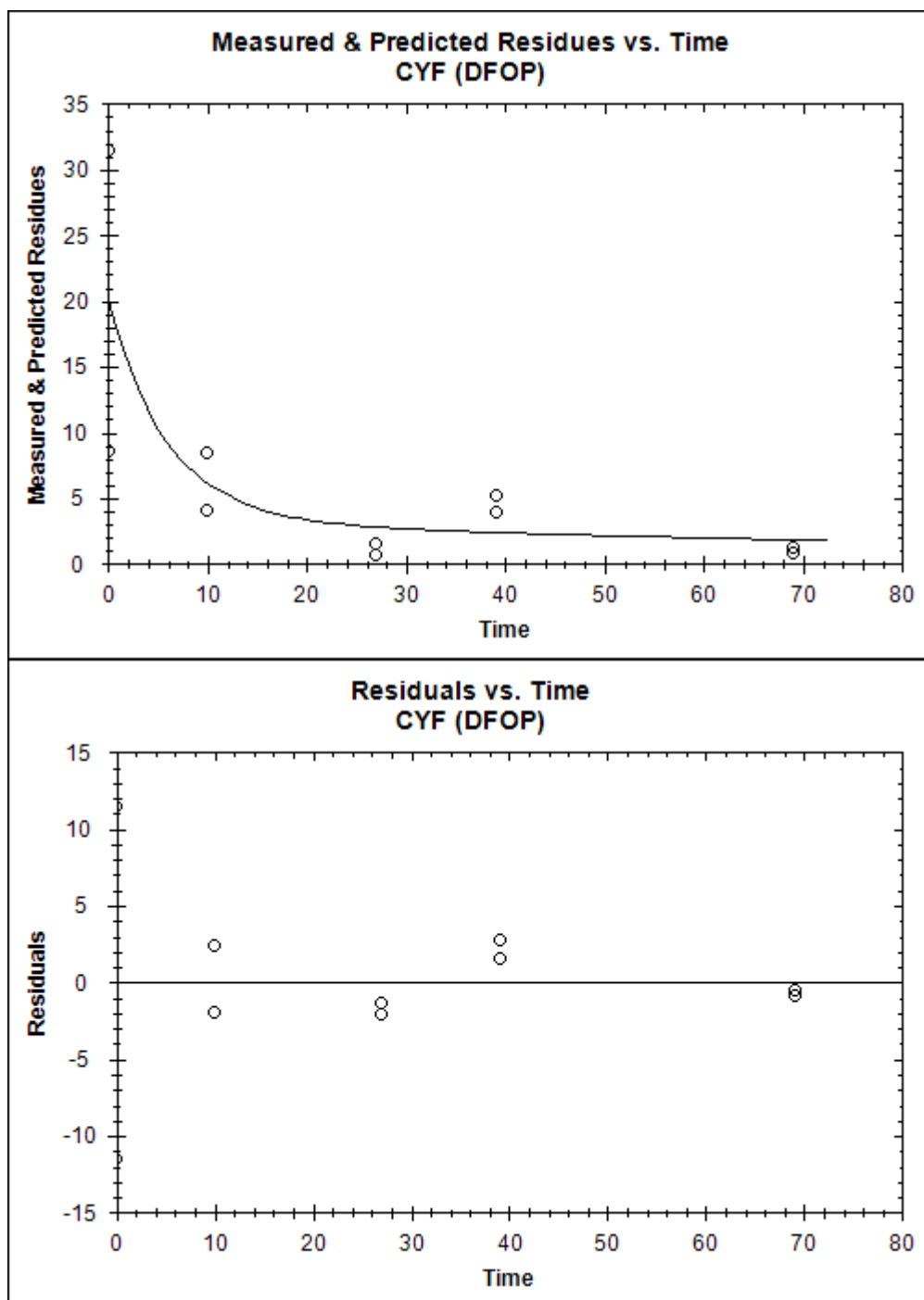
              CYF
      DT50 :      5.2524
      DT90 :      57.685
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment CYF
      time observed err-std predicted residual
0.0000      8.6000      5.3821      20.0709      -11.4709
0.0000     31.5000      5.3821      20.0709      11.4291
10.0000      4.1000      5.3821      6.1078      -2.0078
10.0000      8.5000      5.3821      6.1078      2.3922
27.0000      1.5000      5.3821      2.7947      -1.2947
27.0000      0.7000      5.3821      2.7947      -2.0947
39.0000      5.2000      5.3821      2.3848      2.8152

```

39.0000	4.0000	5.3821	2.3848	1.6152
69.0000	0.9000	5.3821	1.8172	-0.9172
69.0000	1.3000	5.3821	1.8172	-0.5172



11.6.4 Lienden

11.6.4.1 SFO

```
# Trial      : LiendensCYF
# File name  : LiendensCYF IRLS SFO  CYF.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_CYF
# Created    : on 18 Oct 2013
#            : at 11:37
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      21.3              0              Inf      False
k      CYF      :       0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      22.12      22.12
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 8
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  CYF      :      12.14280      4.94822      19.337      3.67077
0.00537
k      CYF      :       0.08635     -0.04562      0.218      0.06734
0.11780

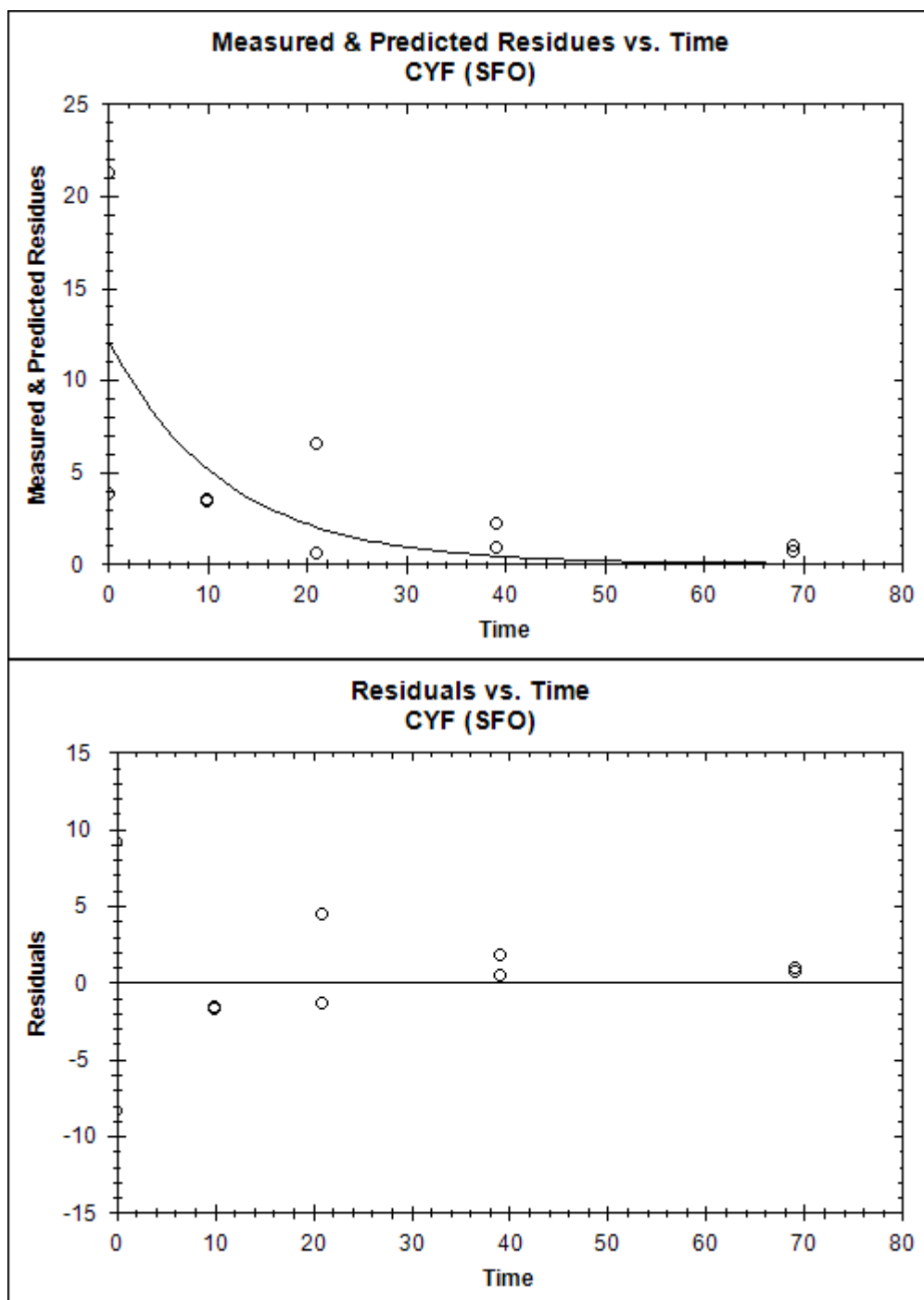
# -----
# DT50 and DT90 values
# -----

      DT50 :      8.0268
      DT90 :      26.664
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment CYF
      time observed err-std predicted residual
0.0000  21.3000  4.3147  12.1428  9.1572
0.0000  3.8000  4.3147  12.1428 -8.3428
10.0000  3.5000  4.3147  5.1202 -1.6202
10.0000  3.4000  4.3147  5.1202 -1.7202
21.0000  6.5000  4.3147  1.9804  4.5196
21.0000  0.6000  4.3147  1.9804 -1.3804
39.0000  0.9000  4.3147  0.4185  0.4815
```

39.0000	2.2000	4.3147	0.4185	1.7815
69.0000	0.7000	4.3147	0.0314	0.6686
69.0000	1.0000	4.3147	0.0314	0.9686



11.6.4.2HS

```

# Trial      : LiendensCYF
# File name  : LiendensCYF IRLS HS   CYF.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_CYF
# Created    : on 18 Oct 2013
#            : at 11:38
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      21.30              0              Inf      False
k1    CYF      :       0.10              0              Inf      False
k2    CYF      :       0.01              0              Inf      False
tb    CYF      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

              CYF      All
      Chi2Err% :      9.326      9.326
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  CYF      :      12.55010      5.05827      20.042      3.82243
0.00838
k1    CYF      :       0.19915     -17.73746      18.136      9.15150
0.49167
k2    CYF      :       0.02414     -0.16473       0.213      0.09636
0.40528
tb    CYF      :       5.48288    -530.87377     541.840     273.65638
0.49233

# -----
# DT50 and DT90 values
# -----

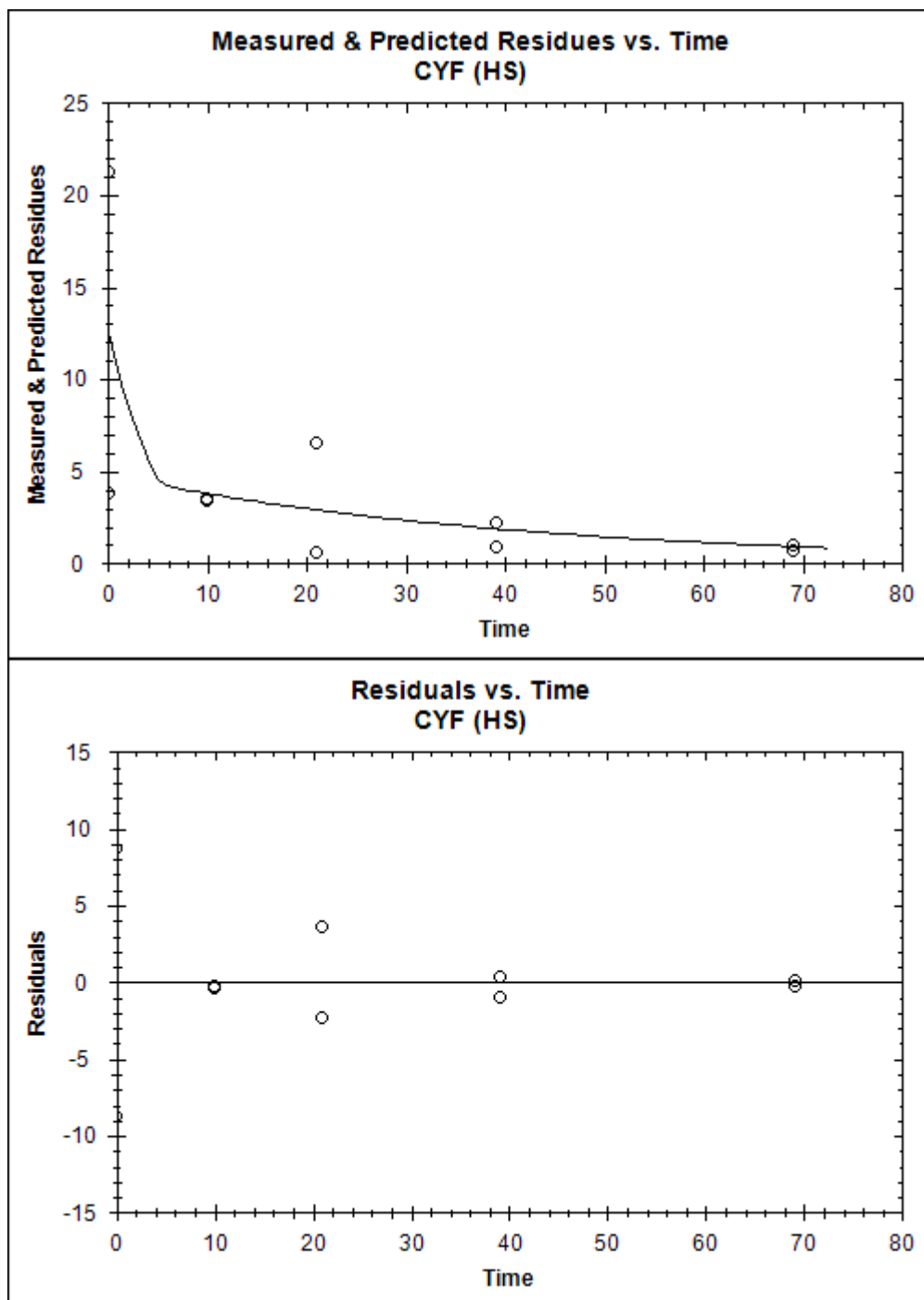
              CYF
      DT50 :       3.4805
      DT90 :       55.636
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment CYF
      time observed err-std predicted residual
0.0000  21.3000  4.1559  12.5501  8.7499
0.0000   3.8000  4.1559  12.5501 -8.7501

```

10.0000	3.5000	4.1559	3.7764	-0.2764
10.0000	3.4000	4.1559	3.7764	-0.3764
21.0000	6.5000	4.1559	2.8957	3.6043
21.0000	0.6000	4.1559	2.8957	-2.2957
39.0000	0.9000	4.1559	1.8752	-0.9752
39.0000	2.2000	4.1559	1.8752	0.3248
69.0000	0.7000	4.1559	0.9090	-0.2090
69.0000	1.0000	4.1559	0.9090	0.0910



11.6.4.3FOMC

```

# Trial      : LiendensCYF
# File name  : LiendensCYF IRLS FOMC CYF.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_CYF
# Created    : on 18 Oct 2013
#            : at 11:38
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      21.3              0              Inf      False
alpha CYF      :       0.1              0              Inf      False
beta  CYF      :       0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      CYF      All
      Chi2Err% :      10.90      10.90
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  CYF      :      12.544      6.057      19.030      3.310      0.0034
alpha CYF      :       0.619     -2.304      3.542      1.491      0.3453
beta  CYF      :       1.758     -20.277     23.794     11.243      0.4401

# -----
# DT50 and DT90 values
# -----

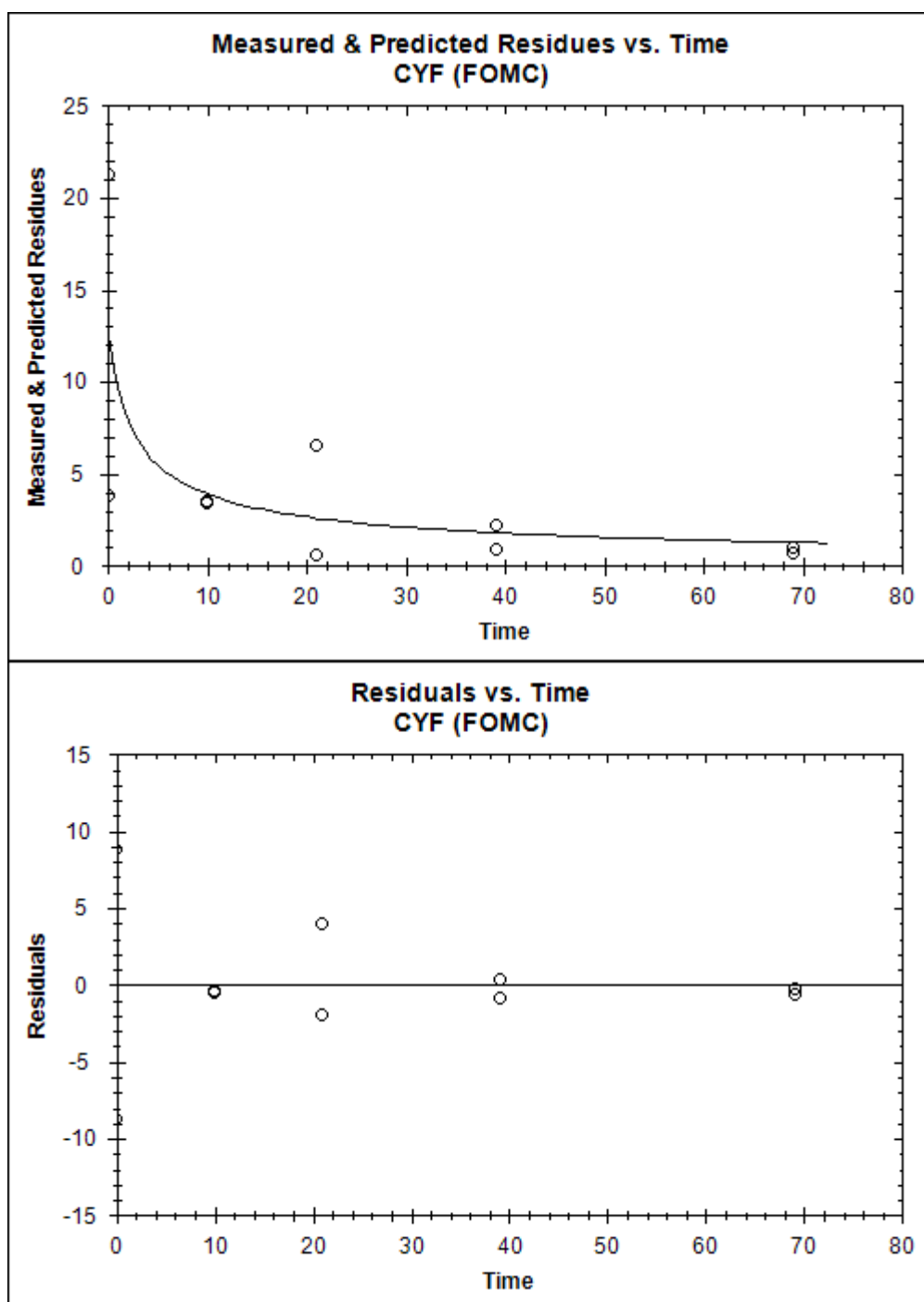
      CYF
      DT50 :      3.6300
      DT90 :      70.798
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment CYF
      time observed err-std predicted residual
0.0000  21.3000  4.1734  12.5436  8.7564
0.0000   3.8000  4.1734  12.5436 -8.7436
10.0000  3.5000  4.1734   3.8693 -0.3693
10.0000  3.4000  4.1734   3.8693 -0.4693
21.0000  6.5000  4.1734   2.5710  3.9290
21.0000  0.6000  4.1734   2.5710 -1.9710
39.0000  0.9000  4.1734   1.7925 -0.8925
39.0000  2.2000  4.1734   1.7925  0.4075
69.0000  0.7000  4.1734   1.2740 -0.5740

```

69.0000 1.0000 4.1734 1.2740 -0.2740



11.6.4.4DFOP

```

# Trial      : LiendensCYF
# File name  : LiendensCYF IRLS DFOP CYF.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_s_CYF
# Created    : on 18 Oct 2013
#            : at 11:38
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment Cyfluthrin
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  CYF      :      21.30              0              Inf      False
k1    CYF      :       0.10              0              Inf      False
k2    CYF      :       0.01              0              Inf      False
g     CYF      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              CYF      All
      Chi2Err% :      9.326      9.326
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  CYF      :      12.55000      5.66185      19.438      3.51443
0.00589
k1    CYF      :       1.13234     -65.51852      67.783      34.00617
0.48726
k2    CYF      :       0.02414     -0.08470       0.133      0.05553
0.33950
g     CYF      :       0.61697     -0.37639       1.610      0.50683
0.13459

# -----
# DT50 and DT90 values
# -----

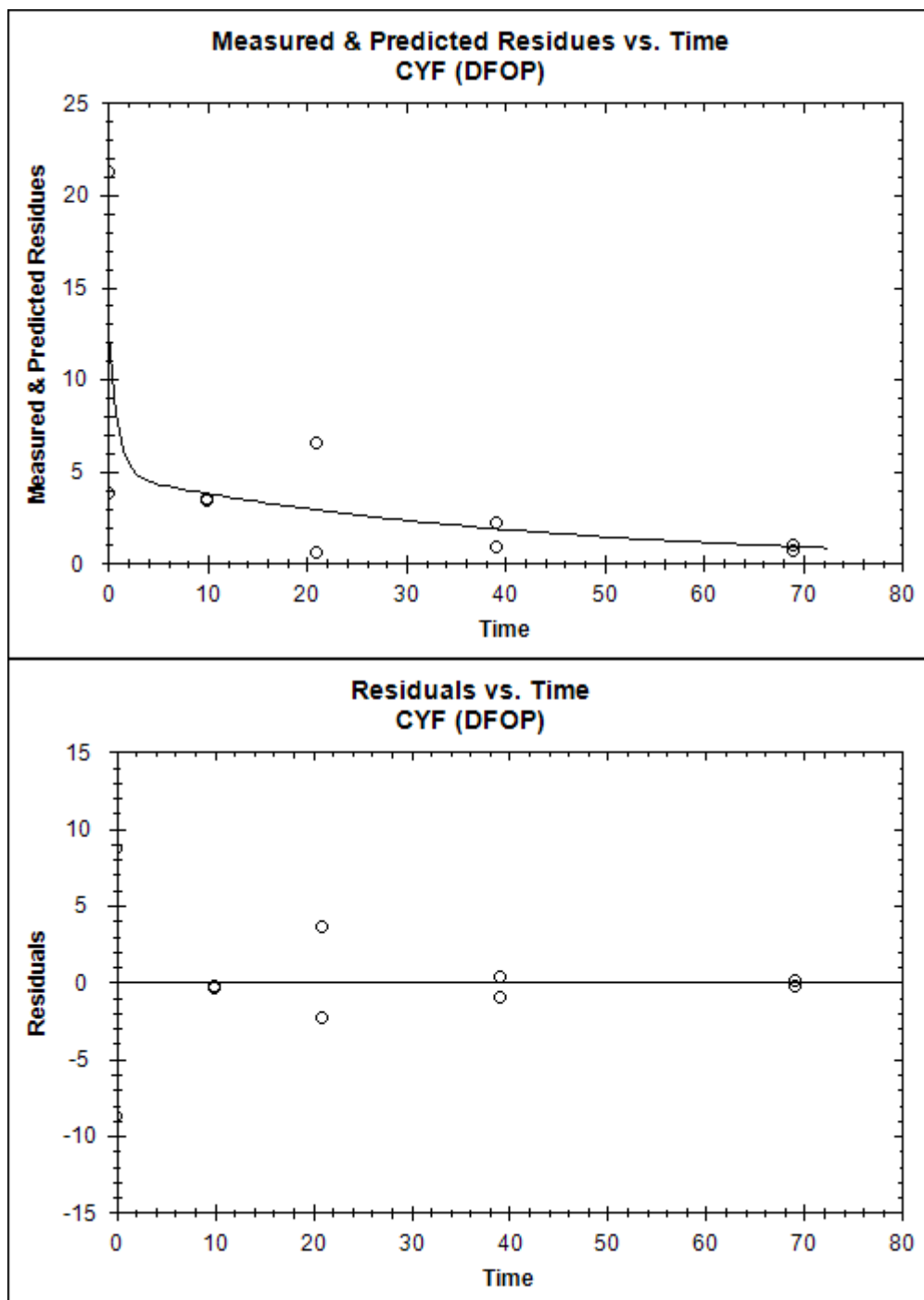
              CYF
      DT50 :       1.3786
      DT90 :       55.638
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment CYF
      time observed err-std predicted residual
0.0000  21.3000  4.1559  12.5500  8.7500
0.0000   3.8000  4.1559  12.5500 -8.7500

```

10.0000	3.5000	4.1559	3.7762	-0.2762
10.0000	3.4000	4.1559	3.7762	-0.3762
21.0000	6.5000	4.1559	2.8956	3.6044
21.0000	0.6000	4.1559	2.8956	-2.2956
39.0000	0.9000	4.1559	1.8752	-0.9752
39.0000	2.2000	4.1559	1.8752	0.3248
69.0000	0.7000	4.1559	0.9090	-0.2090
69.0000	1.0000	4.1559	0.9090	0.0910



11.7 Beta-Cyfluthrin (Isomers II+IV) Dissipation Sediment Phase

11.7.1 Barmen

11.7.1.1 SFO

```

# Trial      : Barmensbeta
# File name  : Barmensbeta IRLS SFO Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_s_beta
# Created    : on 17 Sep 2013
#            : at 10:16
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : Barmener See sediment
# # beta-Cyfluthrin Anteil Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      30.76              0              Inf      False
k      Par      :       0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      16.50      Par      All
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 17
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      26.31455      23.08300      29.546      1.64878      5.76e-12
k      Par      :       0.13073       0.08743       0.174      0.02209      8.44e-06

# -----
# DT50 and DT90 values
# -----

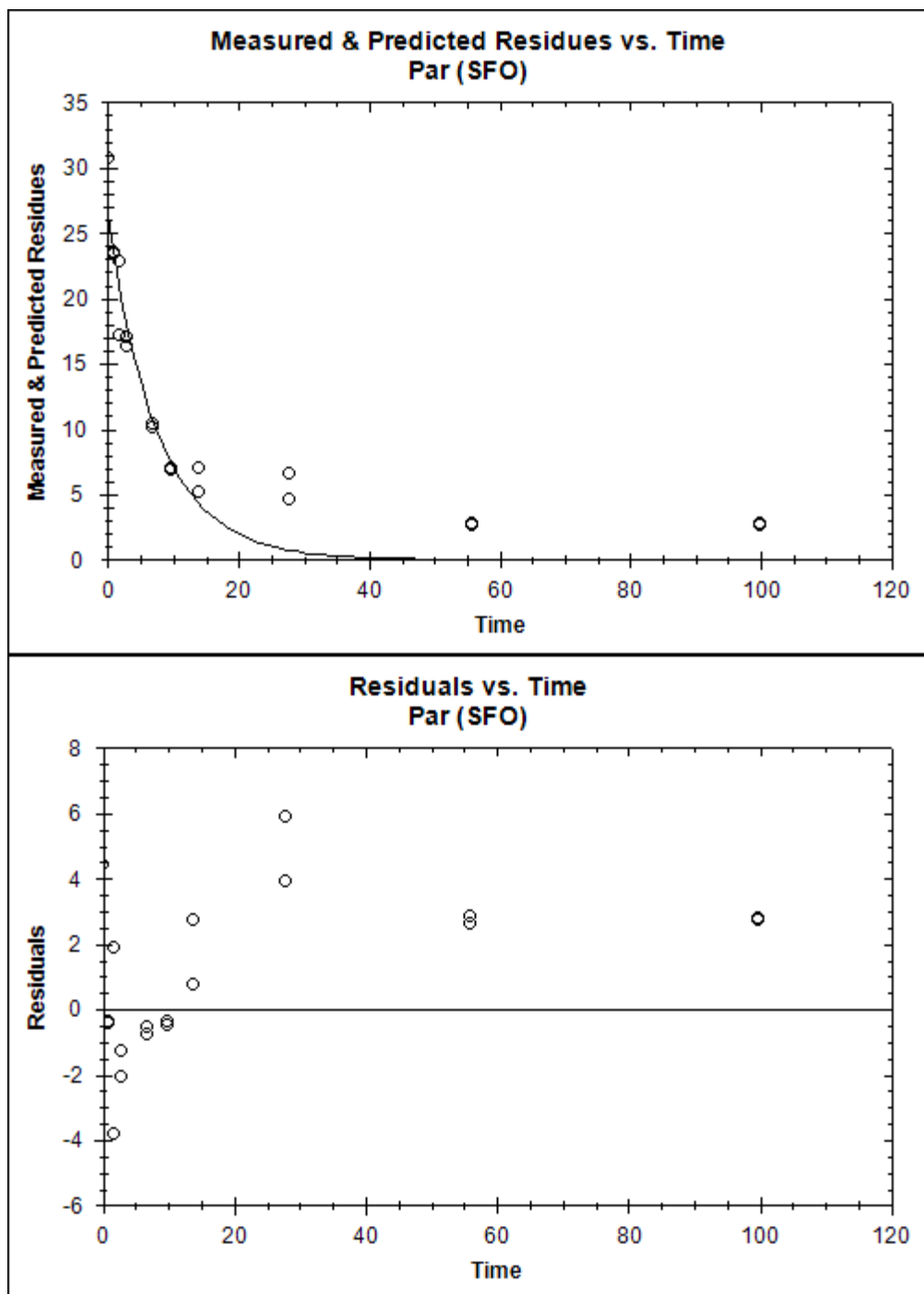
      Par
      DT50 :      5.3023
      DT90 :      17.614
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 30.7600 2.6474 26.3146 4.4454
0.0000 NA 2.6474 26.3146 NA
0.7500 23.4600 2.6474 23.8570 -0.3970
0.7500 23.5000 2.6474 23.8570 -0.3570
1.7500 17.1500 2.6474 20.9335 -3.7835
1.7500 22.8200 2.6474 20.9335 1.8865

```

2.7500	16.3100	2.6474	18.3683	-2.0583
2.7500	17.0800	2.6474	18.3683	-1.2883
6.7500	10.1300	2.6474	10.8886	-0.7586
6.7500	10.3800	2.6474	10.8886	-0.5086
9.7500	6.8700	2.6474	7.3562	-0.4862
9.7500	6.9900	2.6474	7.3562	-0.3662
13.7500	7.0900	2.6474	4.3607	2.7293
13.7500	5.1400	2.6474	4.3607	0.7793
27.7500	4.6200	2.6474	0.6994	3.9206
27.7500	6.5900	2.6474	0.6994	5.8906
55.7500	2.6400	2.6474	0.0180	2.6220
55.7500	2.8500	2.6474	0.0180	2.8320
99.7500	2.7200	2.6474	0.0001	2.7199
99.7500	2.7800	2.6474	0.0001	2.7799



11.7.1.2_HS

```

# Trial      : Barmensbeta
# File name  : Barmensbeta IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Barmen_s_beta
# Created    : on 17 Sep 2013
#            : at 10:16
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : Barmener See sediment
# # beta-Cyfluthrin Anteil Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      30.76              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
tb    Par      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :      8.022      8.022
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 15
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      29.127237      26.519029      31.735      1.330743      4.25e-13
k1    Par      :       0.214831      0.153430      0.276      0.031328      2.72e-06
k2    Par      :       0.018809      0.005978      0.032      0.006547      0.0058
tb    Par      :       5.740554      3.924127      7.557      0.926765      8.59e-06

# -----
# DT50 and DT90 values
# -----

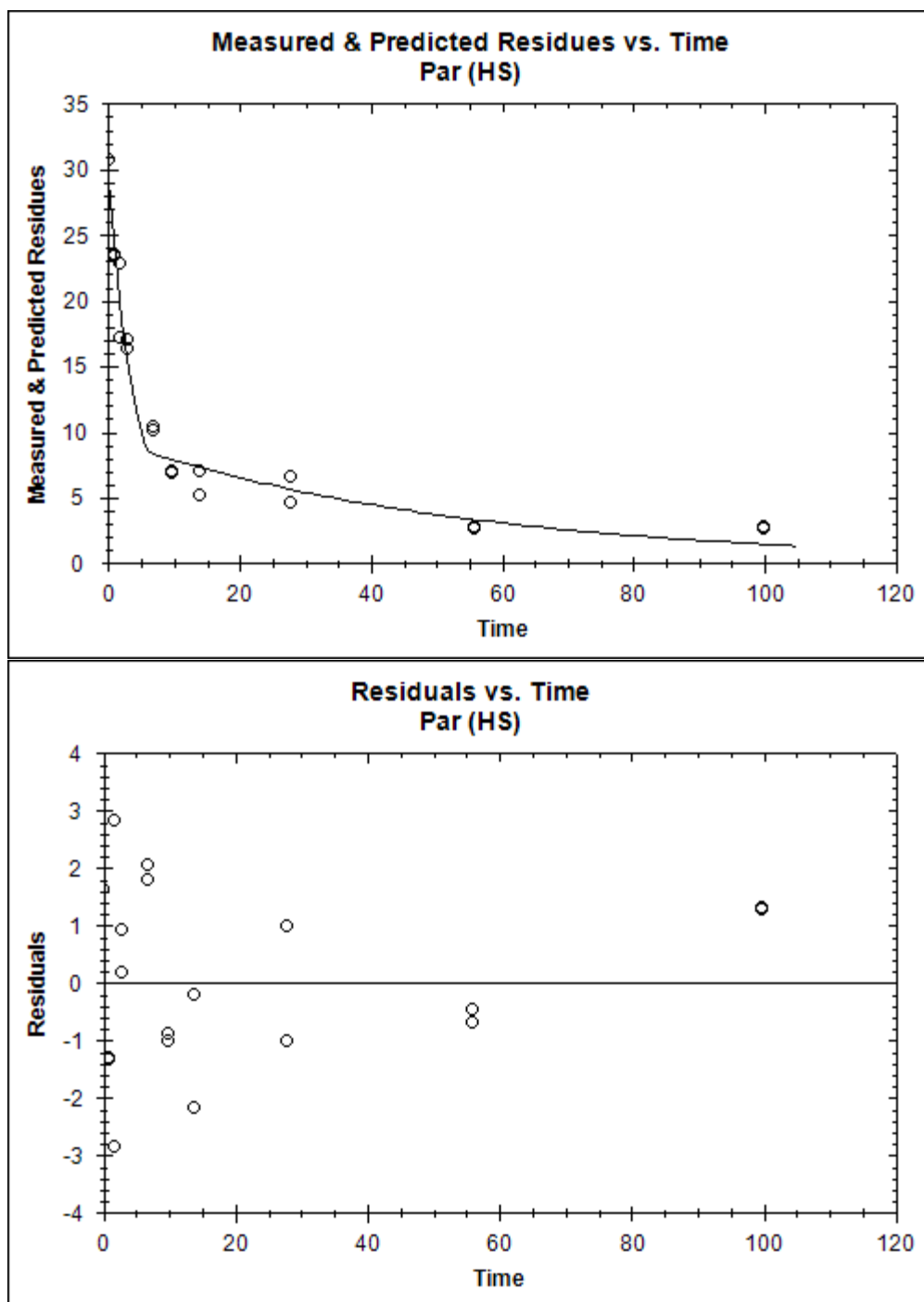
              Par
      DT50 :      3.2265
      DT90 :      62.592
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 30.7600 1.5055 29.1272 1.6328
0.0000 NA 1.5055 29.1272 NA
0.7500 23.4600 1.5055 24.7927 -1.3327
0.7500 23.5000 1.5055 24.7927 -1.2927
1.7500 17.1500 1.5055 19.9997 -2.8497
1.7500 22.8200 1.5055 19.9997 2.8203
2.7500 16.3100 1.5055 16.1333 0.1767

```

2.7500	17.0800	1.5055	16.1333	0.9467
6.7500	10.1300	1.5055	8.3264	1.8036
6.7500	10.3800	1.5055	8.3264	2.0536
9.7500	6.8700	1.5055	7.8696	-0.9996
9.7500	6.9900	1.5055	7.8696	-0.8796
13.7500	7.0900	1.5055	7.2992	-0.2092
13.7500	5.1400	1.5055	7.2992	-2.1592
27.7500	4.6200	1.5055	5.6094	-0.9894
27.7500	6.5900	1.5055	5.6094	0.9806
55.7500	2.6400	1.5055	3.3127	-0.6727
55.7500	2.8500	1.5055	3.3127	-0.4627
99.7500	2.7200	1.5055	1.4480	1.2720
99.7500	2.7800	1.5055	1.4480	1.3320



11.7.1.3 FOMC

```

# Trial      : Barmensbeta
# File name  : Barmensbeta IRLS FOMC Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_s_beta
# Created    : on 17 Sep 2013
#            : at 10:17
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : Barmener See sediment
# # beta-Cyfluthrin Anteil Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      30.76      0      Inf      False
alpha Par      :      0.10      0      Inf      False
beta  Par      :      0.10      0      Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      5.434      5.434
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 16
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      30.70972      28.14288      33.277      1.30963      4.06e-14
alpha Par      :      0.69435      0.51551      0.873      0.09125      5.27e-07
beta  Par      :      1.79160      0.75043      2.833      0.53122      0.00194

# -----
# DT50 and DT90 values
# -----

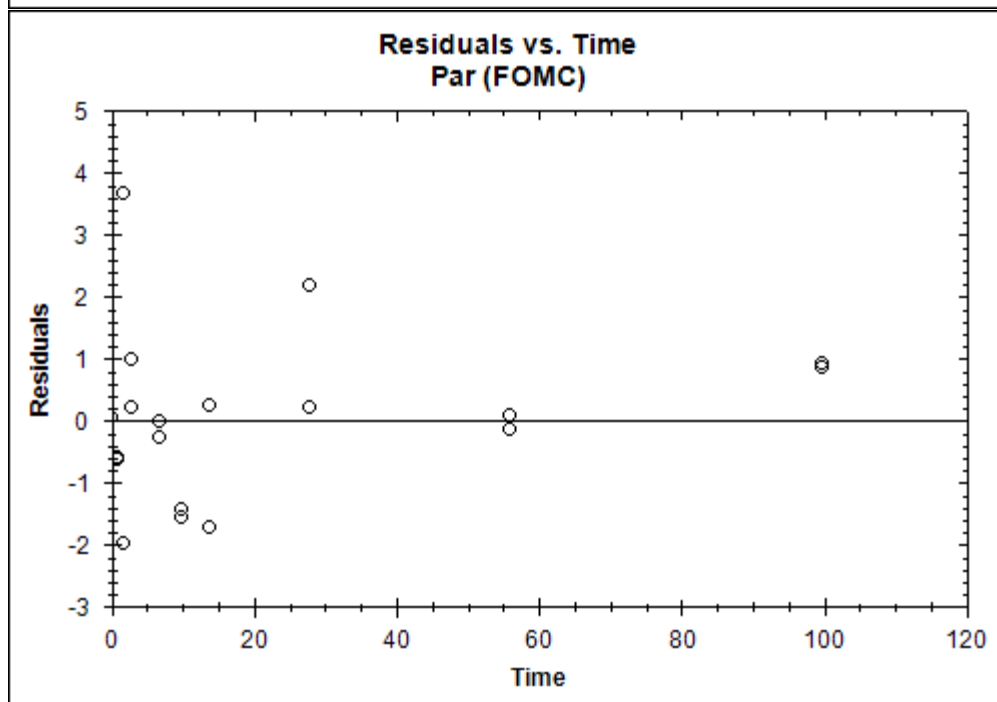
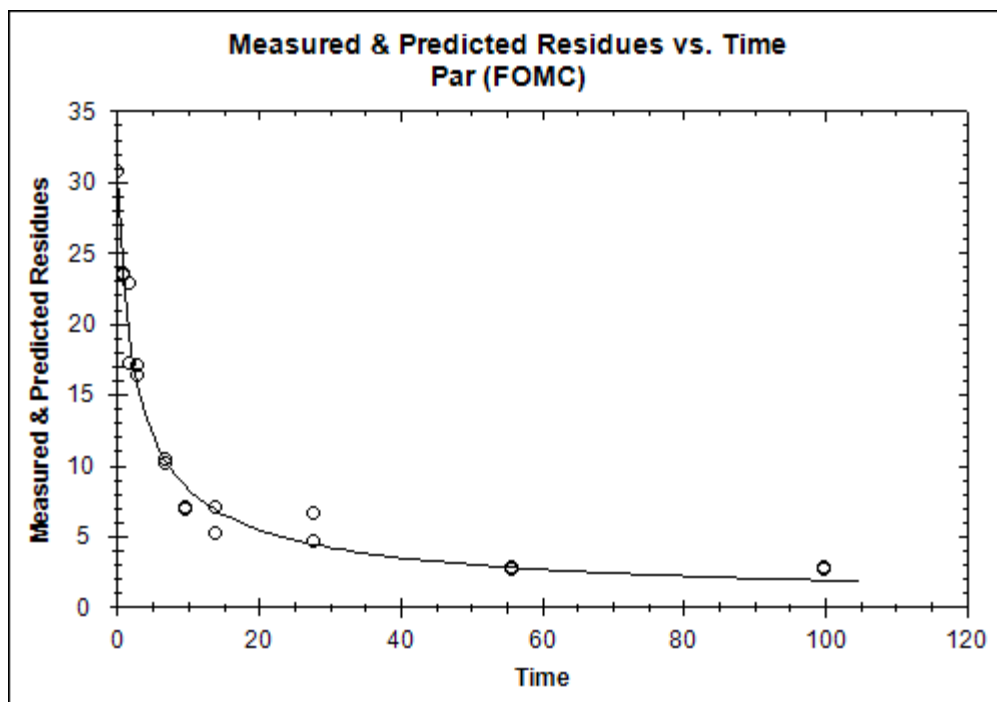
      Par
      DT50 :      3.0700
      DT90 :      47.575
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 30.7600 1.3242 30.7097 0.0503
0.0000 NA 1.3242 30.7097 NA
0.7500 23.4600 1.3242 24.0895 -0.6295
0.7500 23.5000 1.3242 24.0895 -0.5895
1.7500 17.1500 1.3242 19.1327 -1.9827
1.7500 22.8200 1.3242 19.1327 3.6873
2.7500 16.3100 1.3242 16.0983 0.2117
2.7500 17.0800 1.3242 16.0983 0.9817
6.7500 10.1300 1.3242 10.3824 -0.2524
6.7500 10.3800 1.3242 10.3824 -0.0024

```

9.7500	6.8700	1.3242	8.4242	-1.5542
9.7500	6.9900	1.3242	8.4242	-1.4342
13.7500	7.0900	1.3242	6.8517	0.2383
13.7500	5.1400	1.3242	6.8517	-1.7117
27.7500	4.6200	1.3242	4.3865	0.2335
27.7500	6.5900	1.3242	4.3865	2.2035
55.7500	2.6400	1.3242	2.7610	-0.1210
55.7500	2.8500	1.3242	2.7610	0.0890
99.7500	2.7200	1.3242	1.8612	0.8588
99.7500	2.7800	1.3242	1.8612	0.9188



11.7.1.4 DFOP

```

# Trial      : Barmensbeta
# File name  : Barmensbeta IRLS DFOP Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Barmen_s_beta
# Created    : on 17 Sep 2013
#            : at 10:16
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : Barmener See sediment
# # beta-Cyfluthrin Anteil Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      30.76      0      Inf      False
k1    Par      :      0.10      0      Inf      False
k2    Par      :      0.01      0      Inf      False
g     Par      :      0.50      0      1      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      5.628      5.628
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 15
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      29.243244      27.023207      31.463      1.132693      3.80e-14
k1    Par      :      0.303923      0.201684      0.406      0.052164      1.67e-05
k2    Par      :      0.011985      0.002184      0.022      0.005001      0.015
g     Par      :      0.757004      0.672230      0.842      0.043253      1.08e-11

# -----
# DT50 and DT90 values
# -----

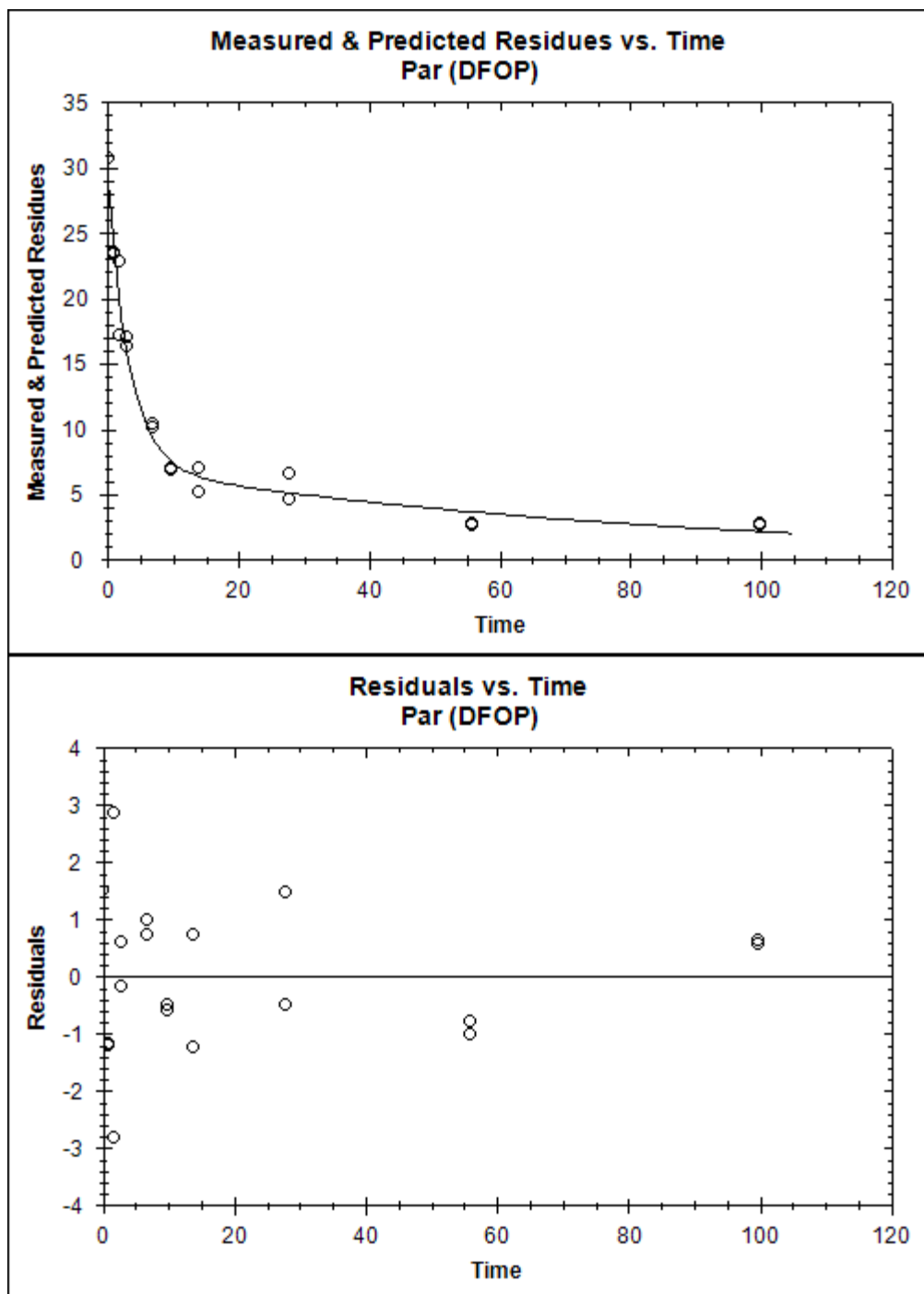
      Par
      DT50 :      3.4314
      DT90 :      74.084
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 30.7600 1.2670 29.2432 1.5168
0.0000 NA 1.2670 29.2432 NA
0.7500 23.4600 1.2670 24.6674 -1.2074
0.7500 23.5000 1.2670 24.6674 -1.1674
1.7500 17.1500 1.2670 19.9643 -2.8143
1.7500 22.8200 1.2670 19.9643 2.8557
2.7500 16.3100 1.2670 16.4728 -0.1628
2.7500 17.0800 1.2670 16.4728 0.6072

```

6.7500	10.1300	1.2670	9.3994	0.7306
6.7500	10.3800	1.2670	9.3994	0.9806
9.7500	6.8700	1.2670	7.4657	-0.5957
9.7500	6.9900	1.2670	7.4657	-0.4757
13.7500	7.0900	1.2670	6.3654	0.7246
13.7500	5.1400	1.2670	6.3654	-1.2254
27.7500	4.6200	1.2670	5.1003	-0.4803
27.7500	6.5900	1.2670	5.1003	1.4897
55.7500	2.6400	1.2670	3.6429	-1.0029
55.7500	2.8500	1.2670	3.6429	-0.7929
99.7500	2.7200	1.2670	2.1500	0.5700
99.7500	2.7800	1.2670	2.1500	0.6300



11.7.2 Genkel

11.7.2.1 SFO

```
# Trial      : Genkelsbeta
# File name  : Genkelsbeta IRLS SFO  Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Genkel_s_beta
# Created    : on 17 Sep 2013
#            : at 10:18
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : sediment
# # beta-Cyfluthrin Anteil sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.87              0              Inf      False
k      Par      :      0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :      18.62      18.62
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 18
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      23.24591      19.73235      26.759      1.79267      7.17e-11
k      Par      :      0.04834      0.01854      0.078      0.01521      0.00260

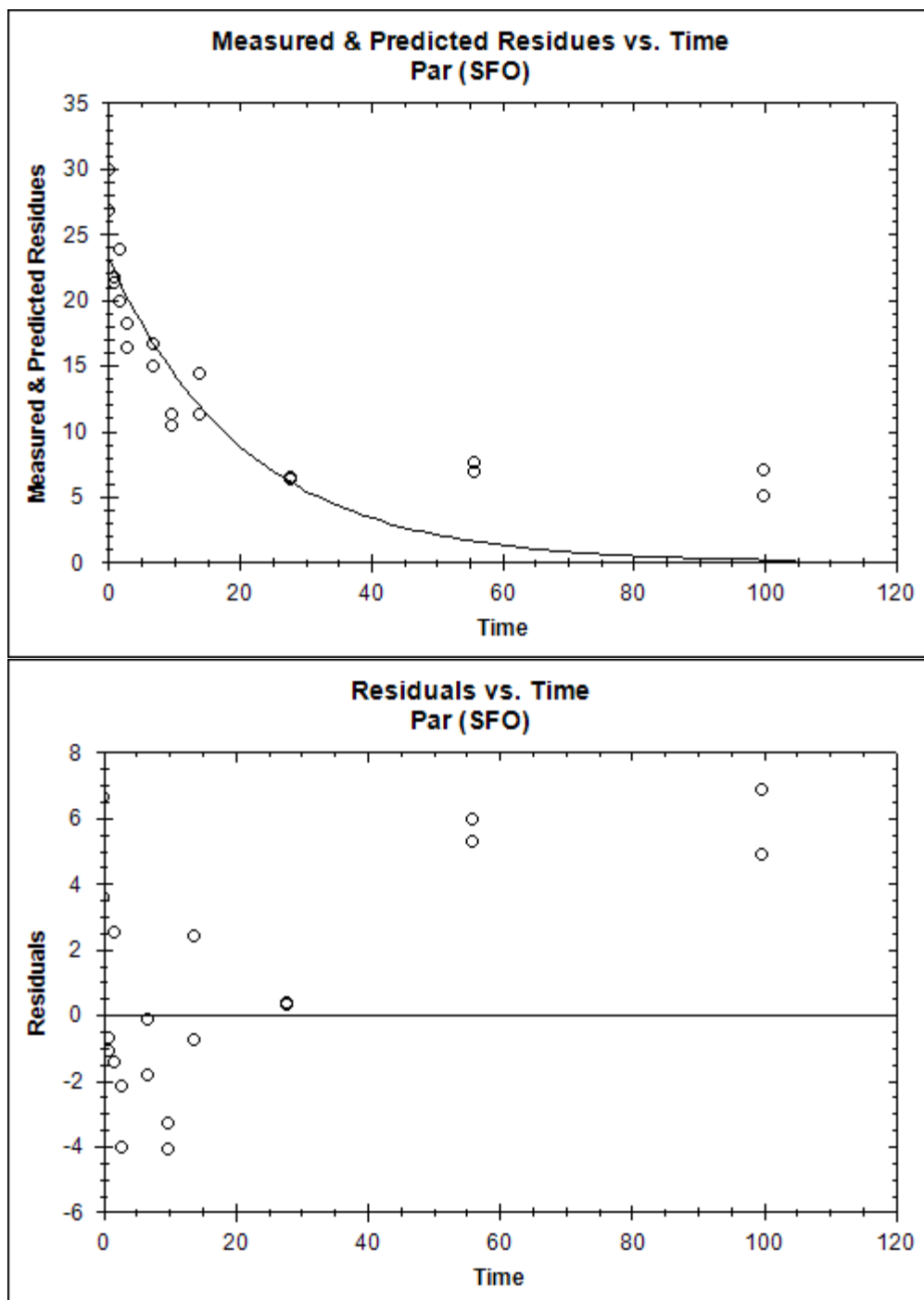
# -----
# DT50 and DT90 values
# -----

              Par
      DT50 :      14.338
      DT90 :      47.630
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000  29.8700  3.5977  23.2459  6.6241
0.0000  26.8400  3.5977  23.2459  3.5941
0.7500  21.3000  3.5977  22.4182 -1.1182
0.7500  21.7400  3.5977  22.4182 -0.6782
1.7500  19.9500  3.5977  21.3602 -1.4102
1.7500  23.8700  3.5977  21.3602  2.5098
2.7500  18.2100  3.5977  20.3521 -2.1421
2.7500  16.3400  3.5977  20.3521 -4.0121
6.7500  16.6300  3.5977  16.7737 -0.1437
6.7500  14.9600  3.5977  16.7737 -1.8137
```

9.7500	11.2100	3.5977	14.5092	-3.2992
9.7500	10.4400	3.5977	14.5092	-4.0692
13.7500	14.3800	3.5977	11.9581	2.4219
13.7500	11.2200	3.5977	11.9581	-0.7381
27.7500	6.4700	3.5977	6.0775	0.3925
27.7500	6.3900	3.5977	6.0775	0.3125
55.7500	6.8300	3.5977	1.5699	5.2601
55.7500	7.5400	3.5977	1.5699	5.9701
99.7500	5.0700	3.5977	0.1871	4.8829
99.7500	7.0300	3.5977	0.1871	6.8429



11.7.2.2_HS

```

# Trial      : Genkelsbeta
# File name  : Genkelsbeta IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory_wat_sed_CYF\Sediment\Genkel_s_beta
# Created    : on 16 Oct 2013
#            : at 12:27
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : Barmener See sediment
# # beta-Cyfluthrin Anteil Barmener See sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.87              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
tb    Par      :       9.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      11.84      11.84
      Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 16
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      2.540e+01      2.288e+01      27.910      1.282e+00      5.54e-13
k1    Par      :      8.902e-02      4.733e-02      0.131      2.127e-02      0.000350
k2    Par      :      8.506e-03      8.643e-04      0.016      3.899e-03      0.022199
tb    Par      :      9.497e+00      4.531e+00      14.464      2.534e+00      0.000877

# -----
# DT50 and DT90 values
# -----

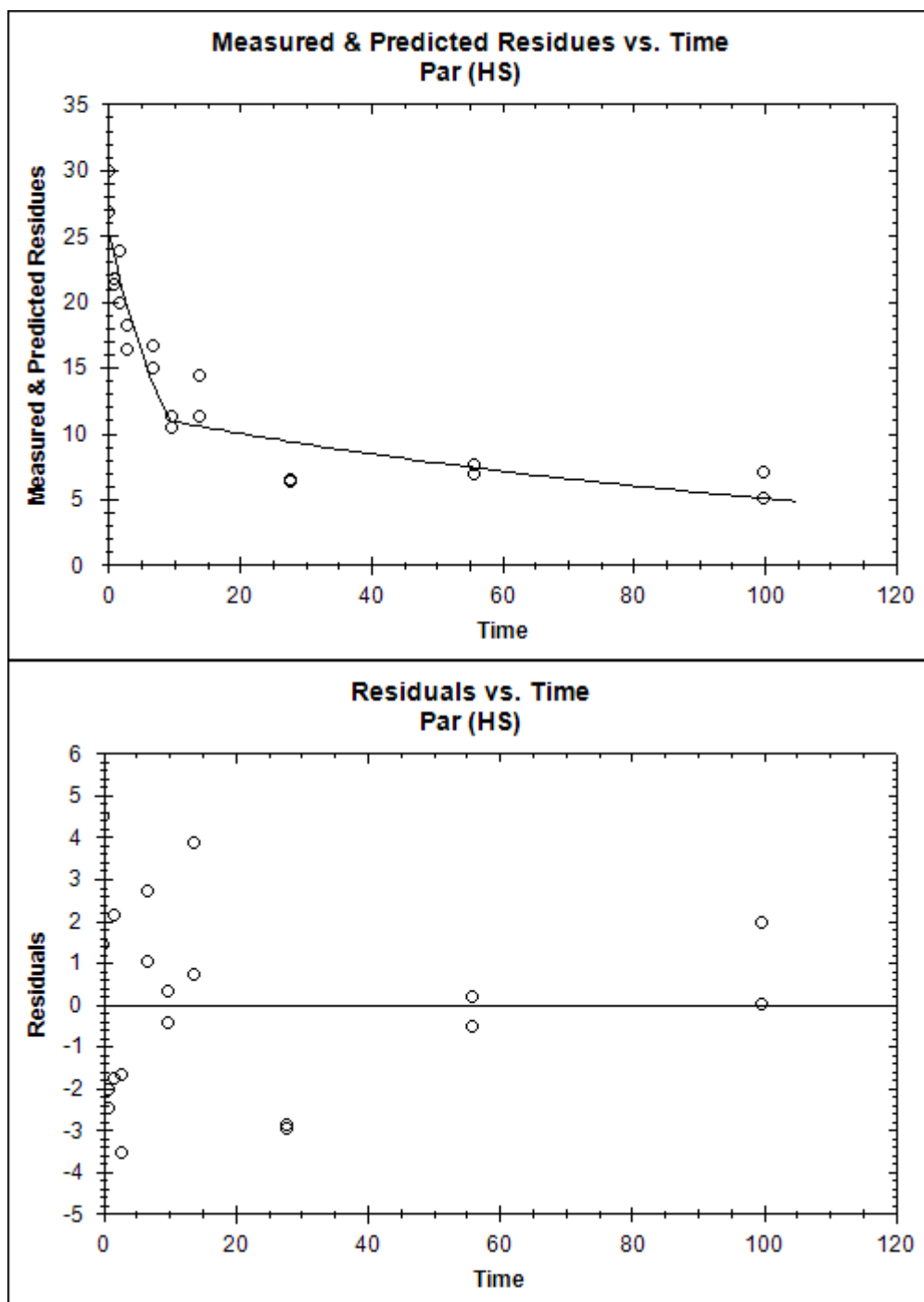
      Par
      DT50 :      7.7865
      DT90 :      180.80
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 29.8700 2.2413 25.3972 4.4728
0.0000 26.8400 2.2413 25.3972 1.4428
0.7500 21.3000 2.2413 23.7569 -2.4569
0.7500 21.7400 2.2413 23.7569 -2.0169
1.7500 19.9500 2.2413 21.7335 -1.7835
1.7500 23.8700 2.2413 21.7335 2.1365
2.7500 18.2100 2.2413 19.8824 -1.6724

```

2.7500	16.3400	2.2413	19.8824	-3.5424
6.7500	16.6300	2.2413	13.9260	2.7040
6.7500	14.9600	2.2413	13.9260	1.0340
9.7500	11.2100	2.2413	10.8812	0.3288
9.7500	10.4400	2.2413	10.8812	-0.4412
13.7500	14.3800	2.2413	10.5172	3.8628
13.7500	11.2200	2.2413	10.5172	0.7028
27.7500	6.4700	2.2413	9.3364	-2.8664
27.7500	6.3900	2.2413	9.3364	-2.9464
55.7500	6.8300	2.2413	7.3577	-0.5277
55.7500	7.5400	2.2413	7.3577	0.1823
99.7500	5.0700	2.2413	5.0605	0.0095
99.7500	7.0300	2.2413	5.0605	1.9695



11.7.2.3 FOMC

```

# Trial      : Genkelsbeta
# File name  : Genkelsbeta IRLS FOMC Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Genkel_s_beta
# Created    : on 17 Sep 2013
#            : at 10:18
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : See sediment
# # beta-Cyfluthrin Anteil sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.87              0              Inf      False
alpha Par      :       0.10              0              Inf      False
beta  Par      :       0.10              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Par      All
      Chi2Err% :      8.436      8.436
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 17
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      27.82896      24.97794      30.680      1.45463      3.09e-13
alpha Par      :       0.36741      0.24652      0.488      0.06168      7.81e-06
beta  Par      :       1.23750      -0.04850      2.523      0.65613      0.0382

# -----
# DT50 and DT90 values
# -----

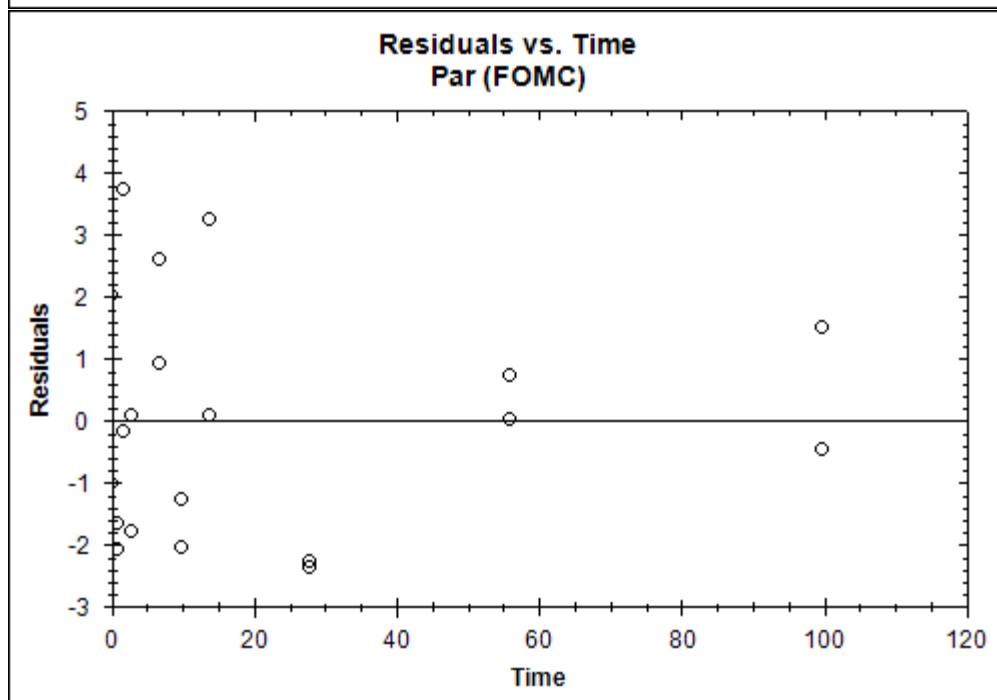
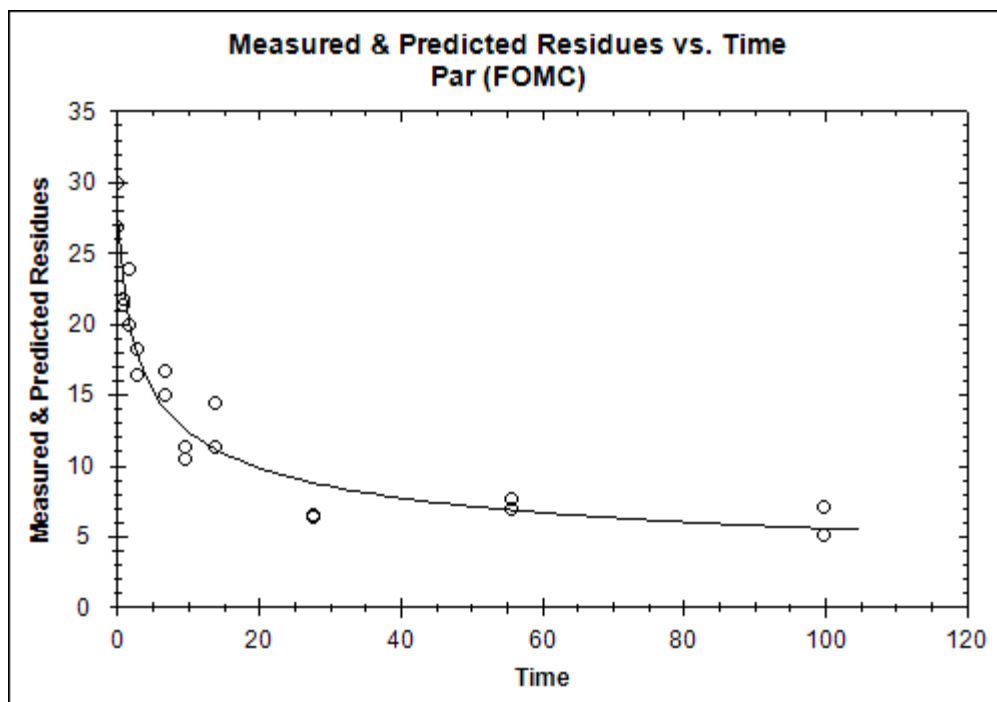
      Par
      DT50 :       6.9259
      DT90 :      650.81
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 29.8700 1.8292 27.8290 2.0410
0.0000 26.8400 1.8292 27.8290 -0.9890
0.7500 21.3000 1.8292 23.3829 -2.0829
0.7500 21.7400 1.8292 23.3829 -1.6429
1.7500 19.9500 1.8292 20.1310 -0.1810
1.7500 23.8700 1.8292 20.1310 3.7390
2.7500 18.2100 1.8292 18.1048 0.1052
2.7500 16.3400 1.8292 18.1048 -1.7648
6.7500 16.6300 1.8292 14.0263 2.6037
6.7500 14.9600 1.8292 14.0263 0.9337

```

9.7500	11.2100	1.8292	12.4756	-1.2656
9.7500	10.4400	1.8292	12.4756	-2.0356
13.7500	14.3800	1.8292	11.1307	3.2493
13.7500	11.2200	1.8292	11.1307	0.0893
27.7500	6.4700	1.8292	8.7350	-2.2650
27.7500	6.3900	1.8292	8.7350	-2.3450
55.7500	6.8300	1.8292	6.8140	0.0160
55.7500	7.5400	1.8292	6.8140	0.7260
99.7500	5.0700	1.8292	5.5221	-0.4521
99.7500	7.0300	1.8292	5.5221	1.5079



11.7.2.4 DFOP

```

# Trial      : Genkelsbeta
# File name  : Genkelsbeta IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Genkel_s_beta
# Created    : on 17 Sep 2013
#            : at 10:18
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Sneikus
# # label: 14C cyclopropy
# # soil : sediment
# # beta-Cyfluthrin Anteil sediment
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      29.87              0              Inf      False
k1    Par      :       0.10              0              Inf      False
k2    Par      :       0.01              0              Inf      False
g     Par      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

              Par      All
      Chi2Err% :    10.46    10.46
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 16
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :    26.215675    22.995862    29.435    1.642792    1.50e-11
k1    Par      :     0.208486    -0.058843     0.476    0.136395    0.072952
k2    Par      :     0.006416    -0.005863     0.019    0.006265    0.160521
g     Par      :     0.603250     0.339537     0.867    0.134550    0.000188

# -----
# DT50 and DT90 values
# -----

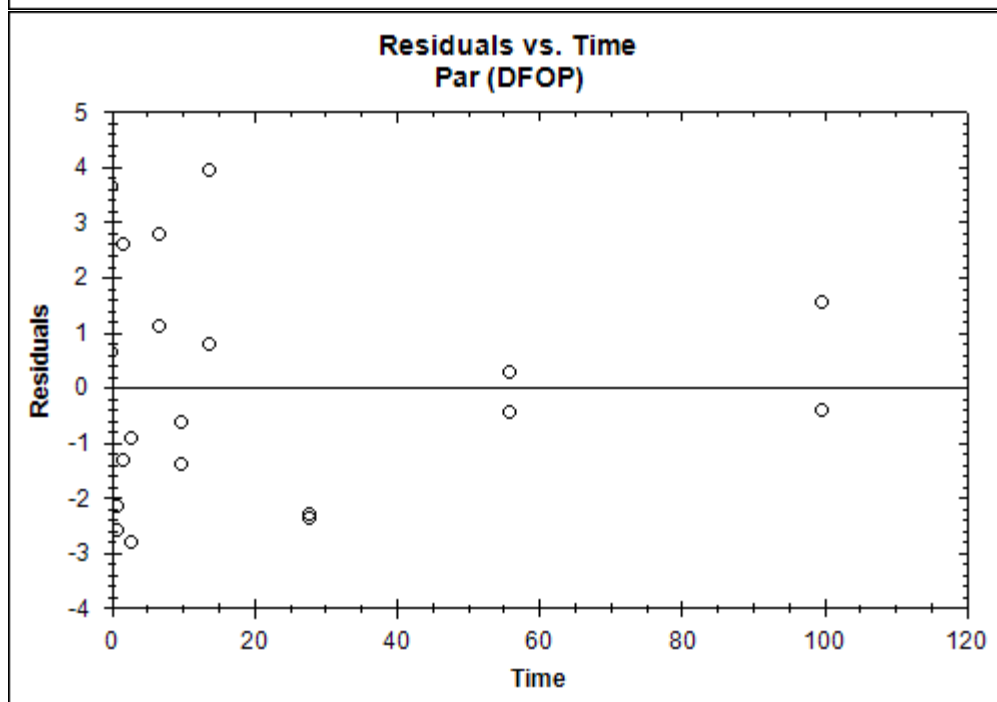
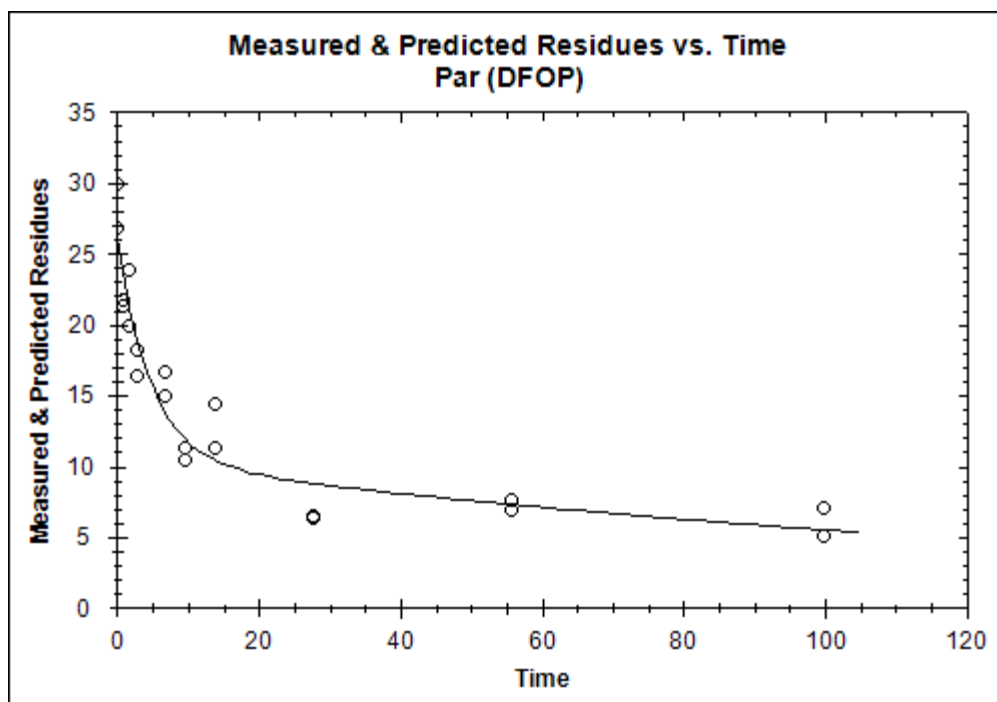
              Par
      DT50 :      7.6558
      DT90 :     214.81
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment Par
      time observed err-std predicted residual
0.0000 29.8700 2.0434 26.2157 3.6543
0.0000 26.8400 2.0434 26.2157 0.6243
0.7500 21.3000 2.0434 23.8765 -2.5765
0.7500 21.7400 2.0434 23.8765 -2.1365
1.7500 19.9500 2.0434 21.2650 -1.3150
1.7500 23.8700 2.0434 21.2650 2.6050
2.7500 18.2100 2.0434 19.1329 -0.9229

```

2.7500	16.3400	2.0434	19.1329	-2.7929
6.7500	16.6300	2.0434	13.8318	2.7982
6.7500	14.9600	2.0434	13.8318	1.1282
9.7500	11.2100	2.0434	11.8417	-0.6317
9.7500	10.4400	2.0434	11.8417	-1.4017
13.7500	14.3800	2.0434	10.4225	3.9575
13.7500	11.2200	2.0434	10.4225	0.7975
27.7500	6.4700	2.0434	8.7534	-2.2834
27.7500	6.3900	2.0434	8.7534	-2.3634
55.7500	6.8300	2.0434	7.2737	-0.4437
55.7500	7.5400	2.0434	7.2737	0.2663
99.7500	5.0700	2.0434	5.4847	-0.4147
99.7500	7.0300	2.0434	5.4847	1.5453



11.8 FPB-Aldehyd (FCR 1260) Dissipation Sediment Phase

11.8.1 Ijzendoorn

11.8.1.1 SFO

```

# Trial      : IjzendoornsFCR1260
# File name  : IjzendoornsFCR1260 IRLS SFO  FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 10:56
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      15.70              0              Inf      False
k      FCR1260      :       0.01              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
      Chi2Err% :      15.09      15.09
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 8
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260      :      15.64707      14.26449      17.03      0.70541      9.02e-09
k      FCR1260      :       0.24839       0.13709       0.36      0.05678      0.00118

# -----
# DT50 and DT90 values
# -----

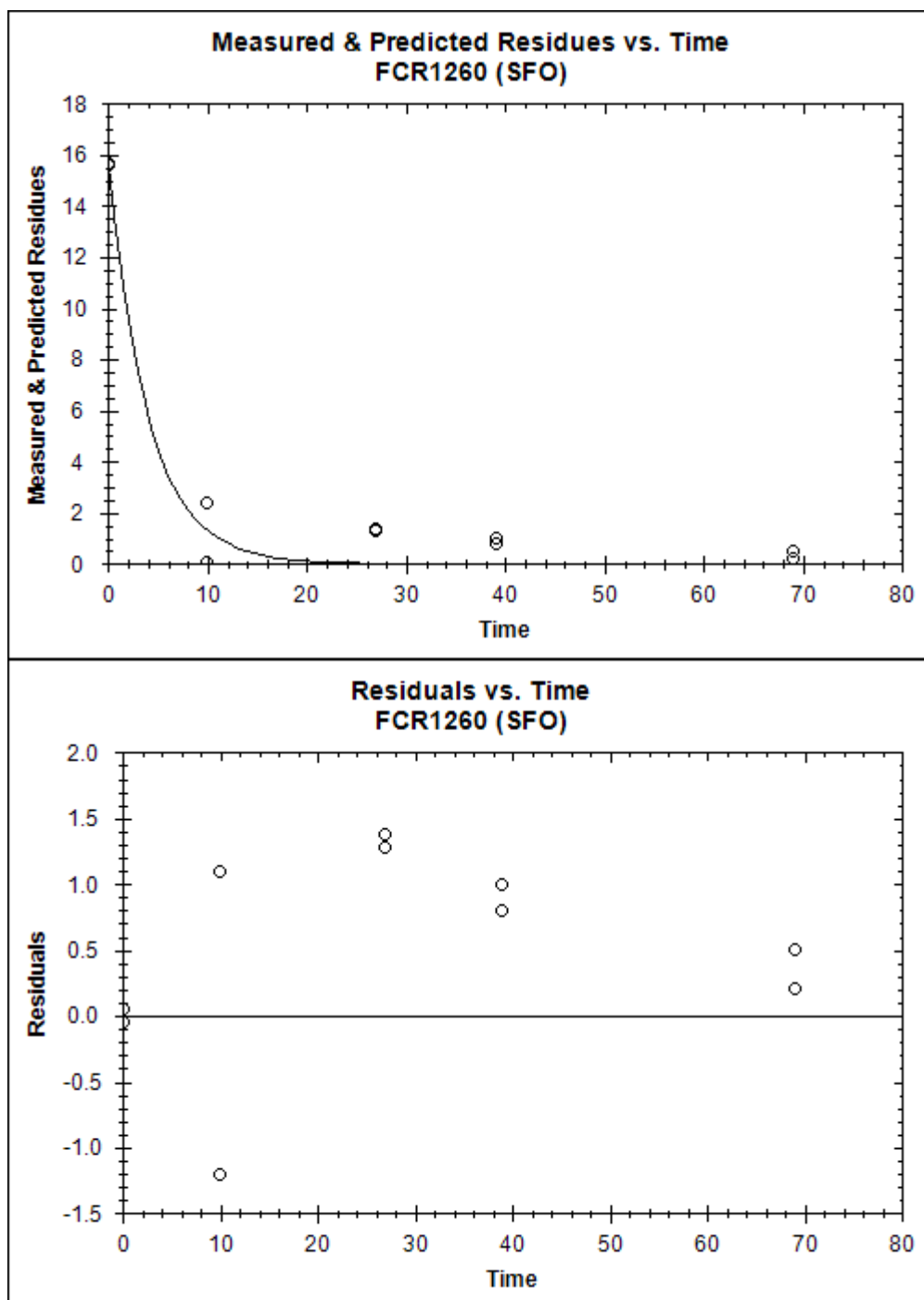
      FCR1260
      DT50 :       2.7906
      DT90 :       9.2702
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  15.7000  0.9017  15.6471  0.0529
0.0000  15.6000  0.9017  15.6471 -0.0471
10.0000  0.1000  0.9017   1.3053 -1.2053
10.0000  2.4000  0.9017   1.3053  1.0947
27.0000  1.4000  0.9017   0.0191  1.3809
27.0000  1.3000  0.9017   0.0191  1.2809

```

39.0000	0.8000	0.9017	0.0010	0.7990
39.0000	1.0000	0.9017	0.0010	0.9990
69.0000	0.2000	0.9017	0.0000	0.2000
69.0000	0.5000	0.9017	0.0000	0.5000



11.8.1.2HS

```

# Trial      : IjzendoornsFCR1260
# File name  : IjzendoornsFCR1260 IRLS HS   FCR1260.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 10:29
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      15.70              0              Inf      False
k1    FCR1260      :       0.10              0              Inf      False
k2    FCR1260      :       0.01              0              Inf      False
tb    FCR1260      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

              FCR1260      All
      Chi2Err% :       4.909      4.909
      Kinetic model :       HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260      :      15.649994      14.672535      16.627      0.498713      3.48e-08
k1    FCR1260      :       0.392596       0.169606       0.616      0.113773      0.00681
k2    FCR1260      :       0.016474      -0.009769       0.043      0.013390      0.13230
tb    FCR1260      :       5.959941       2.487035       9.433      1.771924      0.00758

# -----
# DT50 and DT90 values
# -----

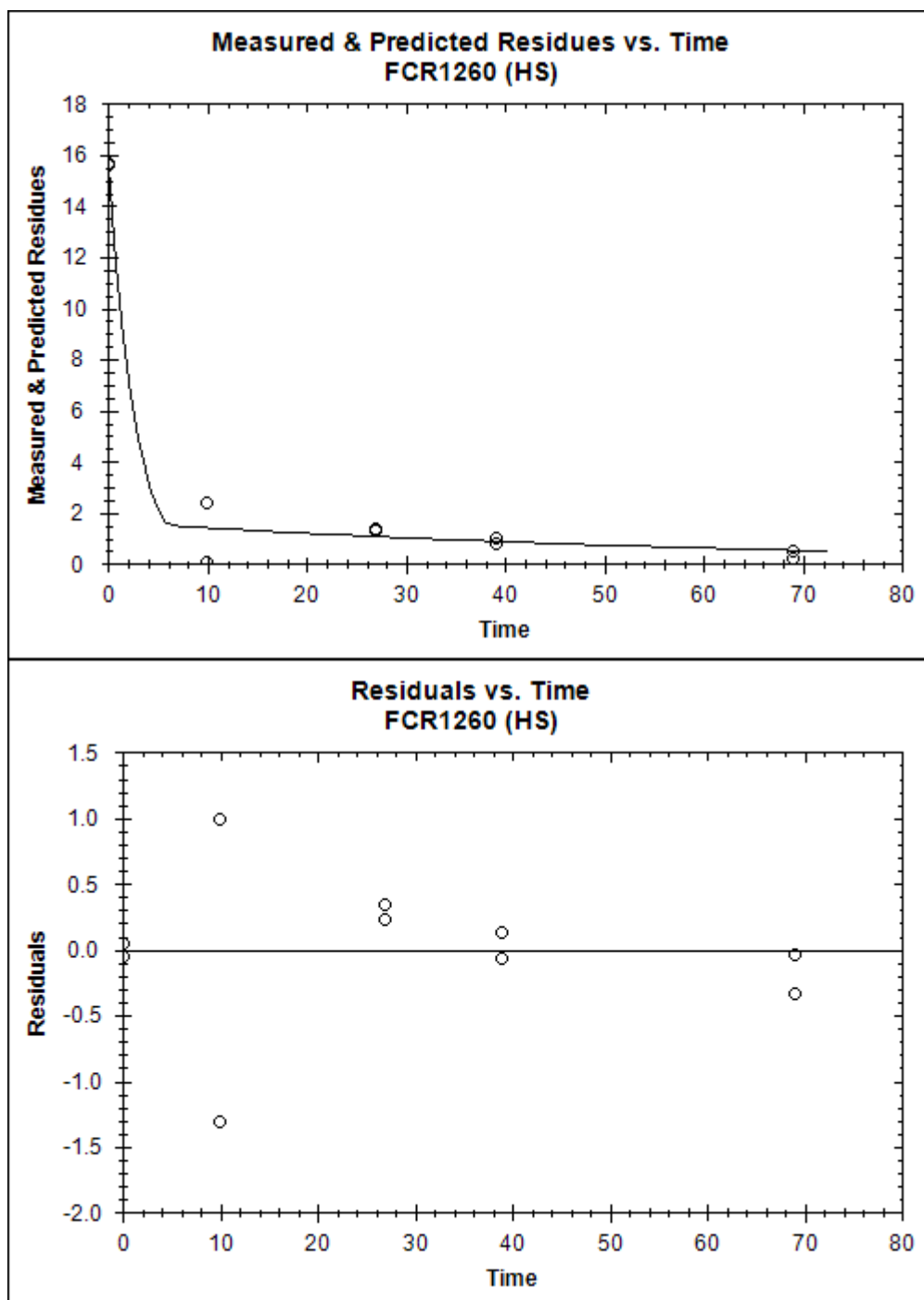
              FCR1260
      DT50 :       1.7655
      DT90 :       5.8650
      Kinetic model :       HS

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  15.7000  0.5479  15.6500  0.0500
0.0000  15.6000  0.5479  15.6500 -0.0500
10.0000  0.1000  0.5479   1.4107 -1.3107
10.0000  2.4000  0.5479   1.4107  0.9893
27.0000  1.4000  0.5479   1.0661  0.3339
27.0000  1.3000  0.5479   1.0661  0.2339
39.0000  0.8000  0.5479   0.8749 -0.0749

```

39.0000	1.0000	0.5479	0.8749	0.1251
69.0000	0.2000	0.5479	0.5337	-0.3337
69.0000	0.5000	0.5479	0.5337	-0.0337



11.8.1.3FOMC

```

# Trial      : IjzendoornsFCR1260
# File name  : IjzendoornsFCR1260 IRLS FOMC FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 10:29
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      15.7              0              Inf      False
alpha FCR1260      :       0.1              0              Inf      False
beta  FCR1260      :       0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      5.566      5.566
Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260 :      15.65073      14.27841      17.023      0.70018      4.54e-08
alpha FCR1260 :       0.37062       0.09480       0.646      0.14073       0.0169
beta  FCR1260 :       0.01462      -0.07009       0.099      0.04322       0.3726

# -----
# DT50 and DT90 values
# -----

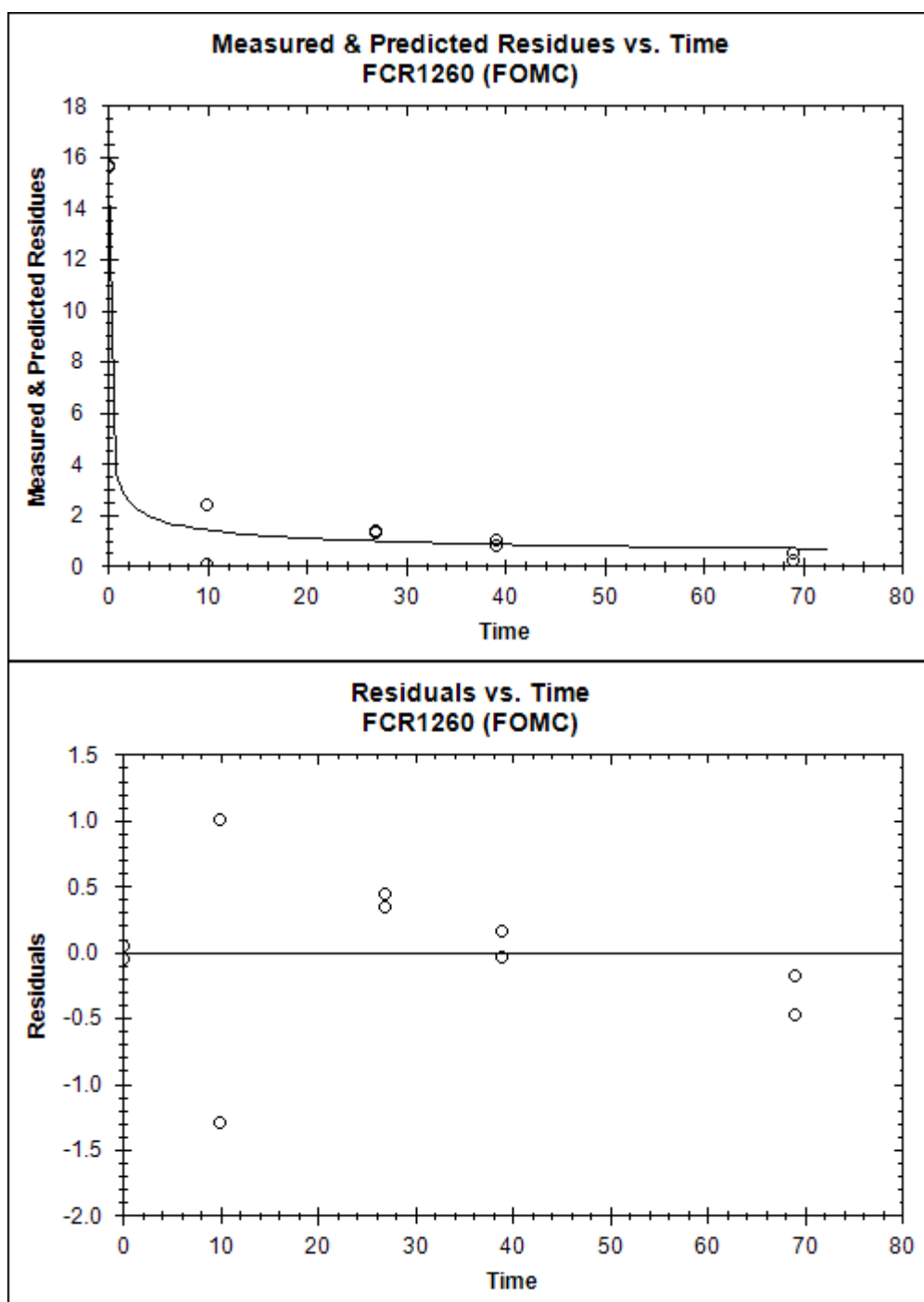
      FCR1260
DT50 :       0.0803
DT90 :       7.2812
Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  15.7000  0.5731  15.6507  0.0493
0.0000  15.6000  0.5731  15.6507 -0.0507
10.0000  0.1000  0.5731  1.3917 -1.2917
10.0000  2.4000  0.5731  1.3917  1.0083
27.0000  1.4000  0.5731  0.9634  0.4366
27.0000  1.3000  0.5731  0.9634  0.3366
39.0000  0.8000  0.5731  0.8407 -0.0407
39.0000  1.0000  0.5731  0.8407  0.1593
69.0000  0.2000  0.5731  0.6805 -0.4805

```

69.0000 0.5000 0.5731 0.6805 -0.1805



11.8.1.4DFOP

```
# Trial      : IjzendoornsFCR1260
# File name  : IjzendoornsFCR1260 IRLS DFOP FCR1260.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 10:29
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FCR1260
# #
```

```
# =====
# Results of the kinetic evaluation
# =====
```

```
# -----
# Initial values
# -----
```

		Initial Value	Lower Bound	Upper Bound	Fixed
M(0)	FCR1260	: 15.70	0	Inf	False
k1	FCR1260	: 0.10	0	Inf	False
k2	FCR1260	: 0.01	0	Inf	False
g	FCR1260	: 0.50	0	1	False

```
# -----
# Chi2 error estimation
# -----
```

	FCR1260	All
Chi2Err% :	4.909	4.909
Kinetic model :	DFOP	

```
# -----
# Parameter estimation
# -----
```

Degrees of Freedom : 6						
Parameter		Estimate	Lower CI	Upper CI	St.Dev	Prob > t
M(0)	FCR1260	: 15.64999	14.75022	16.550	0.45907	2.12e-08
k1	FCR1260	: 1.56588	-79.33793	82.470	41.27821	0.485
k2	FCR1260	: 0.01647	-0.01182	0.045	0.01444	0.149
g	FCR1260	: 0.89372	0.80003	0.987	0.04780	7.56e-07

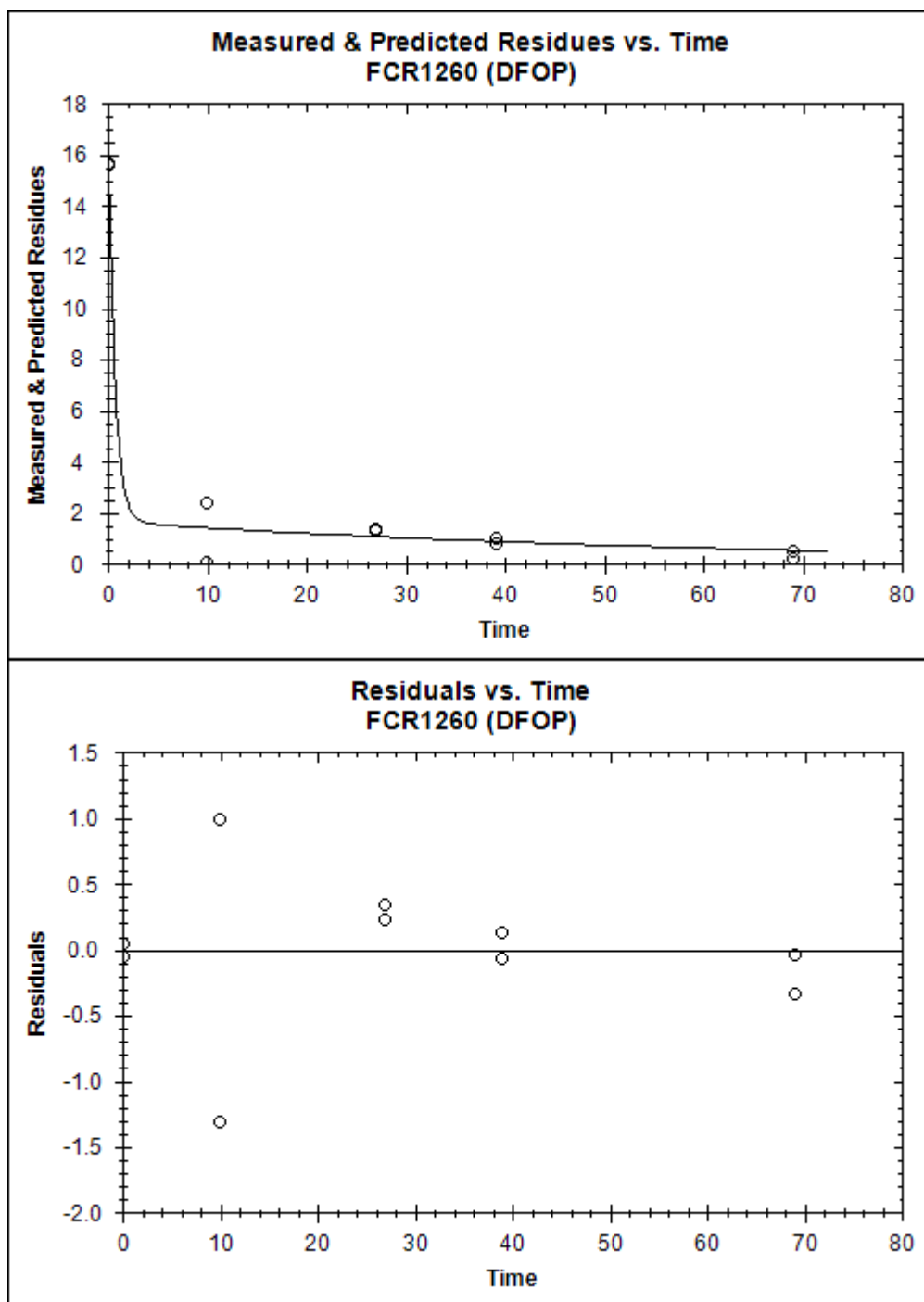
```
# -----
# DT50 and DT90 values
# -----
```

	FCR1260
DT50 :	0.5220
DT90 :	4.3226
Kinetic model :	DFOP

```
# -----
# Measured vs. predicted values
# -----
```

Compartment FCR1260					
time	observed	err-std	predicted	residual	
0.0000	15.7000	0.5479	15.6500	0.0500	
0.0000	15.6000	0.5479	15.6500	-0.0500	
10.0000	0.1000	0.5479	1.4106	-1.3106	
10.0000	2.4000	0.5479	1.4106	0.9894	
27.0000	1.4000	0.5479	1.0660	0.3340	
27.0000	1.3000	0.5479	1.0660	0.2340	
39.0000	0.8000	0.5479	0.8748	-0.0748	

39.0000	1.0000	0.5479	0.8748	0.1252
69.0000	0.2000	0.5479	0.5337	-0.3337
69.0000	0.5000	0.5479	0.5337	-0.0337



11.8.2 Lienden

11.8.2.1 SFO

```
# Trial      : LiendensFCR1260
# File name  : LiendensFCR1260 IRLS SFO  FCR1260.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:39
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----
```

		Initial Value	Lower Bound	Upper Bound	Fixed
M(0)	FCR1260	11.3	0	Inf	False
k	FCR1260	0.1	0	Inf	False

```
# -----
# Chi2 error estimation
# -----
```

	FCR1260	All
Chi2Err%	26.05	26.05
Kinetic model	SFO	

```
# -----
# Parameter estimation
# -----
```

Degrees of Freedom : 8						
Parameter		Estimate	Lower CI	Upper CI	St.Dev	Prob > t
M(0)	FCR1260	8.73308	5.87035	11.596	1.46061	0.000166
k	FCR1260	0.06211	0.01812	0.106	0.02245	0.012204

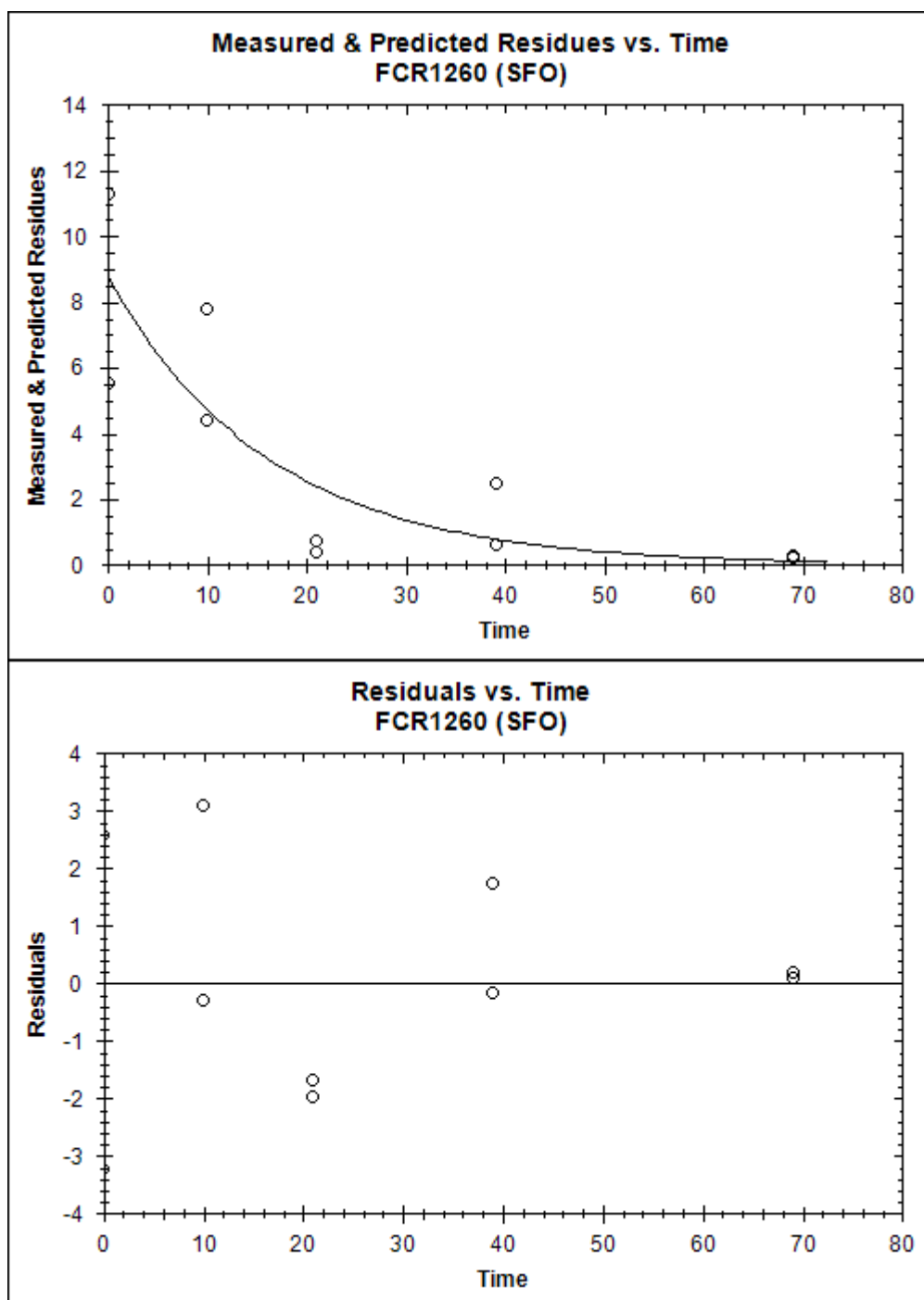
```
# -----
# DT50 and DT90 values
# -----
```

	FCR1260
DT50	11.159
DT90	37.070
Kinetic model	SFO

```
# -----
# Measured vs. predicted values
# -----
```

Compartment FCR1260					
time	observed	err-std	predicted	residual	
0.0000	11.3000	1.9104	8.7331	2.5669	
0.0000	5.5000	1.9104	8.7331	-3.2331	
10.0000	7.8000	1.9104	4.6926	3.1074	
10.0000	4.4000	1.9104	4.6926	-0.2926	
21.0000	0.7000	1.9104	2.3696	-1.6696	
21.0000	0.4000	1.9104	2.3696	-1.9696	
39.0000	2.5000	1.9104	0.7747	1.7253	
39.0000	0.6000	1.9104	0.7747	-0.1747	

69.0000	0.3000	1.9104	0.1202	0.1798
69.0000	0.2000	1.9104	0.1202	0.0798



11.8.2.HS

```

# Trial      : LiendensFCR1260
# File name  : LiendensFCR1260 IRLS HS   FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:39
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      11.30              0              Inf      False
k1    FCR1260      :       0.10              0              Inf      False
k2    FCR1260      :       0.01              0              Inf      False
tb    FCR1260      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      23.57      23.57
Kinetic model :      HS

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FCR1260      :      8.399997      5.496858      11.303      1.481221
0.000647
k1    FCR1260      :      0.007661     -0.142598      0.158      0.076664
0.461829
k2    FCR1260      :      0.202712     -0.299761      0.705      0.256368
0.229609
tb    FCR1260      :      8.746513      3.843885     13.649      2.501387
0.006439

# -----
# DT50 and DT90 values
# -----

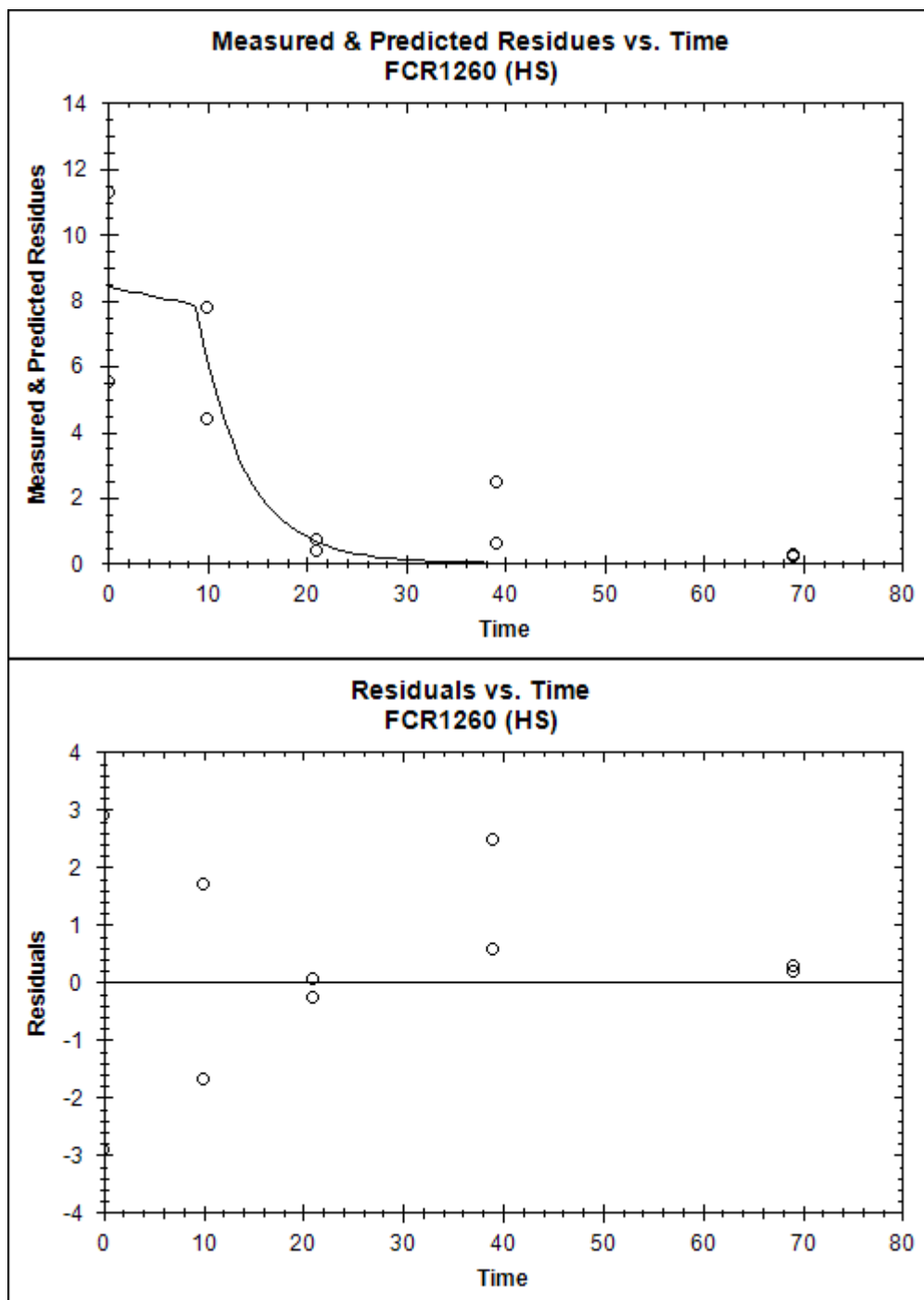
      FCR1260
DT50 :      11.835
DT90 :      19.775
Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
time observed err-std predicted residual
0.0000  11.3000  1.7118      8.4000  2.9000
0.0000   5.5000  1.7118      8.4000 -2.9000

```

10.0000	7.8000	1.7118	6.0929	1.7071
10.0000	4.4000	1.7118	6.0929	-1.6929
21.0000	0.7000	1.7118	0.6553	0.0447
21.0000	0.4000	1.7118	0.6553	-0.2553
39.0000	2.5000	1.7118	0.0171	2.4829
39.0000	0.6000	1.7118	0.0171	0.5829
69.0000	0.3000	1.7118	0.0000	0.3000
69.0000	0.2000	1.7118	0.0000	0.2000



11.8.2.3 FOMC

```

# Trial      : LiendensFCR1260
# File name  : LiendensFCR1260 IRLS FOMC FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:39
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      11.3              0              Inf      False
alpha FCR1260      :       0.1              0              Inf      False
beta  FCR1260      :       0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      30.29      30.29
Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FCR1260:      8.925e+00      6.242e+00      11.61      1.369e+00      0.000164
alpha FCR1260:      3.955e+02      -8.331e+03      9122.05      4.452e+03      0.465857
beta  FCR1260:      5.700e+03      -1.203e+05      131698.89      6.429e+04      0.465917

# -----
# DT50 and DT90 values
# -----

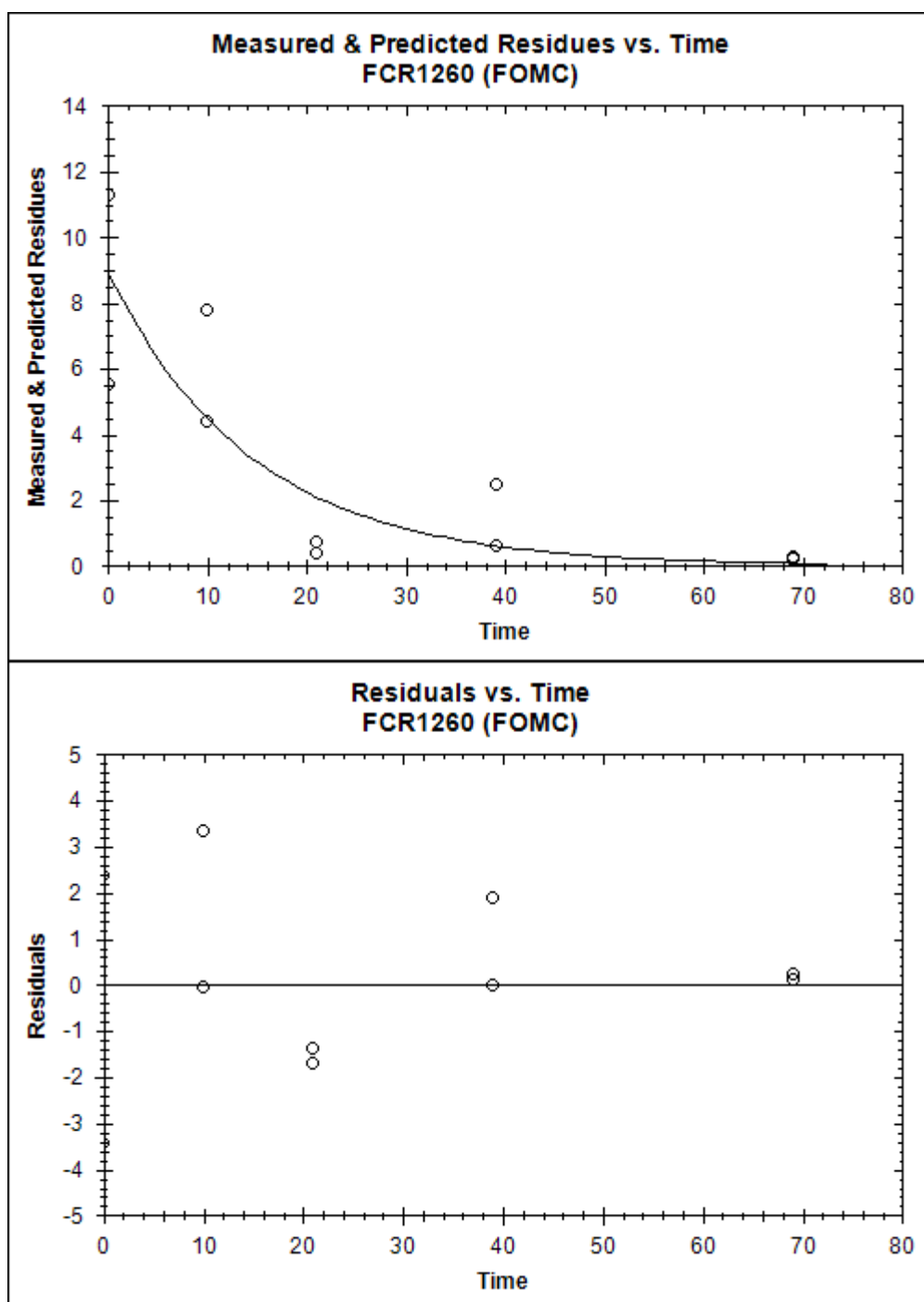
      FCR1260
DT50 :      9.9991
DT90 :      33.284
Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  11.3000  1.9219      8.9255  2.3745
0.0000   5.5000  1.9219      8.9255 -3.4255
10.0000  7.8000  1.9219      4.4625  3.3375
10.0000  4.4000  1.9219      4.4625 -0.0625
21.0000  0.7000  1.9219      2.0846 -1.3846
21.0000  0.4000  1.9219      2.0846 -1.6846
39.0000  2.5000  1.9219      0.6018  1.8982
39.0000  0.6000  1.9219      0.6018 -0.0018
69.0000  0.3000  1.9219      0.0766  0.2234

```

69.0000 0.2000 1.9219 0.0766 0.1234



11.8.2.4 DFOP

```

# Trial      : LiendensFCR1260
# File name  : LiendensFCR1260 IRLS DFOP FCR1260.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_FCR1260
# Created    : on 18 Oct 2013
#            : at 11:39
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FCR1260
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FCR1260      :      11.30           0           Inf      False
k1    FCR1260      :       0.10           0           Inf      False
k2    FCR1260      :       0.01           0           Inf      False
g     FCR1260      :       0.50           0            1      False

# -----
# Chi2 error estimation
# -----

      FCR1260      All
Chi2Err% :      37.08      37.08
Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FCR1260      :      8.747e+00      5.596e+00      11.899      1.608e+00
0.000801
k1    FCR1260      :      6.455e-02      -1.067e-02      0.140      3.838e-02
0.071791
k2    FCR1260      :      2.825e-07      -1.313e+00      1.313      6.700e-01
0.500000
g     FCR1260      :      9.834e-01      5.386e-02      1.913      4.743e-01
0.041740

# -----
# DT50 and DT90 values
# -----

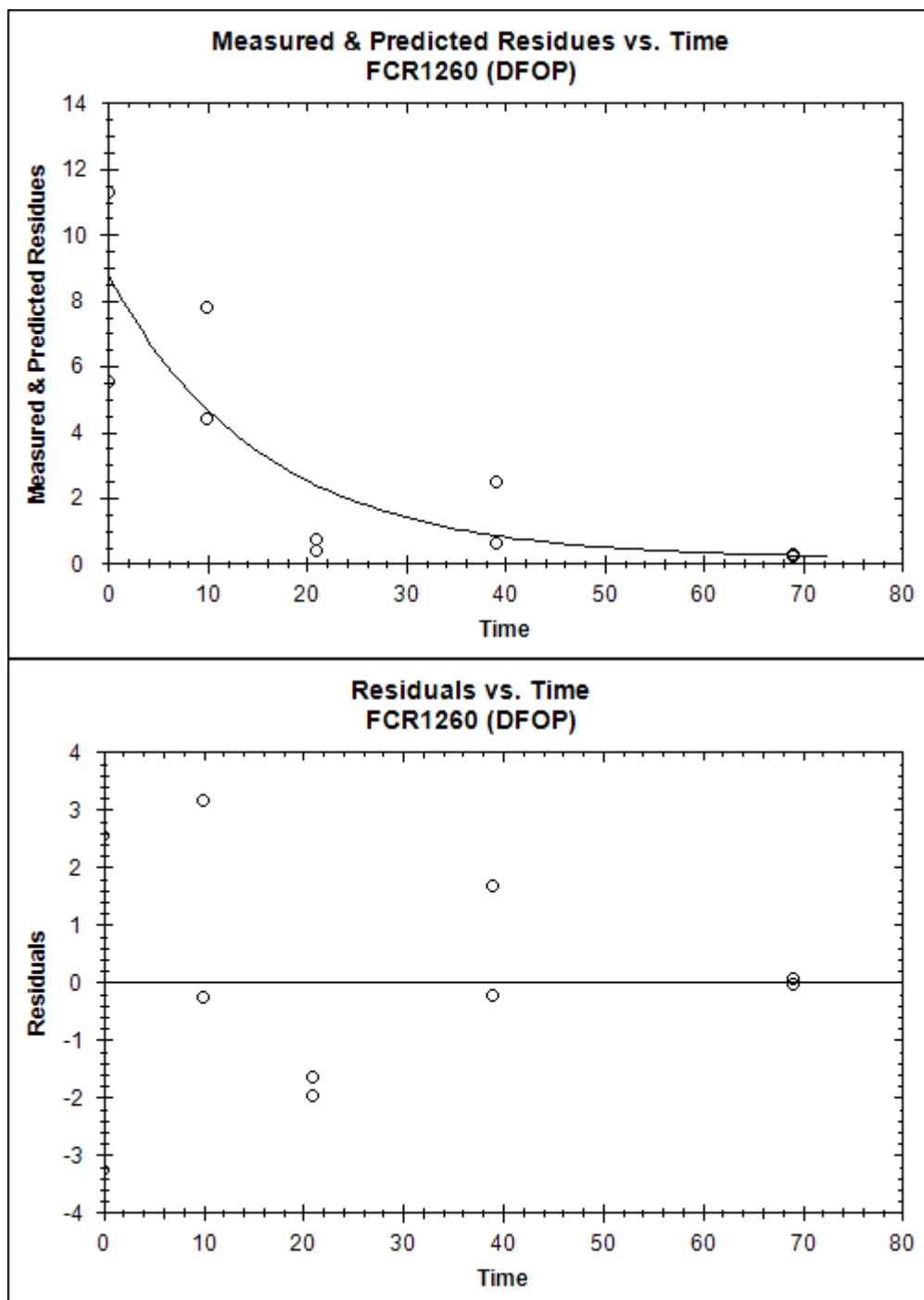
      FCR1260
DT50 :      11.001
DT90 :      38.220
Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment FCR1260
      time observed err-std predicted residual
0.0000  11.3000  1.9092      8.7473  2.5527
0.0000   5.5000  1.9092      8.7473 -3.2473

```

10.0000	7.8000	1.9092	4.6560	3.1440
10.0000	4.4000	1.9092	4.6560	-0.2560
21.0000	0.7000	1.9092	2.3627	-1.6627
21.0000	0.4000	1.9092	2.3627	-1.9627
39.0000	2.5000	1.9092	0.8389	1.6611
39.0000	0.6000	1.9092	0.8389	-0.2389
69.0000	0.3000	1.9092	0.2451	0.0549
69.0000	0.2000	1.9092	0.2451	-0.0451



11.9 FPB-Acid (FCR 3191) Dissipation Sediment Phase

11.9.1 Ijzendoorn

11.9.1.1 SFO

```

# Trial      : IjzendoornsFPB
# File name  : IjzendoornsFPB IRLS SFO  FPB.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FPB
# Created    : on 18 Oct 2013
#            : at 11:01
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

M(0)  FPB      :      17.80      0      Inf      Fixed
k      FPB      :      0.01      0      Inf      False

# -----
# Chi2 error estimation
# -----

Chi2Err% :      6.418      6.418
Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      15.39259      13.25917      17.526      1.08850      3.91e-06
k      FPB      :      0.12347      0.06288      0.184      0.03091      0.00358

# -----
# DT50 and DT90 values
# -----

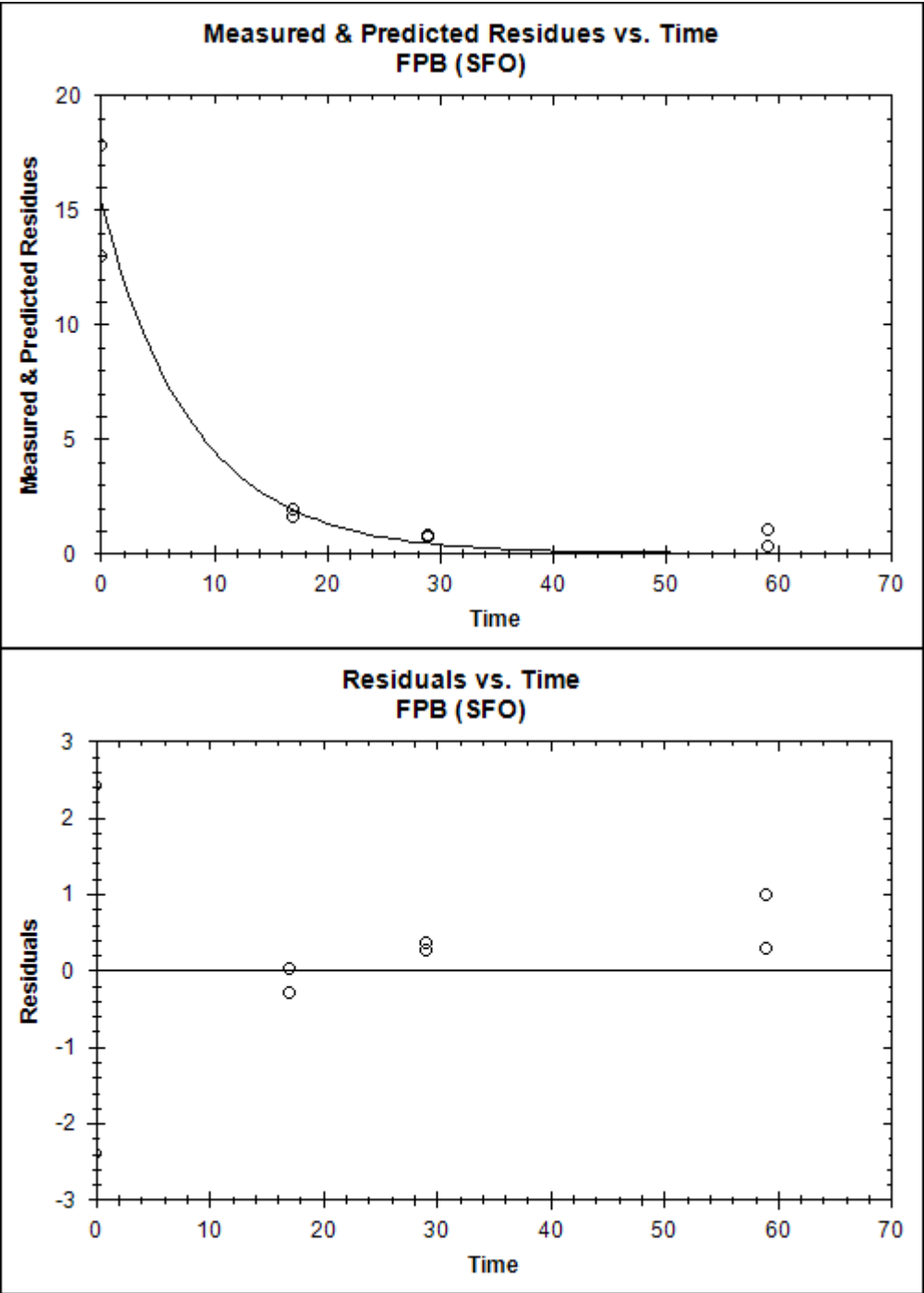
DT50 :      5.6141
DT90 :      18.650
Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

Compartment FPB
time observed err-std predicted residual
0.0000 17.8000 1.2687 15.3926 2.4074
0.0000 13.0000 1.2687 15.3926 -2.3926
17.0000 1.6000 1.2687 1.8869 -0.2869
17.0000 1.9000 1.2687 1.8869 0.0131
29.0000 0.7000 1.2687 0.4289 0.2711

```

29.0000	0.8000	1.2687	0.4289	0.3711
59.0000	0.3000	1.2687	0.0106	0.2894
59.0000	1.0000	1.2687	0.0106	0.9894



11.9.1.2HS

```

# Trial      : IjzendoornsFPB
# File name  : IjzendoornsFPB IRLS HS   FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FPB
# Created    : on 18 Oct 2013
#            : at 10:31
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      17.80              0              Inf      False
k1    FPB      :       0.10              0              Inf      False
k2    FPB      :       0.01              0              Inf      False
tb    FPB      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      Inf      All
      Kinetic model :      HS      Inf

# -----
# Parameter estimation
# -----

Degrees of Freedom : 4
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      15.40001      13.00442      17.796      1.22226      0.000114
k1    FPB      :       0.26857      -0.39388      0.931      0.33799      0.235662
k2    FPB      :       0.03281      -0.12049      0.186      0.07822      0.348202
tb    FPB      :       7.25593      -17.04804      31.560      12.40021      0.294934

# -----
# DT50 and DT90 values
# -----

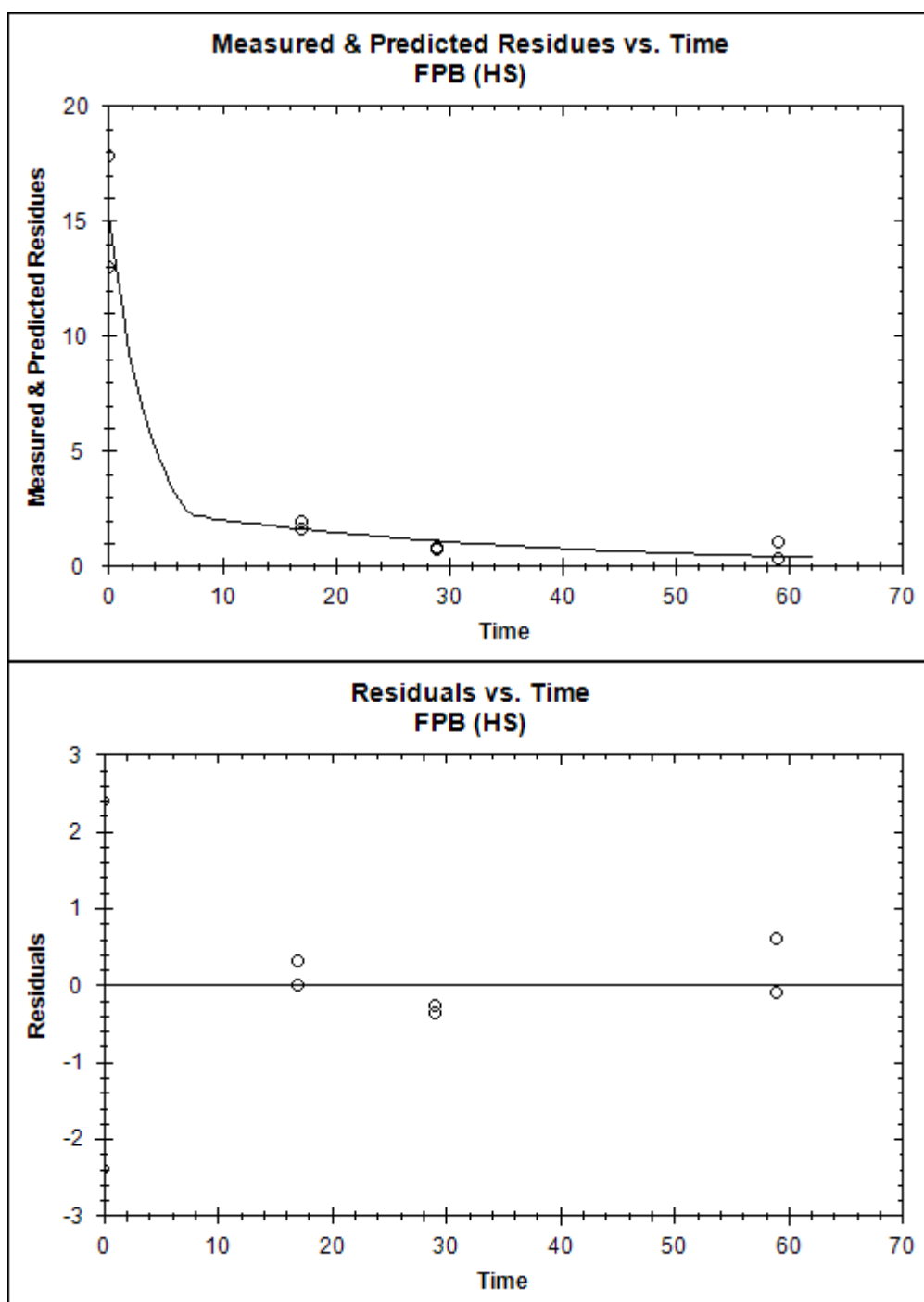
      DT50 :      2.5809
      DT90 :      18.040
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 17.8000 1.2348 15.4000 2.4000
0.0000 13.0000 1.2348 15.4000 -2.4000
17.0000 1.6000 1.2348 1.5935 0.0065
17.0000 1.9000 1.2348 1.5935 0.3065
29.0000 0.7000 1.2348 1.0748 -0.3748
29.0000 0.8000 1.2348 1.0748 -0.2748
59.0000 0.3000 1.2348 0.4017 -0.1017

```

59.0000 1.0000 1.2348 0.4017 0.5983



11.9.1.3 FOMC

```

# Trial      : IjzendoornsFPB
# File name  : IjzendoornsFPB IRLS FOMC FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FPB
# Created    : on 18 Oct 2013
#            : at 10:32
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      17.8              0              Inf      False
alpha FPB      :      0.1              0              Inf      False
beta  FPB      :      0.1              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      3.367      3.367
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 5
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      15.4003      13.5039      17.297      0.9676      8.91e-06
alpha FPB      :      1.1162      -3.7859      6.018      2.5011      0.337
beta  FPB      :      2.6824      -25.9911      31.356      14.6296      0.431

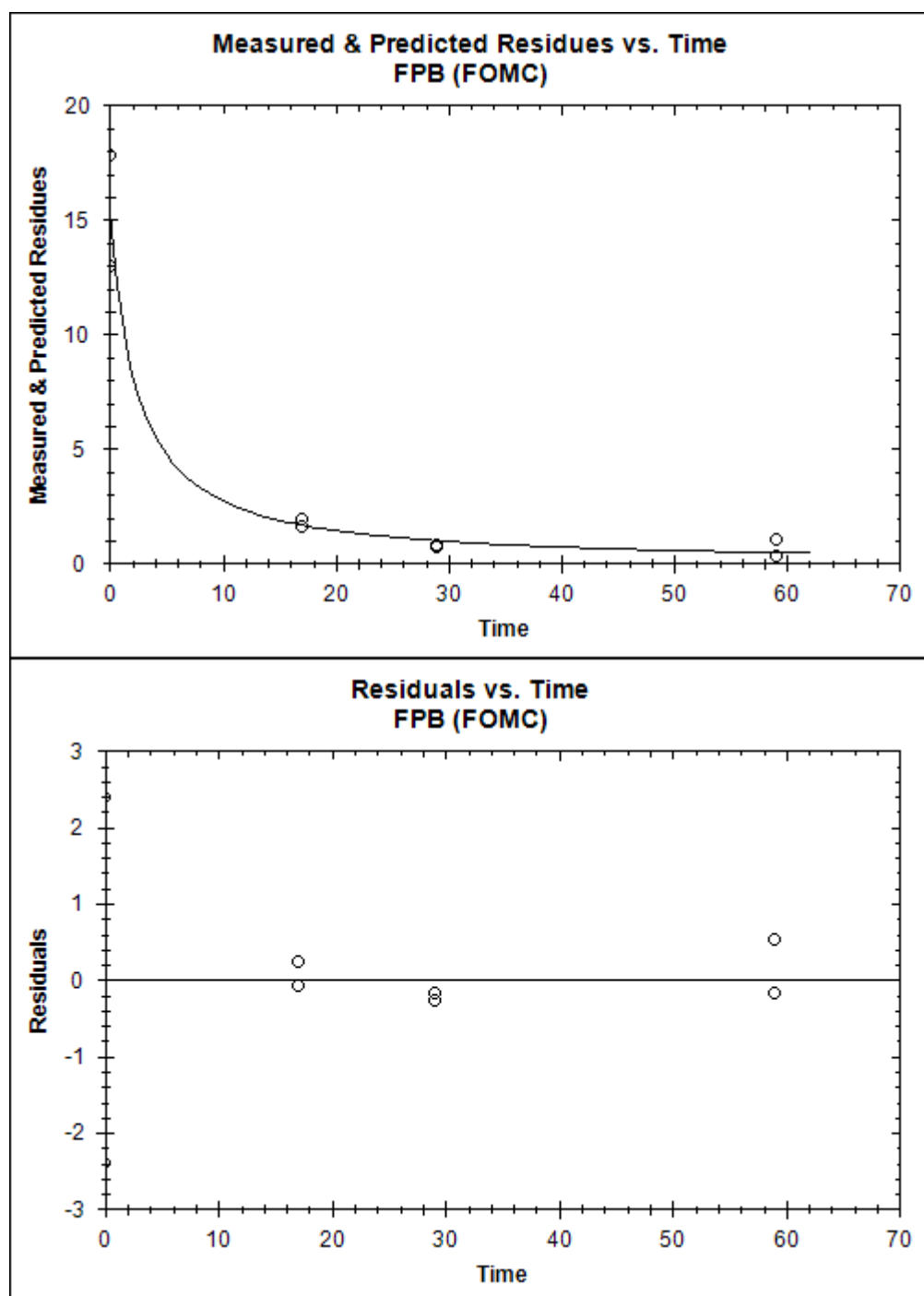
# -----
# DT50 and DT90 values
# -----

      DT50 :      2.3088
      DT90 :      18.423
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

Compartment FPB
time observed err-std predicted residual
0.0000 17.8000 1.2249 15.4003 2.3997
0.0000 13.0000 1.2249 15.4003 -2.4003
17.0000 1.6000 1.2249 1.6648 -0.0648
17.0000 1.9000 1.2249 1.6648 0.2352
29.0000 0.7000 1.2249 0.9786 -0.2786
29.0000 0.8000 1.2249 0.9786 -0.1786
59.0000 0.3000 1.2249 0.4652 -0.1652
59.0000 1.0000 1.2249 0.4652 0.5348

```



11.9.1.4DFOP

```

# Trial      : IjzendoornsFPB
# File name  : IjzendoornsFPB IRLS DFOP FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Ijzendoorn\Ijzendoorn_s_FPB
# Created    : on 18 Oct 2013
#            : at 10:31
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Ijzendoorn s
# # Ijzendoorn sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      17.80              0              Inf      False
k1    FPB      :       0.10              0              Inf      False
k2    FPB      :       0.01              0              Inf      False
g      FPB      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      Inf      All
      Kinetic model :      DFOP      Inf

# -----
# Parameter estimation
# -----

Degrees of Freedom : 4
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      1.540e+01      1.290e+01      17.898      1.274e+00      0.000134
k1    FPB      :      1.516e-01      -1.530e-01      0.456      1.554e-01      0.192265
k2    FPB      :      6.464e-07      -2.543e-01      0.254      1.298e-01      0.499998
g      FPB      :      9.601e-01      4.476e-01      1.473      2.615e-01      0.010680

# -----
# DT50 and DT90 values
# -----

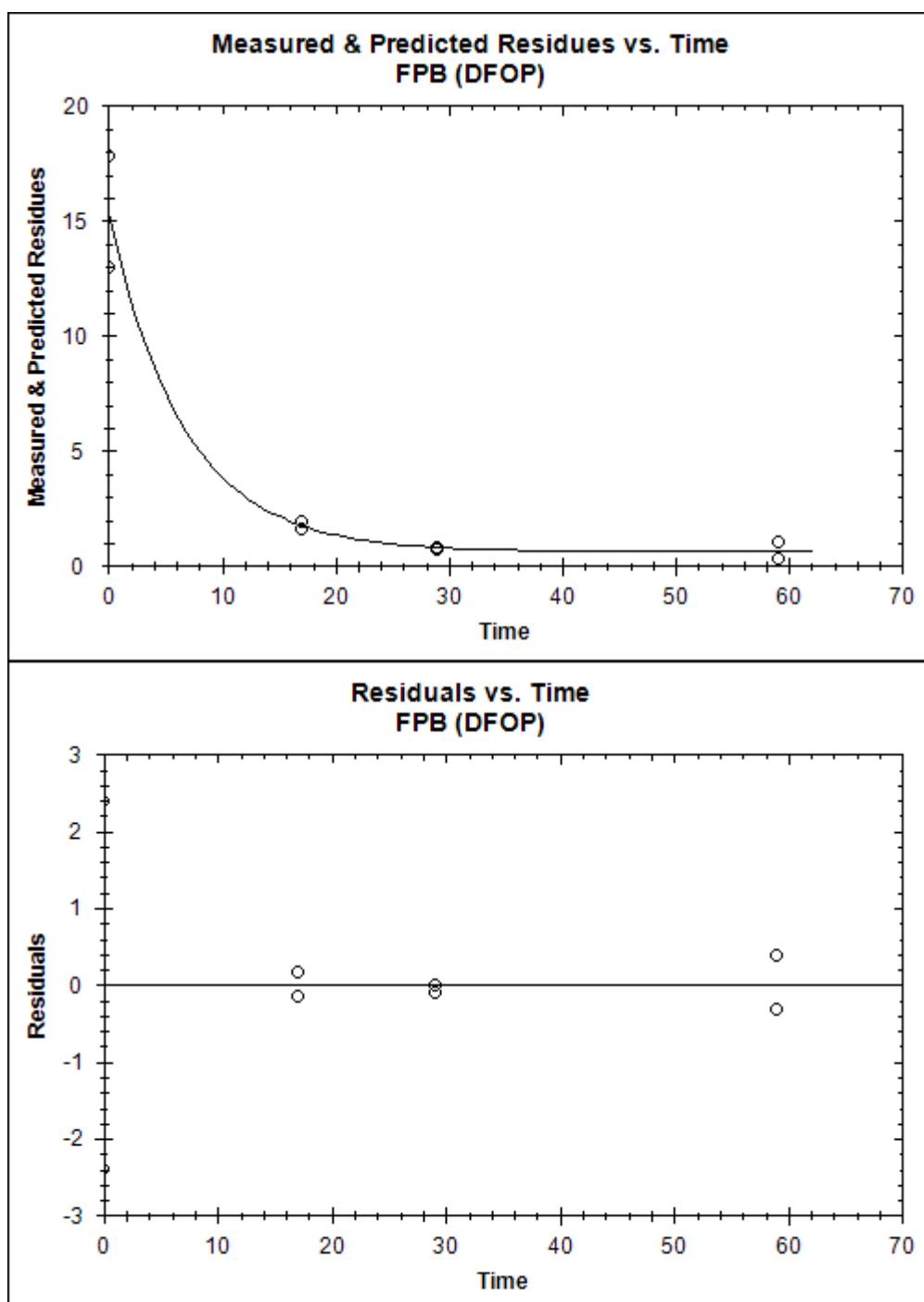
      DT50 :      4.8517
      DT90 :      18.275
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 17.8000 1.2156 15.4004 2.3996
0.0000 13.0000 1.2156 15.4004 -2.4004
17.0000 1.6000 1.2156 1.7374 -0.1374
17.0000 1.9000 1.2156 1.7374 0.1626
29.0000 0.7000 1.2156 0.7962 -0.0962
29.0000 0.8000 1.2156 0.7962 0.0038
59.0000 0.3000 1.2156 0.6160 -0.3160

```

59.0000 1.0000 1.2156 0.6160 0.3840



11.9.2 Lienden

11.9.2.1 SFO

```
# Trial      : LiendensFPB
# File name  : LiendensFPB IRLS SFO  FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_FPB
# Created    : on 18 Oct 2013
#            : at 11:41
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm : solnp
# Comments    :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      18.20              0              Inf      False
k      FPB      :       0.01              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      13.27      13.27
      Kinetic model :      SFO

# -----
# Parameter estimation
# -----

Degrees of Freedom : 8
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FPB      :      24.23032      19.71759      28.743      2.30245
2.90e-06
k      FPB      :       0.16910      0.06565      0.273      0.05278
0.00627

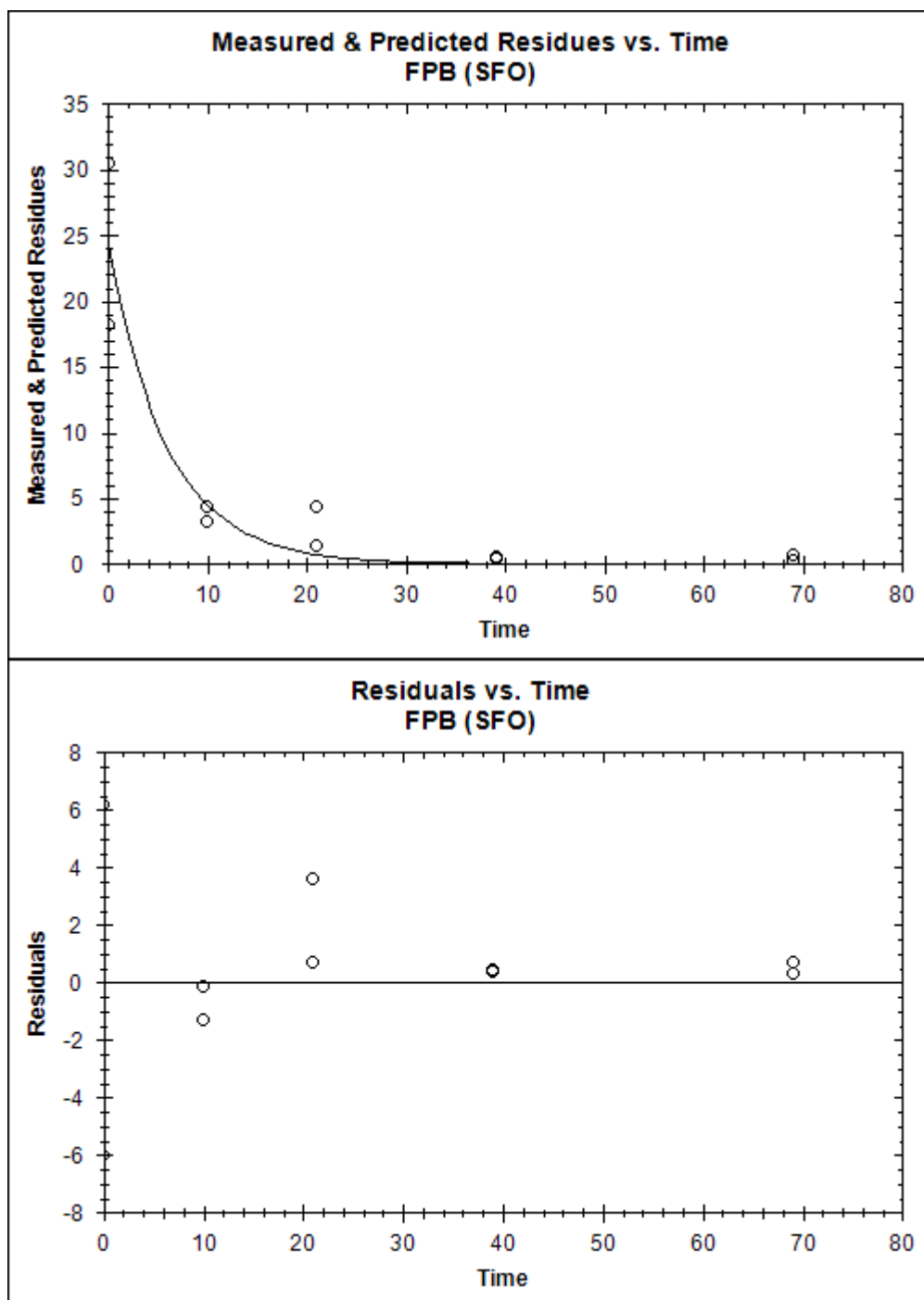
# -----
# DT50 and DT90 values
# -----

      DT50 :      4.0991
      DT90 :      13.617
      Kinetic model :      SFO

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 18.2000 3.0081 24.2303 -6.0303
0.0000 30.4000 3.0081 24.2303 6.1697
10.0000 4.3000 3.0081 4.4666 -0.1666
10.0000 3.2000 3.0081 4.4666 -1.2666
21.0000 1.4000 3.0081 0.6953 0.7047
21.0000 4.3000 3.0081 0.6953 3.6047
39.0000 0.4000 3.0081 0.0331 0.3669
```

39.0000	0.5000	3.0081	0.0331	0.4669
69.0000	0.7000	3.0081	0.0002	0.6998
69.0000	0.3000	3.0081	0.0002	0.2998



11.9.2.2HS

```

# Trial      : LiendensFPB
# File name  : LiendensFPB IRLS HS   FPB.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_s_FPB
# Created    : on 18 Oct 2013
#            : at 11:41
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments      :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      18.20              0              Inf      False
k1    FPB      :       0.10              0              Inf      False
k2    FPB      :       0.01              0              Inf      False
tb    FPB      :       3.00              0              Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      6.518      6.518
      Kinetic model :      HS      All

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FPB      :      24.29998      19.48495      29.115      2.45669
3.08e-05
k1    FPB      :       0.25001      -0.51500      1.015      0.39032
0.273
k2    FPB      :       0.04658      -0.08428      0.177      0.06677
0.256
tb    FPB      :       6.67825      -19.39498      32.751      13.30291
0.317

# -----
# DT50 and DT90 values
# -----

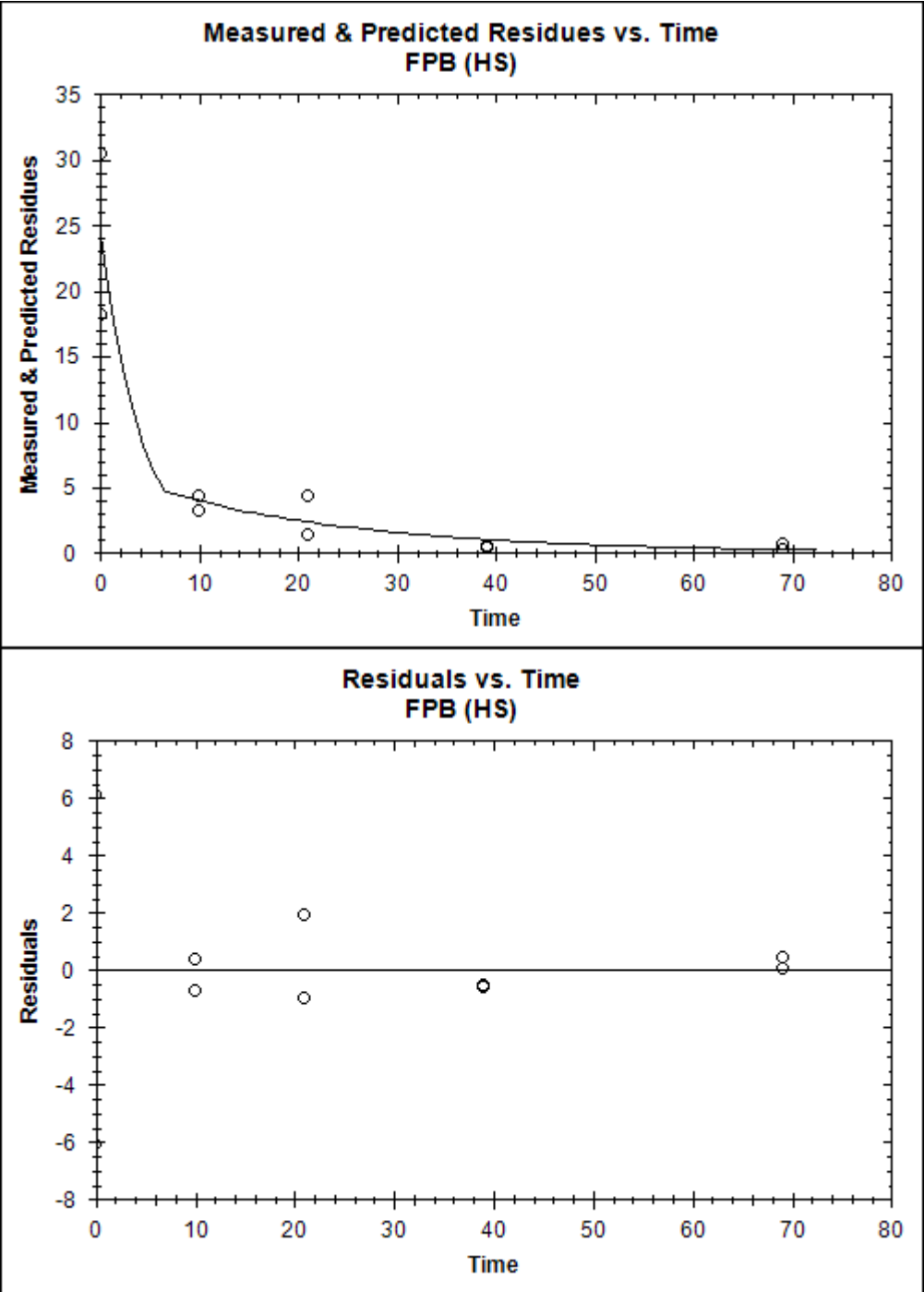
      DT50 :      2.7725
      DT90 :      20.266
      Kinetic model :      HS

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 18.2000 2.8397 24.3000 -6.1000
0.0000 30.4000 2.8397 24.3000 6.1000

```

10.0000	4.3000	2.8397	3.9200	0.3800
10.0000	3.2000	2.8397	3.9200	-0.7200
21.0000	1.4000	2.8397	2.3483	-0.9483
21.0000	4.3000	2.8397	2.3483	1.9517
39.0000	0.4000	2.8397	1.0154	-0.6154
39.0000	0.5000	2.8397	1.0154	-0.5154
69.0000	0.7000	2.8397	0.2510	0.4490
69.0000	0.3000	2.8397	0.2510	0.0490



11.9.2.3 FOMC

```

# Trial      : LiendensFPB
# File name  : LiendensFPB IRLS FOMC FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\Lienden\Lienden_s_FPB
# Created    : on 18 Oct 2013
#            : at 11:41
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      18.2          0          Inf      False
alpha FPB      :       0.1          0          Inf      False
beta  FPB      :       0.1          0          Inf      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      6.97      6.97
      Kinetic model :      FOMC

# -----
# Parameter estimation
# -----

Degrees of Freedom : 7
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      24.298      19.771      28.825      2.310      7.65e-06
alpha FPB      :       1.062      -2.062      4.185      1.594      0.263
beta  FPB      :       2.230     -13.045     17.506      7.794      0.392

# -----
# DT50 and DT90 values
# -----

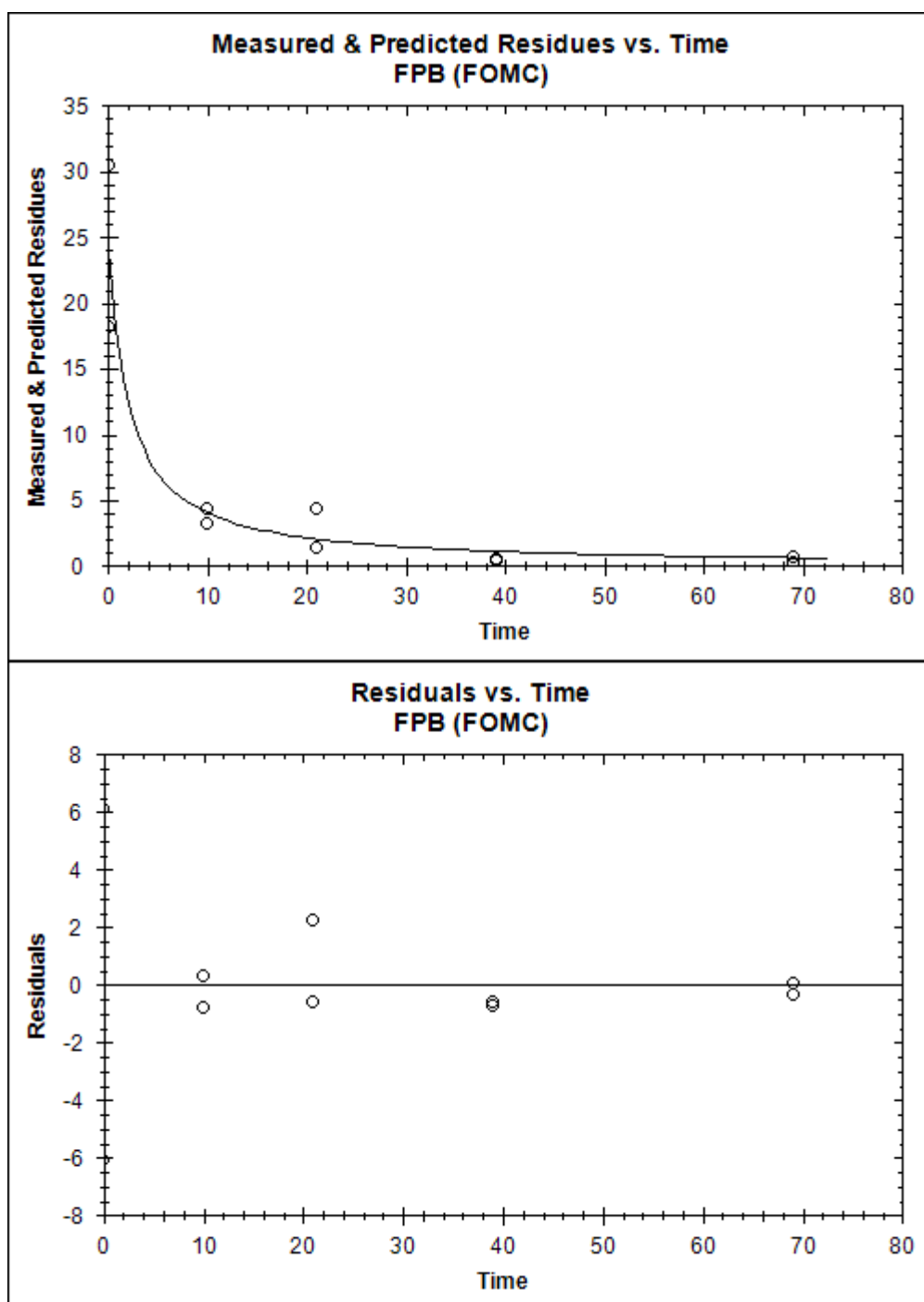
      DT50 :      2.0538
      DT90 :      17.274
      Kinetic model :      FOMC

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000 18.2000 2.8579 24.2978 -6.0978
0.0000 30.4000 2.8579 24.2978 6.1022
10.0000 4.3000 2.8579 3.9884 0.3116
10.0000 3.2000 2.8579 3.9884 -0.7884
21.0000 1.4000 2.8579 2.0182 -0.6182
21.0000 4.3000 2.8579 2.0182 2.2818
39.0000 0.4000 2.8579 1.0975 -0.6975
39.0000 0.5000 2.8579 1.0975 -0.5975
69.0000 0.7000 2.8579 0.6141 0.0859

```

69.0000 0.3000 2.8579 0.6141 -0.3141



11.9.2.4DFOP

```

# Trial      : LiendensFPB
# File name  : LiendensFPB IRLS DFOP FPB.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\Lienden\Lienden_s_FPB
# Created    : on 18 Oct 2013
#            : at 11:41
#            : by EZCIA on ADEMONC6031(4CPUs)
# KinGUIII version : 2.2012.1030.1351
# Viewer version  : 2.2012.1205.1116 (Network Deployed)
# Sourcefunctions : 1.2013.0411.1519
# Opt. Algorithm  : solnp
# Comments     :
# # study ID: Anderson
# # label: 14C
# # soil :Lienden s
# # Lienden sediment FPB-acid
# #

# =====
# Results of the kinetic evaluation
# =====

# -----
# Initial values
# -----

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      18.20              0              Inf      False
k1    FPB      :       0.10              0              Inf      False
k2    FPB      :       0.01              0              Inf      False
g     FPB      :       0.50              0              1      False

# -----
# Chi2 error estimation
# -----

      Chi2Err% :      6.518      6.518
      Kinetic model :      DFOP

# -----
# Parameter estimation
# -----

Degrees of Freedom : 6
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob
> t
M(0)  FPB      :      24.30000      19.44292      29.157      2.47815
3.24e-05
k1    FPB      :       1.27844     -84.42530      86.982      43.72720
0.4888
k2    FPB      :       0.04658     -0.06767       0.161      0.05829
0.2273
g     FPB      :       0.74298       0.20498       1.281      0.27449
0.0176

# -----
# DT50 and DT90 values
# -----

      DT50 :      0.8431
      DT90 :      20.266
      Kinetic model :      DFOP

# -----
# Measured vs. predicted values
# -----

      Compartment FPB
      time observed err-std predicted residual
0.0000  18.2000  2.8397  24.3000  -6.1000
0.0000  30.4000  2.8397  24.3000   6.1000

```

10.0000	4.3000	2.8397	3.9201	0.3799
10.0000	3.2000	2.8397	3.9201	-0.7201
21.0000	1.4000	2.8397	2.3484	-0.9484
21.0000	4.3000	2.8397	2.3484	1.9516
39.0000	0.4000	2.8397	1.0154	-0.6154
39.0000	0.5000	2.8397	1.0154	-0.5154
69.0000	0.7000	2.8397	0.2511	0.4489
69.0000	0.3000	2.8397	0.2511	0.0489

