

# **Renewal Assessment Report**

## **beta-Cyfluthrin**

**Volume 3 – B.8 Environmental fate and behaviour**

### **Appendix 1**

**Rapporteur Member State: Germany**

**Co-Rapporteur Member State: Hungary**

## **Appendix 1:**

### **KinGUI results from the study**

#### **Kinetic Evaluation of Aerobic Metabolism of Beta-Cyfluthrin and its Metabolites in Soil According to FOCUS Kinetics**

**Beta-Cyfluthrin (FCR 4545)**

**DCVA (AE0433590)**

**FPB-acid (AE F105561)**

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Date: 26 November 2013

Report No. EnSa-13-0876

## 11.3 KinGUII Results Beta-Cyfluthrin

### 11.3.1 Grand Forks County ND (BETA-CYF, DCVA)

#### 11.3.1.1 SFO

```
# Trial      : NDsandyclayloam
# File name  : NDsandyclayloam IRLS SFO Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\NDsandyclayloam
# Created    : on 30 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. Algorithms : solnp; L-BFGS-B
# Comments    :
# # study ID:
# # label: 14C cyclopropyl
# # soil : ND-sandy clay loam
# # ND-sandy clay loam
# #

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

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0) Par      :      103.9              0              Inf      False
k   Par      :         0.1              0              Inf      False
k   Met      :         0.1              0              Inf      False
FF  Par -> Met :         0.1              0              1      False
M(0) Met      :         0                  0              1      True

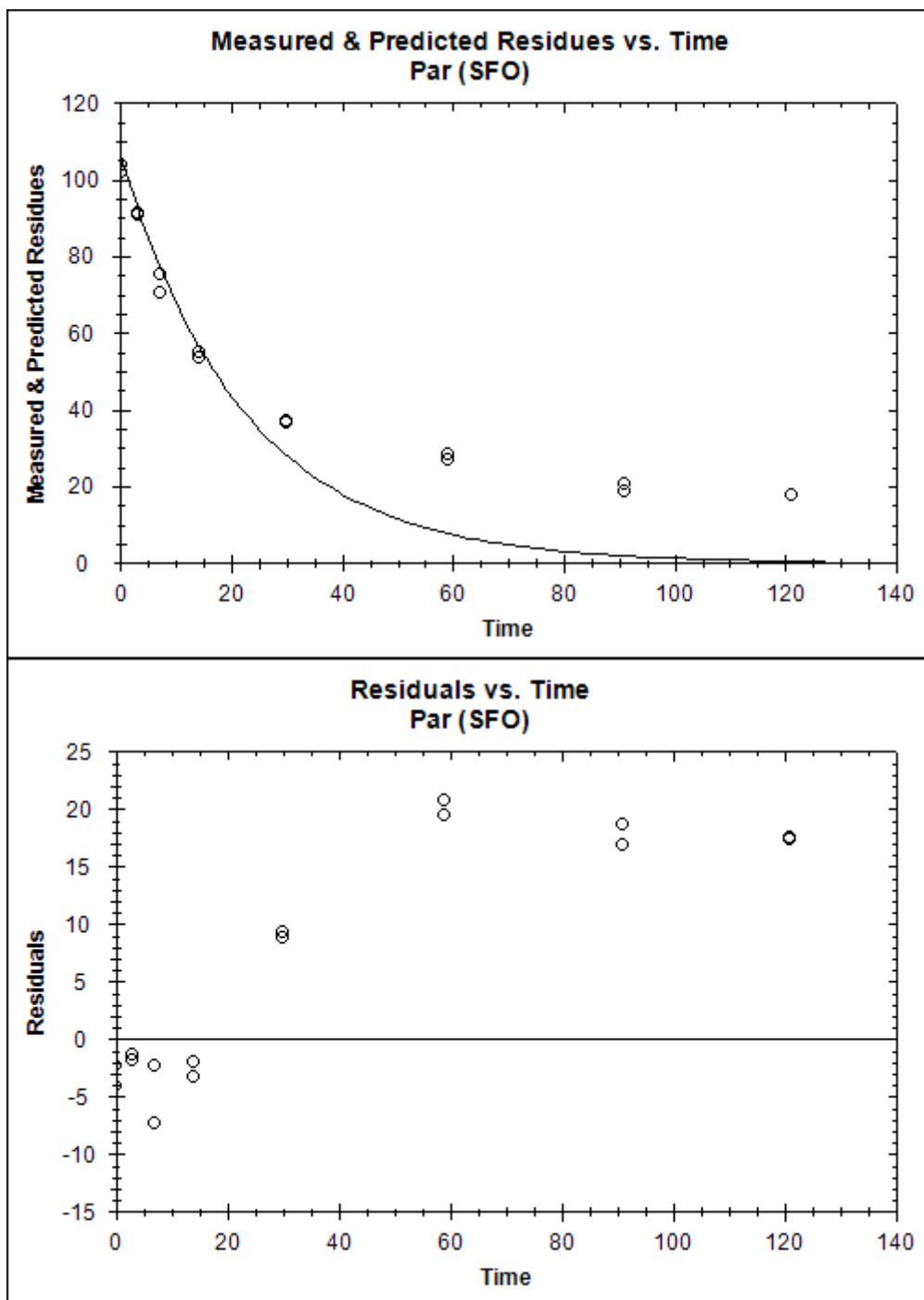
# -----
# Chi2 error estimation
# -----
# -----
#           Par      Met      All
#           Chi2Err% :      18.048      6.738      24.429
#           Kinetic model :      SFO      SFO

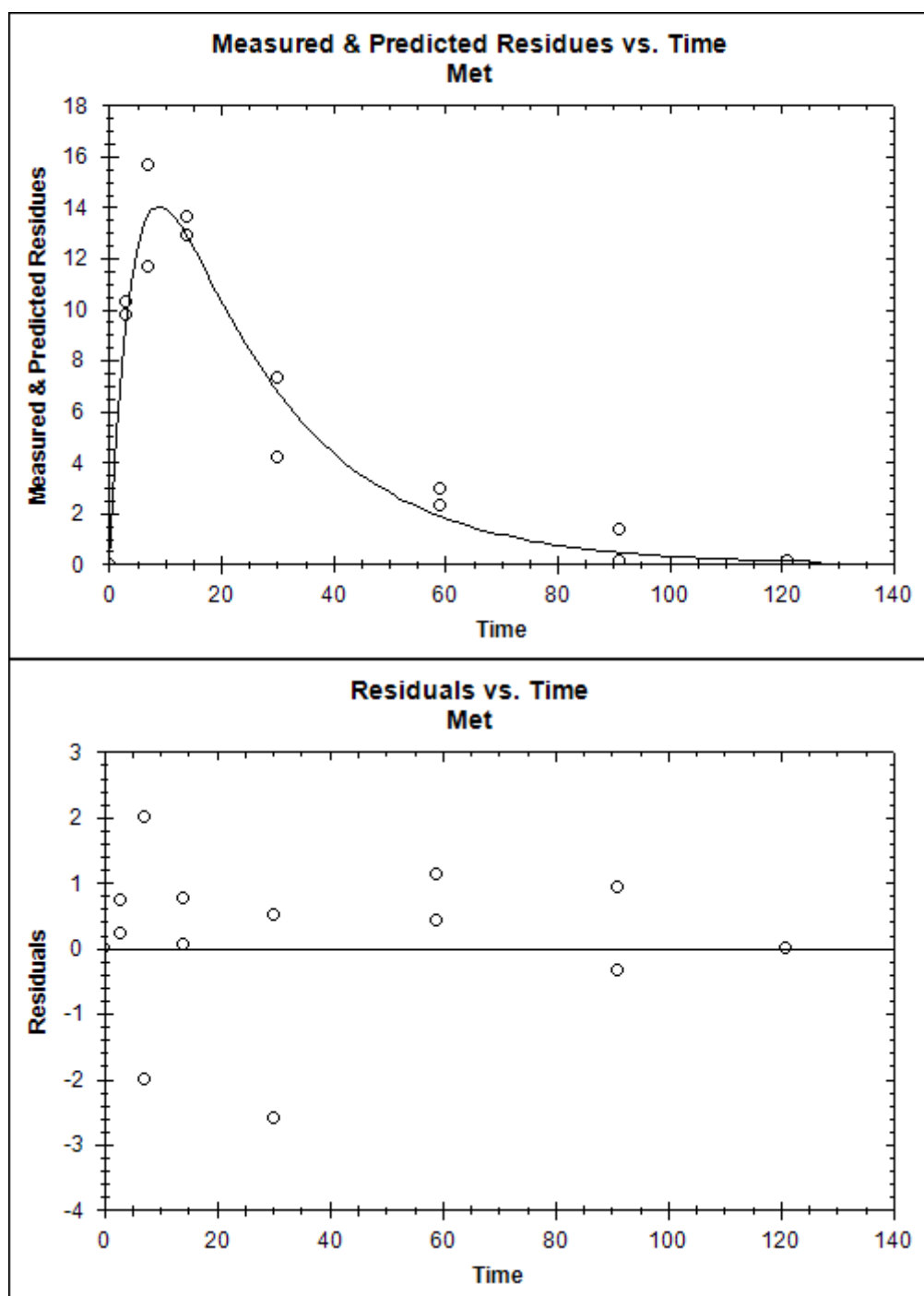
# -----
# Parameter estimation
# -----
# -----
# Degrees of Freedom : 28
# Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0) Par      :      1.062e+02      9.462e+01      117.777      5.908e+00      < 2e-16
k   Par      :      4.456e-02      3.309e-02      0.056      5.853e-03      1.36e-08
k   Met      :      2.267e-01      1.575e-01      0.296      3.535e-02      3.03e-07
FF  Par -> Met :      1.000e+00

# -----
# DT50 and DT90 values
# -----
# -----
#           Par      Met
#           DT50 :      15.556      3.0570
#           DT90 :      51.678      10.155
#           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 103.9000 12.0454 106.1986 -2.2986 0.0000 1.0790 0.0000 0.0000
0.0000 102.2000 12.0454 106.1986 -3.9986 0.0000 1.0790 0.0000 0.0000
3.0000 91.6000 12.0454 92.9109 -1.3109 9.8000 1.0790 9.5676 0.2324
```

3.0000	91.1000	12.0454	92.9109	-1.8109	10.3000	1.0790	9.5676	0.7324
7.0000	70.4000	12.0454	77.7434	-7.3434	15.7000	1.0790	13.7019	1.9981
7.0000	75.4000	12.0454	77.7434	-2.3434	11.7000	1.0790	13.7019	-2.0019
14.0000	55.0000	12.0454	56.9126	-1.9126	13.6000	1.0790	12.8326	0.7674
14.0000	53.6000	12.0454	56.9126	-3.3126	12.9000	1.0790	12.8326	0.0674
30.0000	37.3000	12.0454	27.8995	9.4005	7.3000	1.0790	6.7943	0.5057
30.0000	36.8000	12.0454	27.8995	8.9005	4.2000	1.0790	6.7943	-2.5943
59.0000	28.4000	12.0454	7.6635	20.7365	3.0000	1.0790	1.8742	1.1258
59.0000	27.1000	12.0454	7.6635	19.4365	2.3000	1.0790	1.8742	0.4258
91.0000	20.6000	12.0454	1.8416	18.7584	1.4000	1.0790	0.4504	0.9496
91.0000	18.7000	12.0454	1.8416	16.8584	0.1300	1.0790	0.4504	-0.3204
121.0000	18.0000	12.0454	0.4838	17.5162	0.1300	1.0790	0.1183	0.0117
121.0000	17.9000	12.0454	0.4838	17.4162	0.1300	1.0790	0.1183	0.0117





## 11.3.1.2 HS

```

# Trial      : NDSandyclayloam
# File name  : NDSandyclayloam IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\NDSandyclayloam
# Created    : on 30 Oct 2013
#            : at 10:25
#            : 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:
# # label: 14C cyclopropyl
# # soil : ND-sandy clay loam
# # ND-sandy clay loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      103.90           0           Inf      False
k1    Par      :       0.10           0           Inf      False
k2    Par      :       0.01           0           Inf      False
tb    Par      :       3.00           0           Inf      False
k      Met      :       0.10           0           Inf      False
FF    Par -> Met :       0.10           0           1      False
M(0)  Met      :           0              True

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

      Chi2Err% :       5.047      Par      Met      All
Kinetic model :       HS          SFO      6.641

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

Degrees of Freedom : 26
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :  1.047e+02  1.005e+02  108.932  2.148e+00  < 2e-16
k1    Par      :  5.369e-02  4.457e-02  0.063   4.653e-03  4.96e-12
k2    Par      :  1.291e-02  1.056e-02  0.015   1.199e-03  2.22e-11
tb    Par      :  1.264e+01  1.061e+01  14.669  1.036e+00  1.44e-12
k      Met      :  1.286e-01  7.324e-02  0.184   2.823e-02  5.45e-05
FF    Par -> Met :  0.6782      1.142e-01

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

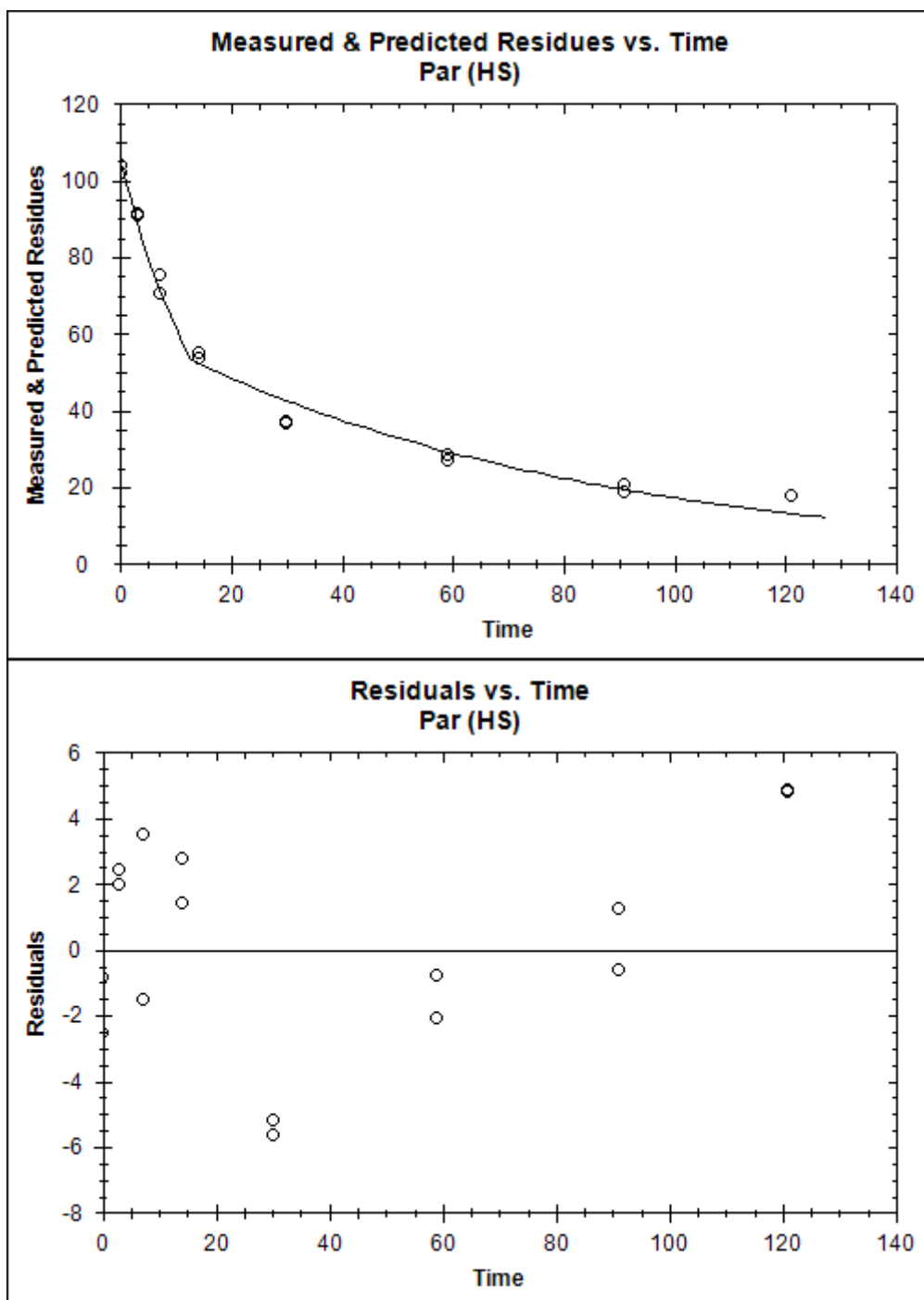
      DT50 :       13.767      Par      Met
      DT90 :       138.46      HS          SFO
Kinetic model :       HS          SFO

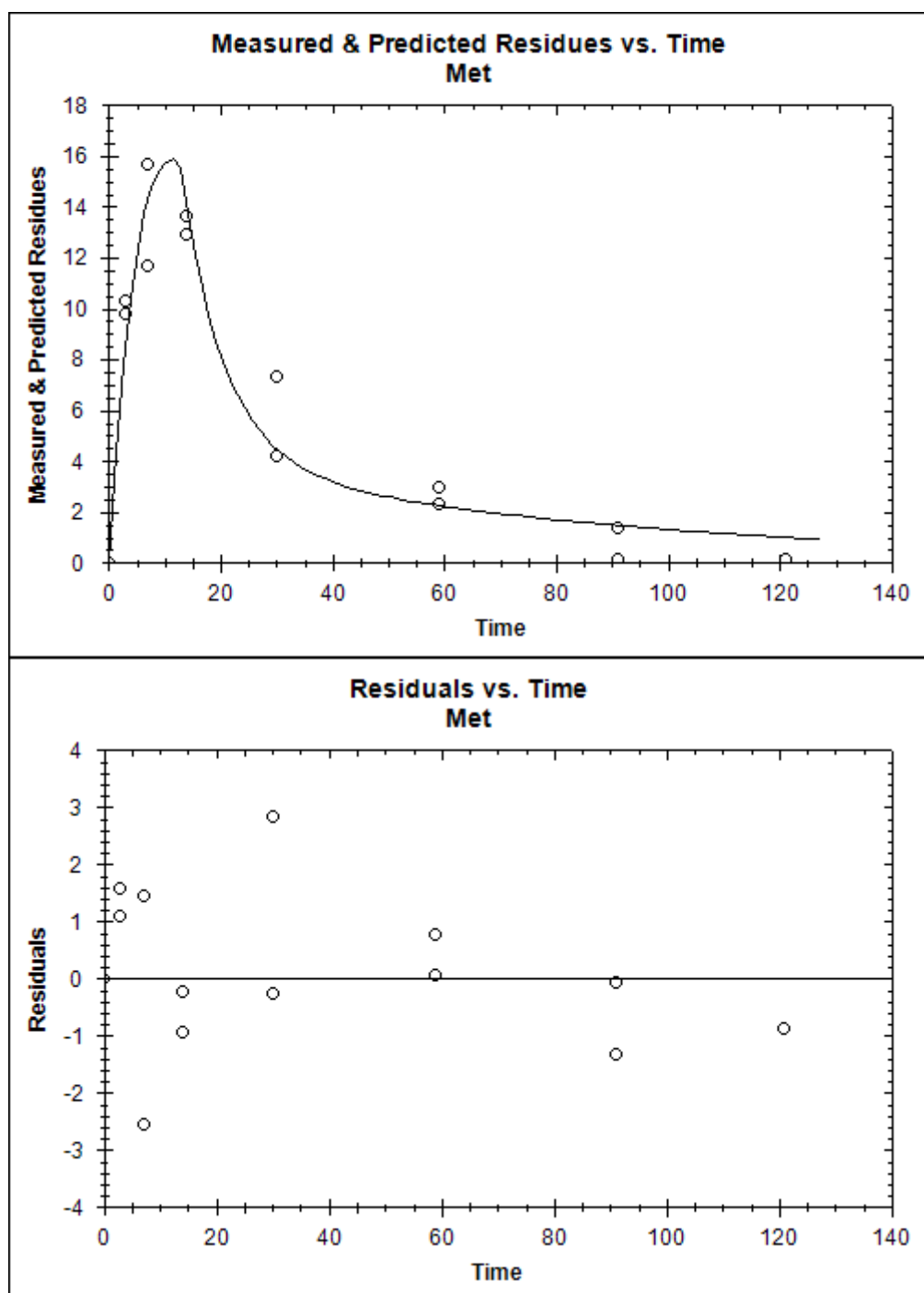
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000 103.9000 3.0975 104.7214 -0.8214 0.0000 1.2539 0.0000 0.0000
0.0000 102.2000 3.0975 104.7214 -2.5214 0.0000 1.2539 0.0000 0.0000
3.0000 91.6000 3.0975 89.1420 2.4580 9.8000 1.2539 8.7215 1.0785
3.0000 91.1000 3.0975 89.1420 1.9580 10.3000 1.2539 8.7215 1.5785

```

7.0000	70.4000	3.0975	71.9137	-1.5137	15.7000	1.2539	14.2660	1.4340
7.0000	75.4000	3.0975	71.9137	3.4863	11.7000	1.2539	14.2660	-2.5660
14.0000	55.0000	3.0975	52.2032	2.7968	13.6000	1.2539	13.8451	-0.2451
14.0000	53.6000	3.0975	52.2032	1.3968	12.9000	1.2539	13.8451	-0.9451
30.0000	37.3000	3.0975	42.4629	-5.1629	7.3000	1.2539	4.4782	2.8218
30.0000	36.8000	3.0975	42.4629	-5.6629	4.2000	1.2539	4.4782	-0.2782
59.0000	28.4000	3.0975	29.2046	-0.8046	3.0000	1.2539	2.2406	0.7594
59.0000	27.1000	3.0975	29.2046	-2.1046	2.3000	1.2539	2.2406	0.0594
91.0000	20.6000	3.0975	19.3231	1.2769	1.4000	1.2539	1.4628	-0.0628
91.0000	18.7000	3.0975	19.3231	-0.6231	0.1300	1.2539	1.4628	-1.3328
121.0000	18.0000	3.0975	13.1193	4.8807	0.1300	1.2539	0.9929	-0.8629
121.0000	17.9000	3.0975	13.1193	4.7807	0.1300	1.2539	0.9929	-0.8629







## 11.3.1.3 FOMC

```

# Trial      : NDSandyclayloam
# File name  : NDSandyclayloam IRLS FOMC Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\CYF_met\NDSandyclayloam
# Created    : on 30 Oct 2013
#            : at 10:34
#            : 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. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID:
# # label: 14C cyclopropyl
# # soil : ND-sandy clay loam
# # ND-sandy clay loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      103.9              0              Inf      False
alpha Par      :       0.1              0              Inf      False
beta  Par      :       0.1              0              Inf      False
k      Met      :       0.1              0              Inf      False
FF     Par -> Met :       0.1              0              1      False
M(0)  Met      :              0                      True

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

      Par      Met      All
Chi2Err% :      3.263      4.983      4.367
Kinetic model :      FOMC      SFO

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

Degrees of Freedom : 27
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      105.01762      101.89713      108.138      1.59211      < 2e-16
alpha Par      0.74167      0.62424      0.859      0.05992      6.07e-13
beta  Par      10.78763      7.44972      14.126      1.70304      4.41e-07
k      Met      0.12573      0.09451      0.157      0.01593      8.72e-09
FF     Par -> Met      0.6913      0.07582

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

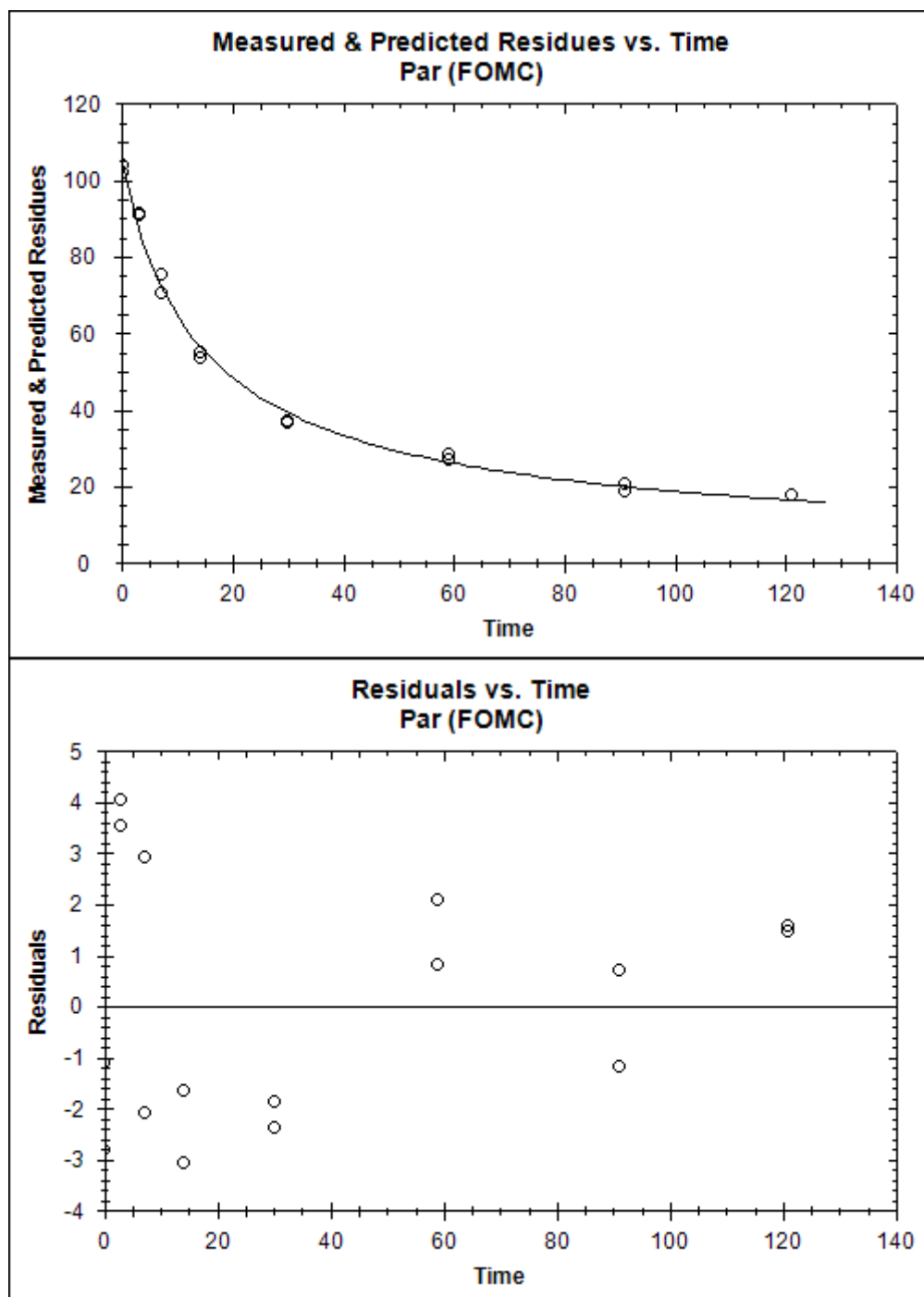
      Par      Met
DT50 :      16.679      5.5130
DT90 :      229.78      18.314
Kinetic model :      FOMC      SFO

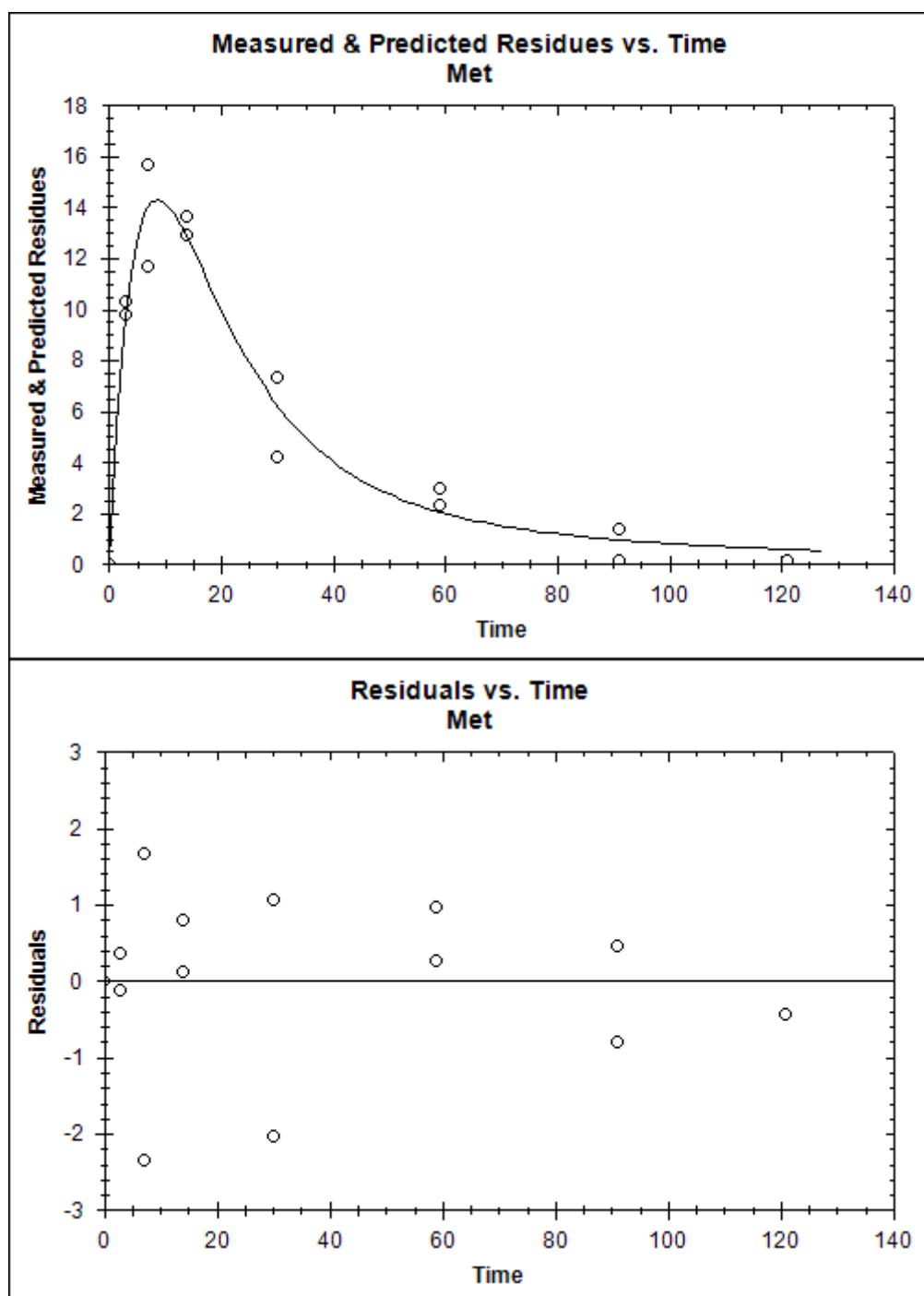
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000 103.9000 2.2922 105.0176 -1.1176 0.0000 1.0195 0.0000 0.0000
0.0000 102.2000 2.2922 105.0176 -2.8176 0.0000 1.0195 0.0000 0.0000
3.0000 91.6000 2.2922 87.5441 4.0559 9.8000 1.0195 9.9286 -0.1286
3.0000 91.1000 2.2922 87.5441 3.5559 10.3000 1.0195 9.9286 0.3714
7.0000 70.4000 2.2922 72.4731 -2.0731 15.7000 1.0195 14.0419 1.6581
7.0000 75.4000 2.2922 72.4731 2.9269 11.7000 1.0195 14.0419 -2.3419

```

14.0000	55.0000	2.2922	56.6617	-1.6617	13.6000	1.0195	12.7931	0.8069
14.0000	53.6000	2.2922	56.6617	-3.0617	12.9000	1.0195	12.7931	0.1069
30.0000	37.3000	2.2922	39.1626	-1.8626	7.3000	1.0195	6.2445	1.0555
30.0000	36.8000	2.2922	39.1626	-2.3626	4.2000	1.0195	6.2445	-2.0445
59.0000	28.4000	2.2922	26.2952	2.1048	3.0000	1.0195	2.0251	0.9749
59.0000	27.1000	2.2922	26.2952	0.8048	2.3000	1.0195	2.0251	0.2749
91.0000	20.6000	2.2922	19.8749	0.7251	1.4000	1.0195	0.9398	0.4602
91.0000	18.7000	2.2922	19.8749	-1.1749	0.1300	1.0195	0.9398	-0.8098
121.0000	18.0000	2.2922	16.4098	1.5902	0.1300	1.0195	0.5729	-0.4429
121.0000	17.9000	2.2922	16.4098	1.4902	0.1300	1.0195	0.5729	-0.4429





## 11.3.1.4 DFOP

```

# Trial      : NDSandyclayloam
# File name  : NDSandyclayloam IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\NDSandyclayloam
# Created    : on 30 Oct 2013
#            : at 10:22
#            : 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:
# # label: 14C cyclopropyl
# # soil : ND-sandy clay loam
# # ND-sandy clay loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      103.90           0           Inf      False
k1    Par      :       0.10           0           Inf      False
k2    Par      :       0.01           0           Inf      False
g     Par      :       0.50           0           1      False
k     Met      :       0.10           0           Inf      False
FF    Par -> Met :       0.10           0           1      False
M(0)  Met      :           0              True

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

      Chi2Err% :      2.222      6.891      3.048
      Kinetic model :      DFOP      SFO

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

Degrees of Freedom : 26
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      1.043e+02      1.021e+02      106.604      1.160e+00      < 2e-16
k1    Par      8.478e-02      6.939e-02      0.100      7.855e-03      2.11e-11
k2    Par      6.815e-03      4.471e-03      0.009      1.196e-03      2.69e-06
g     Par      6.247e-01      5.536e-01      0.696      3.627e-02      4.87e-16
k     Met      1.463e-01      1.057e-01      0.187      2.073e-02      8.55e-08
FF    Par -> Met      0.7659              8.698e-02

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

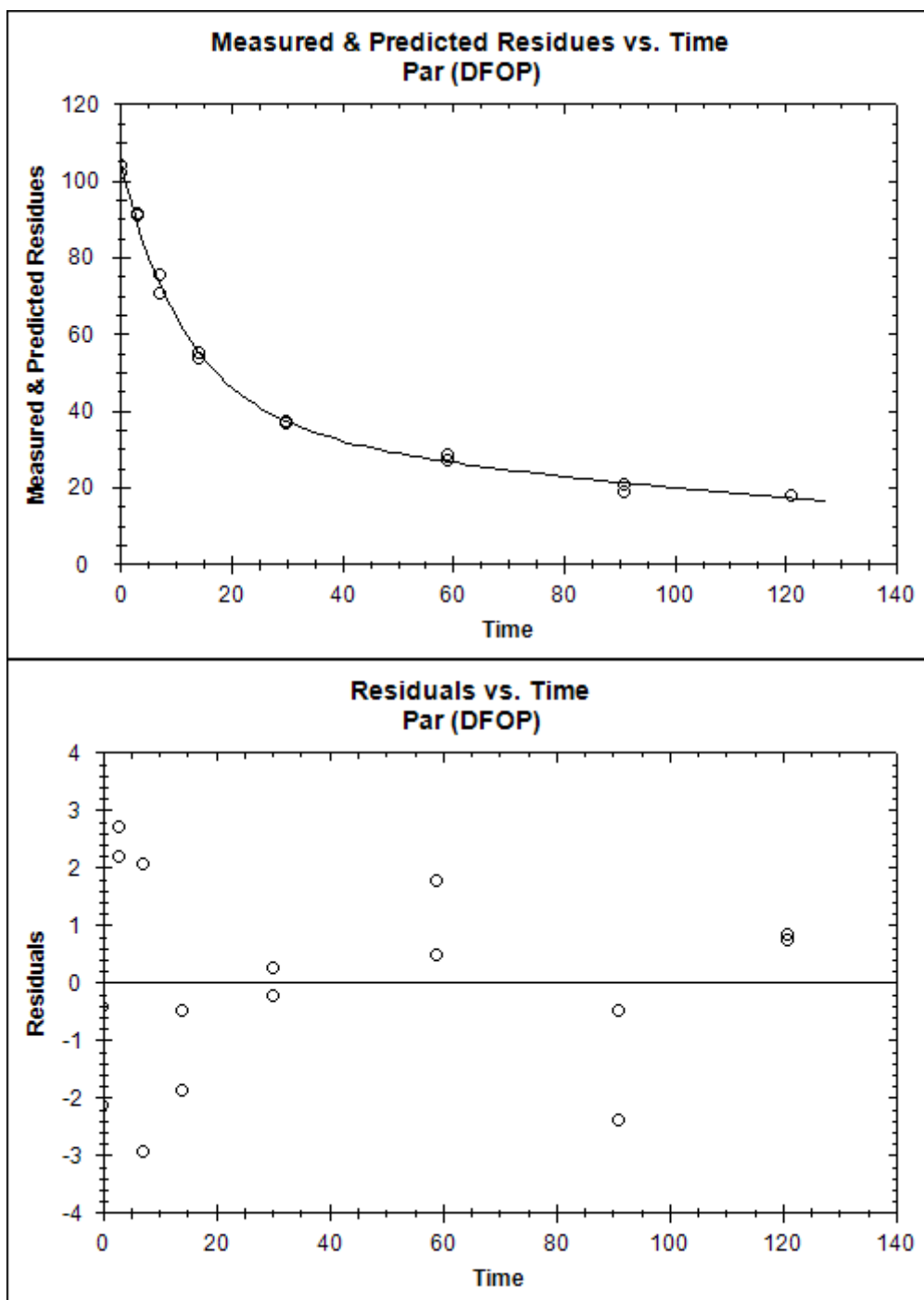
      DT50 :      15.839      4.7383
      DT90 :      194.06      15.740
      Kinetic model :      DFOP      SFO

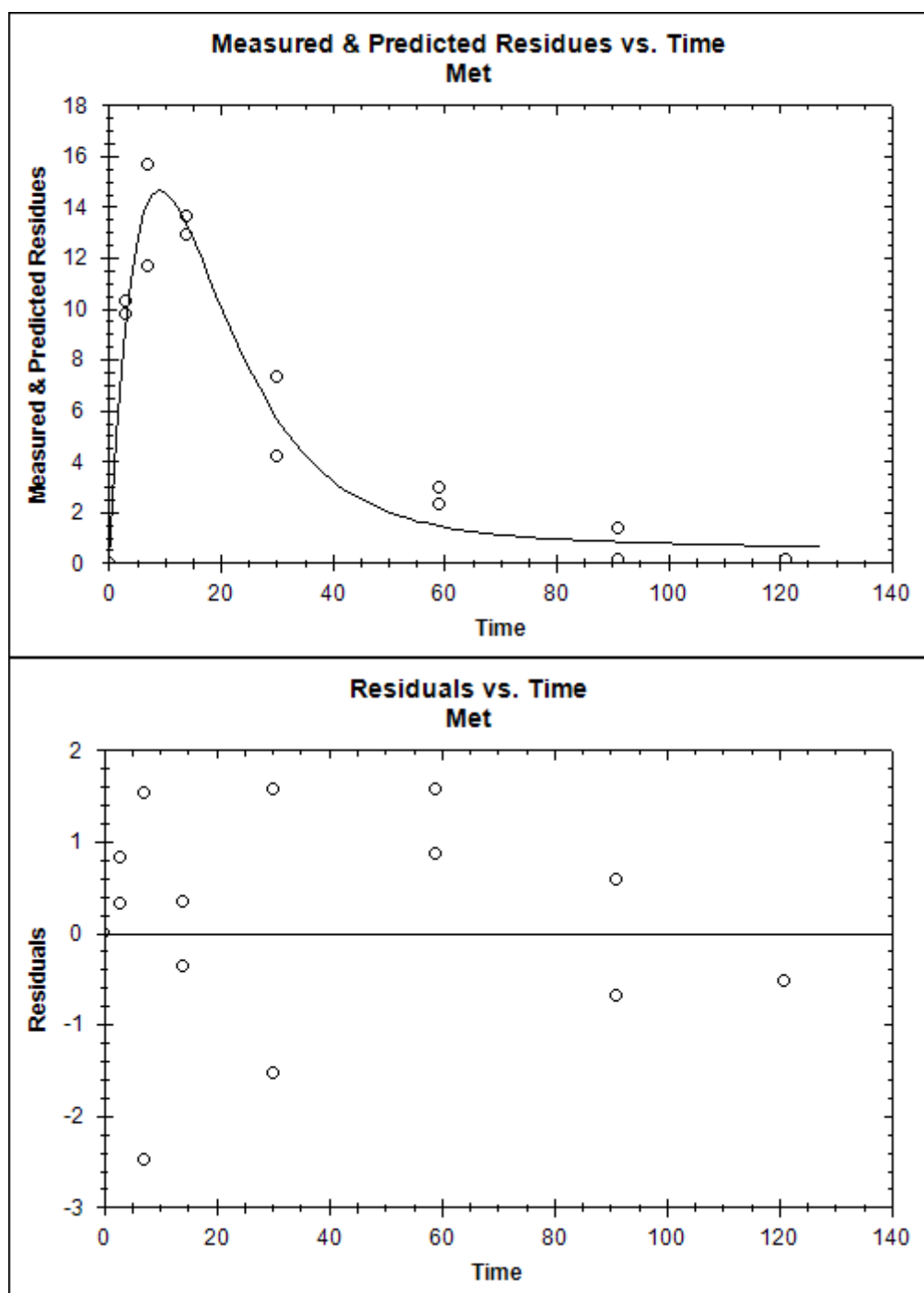
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000 103.9000 1.6609 104.3307 -0.4307 0.0000 1.0847 0.0000 0.0000
0.0000 102.2000 1.6609 104.3307 -2.1307 0.0000 1.0847 0.0000 0.0000
3.0000 91.6000 1.6609 88.9014 2.6986 9.8000 1.0847 9.4815 0.3185
3.0000 91.1000 1.6609 88.9014 2.1986 10.3000 1.0847 9.4815 0.8185

```

7.0000	70.4000	1.6609	73.3344	-2.9344	15.7000	1.0847	14.1692	1.5308
7.0000	75.4000	1.6609	73.3344	-2.0656	11.7000	1.0847	14.1692	-2.4692
14.0000	55.0000	1.6609	55.4803	-0.4803	13.6000	1.0847	13.2654	0.3346
14.0000	53.6000	1.6609	55.4803	-1.8803	12.9000	1.0847	13.2654	-0.3654
30.0000	37.3000	1.6609	37.0372	0.2628	7.3000	1.0847	5.7302	1.5698
30.0000	36.8000	1.6609	37.0372	-0.2372	4.2000	1.0847	5.7302	-1.5302
59.0000	28.4000	1.6609	26.6294	1.7706	3.0000	1.0847	1.4304	1.5696
59.0000	27.1000	1.6609	26.6294	0.4706	2.3000	1.0847	1.4304	0.8696
91.0000	20.6000	1.6609	21.0882	-0.4882	1.4000	1.0847	0.8188	0.5812
91.0000	18.7000	1.6609	21.0882	-2.3882	0.1300	1.0847	0.8188	-0.6888
121.0000	18.0000	1.6609	17.1673	0.8327	0.1300	1.0847	0.6449	-0.5149
121.0000	17.9000	1.6609	17.1673	0.7327	0.1300	1.0847	0.6449	-0.5149





## 11.3.2 Carlyle IL(BETA-CYF, DCVA)

### 11.3.2.1 SFO

```
# Trial      : ILSiltloam
# File name  : ILSiltloam IRLS SFO Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\CYF_met\ILSiltloam
# Created    : on 30 Oct 2013
#            : at 10:39
#            : 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. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID:
# # label: 14C cyclopropyl
# # soil : IL-silt loam
# # IL-silt loam
# #

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

# -----
# Initial values
# -----
# -----
# Initial Value      Lower Bound      Upper Bound      Fixed
M(0) Par      :      95.3              0              Inf      False
k   Par      :       0.1              0              Inf      False
k   Met      :       0.1              0              Inf      False
FF  Par -> Met :       0.1              0              1      False
M(0) Met      :       0                0              0      True

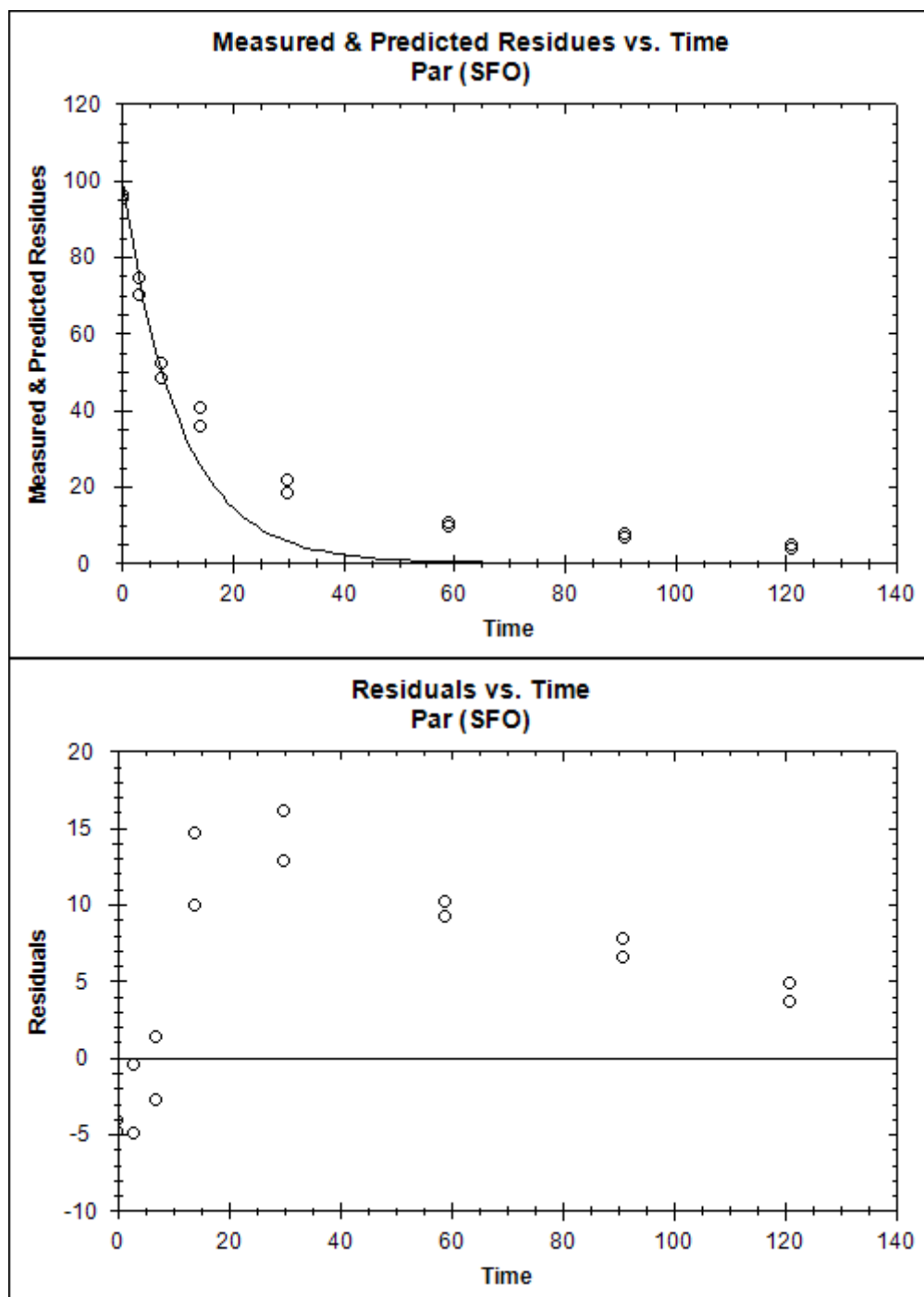
# -----
# Chi2 error estimation
# -----
# -----
# Par      Met      All
Chi2Err% :      17.82      3.36      22.97
Kinetic model :      SFO      SFO

# -----
# Parameter estimation
# -----
# -----
# Degrees of Freedom : 24
# Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0) Par      :      1.001e+02      9.060e+01      109.600      4.848e+00      < 2e-16
k   Par      :      9.670e-02      8.085e-02      0.113      8.089e-03      6.76e-12
k   Met      :      6.183e-01      4.526e-01      0.784      8.455e-02      7.45e-08
FF  Par -> Met :      1.000e+00

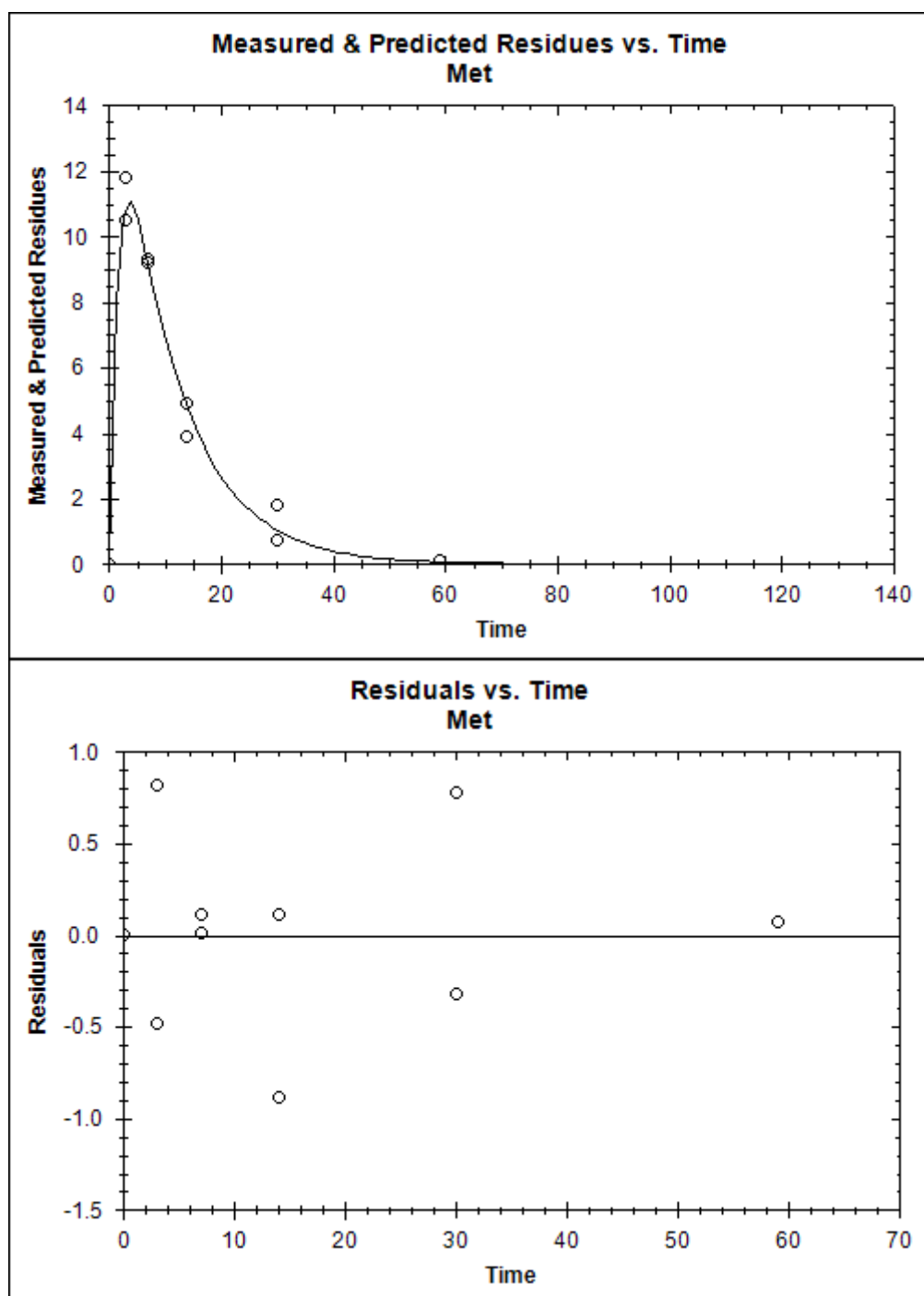
# -----
# DT50 and DT90 values
# -----
# -----
# Par      Met
DT50 :      7.1681      1.1211
DT90 :      23.812      3.7242
Kinetic model :      SFO      SFO

# -----
# Measured vs. predicted values
# -----
# -----
# Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000 95.3000 8.4516 100.0987 -4.7987 0.0000 0.4512 0.0000 0.0000
0.0000 96.0000 8.4516 100.0987 -4.0987 0.0000 0.4512 0.0000 0.0000
3.0000 69.9000 8.4516 74.8929 -4.9929 11.8000 0.4512 10.9808 0.8192
3.0000 74.4000 8.4516 74.8929 -0.4929 10.5000 0.4512 10.9808 -0.4808
7.0000 48.1000 8.4516 50.8694 -2.7694 9.3000 0.4512 9.1861 0.1139
7.0000 52.2000 8.4516 50.8694 1.3306 9.2000 0.4512 9.1861 0.0139
```

14.0000	40.5000	8.4516	25.8515	14.6485	3.9000	0.4512	4.7895	-0.8895
14.0000	35.8000	8.4516	25.8515	9.9485	4.9000	0.4512	4.7895	0.1105
30.0000	18.4000	8.4516	5.5024	12.8976	0.7000	0.4512	1.0201	-0.3201
30.0000	21.6000	8.4516	5.5024	16.0976	1.8000	0.4512	1.0201	0.7799
59.0000	10.5000	8.4516	0.3332	10.1668	0.1300	0.4512	0.0618	0.0682
59.0000	9.6000	8.4516	0.3332	9.2668	0.1300	0.4512	0.0618	0.0682
91.0000	6.6000	8.4516	0.0151	6.5849	NA	0.4512	0.0028	NA
91.0000	7.8000	8.4516	0.0151	7.7849	NA	0.4512	0.0028	NA
121.0000	4.9000	8.4516	0.0008	4.8992	NA	0.4512	0.0002	NA
121.0000	3.7000	8.4516	0.0008	3.6992	NA	0.4512	0.0002	NA







## 11.3.2.2 HS

```

# Trial      : ILsiltloam
# File name  : ILsiltloam IRLS HS   Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\CYF_met\ILsiltloam
# Created    : on 30 Oct 2013
#            : at 10:47
#            : 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:
# # label: 14C cyclopropyl
# # soil : IL-silt loam
# # IL-silt loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      95.30              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% :      6.130      Par      Met      All
Kinetic model :      HS      SFO      6.794      7.595

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

Degrees of Freedom : 22
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :  96.569380  92.106965  101.032  2.276784  < 2e-16
k1    Par      :   0.107284   0.085477   0.129   0.011126  1.17e-09
k2    Par      :   0.035529   0.027889   0.043   0.003898  3.17e-09
tb    Par      :   5.638030   4.636311   6.640   0.511090  9.83e-11
k      Met      :   0.313615   0.190930   0.436   0.062596  2.57e-05
FF    Par -> Met :   0.6579                      0.122962

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

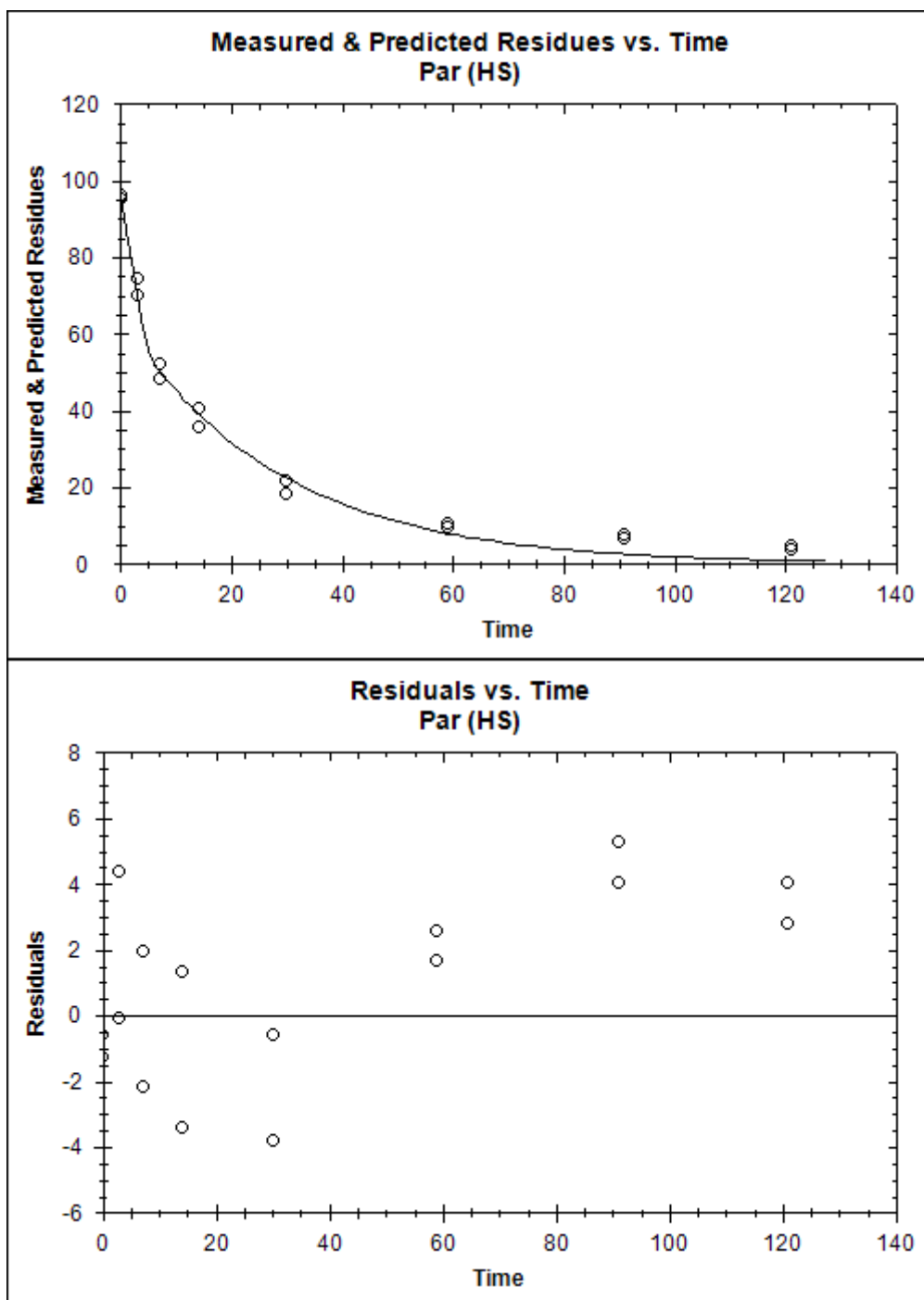
      DT50 :      8.1227      Par      Met
      DT90 :     53.422   2.2102
Kinetic model :      HS      SFO

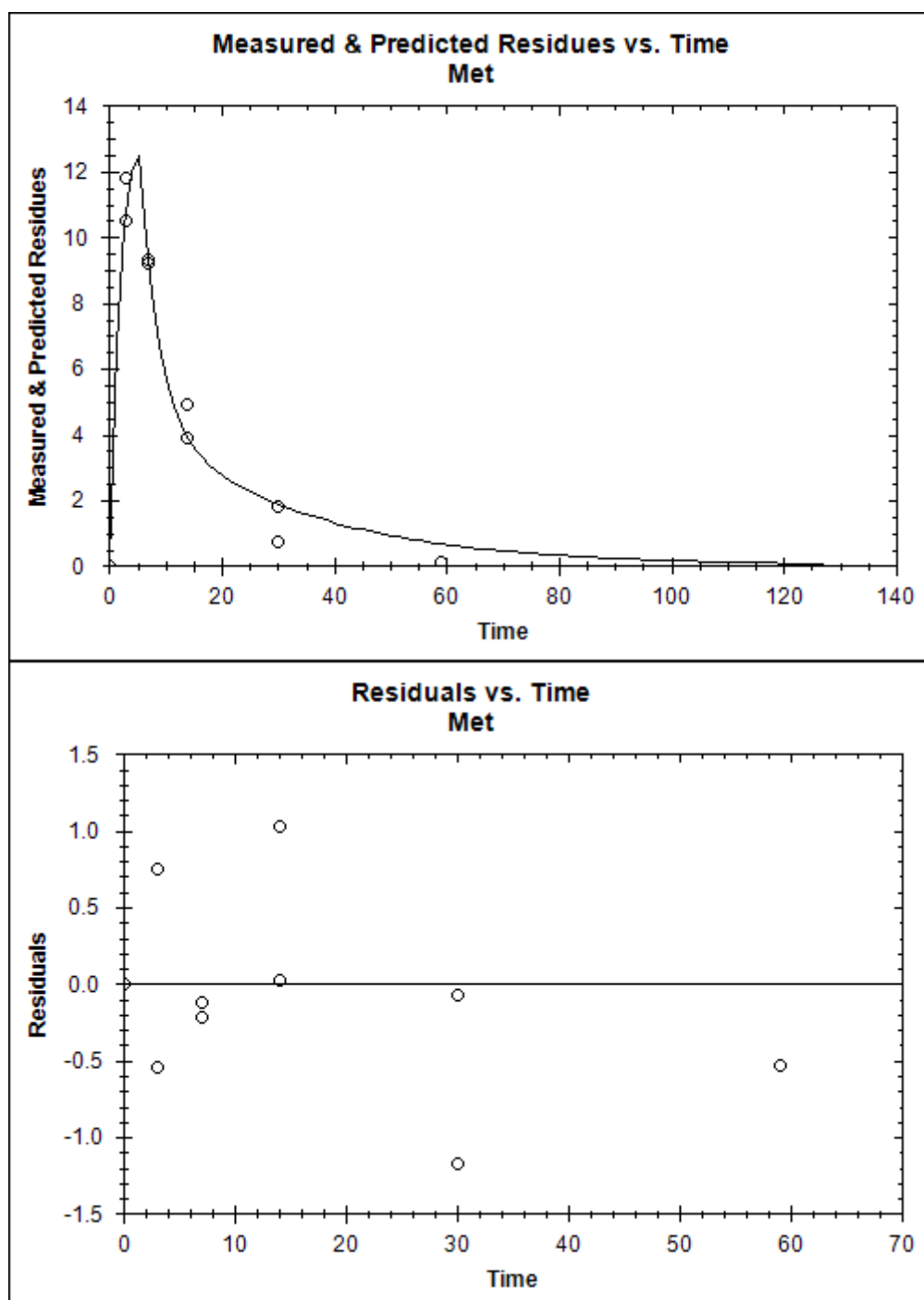
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000  95.3000  2.9075  96.5694 -1.2694  0.0000  0.5732  0.0000  0.0000
0.0000  96.0000  2.9075  96.5694 -0.5694  0.0000  0.5732  0.0000  0.0000
3.0000  69.9000  2.9075  69.9940 -0.0940 11.8000  0.5732 11.0499  0.7501
3.0000  74.4000  2.9075  69.9940  4.4060 10.5000  0.5732 11.0499 -0.5499

```

7.0000	48.1000	2.9075	50.2496	-2.1496	9.3000	0.5732	9.4237	-0.1237
7.0000	52.2000	2.9075	50.2496	1.9504	9.2000	0.5732	9.4237	-0.2237
14.0000	40.5000	2.9075	39.1852	1.3148	3.9000	0.5732	3.8725	0.0275
14.0000	35.8000	2.9075	39.1852	-3.3852	4.9000	0.5732	3.8725	1.0275
30.0000	18.4000	2.9075	22.1943	-3.7943	0.7000	0.5732	1.8693	-1.1693
30.0000	21.6000	2.9075	22.1943	-0.5943	1.8000	0.5732	1.8693	-0.0693
59.0000	10.5000	2.9075	7.9208	2.5792	0.1300	0.5732	0.6658	-0.5358
59.0000	9.6000	2.9075	7.9208	1.6792	0.1300	0.5732	0.6658	-0.5358
91.0000	6.6000	2.9075	2.5410	4.0590	NA	0.5732	0.2136	NA
91.0000	7.8000	2.9075	2.5410	5.2590	NA	0.5732	0.2136	NA
121.0000	4.9000	2.9075	0.8752	4.0248	NA	0.5732	0.0736	NA
121.0000	3.7000	2.9075	0.8752	2.8248	NA	0.5732	0.0736	NA





## 11.3.2.3 FOMC

```

# Trial      : ILsiltloam
# File name  : ILsiltloam IRLS FOMC Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\CYF_met\ILsiltloam
# Created    : on 30 Oct 2013
#            : at 10:54
#            : 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:
# # label: 14C cyclopropyl
# # soil : IL-silt loam
# # IL-silt loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      95.3              0              Inf      False
alpha Par      :       0.1              0              Inf      False
beta  Par      :       0.1              0              Inf      False
k      Met      :       0.1              0              Inf      False
FF     Par -> Met :       0.1              0              1      False
M(0)  Met      :              0                      True

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

      Par      Met      All
Chi2Err% :      3.092      1.936      3.912
Kinetic model :      FOMC      SFO

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

Degrees of Freedom : 23
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      95.77437      92.83843      98.710      1.49796      < 2e-16
alpha Par      :       1.14462      0.92431      1.365      0.11240      2.71e-10
beta  Par      :      10.19575      6.95433      13.437      1.65381      1.37e-06
k      Met      :       0.41950      0.32732      0.512      0.04703      3.16e-09
FF     Par -> Met :       0.8487              0.10026

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

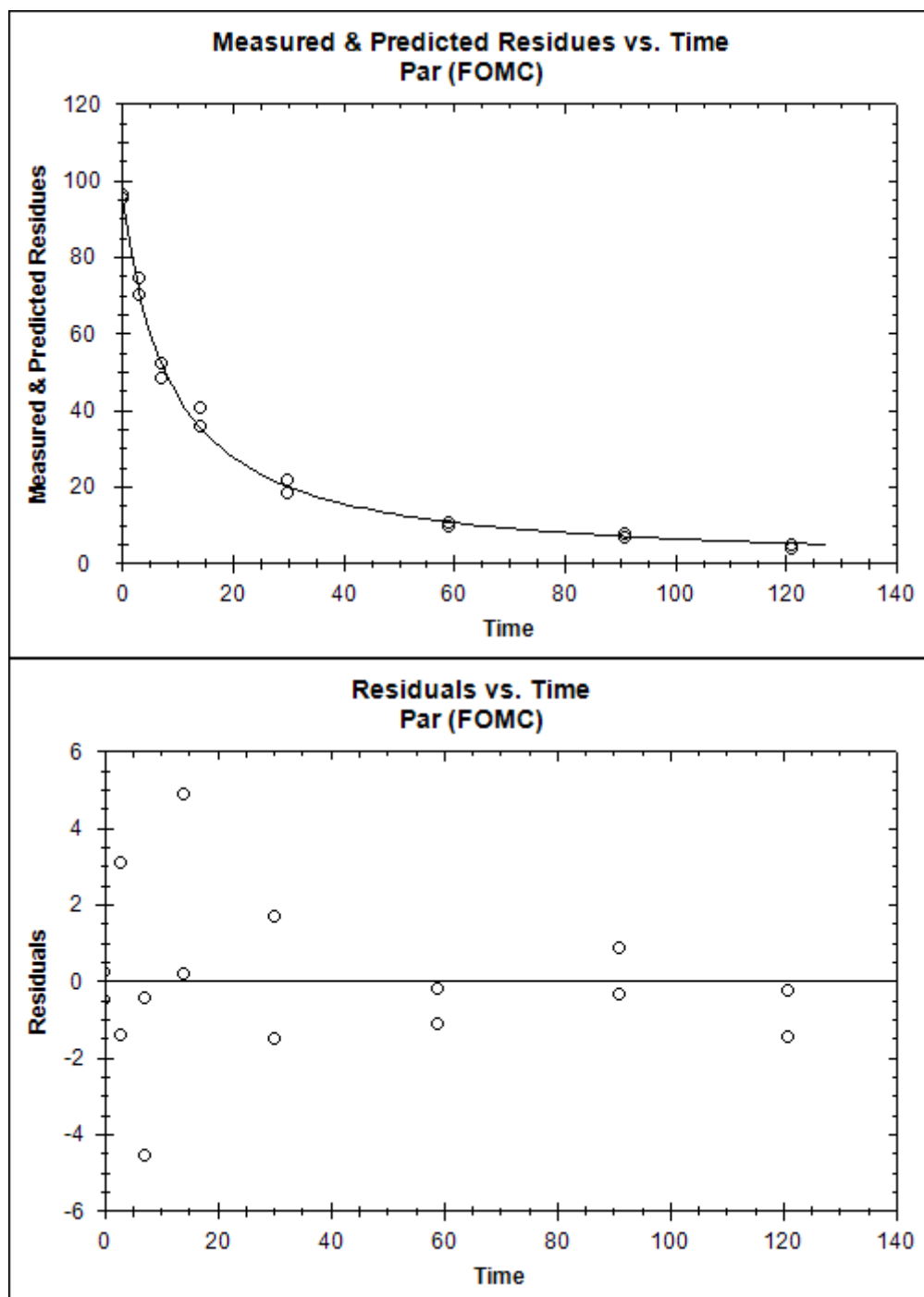
      Par      Met
DT50 :      8.4859      1.6523
DT90 :      66.025      5.4889
Kinetic model :      FOMC      SFO

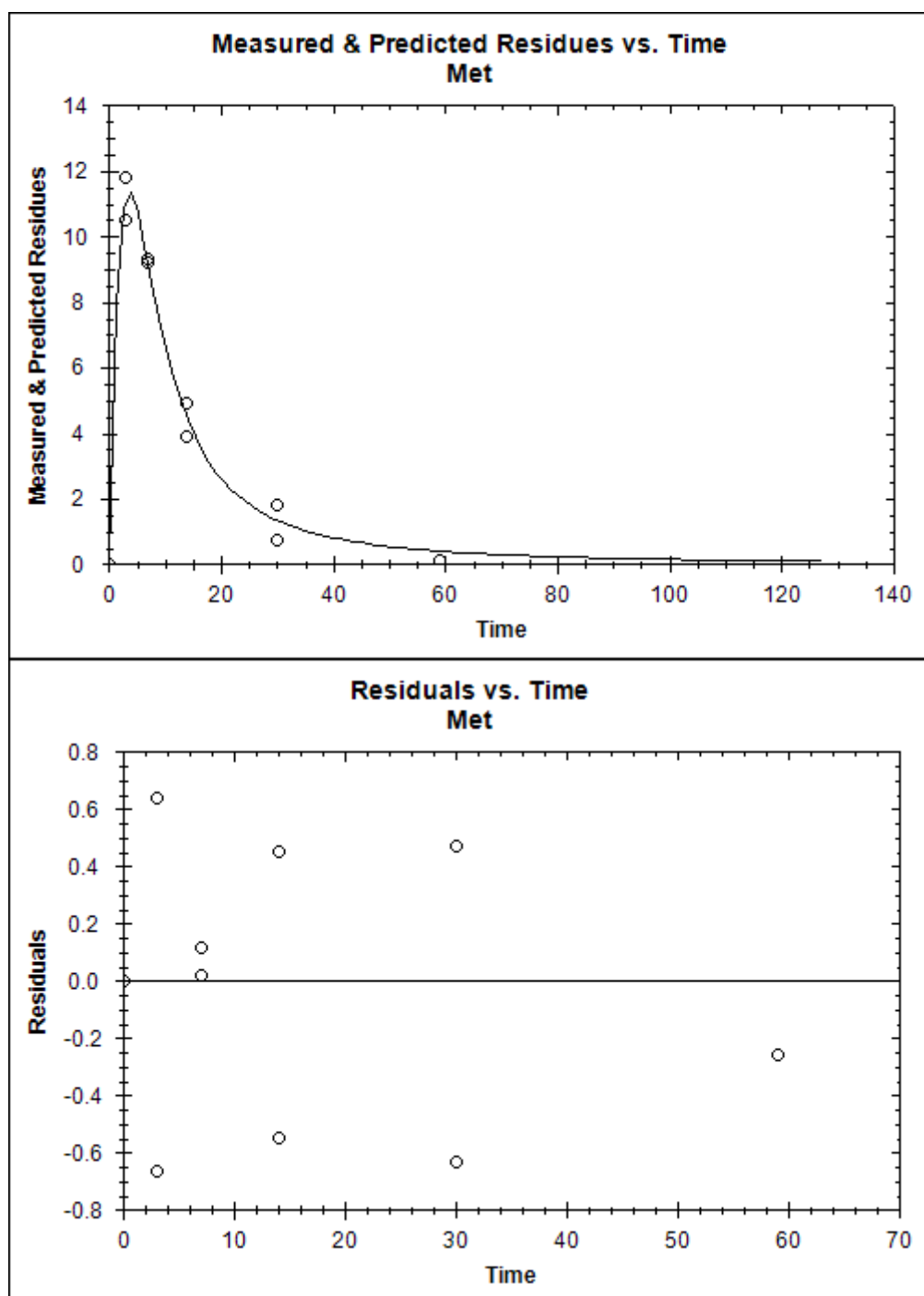
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000  95.3000  2.0323  95.7744 -0.4744  0.0000  0.4199  0.0000  0.0000
0.0000  96.0000  2.0323  95.7744  0.2256  0.0000  0.4199  0.0000  0.0000
3.0000  69.9000  2.0323  71.2910 -1.3910 11.8000  0.4199 11.1646  0.6354
3.0000  74.4000  2.0323  71.2910  3.1090 10.5000  0.4199 11.1646 -0.6646
7.0000  48.1000  2.0323  52.6524 -4.5524  9.3000  0.4199  9.1840  0.1160
7.0000  52.2000  2.0323  52.6524 -0.4524  9.2000  0.4199  9.1840  0.0160

```

14.0000	40.5000	2.0323	35.6164	4.8836	3.9000	0.4199	4.4522	-0.5522
14.0000	35.8000	2.0323	35.6164	0.1836	4.9000	0.4199	4.4522	0.4478
30.0000	18.4000	2.0323	19.9218	-1.5218	0.7000	0.4199	1.3309	-0.6309
30.0000	21.6000	2.0323	19.9218	1.6782	1.8000	0.4199	1.3309	0.4691
59.0000	10.5000	2.0323	10.6983	-0.1983	0.1300	0.4199	0.3878	-0.2578
59.0000	9.6000	2.0323	10.6983	-1.0983	0.1300	0.4199	0.3878	-0.2578
91.0000	6.6000	2.0323	6.9240	-0.3240	NA	0.4199	0.1671	NA
91.0000	7.8000	2.0323	6.9240	0.8760	NA	0.4199	0.1671	NA
121.0000	4.9000	2.0323	5.1439	-0.2439	NA	0.4199	0.0945	NA
121.0000	3.7000	2.0323	5.1439	-1.4439	NA	0.4199	0.0945	NA





## 11.3.2.4 DFOP

```

# Trial      : ILsiltloam
# File name  : ILsiltloam IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\ILsiltloam
# Created    : on 30 Oct 2013
#            : at 10:44
#            : 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. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID:
# # label: 14C cyclopropyl
# # soil : IL-silt loam
# # IL-silt loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      95.30              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                      True

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

      Par      Met      All
Chi2Err% :      3.948      2.639      4.860
Kinetic model :      DFOP      SFO

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

Degrees of Freedom : 22
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      : 95.227919  91.939536  98.516  1.677777  < 2e-16
k1    Par      :  0.148612  0.099672  0.198  0.024970  2.73e-06
k2    Par      :  0.019717  0.011996  0.027  0.003939  2.60e-05
g     Par      :  0.615510  0.474891  0.756  0.071746  9.08e-09
k     Met      :  0.467018  0.311835  0.622  0.079176  3.09e-06
FF    Par -> Met :  0.9349          0.160295

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

      Par      Met
DT50 :      8.4751  1.4842
DT90 :     68.317  4.9304
Kinetic model :      DFOP      SFO

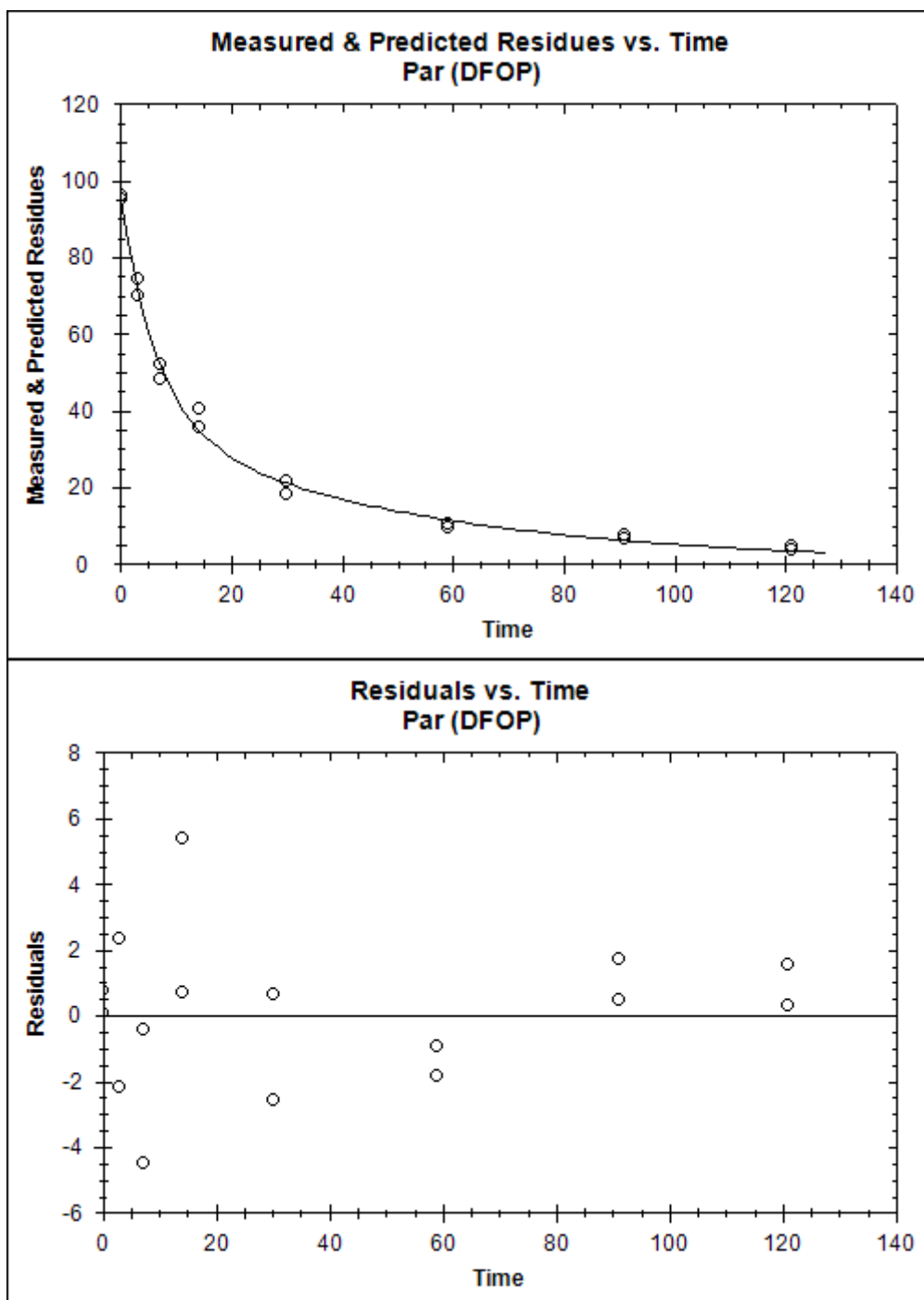
# -----
# Measured vs. predicted values
# -----

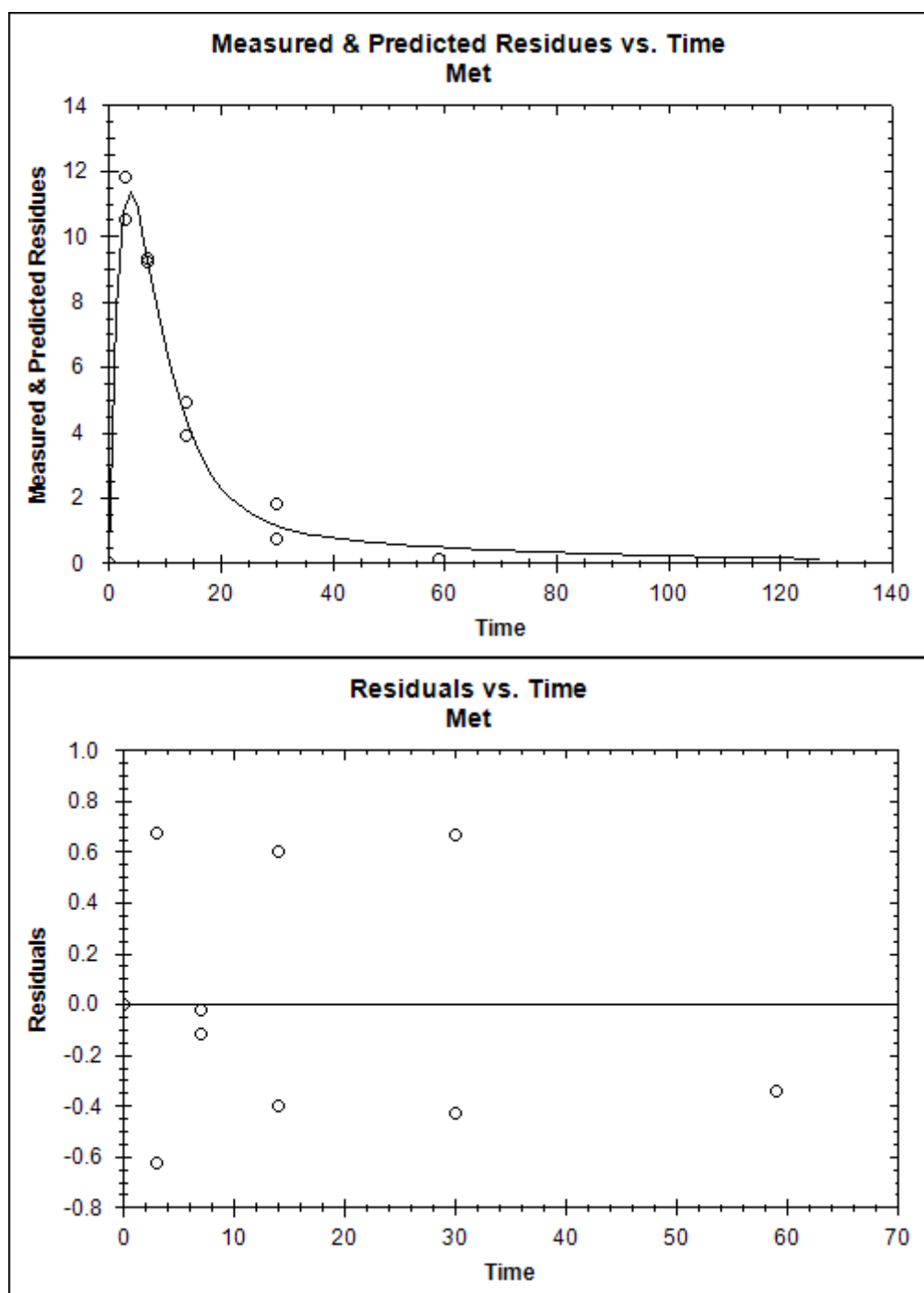
      Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000 95.3000 2.2034 95.2279 0.0721 0.0000 0.4335 0.0000 0.0000
0.0000 96.0000 2.2034 95.2279 0.7721 0.0000 0.4335 0.0000 0.0000
3.0000 69.9000 2.2034 72.0409 -2.1409 11.8000 0.4335 11.1263 0.6737
3.0000 74.4000 2.2034 72.0409 2.3591 10.5000 0.4335 11.1263 -0.6263

```



7.0000	48.1000	2.2034	52.6054	-4.5054	9.3000	0.4335	9.3215	-0.0215
7.0000	52.2000	2.2034	52.6054	-0.4054	9.2000	0.4335	9.3215	-0.1215
14.0000	40.5000	2.2034	35.1008	5.3992	3.9000	0.4335	4.2991	-0.3991
14.0000	35.8000	2.2034	35.1008	0.6992	4.9000	0.4335	4.2991	0.6009
30.0000	18.4000	2.2034	20.9446	-2.5446	0.7000	0.4335	1.1313	-0.4313
30.0000	21.6000	2.2034	20.9446	0.6554	1.8000	0.4335	1.1313	0.6687
59.0000	10.5000	2.2034	11.4495	-0.9495	0.1300	0.4335	0.4754	-0.3454
59.0000	9.6000	2.2034	11.4495	-1.8495	0.1300	0.4335	0.4754	-0.3454
91.0000	6.6000	2.2034	6.0874	0.5126	NA	0.4335	0.2509	NA
91.0000	7.8000	2.2034	6.0874	1.7126	NA	0.4335	0.2509	NA
121.0000	4.9000	2.2034	3.3693	1.5307	NA	0.4335	0.1388	NA
121.0000	3.7000	2.2034	3.3693	0.3307	NA	0.4335	0.1388	NA





### 11.3.3 Madera CA 1 (BETA-CYF, DCVA)

#### 11.3.3.1 SFO

```
# Trial      : CAsandyloam
# File name  : CAsandyloam IRLS SFO Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\CYF_met\CAsandyloam
# Created    : on 16 Oct 2013
#            : at 11:33
#            : 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:
# # label: 14C cyclopropyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

		Initial Value	Lower Bound	Upper Bound	Fixed
M(0)	Par	97.7	0	Inf	False
k	Par	0.1	0	Inf	False
k	Met	0.1	0	Inf	False
FF	Par -> Met	0.1	0	1	False
M(0)	Met	0			True

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

	Par	Met	All
Chi2Err%	20.707	9.975	22.604
Kinetic model	SFO	SFO	

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

Degrees of Freedom : 28

Parameter	Estimate	Lower CI	Upper CI	St.Dev	Prob > t
M(0) Par	102.83043	91.91294	113.748	5.57025	< 2e-16
k Par	0.12480	0.09802	0.152	0.01367	3.43e-10
k Met	0.10748	0.08248	0.132	0.01275	1.82e-09
FF Par -> Met	1.000e+00			0.13328	

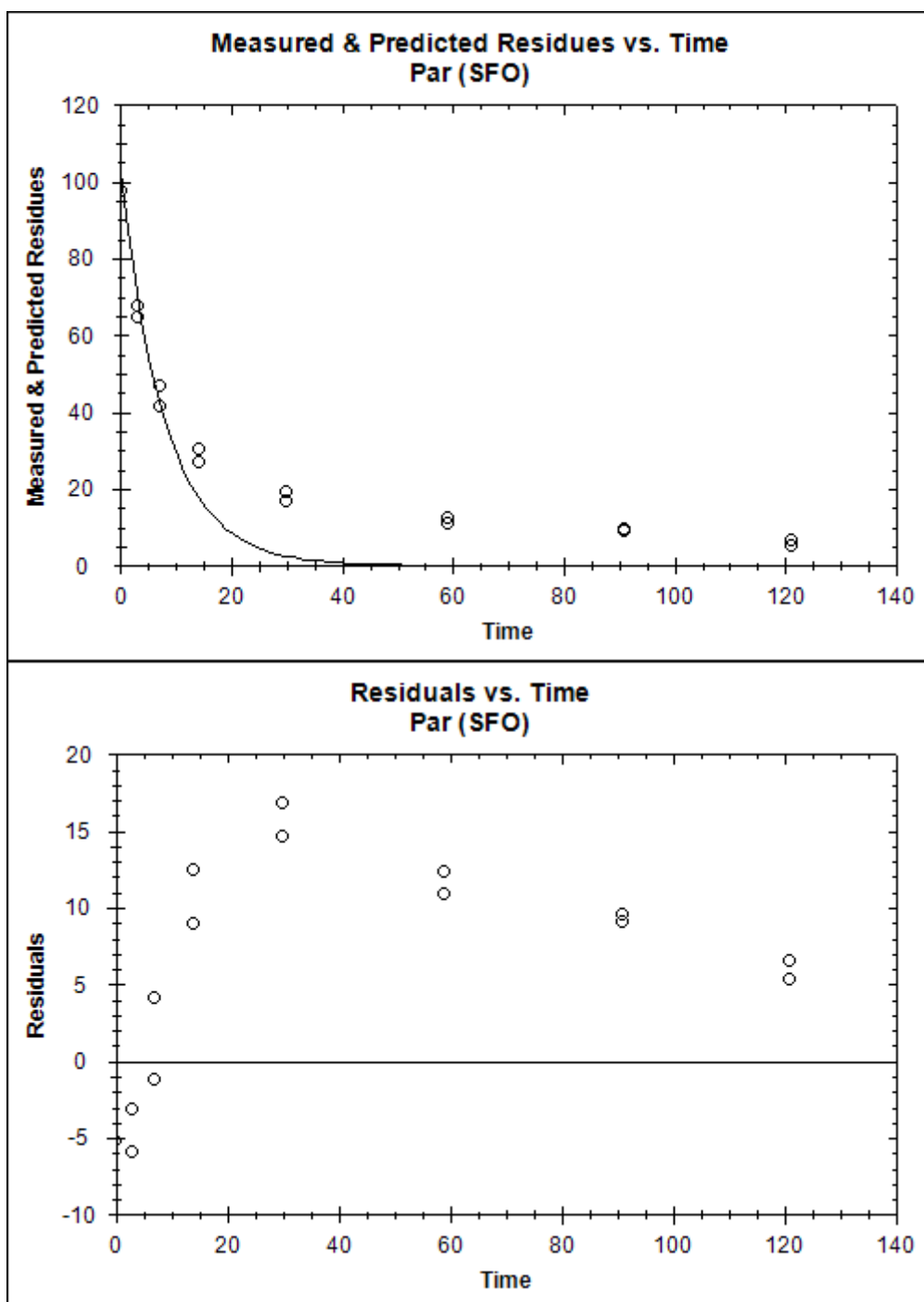
```
# -----
# DT50 and DT90 values
# -----
#
```

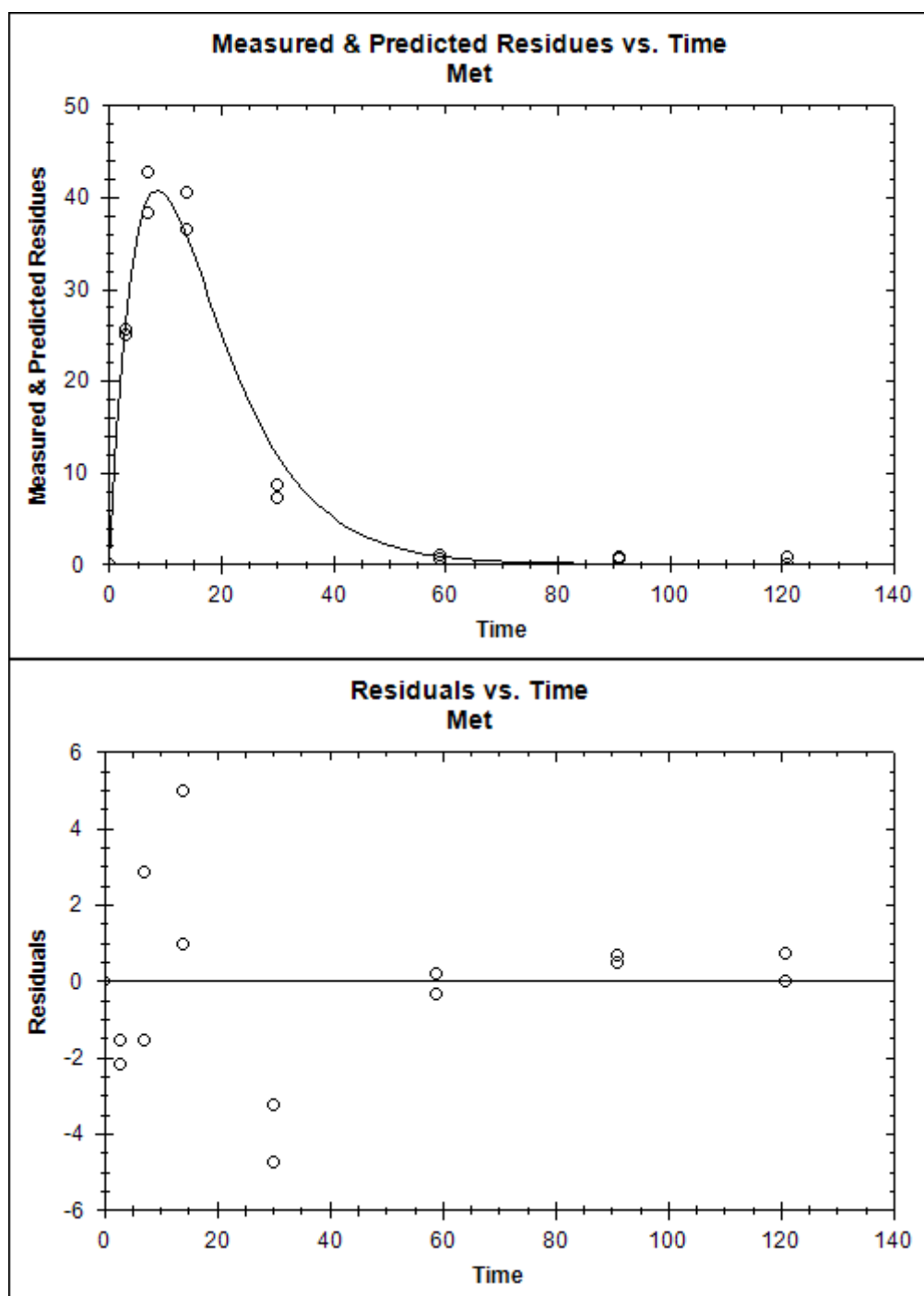
	Par	Met
DT50	5.5539	6.4491
DT90	18.450	21.424
Kinetic model	SFO	SFO

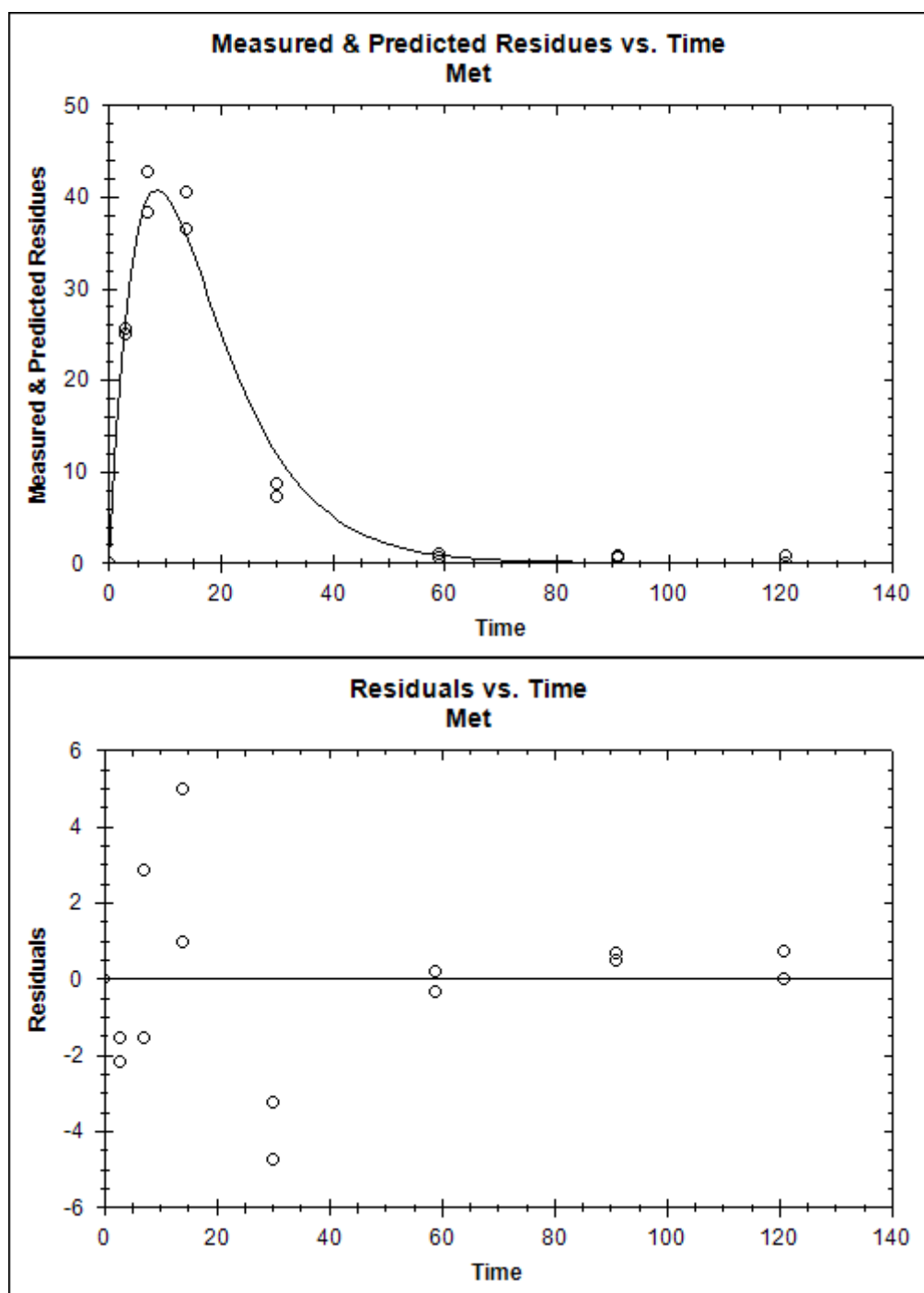
```
# -----
# Measured vs. predicted values
# -----
#
```

time	Compartment Par				Compartment Met			
	observed	err-std	predicted	residual	observed	err-std	predicted	residual
0.0000	97.7000	9.2583	102.8304	-5.1304	0.0000	2.2032	0.0000	0.0000
0.0000	97.6000	9.2583	102.8304	-5.2304	0.0000	2.2032	0.0000	0.0000
3.0000	67.6000	9.2583	70.7161	-3.1161	25.0000	2.2032	27.1764	-2.1764
3.0000	64.8000	9.2583	70.7161	-5.9161	25.6000	2.2032	27.1764	-1.5764
7.0000	41.7000	9.2583	42.9254	-1.2254	42.7000	2.2032	39.8683	2.8317

7.0000	47.1000	9.2583	42.9254	4.1746	38.3000	2.2032	39.8683	-1.5683
14.0000	26.9000	9.2583	17.9187	8.9813	40.4000	2.2032	35.4307	4.9693
14.0000	30.4000	9.2583	17.9187	12.4813	36.4000	2.2032	35.4307	0.9693
30.0000	17.1000	9.2583	2.4327	14.6673	7.2000	2.2032	11.9441	-4.7441
30.0000	19.3000	9.2583	2.4327	16.8673	8.7000	2.2032	11.9441	-3.2441
59.0000	11.0000	9.2583	0.0652	10.9348	0.5000	2.2032	0.8356	-0.3356
59.0000	12.4000	9.2583	0.0652	12.3348	1.0000	2.2032	0.8356	0.1644
91.0000	9.6000	9.2583	0.0012	9.5988	0.5000	2.2032	0.0332	0.4668
91.0000	9.1000	9.2583	0.0012	9.0988	0.7000	2.2032	0.0332	0.6668
121.0000	5.3000	9.2583	0.0000	5.3000	0.7000	2.2032	0.0015	0.6985
121.0000	6.6000	9.2583	0.0000	6.6000	0.0000	2.2032	0.0015	-0.0015







## 11.3.3.2 HS

```

# Trial      : CAsandyloam
# File name  : CAsandyloam IRLS HS   Par.r
# Target path : C:\Emod\KinGUIII\WorkingDirectory\CYF_met\CAsandyloam
# Created    : on 16 Oct 2013
#            : at 12:02
#            : 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:
# # label: 14C cyclopropyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      97.70              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% :      5.728      9.996      7.593
      Kinetic model :      HS      SFO

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

Degrees of Freedom : 26
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :  98.120293    94.563967    101.677    1.814486    < 2e-16
k1    Par      :   0.117052    0.105434     0.129    0.005928    < 2e-16
k2    Par      :   0.012744    0.008764     0.017    0.002030    6.06e-07
tb    Par      :  11.922113   10.403125    13.441    0.775008    7.13e-15
k      Met      :   0.084754    0.069690     0.100    0.007686    1.33e-11
FF    Par -> Met:   1.00e+00    0.000000     0.000    0.067442

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

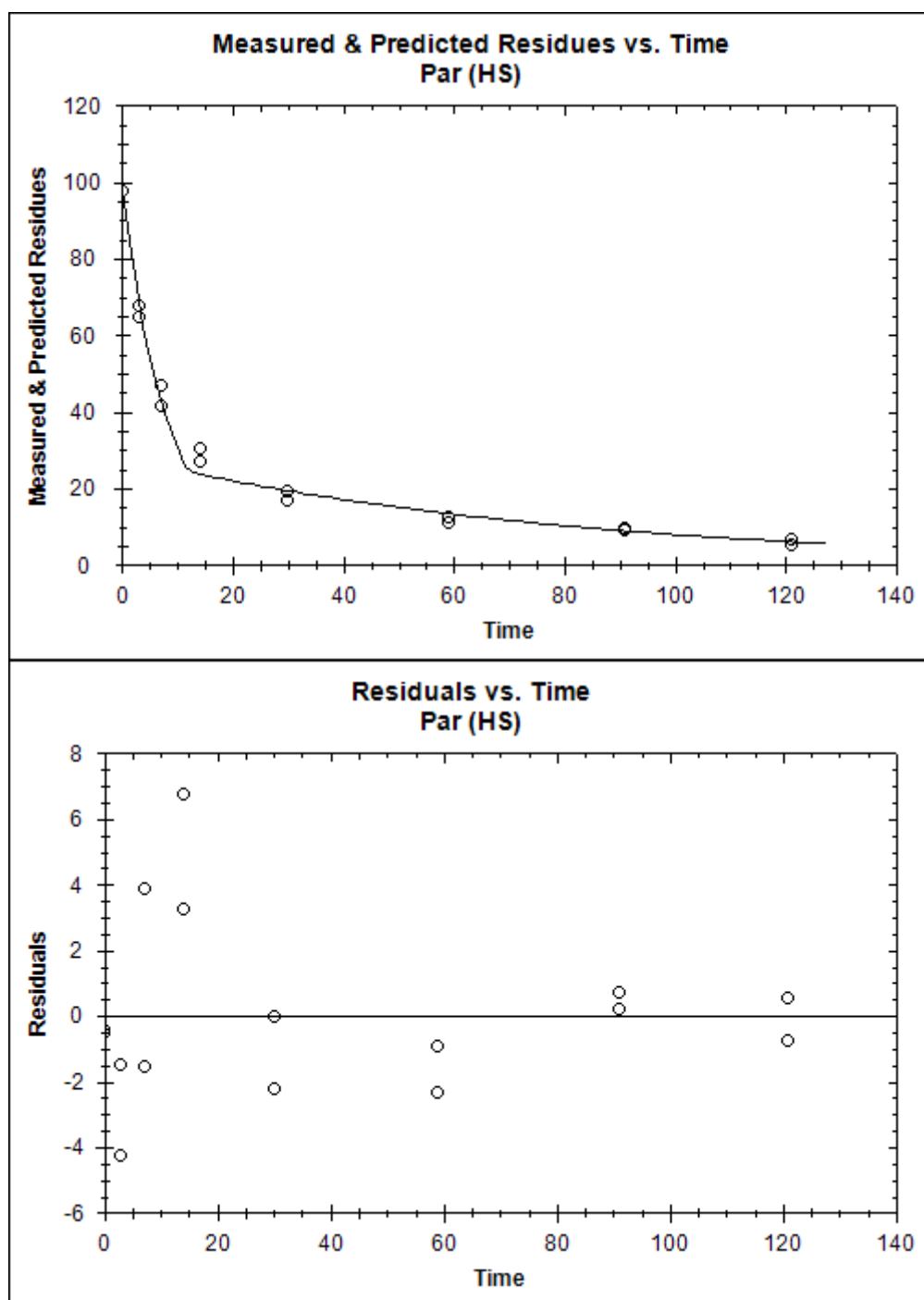
      DT50 :      5.9217      8.1783
      DT90 :     83.102    27.168
      Kinetic model :      HS      SFO

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

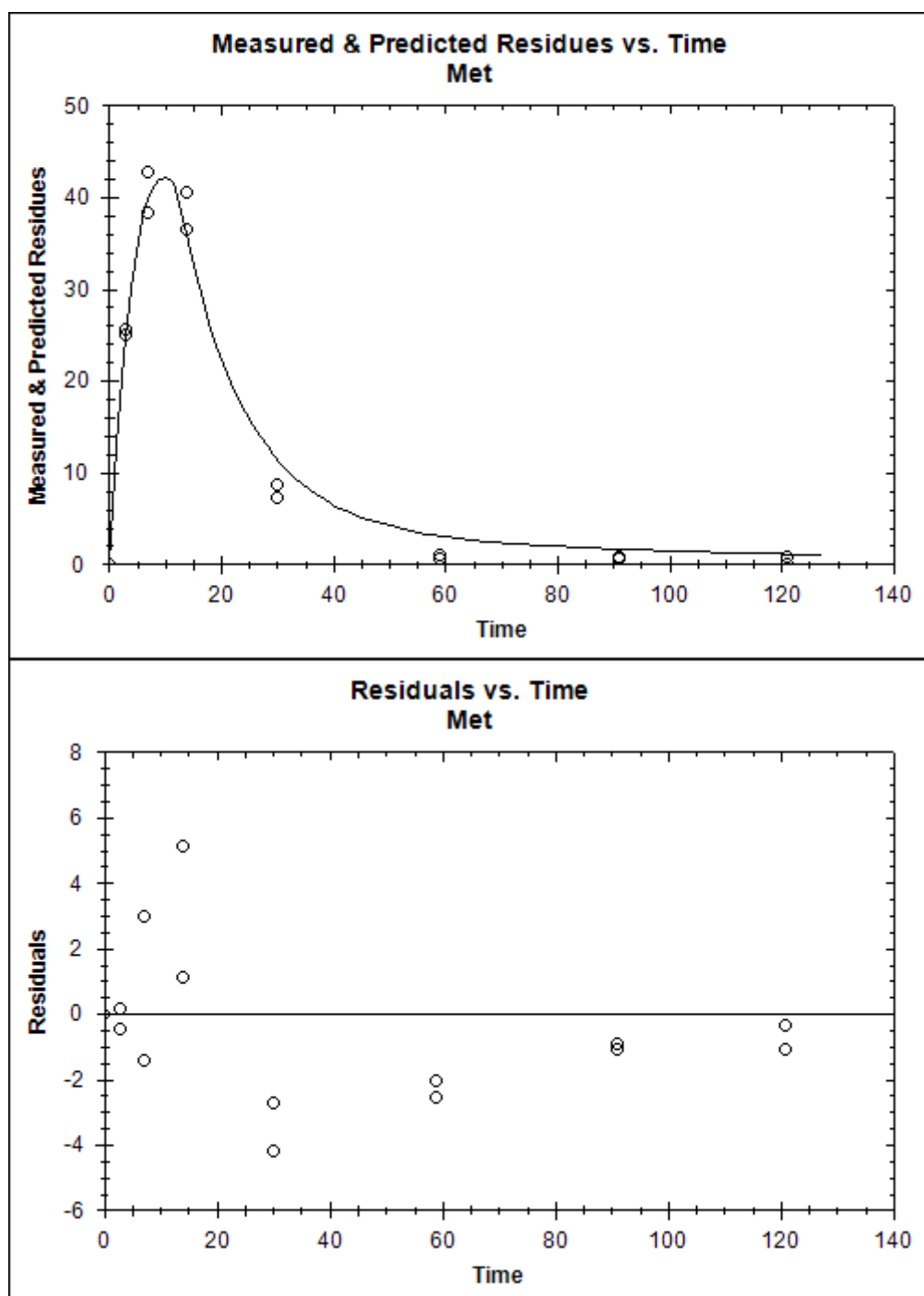
      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000  97.7000  2.5621  98.1203  -0.4203  0.0000  2.2215  0.0000  0.0000
0.0000  97.6000  2.5621  98.1203  -0.5203  0.0000  2.2215  0.0000  0.0000
3.0000  67.6000  2.5621  69.0644  -1.4644  25.0000  2.2215  25.4658  -0.4658
3.0000  64.8000  2.5621  69.0644  -4.2644  25.6000  2.2215  25.4658  0.1342

```

7.0000	41.7000	2.5621	43.2429	-1.5429	42.7000	2.2215	39.7560	2.9440
7.0000	47.1000	2.5621	43.2429	3.8571	38.3000	2.2215	39.7560	-1.4560
14.0000	26.9000	2.5621	23.6701	3.2299	40.4000	2.2215	35.2746	5.1254
14.0000	30.4000	2.5621	23.6701	6.7299	36.4000	2.2215	35.2746	1.1254
30.0000	17.1000	2.5621	19.3040	-2.2040	7.2000	2.2215	11.4261	-4.2261
30.0000	19.3000	2.5621	19.3040	-0.0040	8.7000	2.2215	11.4261	-2.7261
59.0000	11.0000	2.5621	13.3398	-2.3398	0.5000	2.2215	3.0465	-2.5465
59.0000	12.4000	2.5621	13.3398	-0.9398	1.0000	2.2215	3.0465	-2.0465
91.0000	9.6000	2.5621	8.8725	0.7275	0.5000	2.2215	1.6157	-1.1157
91.0000	9.1000	2.5621	8.8725	0.2275	0.7000	2.2215	1.6157	-0.9157
121.0000	5.3000	2.5621	6.0536	-0.7536	0.7000	2.2215	1.0749	-0.3749
121.0000	6.6000	2.5621	6.0536	0.5464	0.0000	2.2215	1.0749	-1.0749







## 11.3.3.3 FOMC

```

# Trial      : CAsandyloam
# File name  : CAsandyloam IRLS FOMC Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\CAsandyloam
# Created    : on 15 Oct 2013
#            : at 11:03
#            : 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:
# # label: 14C cyclopropyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      97.7          0          Inf      False
alpha Par      :       0.1          0          Inf      False
beta  Par      :       0.1          0          Inf      False
k      Met      :       0.1          0          Inf      False
FF     Par -> Met :       0.1          0           1      False
M(0)  Met      :          0          0          0          True

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

      Par      Met      All
Chi2Err% :    2.787    20.593    10.283
Kinetic model :    FOMC      SFO

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

Degrees of Freedom : 27
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :    98.28894    95.68904    100.889    1.32651    < 2e-16
alpha Par      :     0.84074     0.73072     0.951    0.05614    6.68e-15
beta  Par      :     4.60777     3.46489     5.751    0.58311    8.52e-09
k      Met      :     0.08151     0.06068     0.102    0.01063    1.50e-08
FF     Par -> Met :    1.000e+00    0.08795

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

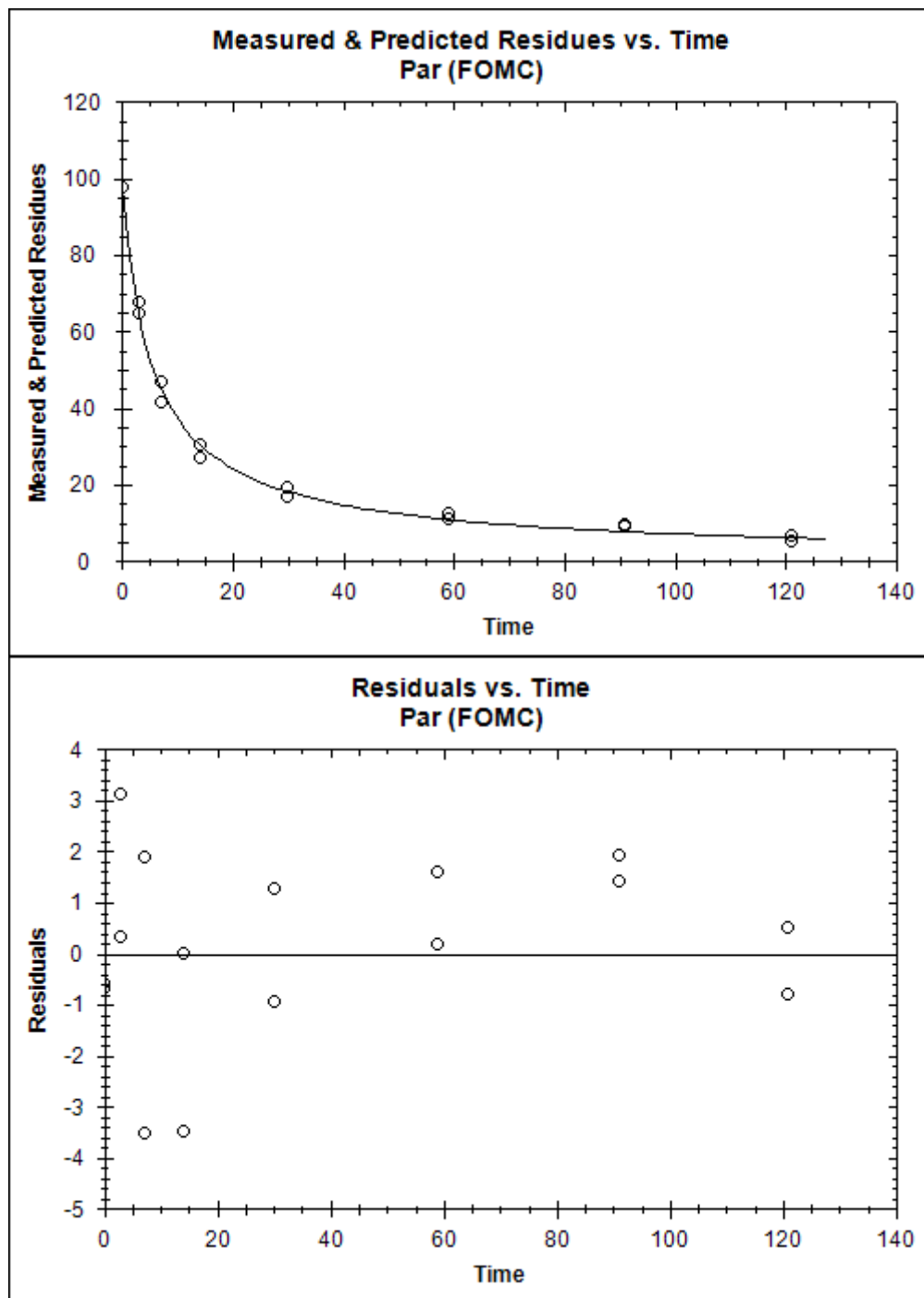
      Par      Met
DT50 :     5.9008    8.5042
DT90 :    66.664    28.250
Kinetic model :    FOMC      SFO

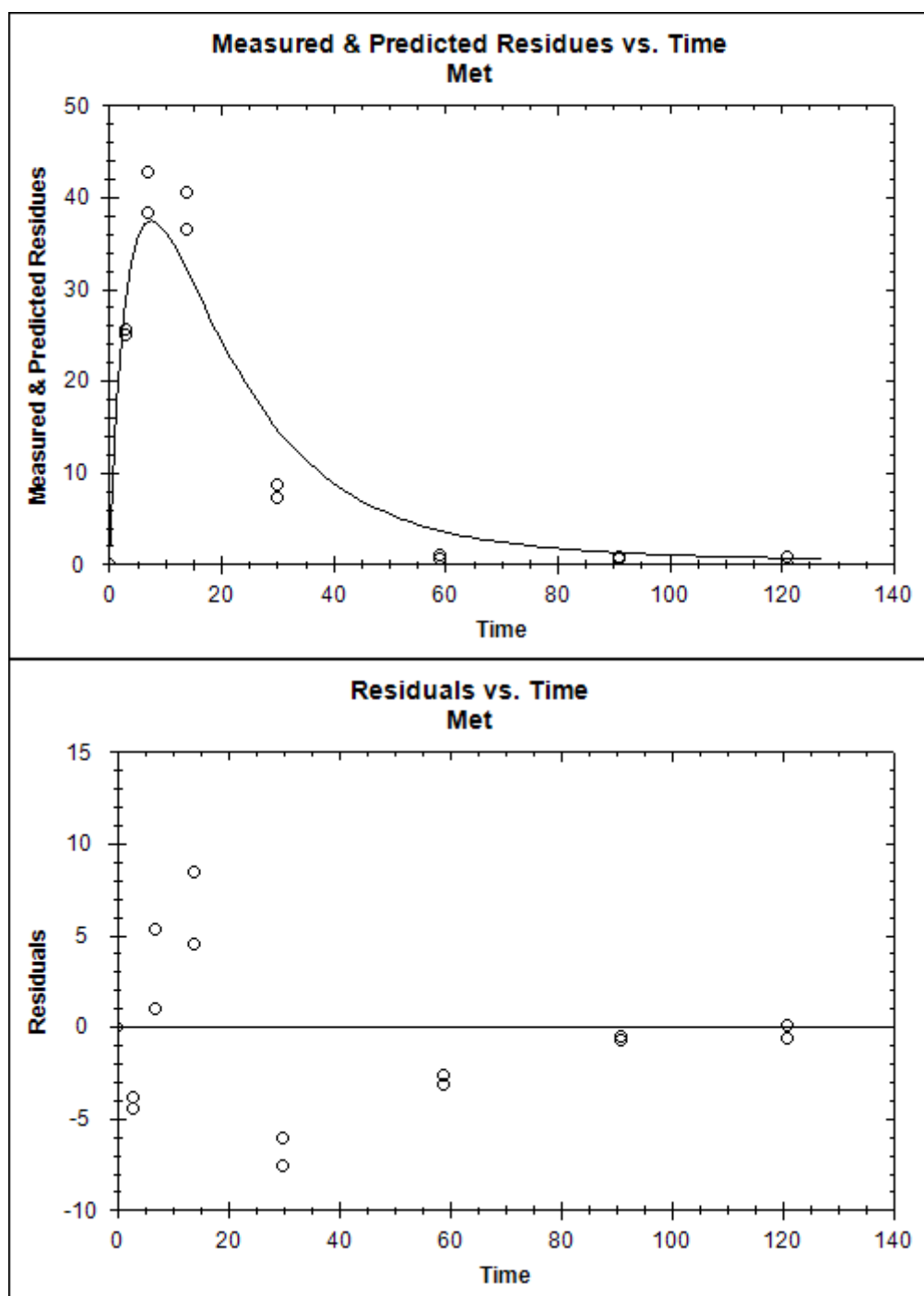
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000  97.7000  1.7746  98.2889 -0.5889  0.0000  4.0907  0.0000  0.0000
0.0000  97.6000  1.7746  98.2889 -0.6889  0.0000  4.0907  0.0000  0.0000
3.0000  67.6000  1.7746  64.4791  3.1209  25.0000  4.0907  29.4369 -4.4369
3.0000  64.8000  1.7746  64.4791  0.3209  25.6000  4.0907  29.4369 -3.8369
7.0000  41.7000  1.7746  45.2012 -3.5012  42.7000  4.0907  37.3547  5.3453
7.0000  47.1000  1.7746  45.2012  1.8988  38.3000  4.0907  37.3547  0.9453

```

14.0000	26.9000	1.7746	30.3979	-3.4979	40.4000	4.0907	31.9396	8.4604
14.0000	30.4000	1.7746	30.3979	0.0021	36.4000	4.0907	31.9396	4.4604
30.0000	17.1000	1.7746	18.0419	-0.9419	7.2000	4.0907	14.7778	-7.5778
30.0000	19.3000	1.7746	18.0419	1.2581	8.7000	4.0907	14.7778	-6.0778
59.0000	11.0000	1.7746	10.8154	0.1846	0.5000	4.0907	3.6395	-3.1395
59.0000	12.4000	1.7746	10.8154	1.5846	1.0000	4.0907	3.6395	-2.6395
91.0000	9.6000	1.7746	7.6780	1.9220	0.5000	4.0907	1.2268	-0.7268
91.0000	9.1000	1.7746	7.6780	1.4220	0.7000	4.0907	1.2268	-0.5268
121.0000	5.3000	1.7746	6.1038	-0.8038	0.7000	4.0907	0.6412	0.0588
121.0000	6.6000	1.7746	6.1038	0.4962	0.0000	4.0907	0.6412	-0.6412





## 11.3.3.4 DFOP

```

# Trial      : CAsandyloam
# File name  : CAsandyloam IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\CAsandyloam
# Created    : on 15 Oct 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:
# # label: 14C cyclopropyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      97.70              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                      True

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

      Chi2Err% :      1.683      Par      Met      All
      Kinetic model :      DFOP      SFO      7.656

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

Degrees of Freedom : 26
      Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      97.801565      95.601004      100.002      1.122756      < 2e-16
k1    Par      :      0.178570      0.156661      0.200      0.011178      2.93e-15
k2    Par      :      0.011758      0.008626      0.015      0.001598      4.09e-08
g     Par      :      0.740232      0.695722      0.785      0.022709      < 2e-16
k     Met      :      0.082568      0.065719      0.099      0.008597      2.44e-10
FF    Par -> Met :      1.000e+00                      0.069631

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

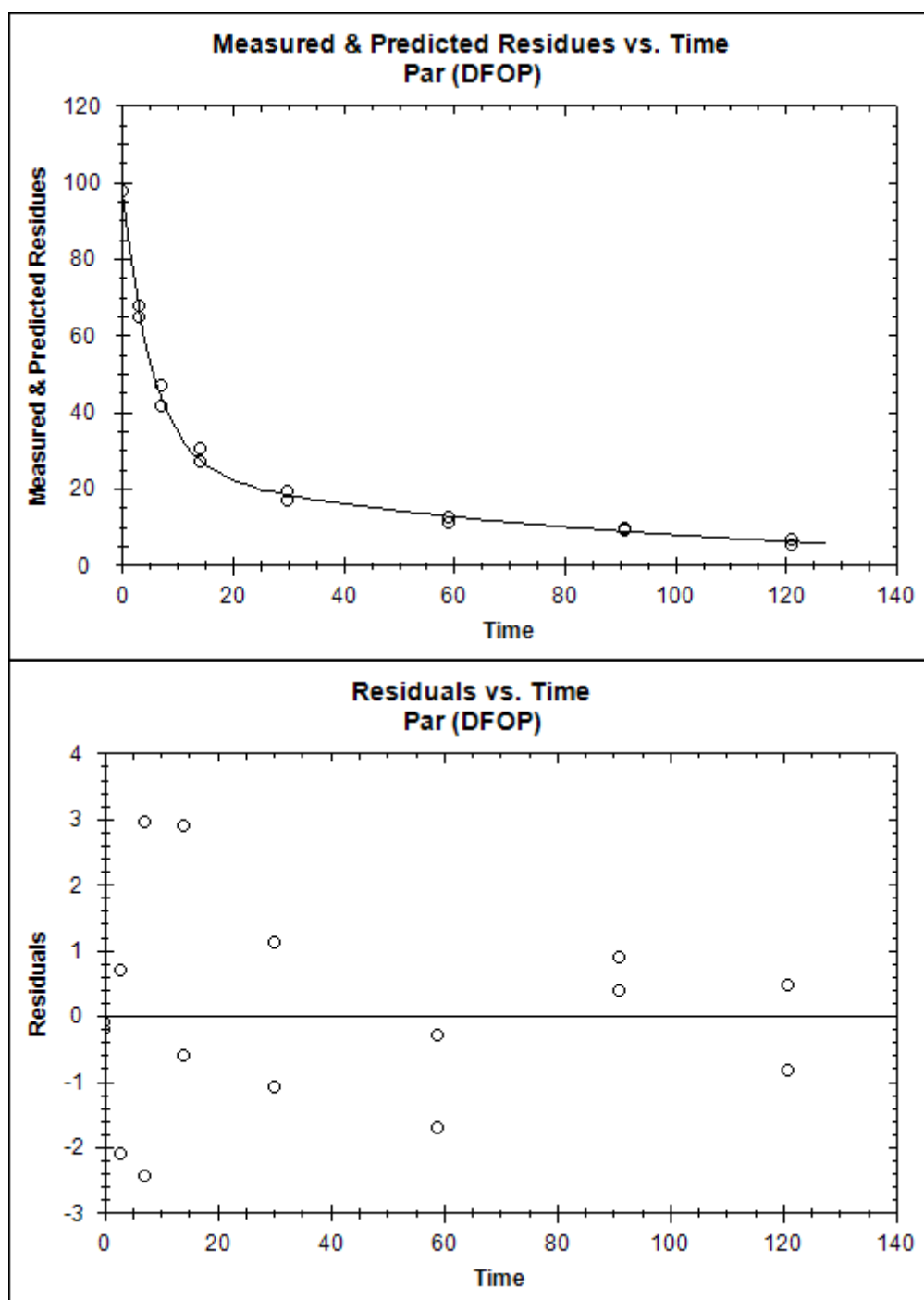
      DT50 :      5.9097      Par      Met
      DT90 :      81.192      8.3949
      Kinetic model :      DFOP      SFO

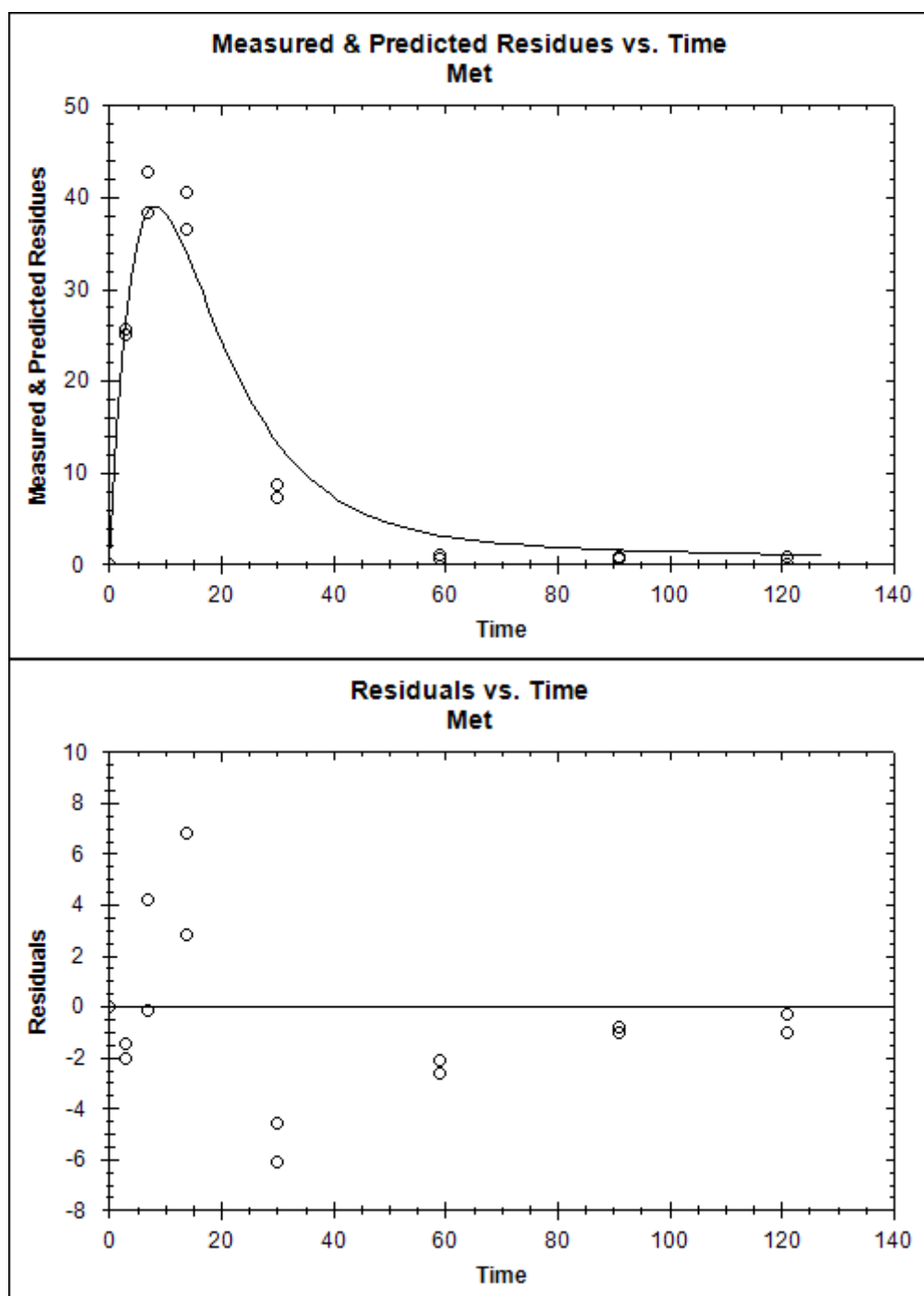
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000 97.7000 1.4937 97.8016 -0.1016 0.0000 3.0703 0.0000 0.0000
0.0000 97.6000 1.4937 97.8016 -0.2016 0.0000 3.0703 0.0000 0.0000
3.0000 67.6000 1.4937 66.8952 0.7048 25.0000 3.0703 27.0833 -2.0833
3.0000 64.8000 1.4937 66.8952 -2.0952 25.6000 3.0703 27.0833 -1.4833

```

7.0000	41.7000	1.4937	44.1405	-2.4405	42.7000	3.0703	38.4858	4.2142
7.0000	47.1000	1.4937	44.1405	2.9595	38.3000	3.0703	38.4858	-0.1858
14.0000	26.9000	1.4937	27.4926	-0.5926	40.4000	3.0703	33.5817	6.8183
14.0000	30.4000	1.4937	27.4926	2.9074	36.4000	3.0703	33.5817	2.8183
30.0000	17.1000	1.4937	18.1957	-1.0957	7.2000	3.0703	13.2857	-6.0857
30.0000	19.3000	1.4937	18.1957	1.1043	8.7000	3.0703	13.2857	-4.5857
59.0000	11.0000	1.4937	12.6978	-1.6978	0.5000	3.0703	3.1039	-2.6039
59.0000	12.4000	1.4937	12.6978	-0.2978	1.0000	3.0703	3.1039	-2.1039
91.0000	9.6000	1.4937	8.7149	0.8851	0.5000	3.0703	1.5182	-1.0182
91.0000	9.1000	1.4937	8.7149	0.3851	0.7000	3.0703	1.5182	-0.8182
121.0000	5.3000	1.4937	6.1245	-0.8245	0.7000	3.0703	1.0229	-0.3229
121.0000	6.6000	1.4937	6.1245	0.4755	0.0000	3.0703	1.0229	-1.0229





**11.3.4 Madera CA 2 (BETA-CYF, FPB-acid)****11.3.4.1 SFO**

```

# Trial      : CAsandyloamFPB
# File name  : CAsandyloamFPB IRLS SFO Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\CAsandyloamFPB
# Created    : on 15 Oct 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:
# # label: 14C fluorophenyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      100.4              0              Inf      False
k      Par      :       0.1              0              Inf      False
k      Met      :       0.1              0              Inf      False
FF      Par -> Met :       0.1              0              1      False
M(0)  Met      :       0                  0              1      True

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

      Par      Met      All
Chi2Err% :    13.19    11.18    17.98
Kinetic model :      SFO      SFO

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

Degrees of Freedom : 28
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :    1.019e+02    9.385e+01    109.955    4.108e+00    < 2e-16
k      Par      :    6.010e-02    4.791e-02     0.072    6.219e-03    1.02e-10
k      Met      :    3.343e-01    2.321e-01     0.437    5.216e-02    3.06e-07
FF      Par -> Met :    1.000e+00    1.873e-01

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

      Par      Met
DT50 :    11.533    2.0734
DT90 :    38.311    6.8878
Kinetic model :      SFO      SFO

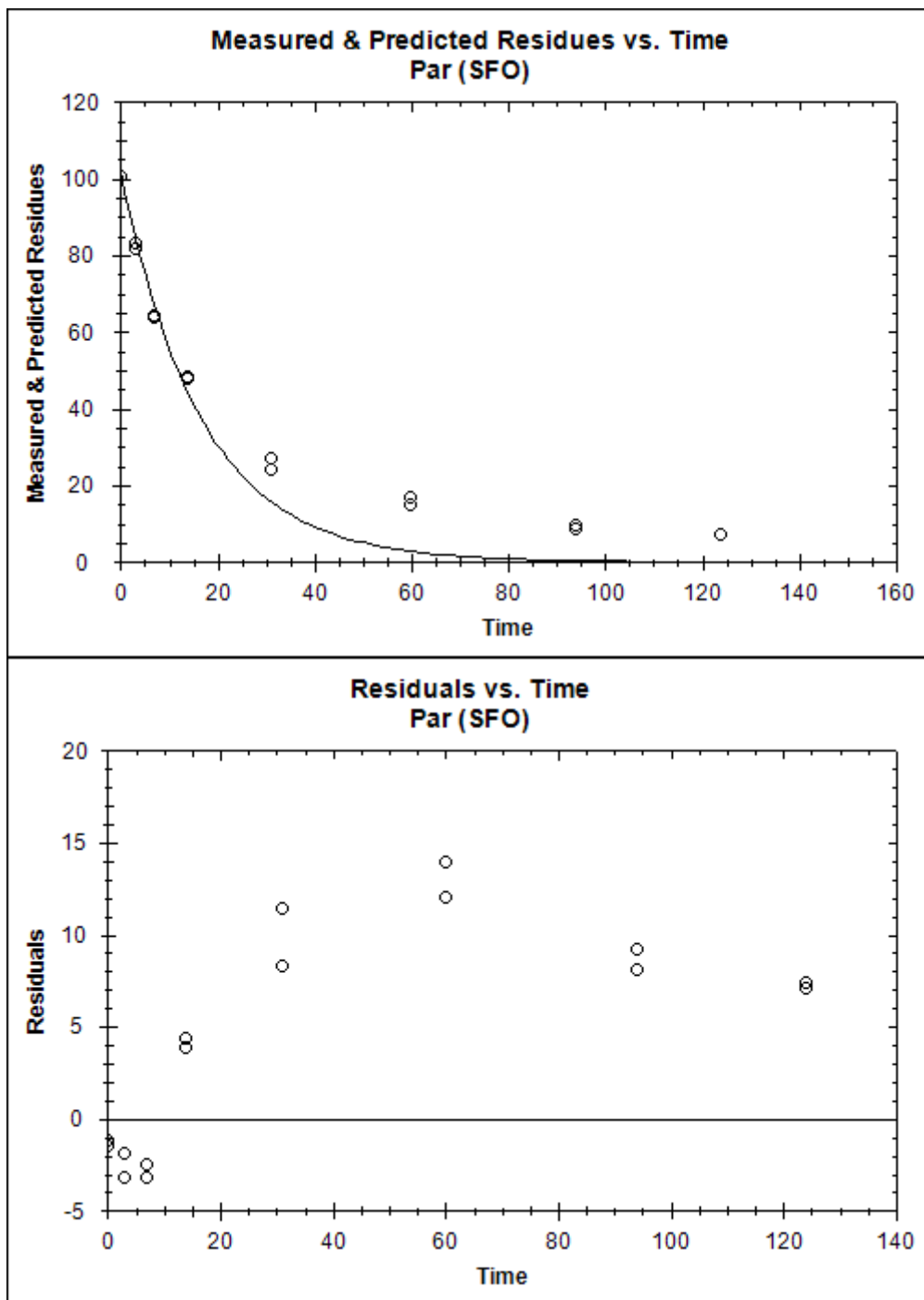
# -----
# Measured vs. predicted values
# -----

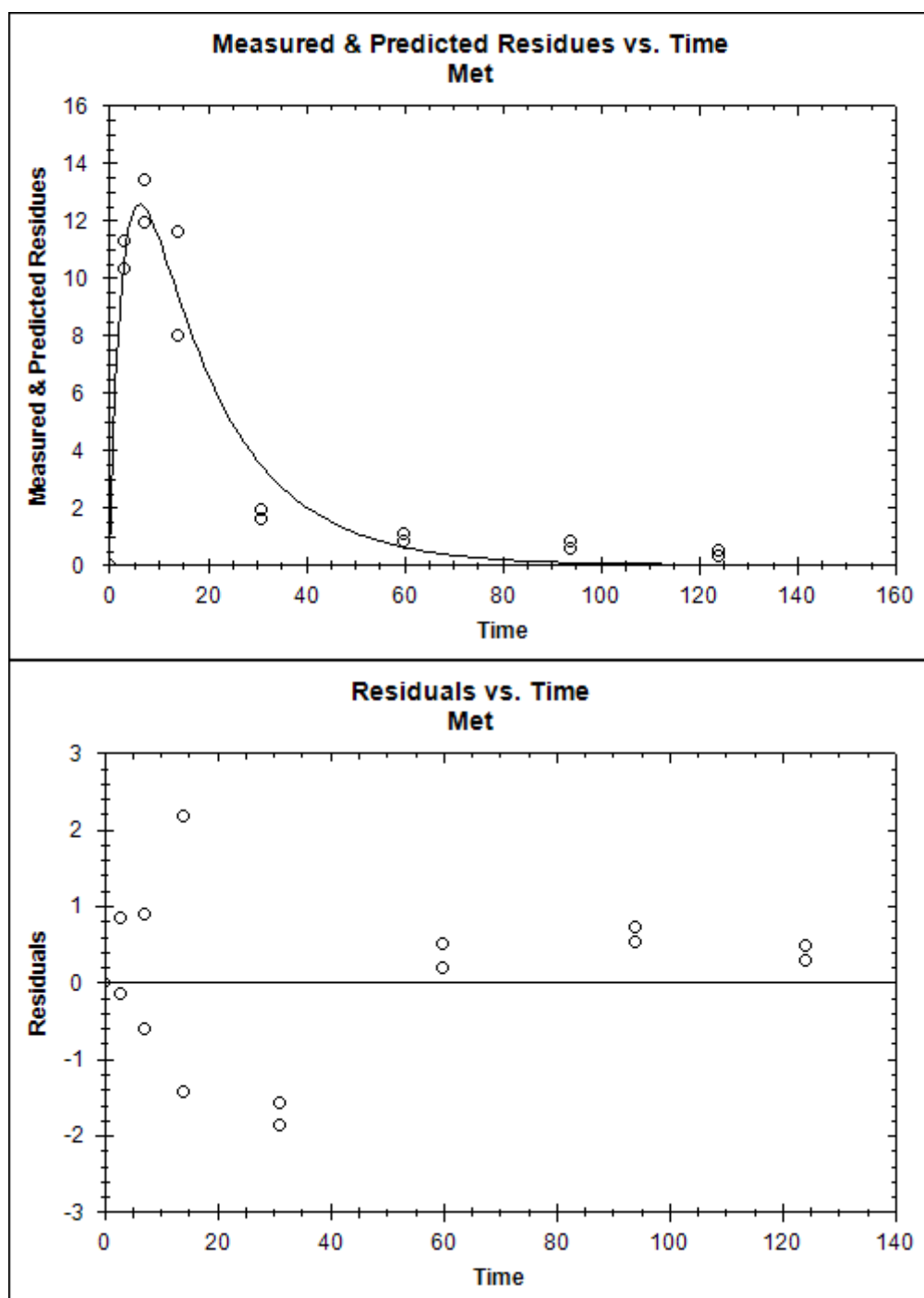
      Compartment Par      Compartment Met
time observed err-std predicted residual observed err-std predicted residual
0.0000 100.4000 7.3286 101.9039 -1.5039 0.0000 1.0002 0.0000 0.0000
0.0000 100.7000 7.3286 101.9039 -1.2039 0.0000 1.0002 0.0000 0.0000
3.0000 83.2000 7.3286 85.0913 -1.8913 11.3000 1.0002 10.4579 0.8421
3.0000 81.9000 7.3286 85.0913 -3.1913 10.3000 1.0002 10.4579 -0.1579
7.0000 64.4000 7.3286 66.9079 -2.5079 11.9000 1.0002 12.5141 -0.6141
7.0000 63.7000 7.3286 66.9079 -3.2079 13.4000 1.0002 12.5141 0.8859

```



14.0000	48.3000	7.3286	43.9302	4.3698	11.6000	1.0002	9.4218	2.1782
14.0000	47.8000	7.3286	43.9302	3.8698	8.0000	1.0002	9.4218	-1.4218
31.0000	27.2000	7.3286	15.8136	11.3864	1.9000	1.0002	3.4655	-1.5655
31.0000	24.1000	7.3286	15.8136	8.2864	1.6000	1.0002	3.4655	-1.8655
60.0000	16.7000	7.3286	2.7674	13.9326	1.1000	1.0002	0.6066	0.4934
60.0000	14.8000	7.3286	2.7674	12.0326	0.8000	1.0002	0.6066	0.1934
94.0000	8.5000	7.3286	0.3586	8.1414	0.6000	1.0002	0.0786	0.5214
94.0000	9.6000	7.3286	0.3586	9.2414	0.8000	1.0002	0.0786	0.7214
124.0000	7.4000	7.3286	0.0591	7.3409	0.5000	1.0002	0.0130	0.4870
124.0000	7.1000	7.3286	0.0591	7.0409	0.3000	1.0002	0.0130	0.2870





## 11.3.4.2 HS

```

# Trial      : CAsandyloamFPB
# File name  : CAsandyloamFPB IRLS HS   Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\CAsandyloamFPB
# Created    : on 16 Oct 2013
#            : at 09:18
#            : 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. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID:
# # label: 14C fluorophenyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      100.40              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% :      7.072      17.327      9.429
      Kinetic model :      HS      SFO

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

Degrees of Freedom : 26
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      1.018e+02      9.677e+01      106.904      2.586e+00      < 2e-16
k1    Par      7.802e-02      5.901e-02      0.097      9.698e-03      7.95e-09
k2    Par      2.934e-02      2.300e-02      0.036      3.235e-03      7.82e-10
tb    Par      6.129e+00      4.547e+00      7.712      8.074e-01      2.33e-08
k      Met      1.751e-01      1.052e-01      0.245      3.565e-02      2.12e-05
FF    Par -> Met      0.6341      1.147e-01

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

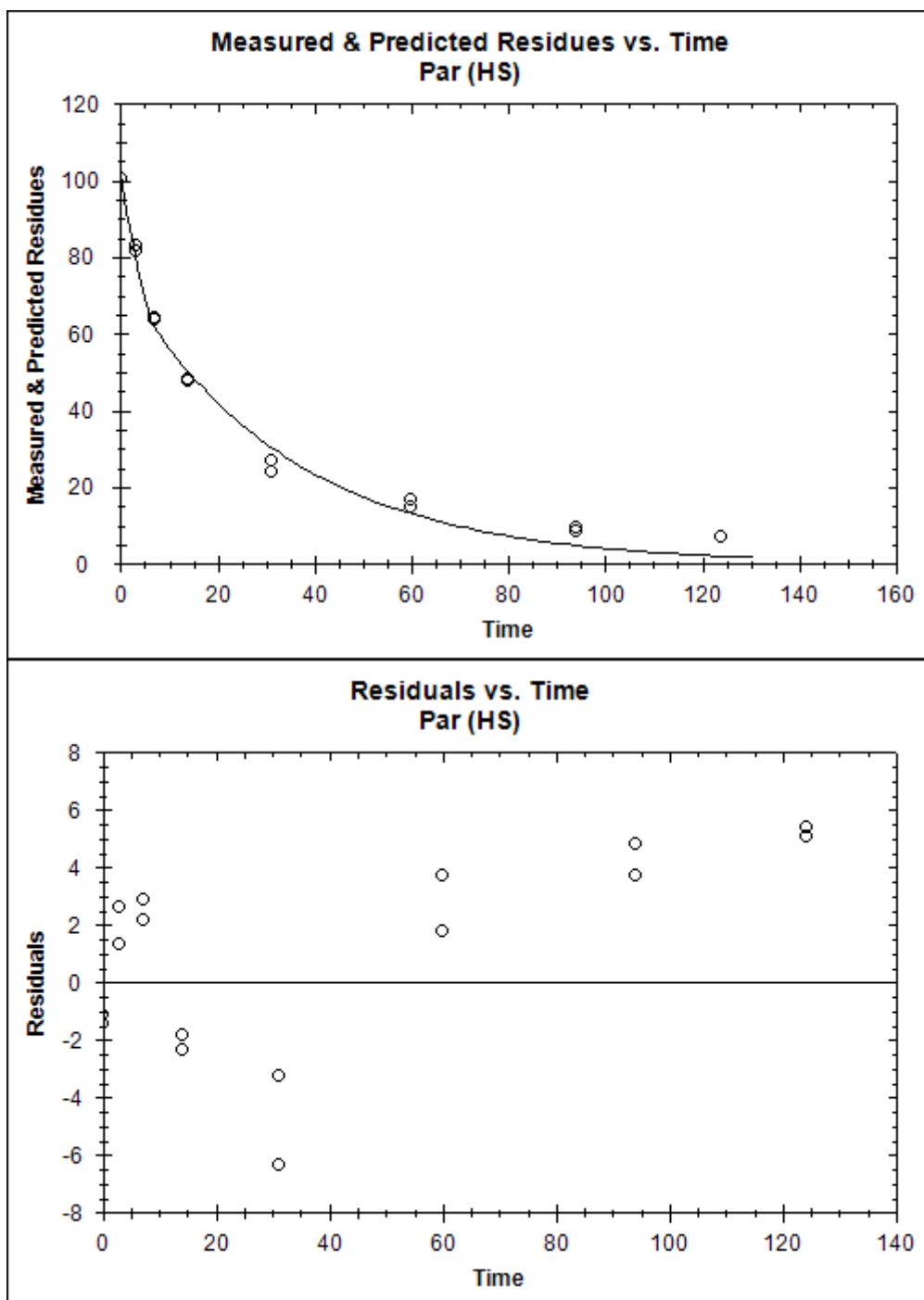
      DT50 :      13.456      3.9584
      DT90 :      68.318      13.150
      Kinetic model :      HS      SFO

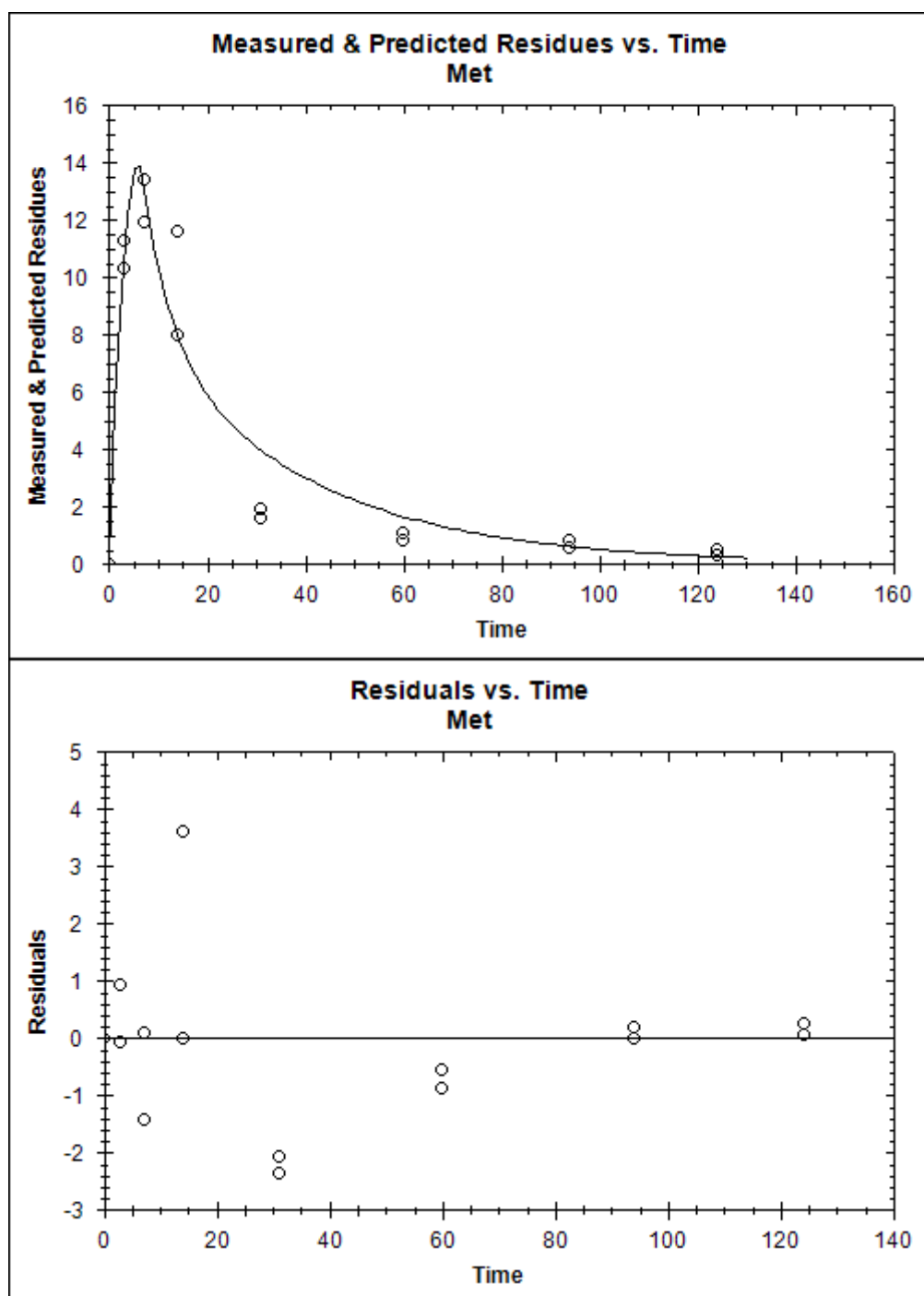
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000 100.4000 3.4753 101.8363 -1.4363 0.0000 1.2955 0.0000 0.0000
0.0000 100.7000 3.4753 101.8363 -1.1363 0.0000 1.2955 0.0000 0.0000
3.0000 83.2000 3.4753 80.5842 2.6158 11.3000 1.2955 10.3752 0.9248
3.0000 81.9000 3.4753 80.5842 1.3158 10.3000 1.2955 10.3752 -0.0752

```

7.0000	64.4000	3.4753	61.5353	2.8647	11.9000	1.2955	13.3215	-1.4215
7.0000	63.7000	3.4753	61.5353	2.1647	13.4000	1.2955	13.3215	0.0785
14.0000	48.3000	3.4753	50.1119	-1.8119	11.6000	1.2955	7.9998	3.6002
14.0000	47.8000	3.4753	50.1119	-2.3119	8.0000	1.2955	7.9998	0.0002
31.0000	27.2000	3.4753	30.4335	-3.2335	1.9000	1.2955	3.9652	-2.0652
31.0000	24.1000	3.4753	30.4335	-6.3335	1.6000	1.2955	3.9652	-2.3652
60.0000	16.7000	3.4753	12.9980	3.7020	1.1000	1.2955	1.6591	-0.5591
60.0000	14.8000	3.4753	12.9980	1.8020	0.8000	1.2955	1.6591	-0.8591
94.0000	8.5000	3.4753	4.7940	3.7060	0.6000	1.2955	0.6117	-0.0117
94.0000	9.6000	3.4753	4.7940	4.8060	0.8000	1.2955	0.6117	0.1883
124.0000	7.4000	3.4753	1.9883	5.4117	0.5000	1.2955	0.2537	0.2463
124.0000	7.1000	3.4753	1.9883	5.1117	0.3000	1.2955	0.2537	0.0463





## 11.3.4.3 FOMC

```

# Trial      : CAsandyloamFPB
# File name  : CAsandyloamFPB IRLS FOMC Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\CAsandyloamFPB
# Created    : on 15 Oct 2013
#            : at 11:36
#            : 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. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID:
# # label: 14C fluorophenyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      100.4          0          Inf      False
alpha Par      :         0.1          0          Inf      False
beta  Par      :         0.1          0          Inf      False
k      Met      :         0.1          0          Inf      False
FF     Par -> Met :         0.1          0          1      False
M(0)  Met      :         0          0          0          True

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

      Par      Met      All
Chi2Err% :      1.570      9.251      2.537
Kinetic model :      FOMC      SFO

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

Degrees of Freedom : 27
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      100.81736      99.30242      102.332      0.77294      < 2e-16
alpha Par      :         1.25130         1.11655         1.386      0.06875      < 2e-16
beta  Par      :         16.60150         13.73361         19.469      1.46324      4.43e-12
k      Met      :         0.23591         0.18051         0.291      0.02827      2.95e-09
FF     Par -> Met:         0.8124         0.08051         0.08051

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

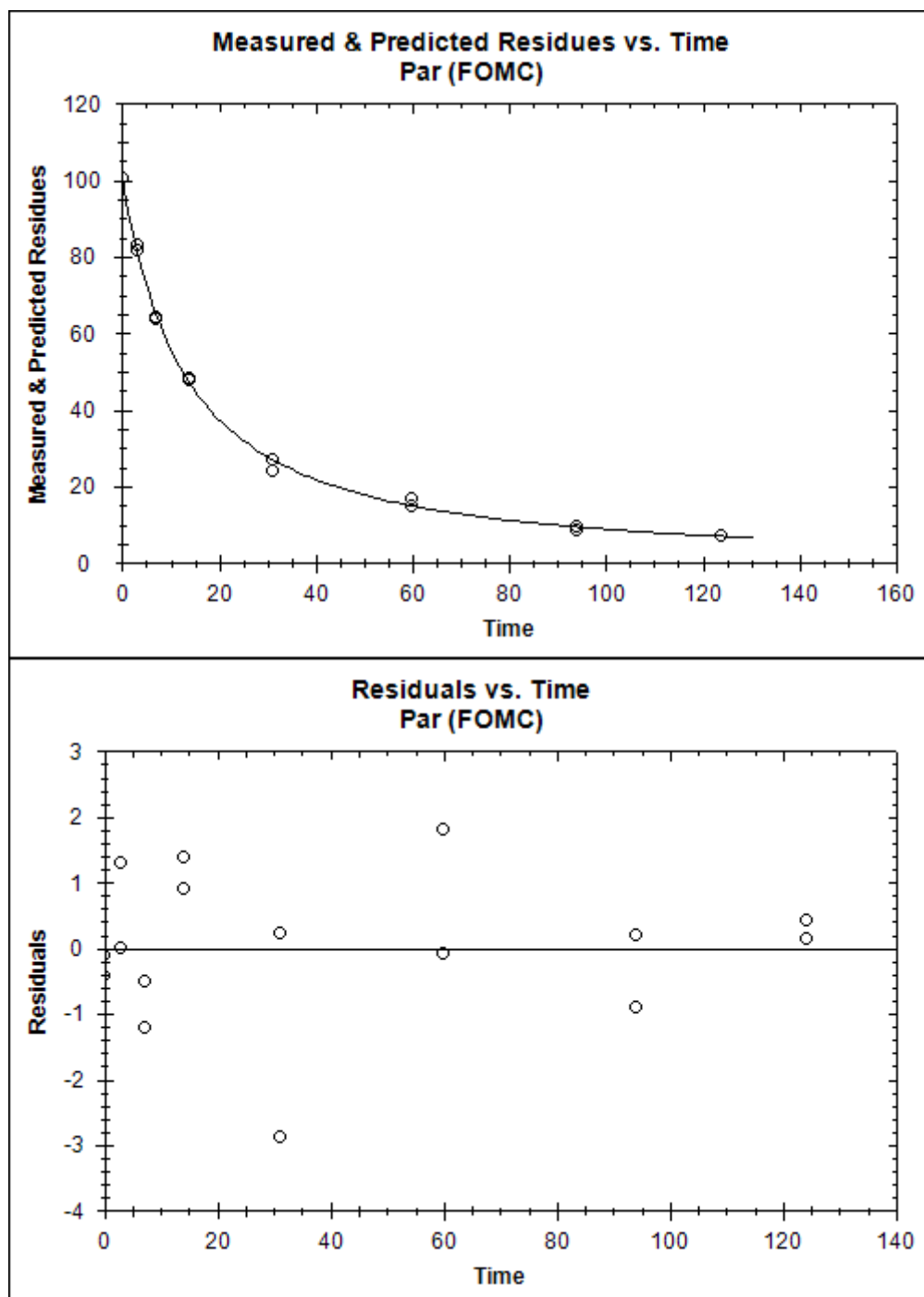
      Par      Met
DT50 :      12.287      2.9381
DT90 :      87.946      9.7603
Kinetic model :      FOMC      SFO

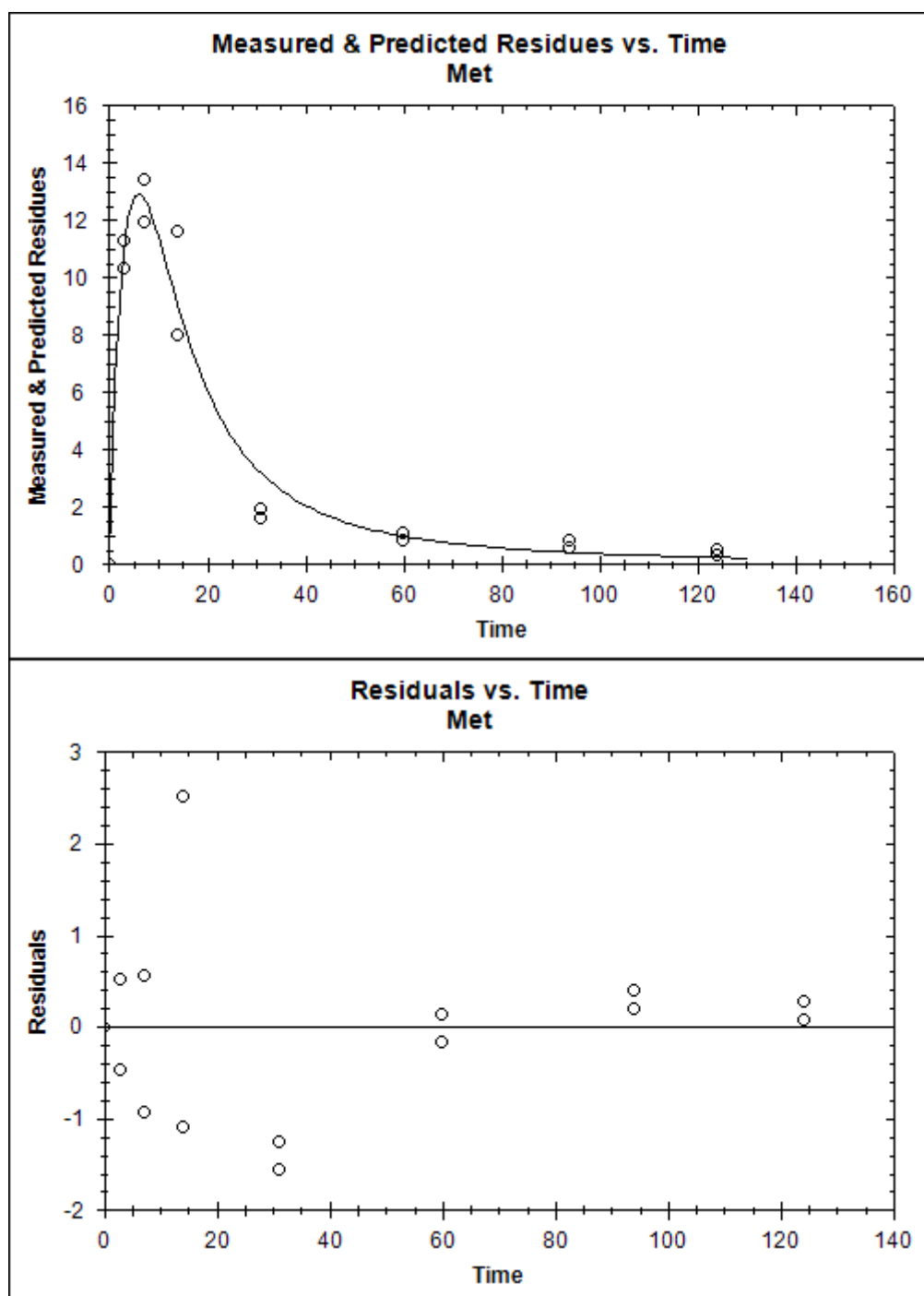
# -----
# Measured vs. predicted values
# -----

      Compartment Par      time observed err-std predicted residual
0.0000 100.4000 1.0935 100.8174 -0.4174
0.0000 100.7000 1.0935 100.8174 -0.1174
3.0000 83.2000 1.0935 81.8963 1.3037
3.0000 81.9000 1.0935 81.8963 0.0037
7.0000 64.4000 1.0935 64.9152 -0.5152
7.0000 63.7000 1.0935 64.9152 -1.2152
      Compartment Met      time observed err-std predicted residual
0.0000 0.9200 0.0000 0.9200 0.0000
0.0000 0.9200 0.0000 0.9200 0.0000
11.3000 0.9200 10.7774 0.5226
10.3000 0.9200 10.7774 -0.4774
11.9000 0.9200 12.8375 -0.9375
13.4000 0.9200 12.8375 0.5625

```

14.0000	48.3000	1.0935	46.9025	1.3975	11.6000	0.9200	9.0859	2.5141
14.0000	47.8000	1.0935	46.9025	0.8975	8.0000	0.9200	9.0859	-1.0859
31.0000	27.2000	1.0935	26.9835	0.2165	1.9000	0.9200	3.1608	-1.2608
31.0000	24.1000	1.0935	26.9835	-2.8835	1.6000	0.9200	3.1608	-1.5608
60.0000	16.7000	1.0935	14.8785	1.8215	1.1000	0.9200	0.9664	0.1336
60.0000	14.8000	1.0935	14.8785	-0.0785	0.8000	0.9200	0.9664	-0.1664
94.0000	8.5000	1.0935	9.3961	-0.8961	0.6000	0.9200	0.4024	0.1976
94.0000	9.6000	1.0935	9.3961	0.2039	0.8000	0.9200	0.4024	0.3976
124.0000	7.4000	1.0935	6.9587	0.4413	0.5000	0.9200	0.2294	0.2706
124.0000	7.1000	1.0935	6.9587	0.1413	0.3000	0.9200	0.2294	0.0706







## 11.3.4.4 DFOP

```

# Trial      : CAsandyloamFPB
# File name  : CAsandyloamFPB IRLS DFOP Par.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\CYF_met\CAsandyloamFPB
# Created    : on 15 Oct 2013
#            : at 11:32
#            : 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. Algorithms : solnp; L-BFGS-B
# Comments      :
# # study ID:
# # label: 14C fluorophenyl
# # soil : CA-sandy loam
# # CA-sandy loam
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  Par      :      100.40              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                      True

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

      Chi2Err% :      1.940      Par      Met      All
      Kinetic model :      DFOP      SFO      2.749

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

Degrees of Freedom : 26
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  Par      :      1.002e+02      9.855e+01      101.873      8.479e-01      < 2e-16
k1    Par      :      9.412e-02      7.943e-02      0.109      7.493e-03      7.56e-13
k2    Par      :      1.343e-02      1.020e-02      0.017      1.647e-03      6.21e-09
g     Par      :      6.555e-01      5.776e-01      0.733      3.974e-02      1.37e-15
k     Met      :      2.664e-01      1.999e-01      0.333      3.393e-02      1.25e-08
FF    Par -> Met :      0.90043                      9.839e-02

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

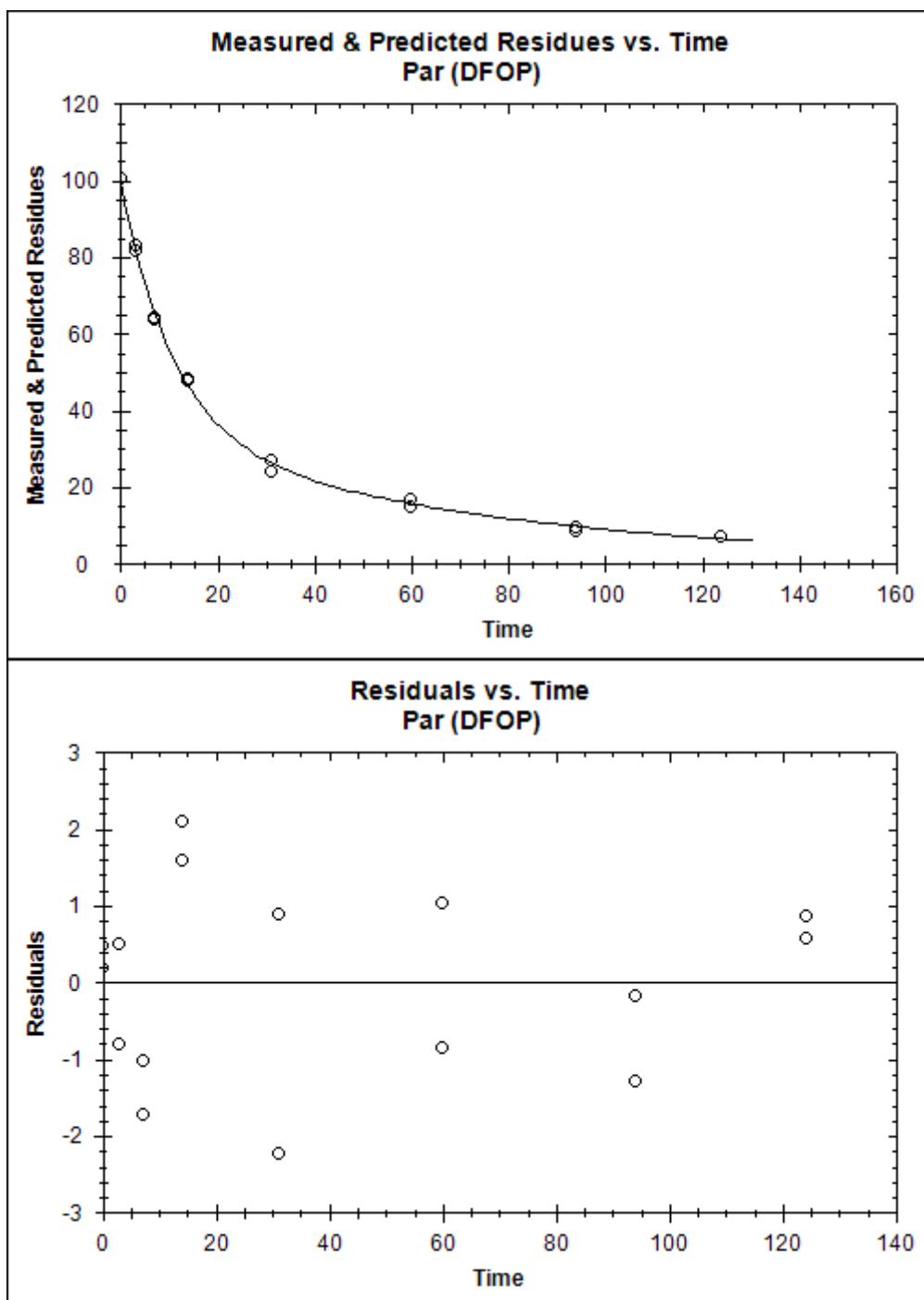
      DT50 :      12.216      Par      Met
      DT90 :      92.209      2.6015
      Kinetic model :      DFOP      SFO      8.6420

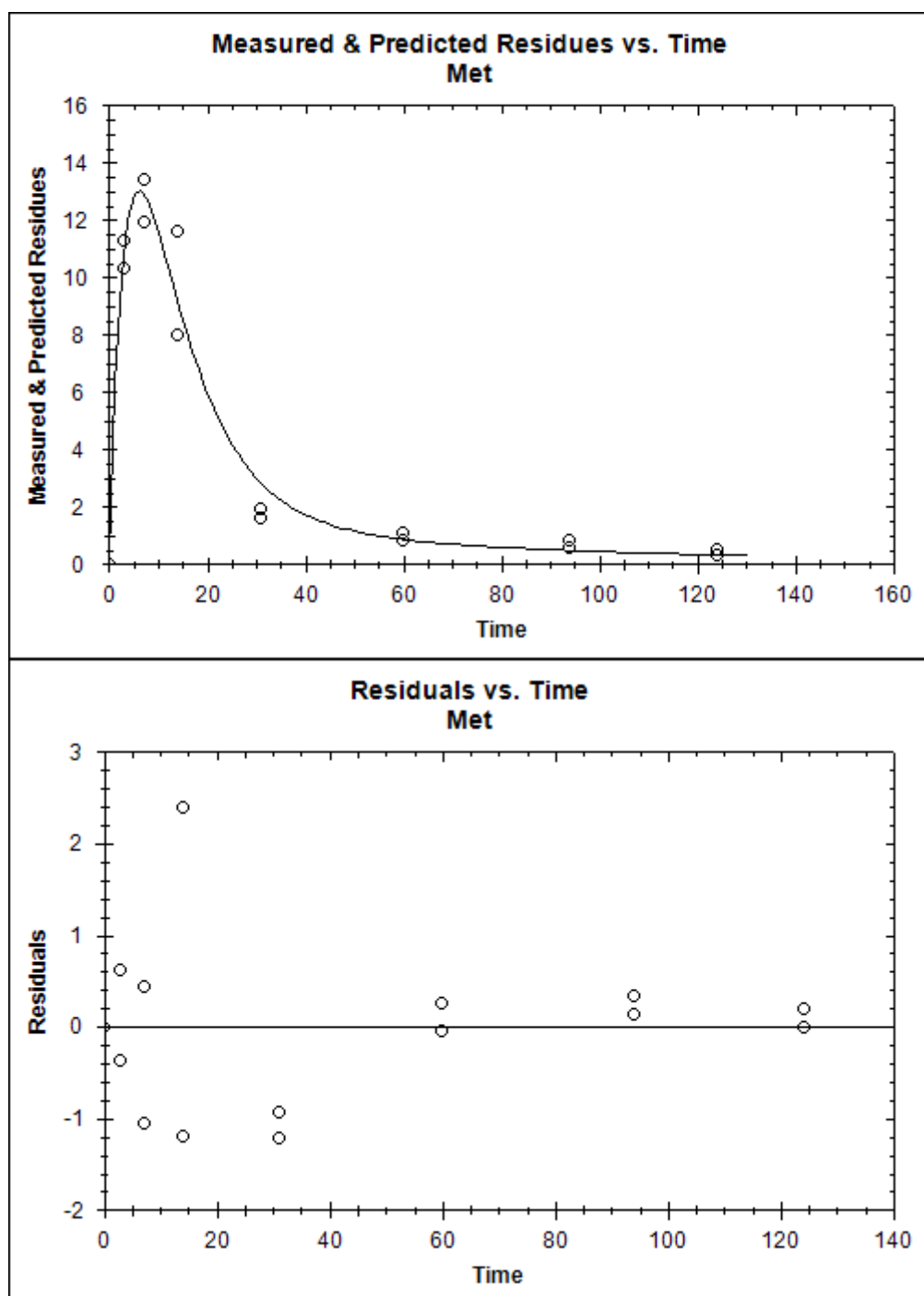
# -----
# Measured vs. predicted values
# -----

      Compartment Par      Compartment Met
      time observed err-std predicted residual observed err-std predicted residual
0.0000 100.4000 1.1836 100.2114 0.1886 0.0000 0.8524 0.0000 0.0000
0.0000 100.7000 1.1836 100.2114 0.4886 0.0000 0.8524 0.0000 0.0000
3.0000 83.2000 1.1836 82.6893 0.5107 11.3000 0.8524 10.6755 0.6245
3.0000 81.9000 1.1836 82.6893 -0.7893 10.3000 0.8524 10.6755 -0.3755

```

7.0000	64.4000	1.1836	65.4167	-1.0167	11.9000	0.8524	12.9591	-1.0591
7.0000	63.7000	1.1836	65.4167	-1.7167	13.4000	0.8524	12.9591	0.4409
14.0000	48.3000	1.1836	46.1954	2.1046	11.6000	0.8524	9.2024	2.3976
14.0000	47.8000	1.1836	46.1954	1.6046	8.0000	0.8524	9.2024	-1.2024
31.0000	27.2000	1.1836	26.3195	0.8805	1.9000	0.8524	2.8255	-0.9255
31.0000	24.1000	1.1836	26.3195	-2.2195	1.6000	0.8524	2.8255	-1.2255
60.0000	16.7000	1.1836	15.6571	1.0429	1.1000	0.8524	0.8510	0.2490
60.0000	14.8000	1.1836	15.6571	-0.8571	0.8000	0.8524	0.8510	-0.0510
94.0000	8.5000	1.1836	9.7815	-1.2815	0.6000	0.8524	0.4716	0.1284
94.0000	9.6000	1.1836	9.7815	-0.1815	0.8000	0.8524	0.4716	0.3284
124.0000	7.4000	1.1836	6.5328	0.8672	0.5000	0.8524	0.3124	0.1876
124.0000	7.1000	1.1836	6.5328	0.5672	0.3000	0.8524	0.3124	-0.0124





## 11.4 KinGUII Results FPB-acid

### 11.4.1 Hanscheider Hof

#### 11.4.1.1 SFO

```
# Trial      : HanschHof
# File name  : HanschHof IRLS SFO  FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\FPB\HanschHof
# Created    : on 27 Oct 2013
#            : at 07:50
#            : 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:
# # label: lphenoxy
# # soil :Hanscheider Hof
# # Hanscheider Hof
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      93.8              0              Inf      False
k      FPB      :      0.1              0              Inf      False

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

      Chi2Err% :      3.644      3.644
      Kinetic model :      SFO

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

Degrees of Freedom : 12
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      93.61095      91.64541      95.576      1.00285      < 2e-16
k      FPB      :      0.67250      0.62739      0.718      0.02302      8.06e-13

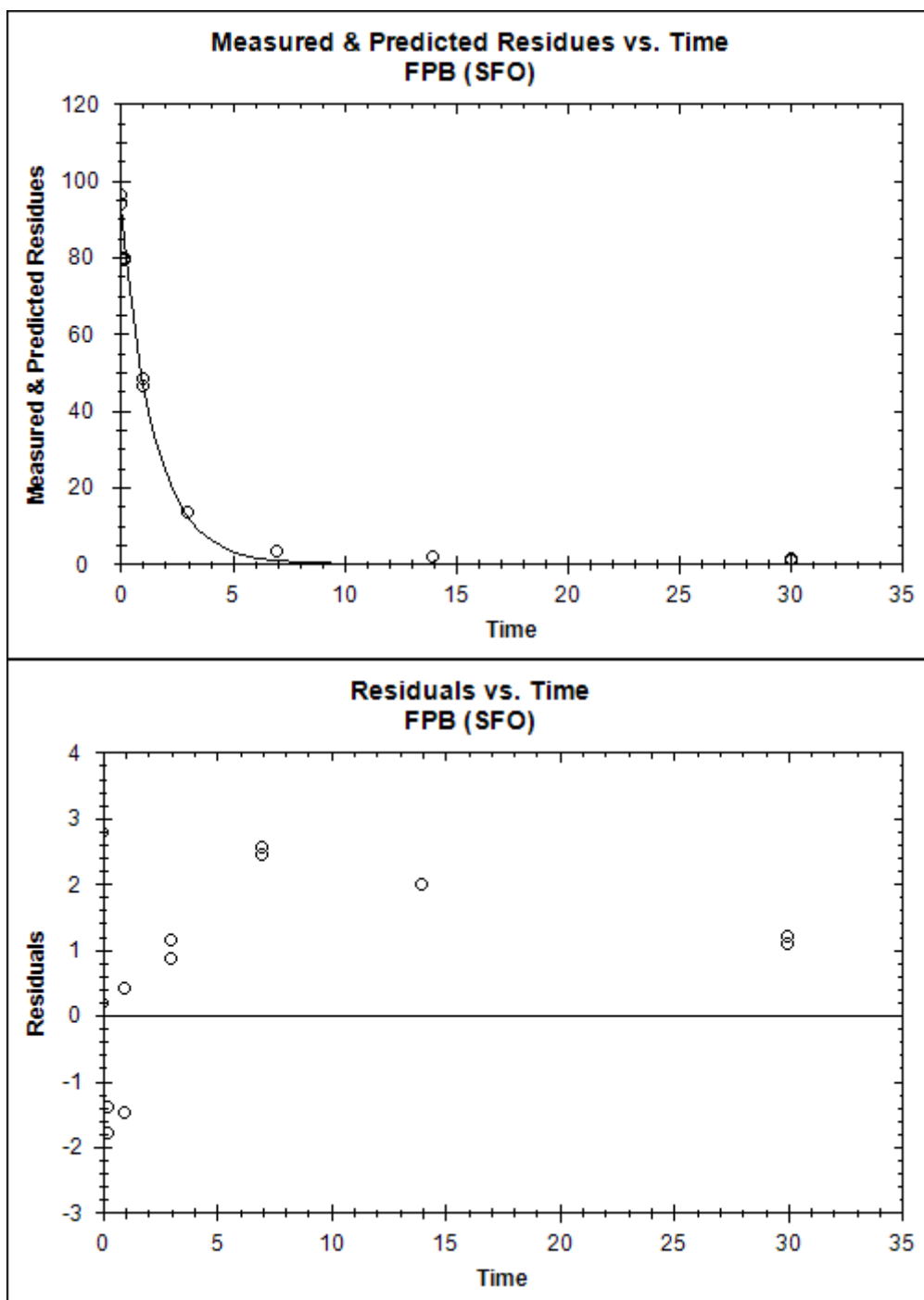
# -----
# DT50 and DT90 values
# -----

      DT50 :      1.0307
      DT90 :      3.4239
      Kinetic model :      SFO

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

      Compartment FPB
      time observed err-std predicted residual
0.0000  93.8000  1.7000  93.6110  0.1890
0.0000  96.4000  1.7000  93.6110  2.7890
0.2100  79.9000  1.7000  81.2818 -1.3818
0.2100  79.5000  1.7000  81.2818 -1.7818
1.0000  46.3000  1.7000  47.7819 -1.4819
1.0000  48.2000  1.7000  47.7819  0.4181
3.0000  13.6000  1.7000  12.4491  1.1509
3.0000  13.3000  1.7000  12.4491  0.8509
7.0000   3.3000  1.7000   0.8450  2.4550
```

7.0000	3.4000	1.7000	0.8450	2.5550
14.0000	2.0000	1.7000	0.0076	1.9924
14.0000	2.0000	1.7000	0.0076	1.9924
30.0000	1.1000	1.7000	0.0000	1.1000
30.0000	1.2000	1.7000	0.0000	1.2000



## 11.4.2 Höfchen am Hohenseh

### 11.4.2.1 SFO

```
# Trial           : Hoefchen
# File name      : Hoefchen IRLS SFO  FPB.r
# Target path    : C:\Emod\KinGUIII\WorkingDirectory\FPB\Hoefchen
# Created       : on 27 Oct 2013
#               : at 07:53
```

```

#                               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:FPB-acid
# # label: phenoxy
# # soil : Hdfchen
# # Hdfchen
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      99.3              0              Inf      False
k      FPB      :      0.1              0              Inf      False

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

      Chi2Err% :      3.689      3.689
      Kinetic model :      SFO

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

Degrees of Freedom : 12
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      101.03817      98.59463      103.482      1.24673      < 2e-16
k      FPB      :      0.80085      0.73639      0.865      0.03289      6.93e-12

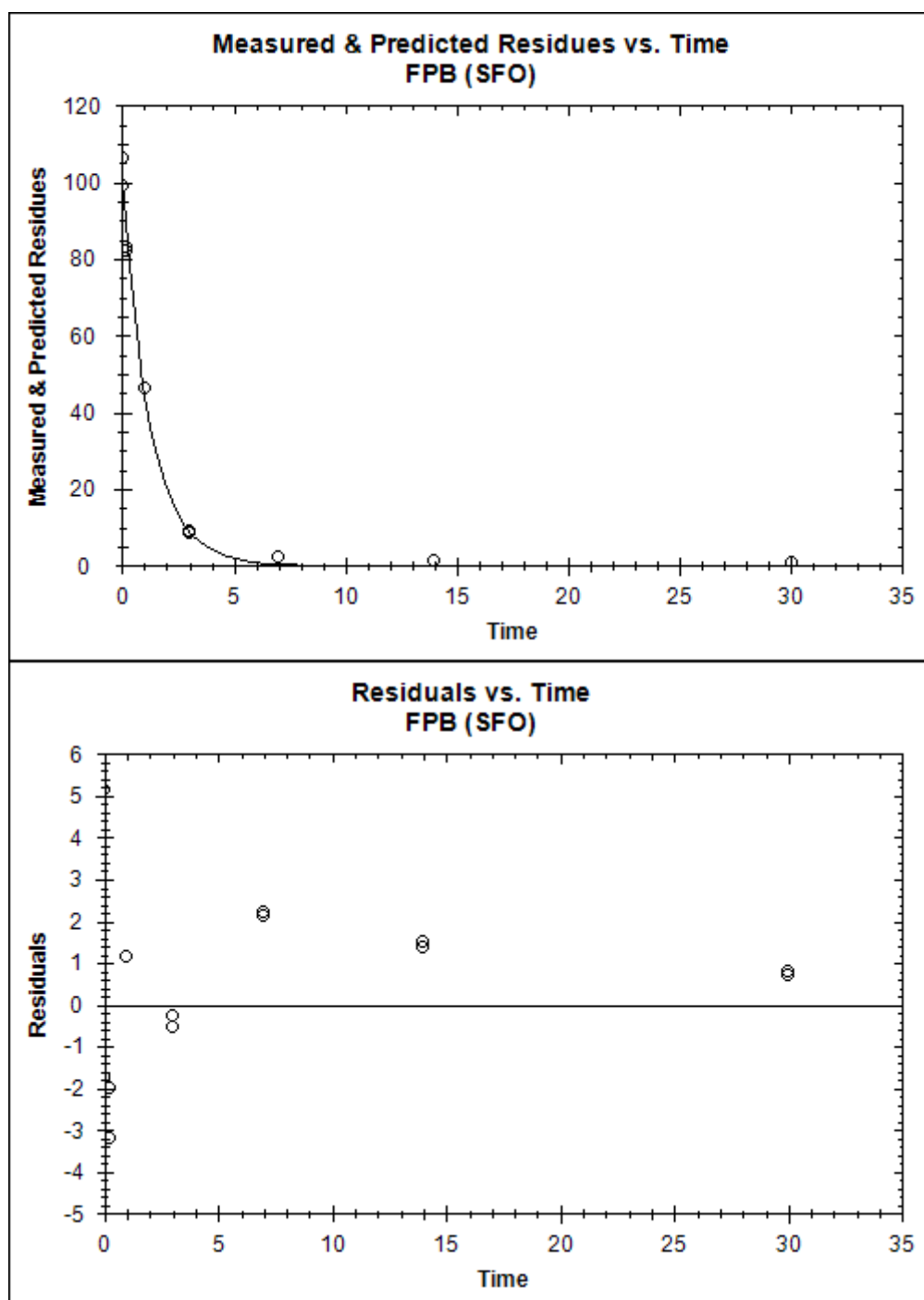
# -----
# DT50 and DT90 values
# -----

      DT50 :      0.8655
      DT90 :      2.8752
      Kinetic model :      SFO

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

      Compartment FPB
      time observed err-std predicted residual
0.0000  99.3000  2.0987  101.0382  -1.7382
0.0000  106.2000  2.0987  101.0382   5.1618
0.2100  82.2000  2.0987   85.3978  -3.1978
0.2100  83.4000  2.0987   85.3978  -1.9978
1.0000  46.5000  2.0987   45.3610   1.1390
1.0000  46.5000  2.0987   45.3610   1.1390
3.0000   8.6000  2.0987   9.1427  -0.5427
3.0000   8.9000  2.0987   9.1427  -0.2427
7.0000   2.6000  2.0987   0.3714   2.2286
7.0000   2.5000  2.0987   0.3714   2.1286
14.0000   1.4000  2.0987   0.0014   1.3986
14.0000   1.5000  2.0987   0.0014   1.4986
30.0000   0.8000  2.0987   0.0000   0.8000
30.0000   0.7000  2.0987   0.0000   0.7000

```



### 11.4.3 Dollendorf II

#### 11.4.3.1 SFO

```
# Trial : Dollendorf
# File name : Dollendorf IRLS SFO FPB.r
# Target path : C:\Emod\KinGUII\WorkingDirectory\FPB\Dollendorf
# Created : on 27 Oct 2013
# : at 07:48
# : 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:FPB-acid
# # label: phenoxy
# # soil : Dollendorf
# # Dollendorf
# #

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

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

      Initial Value      Lower Bound      Upper Bound      Fixed
M(0)  FPB      :      95.6              0              Inf      False
k      FPB      :      0.1              0              Inf      False

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

      Chi2Err% :      3.471      3.471
      Kinetic model :      SFO

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

Degrees of Freedom : 12
Parameter      Estimate      Lower CI      Upper CI      St.Dev      Prob > t
M(0)  FPB      :      95.4887      93.8007      97.18      0.8613      < 2e-16
k      FPB      :      0.7205      0.6809      0.76      0.0202      7.54e-14

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

      DT50 :      0.9620
      DT90 :      3.1957
      Kinetic model :      SFO

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

      Compartment FPB
      time observed err-std predicted residual
0.0000  95.6000  1.4947  95.4887  0.1113
0.0000  94.7000  1.4947  95.4887 -0.7887
0.2100  82.0000  1.4947  82.0803 -0.0803
0.2100  81.2000  1.4947  82.0803 -0.8803
1.0000  48.4000  1.4947  46.4548  1.9452
1.0000  49.0000  1.4947  46.4548  2.5452
3.0000  7.7000  1.4947  10.9948 -3.2948
3.0000  8.3000  1.4947  10.9948 -2.6948
7.0000  1.3000  1.4947  0.6159  0.6841
7.0000  1.2000  1.4947  0.6159  0.5841
14.0000  0.5000  1.4947  0.0040  0.4960
14.0000  0.5000  1.4947  0.0040  0.4960
30.0000  0.3000  1.4947  0.0000  0.3000
30.0000  0.3000  1.4947  0.0000  0.3000

```



