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DEGKINMANAGER 2.0

Calculation of rate constants for water sediment studies according to FOCUS degradation kinetics (Level II)

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Dr. Judith Klein

Dr. Michael Klein

Fraunhofer-Institut für Molekularbiologie und Angewandte Oekologie
in Schmallenberg

Content

1 Summary

The software DegKinManager version 2 (Degradation Kinetics Manager) is developed for the evaluation of water sediment studies at level II. The parent compound can be considered together with a transformation product. It calculates rate constants and DT50 or DegT50 values according to the recommendations of FOCUS Degradation Kinetics (FOCUS 2006/2014).

The software contains four predefined models:

1. Parent without metabolites
2. Parent with a single metabolite in water
3. Parent with a single metabolite in sediment
4. Parent with a single metabolite

These models are recommended for use as a first step to derive regulatory endpoints for parent compounds and metabolites in water-sediment studies (FOCUS 2006 and FOCUS 2014).

The equations represent simple approaches to describe mathematically the experimental data. However, they do not represent the actual chemical reactions.

The quality of the parameters are reported according to the recommendations of FOCUS degradation kinetics (e.g. chi²-test, t-test).

The fitting is done using the Nelder Mead Solver Class by Microsoft Solver Foundation, which is based on the method described in Nelder, J.A. and Mead, R., "A Simplex Method for Function Minimization", Computer Journal 7 (4): 308-313 (Jan., 1965) with the modifications described in Lee, D. and Wiswall, M., "A Parallel Implementation of the Simplex Function Minimization Routine".

We show the performance of DegKinManager 2.0 comparing the results obtained by ModelMaker 4.0.

It is not possible to compare the performance of DegKinManager 2.0 to the performance of the software KinGUI (Mikolasch and Schäfer, 2006) as KinGUI does not consider two phases. Thus, it is not possible using KinGUI to calibrate water-sediment studies on level P2 (FOCUS 2006).

It is not possible to compare the performance of DegKinManager 2.0 to the performance of the software CAKE (Tesella, https://showcase.tessella.com/products/cake/) as CAKE only considers the total system (sum of residues of parent in water and sediment).

This report and the program rely on

FOCUS (2006): "Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration" Report of the FOCUS Work Group on Degradation Kinetics, EC Document Reference Sanco/10058/2005 version 2.0, 434 pp

FOCUS (2014): "Generic guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration". Version 1.1. 18 December 2014

Klein M (2010) Calculation of rates constants according to FOCUS degradation kinetics using DegKinManager and ModelMaker. Project report of UBA project FKZ 360 03 048.

In contrast to Klein M (2010) this DegKinManager 2.0 does not rely on ModelMaker 4.0 and only considers models which differentiate between water and sediment residues (see also water sediment study, compare chapter 2.2 in Klein M (2010)).

2 Mathematical model description

In the following, all four predefined models are explained in detail:

1. Parent without metabolites
2. Parent with a single metabolite in water
3. Parent with a single metabolite in sediment
4. Parent with a single metabolite

The parent substance and the metabolites are defined as compartments. Dissipation processes (flows) are postulated between the compartments according to the proposed route of dissipation (FOCUS 2006).

FOCUS Surface Water modelling requires the use of SFO kinetics, hence we only consider SFO kinetics (single first order). Single first order is recommended by FOCUS 2006 as

1. it approximates the pattern of transfer between the water column and sediment,
2. it eliminates the need for knowledge of the spatial concentration gradients down through the sediment, and
3. it is relatively simple to implement.

The time for a decrease in the concentration by a certain percentage is constant throughout the experiment and independent of the initial concentration of the pesticide (FOCUS 2006).

Mathematically, all these four model variants consist of a linear differential equation system. Thus, all models can be solved analytically. In the following, we are going to describe and explain the underlying mathematical equations, parameters, and the analytical solution of all model variants in detail.

2.1 Parent without metabolites

The degradation of the parent compound in the two compartments follows the same equations as for single-phase models. However, in addition to degradation also distribution between the compartments has to be considered.

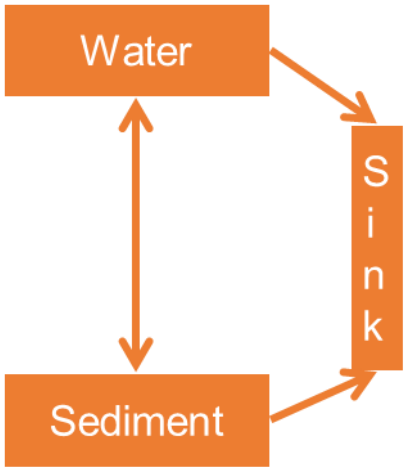

Figure 1: Scheme of the first model variant (parent without metabolites)

We obtain the following linear differential equations describing the change of residue in water and sediment in time:

$$\frac{d}{dt}M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$

$$\frac{d}{dt}M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$

$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$

This model coincides to the model given in BOX 10-2 (page 204) in FOCUS 2014.

In Table 1, an overview of the respecting parameters and their ranges can be seen. The initial residue in sediment is usually set constant equal to zero.

Table 1: Overview of the parameters for the first model variant including their domain and description

Parameters	Domain/Value	Description	Fit
k_{degsed}	$\mathbb{R}_+$	degradation rate in the sediment phase (time^{-1})	yes
k_{degwat}	$\mathbb{R}_+$	degradation rate in the water phase (time^{-1})	yes
k_{des}	$\mathbb{R}_+$	desorption rate (time^{-1})	yes
k_{sorp}	$\mathbb{R}_+\backslash\{0\}$	sorption rate (time^{-1})	yes
M_{sed_0}	$\mathbb{R}_+$	initial residue in the sediment phase (%)	no
M_{wat_0}	$\mathbb{R}_+$	initial residue in the water phase (%)	yes

The analytical solution of this linear differential equation system is described in section A.1.1.

2.2 Parent with a single metabolite in water

For the metabolite, two processes have to be considered: the formation by the parent compound (dependent on the parent degradation kinetics) and the metabolite's degradation. According to FOCUS (2006) only a single phase is considered for the metabolite. Therefore, sorption and desorption is not considered for transformation products.
The calculation of the formation of the metabolite is done according to the equation $k_{formwat} = k_{degwat} \cdot f_{wat}$.For formation fractions below one, parts of the parent compound are transformed into unknown metabolites or bound residues or mineralised. These processes are considered by a single "sink" compartment.

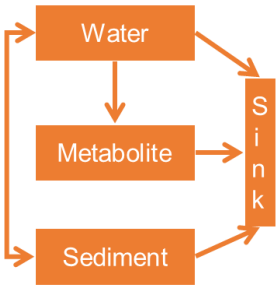

Figure 2: Scheme of the second model variant (parent with a single metabolite in water)

Mathematically, we consider three coupled linear differential equations describing the change of residue of parent in water in time, change of residue of parent in sediment in time and change of residue of the metabolite in water in time.

$$\frac{d}{dt}M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$

$$\frac{d}{dt}M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$

$$\frac{d}{dt}M_{met}(t) = k_{degwat} \cdot f_{wat} \cdot M_{wat}(t) - k_{degmet} \cdot M_{met}(t)$$

$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$
$$M_{met}(0) = M_{met_0} \in \mathbb{R}_+$$

In Table 2, all model parameters including domain and description are presented. In addition to the first model variant, we consider two additional model parameters: the degradation rate of the metabolite $k_{degmet} \in \mathbb{R}_+$and the formation fraction of the metabolite in water $f_{wat} \in [0,1]$.

Table 2: Overview of model parameters of the second model variant

Parameters	Domain/Value	Description	Fit
f_{wat}	$[0,1] \subset \mathbb{R}_+$	formation fraction of the metabolite in water (-)	no
k_{degmet}	$\mathbb{R}_+$	degradation rate of metabolite (time^{-1})	yes
k_{degsed}	$\mathbb{R}_+$	degradation rate in the sediment phase (time^{-1})	yes
k_{degwat}	$\mathbb{R}_+$	degradation rate in the water phase (time^{-1})	yes
k_{des}	$\mathbb{R}_+$	desorption rate (time^{-1})	yes
$k_{formwat}$	$\mathbb{R}_+$	formation rate of the metabolite (time^{-1})	no
k_{sorp}	$\mathbb{R}_+\backslash\{0\}$	sorption rate (time^{-1})	no
M_{met_0}	$\mathbb{R}_+$	initial residue of metabolite (%)	no
M_{sed_0}	$\mathbb{R}_+$	initial residue in the sediment phase (%)	no
M_{wat_0}	$\mathbb{R}_+$	initial residue in the water phase (%)	yes

The analytical solution of this linear differential equation system is described in section A.1.2.

2.3 Parent with a single metabolite in sediment

For the metabolite, two processes have to be considered, the formation by the parent compound (dependent on the parent degradation kinetics) and the metabolite's degradation which following first order kinetics (Figure 3). According to FOCUS (2006) only a single phase is considered for the metabolite. Therefore sorption and desorption are not considered for transformation products.
The calculation of the formation of the metabolite is done according to the equation $k_{formsed} = k_{degsed} \cdot f_{sed}$.
Figure 3 shows the scheme of the third model variant.

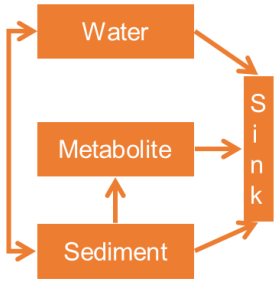

Figure 3: Scheme of the third model variant (parent with a single metabolite in sediment)

The model is similar to the second model variant. However, in this case the metabolite is formed in the sediment.

$$\frac{d}{dt}M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$
$$\frac{d}{dt}M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$
$$\frac{d}{dt}M_{met}(t) = k_{degsed} \cdot f_{sed} \cdot M_{sed}(t) - k_{degmet} \cdot M_{met}(t)$$

$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$
$$M_{met}(0) = M_{met_0} \in \mathbb{R}_+$$

The model parameters are presented in Table 3. In contrast to the second model variant, we consider now the formation fraction of the metabolite in sediment $f_{sed} \in [0,1]$.

Table 3: Overview of all model parameters concerning the third model variant

Parameters	Domain/Value	Description	Fit
f_{sed}	$[0,1] \subset \mathbb{R}_+$	formation fraction of the metabolite in sediment (-)	no
k_{degmet}	$\mathbb{R}_+$	degradation rate of metabolite (time^{-1})	yes
k_{degsed}	$\mathbb{R}_+$	degradation rate in the sediment phase (time^{-1})	yes
k_{degwat}	$\mathbb{R}_+$	degradation rate in the water phase (time^{-1})	yes
k_{des}	$\mathbb{R}_+$	desorption rate (time^{-1})	yes
$k_{formsed}$	$\mathbb{R}_+$	formation rate of the metabolite (time^{-1})	no
k_{sorp}	$\mathbb{R}_+ \backslash \{0\}$	sorption rate (time^{-1})	no
M_{met_0}	$\mathbb{R}_+$	initial residue of metabolite (%)	no
M_{sed_0}	$\mathbb{R}_+$	initial residue in the sediment phase (%)	no
M_{wat_0}	$\mathbb{R}_+$	initial residue in the water phase (%)	yes

The analytical solution of this linear differential equation system is described in section A.1.2A.1.3.

2.4 Parent with a single metabolite

For the metabolite two processes have to be considered, the formation by the parent compound (dependent on the parent degradation kinetics) and the metabolite's degradation which follows first order kinetics. According to FOCUS (2006) only a single phase is considered for the metabolite. Therefore sorption and desorption are not considered for transformation products.
The calculation of the formation of the metabolite is done according to $k_{formwat} = k_{degwat} \cdot f_{wat}$ and $k_{formsed} = k_{degsed} \cdot f_{sed}$.

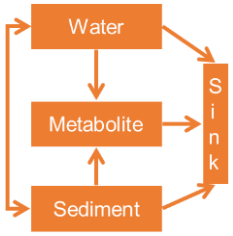

Figure 4: Scheme of the fourth model variant (parent with a single metabolite)

In Figure 4, a scheme of the fourth model variant can be seen. It is the combination of the second and third model variant. Again, we consider three linear differential equations describing the change of parent in water in time, change of parent in sediment in time as well as the change of metabolite in time which is formed in both, water and sediment.

$$\frac{d}{dt}M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$
$$\frac{d}{dt}M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$
$$\frac{d}{dt}M_{met}(t) = k_{degwat} \cdot f_{wat} \cdot M_{wat}(t) + k_{degsed} \cdot f_{sed} \cdot M_{sed}(t) - k_{degmet} \cdot M_{met}(t)$$
$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$
$$M_{met}(0) = M_{met_0} \in \mathbb{R}_+$$

An overview of all model parameters including their domain and description is given in Table 4.

Table 4: Overview of all model parameters of the fourth model variant

Parameters	Domain/Value	Description	Fit
f_{sed}	$[0,1] \subset \mathbb{R}_+$	formation fraction of the metabolite in sediment (-)	no
f_{wat}	$[0,1] \subset \mathbb{R}_+$	formation fraction of the metabolite in water (-)	no
k_{degmet}	$\mathbb{R}_+$	degradation rate of metabolite (time^{-1})	yes
k_{degsed}	$\mathbb{R}_+$	degradation rate in the sediment phase (time^{-1})	yes
k_{degwat}	$\mathbb{R}_+$	degradation rate in the water phase (time^{-1})	yes
k_{des}	$\mathbb{R}_+$	desorption rate (time^{-1})	yes
$k_{formsed}$	$\mathbb{R}_+$	formation rate of the metabolite (time^{-1})	no
$k_{formwat}$	$\mathbb{R}_+$	formation rate of the metabolite (time^{-1})	no
k_{sorp}	$\mathbb{R}_+ \backslash \{0\}$	sorption rate (time^{-1})	yes
M_{met_0}	$\mathbb{R}_+$	initial residue of metabolite (%)	no
M_{sed_0}	$\mathbb{R}_+$	initial residue in the sediment phase (%)	no
M_{wat_0}	$\mathbb{R}_+$	initial residue in the water phase (%)	yes

The analytical solution of this linear differential equation system is described in section A.1.4.

3 Parameter fitting

Considering all model variants, we have a two-dimensional or three-dimensional linear differential equation system. Due to its linearity, we can calculate the solutions of the system exactly with the help of the eigenvalues and corresponding eigenvector. The approach on how to solve the systems exactly is presented in more detail in section A.1 Description of analytical model solution. The resulting analytical solution function is nonlinear.

With help of measured experimental residues in water and sediment, we want to find suitable values for the model parameters. This procedure is also called calibration and can be done with nonlinear optimization algorithms comparing the model predictions and the experimental data with help of an objective function.

The best known objective function is least squares: the quadratic deviation of experimental data and model prediction. This means we want to find values such that the objective function value is as small as possible.

$$\min \sum_{i=1}^{n_{wat}} \left(M_{wat_i} - y_{wat}(t_i)\right)^2 + \sum_{i=1}^{n_{sed}} \left(M_{sed_i} - y_{sed}(t_i)\right)^2 + \sum_{i=1}^{n_{met}} \left(M_{met_i} - y_{met}(t_i)\right)^2$$

There exist several algorithms to solve above minimization problem. We decide between derivative-free (e.g. Nelder-Mead algorithm) and gradient-based methods (e.g. Gauß-Newton). Both approaches lead to local solutions.

In Table 5, all model variants with number of parameters and the respective parameters that have to be calibrated are presented. For the first model variant, we have in total 6 parameters, for the second and third 7 parameters and for the fourth 8 parameters.

Table 5: Overview of the number of model parameters and the parameters that need to be calibrated for all model variants

No	Model	Number of model parameters	Fit parameters
1	Parent without Metabolite	6	k_{degwat} , k_{sorp}, k_{degsed}, k_{des}, M_{wat_0} (M_{sed_0}fixed to 0)
2	Parent with Metabolite in Water	7	f_{wat}, k_{degwat} , k_{sorp}, k_{degsed}, k_{des}, M_{wat_0} ($M_{sed_0}$and M_{met_0}fixed to 0)
3	Parent with Metabolite in Sediment	7	f_{sed}, k_{degwat} , k_{sorp}, k_{degsed}, k_{des}, M_{wat_0} ($M_{sed_0}$and M_{met_0}fixed to 0)
4	Parent with Metabolite	8	f_{wat}, f_{sed}, k_{degwat} , k_{sorp}, k_{degsed}, k_{des}, M_{wat_0} ($M_{sed_0}$and M_{met_0}fixed to 0)

In general, we do not consider all parameters in optimization (over-parameterization of the system). In FOCUS 2006/2014, it is recommended to fix the initial residue in sediment M_{sed_0} (model variant 1-4) and the initial residue of metabolite M_{met_0} (model variant 2-4).

3.1 Data requirements

For the parameterization of the model experimental data is needed. For the first model, parent without metabolite, data on the parent residue in water column and sediment is needed (in %).

In addition for the other models, we need data of the metabolite (%) either in water (model 2, parent with metabolite in water), or in sediment (model 3, parent with metabolite in sediment) or the combined residue of the metabolite in water and sediment (model 3, parent with metabolite).

General recommendations by FOCUS 2006/FOCUS 2014:

- Data quality: The number of data points must be appreciably larger than the number of parameters.
- Replicates: Use true replicates individually in the optimisation.
- Weighting: Initial fit without weights
- Values <LOQ and <LOD: Parent, <LOD set to zero, samples between LOD or LOQ set to measured value or to 0.5 (LOD+LOQ)
- Outliers: include all data points initially
- Time zero concentration: include in optimization initially.

Data taken according to OECD guideline 307 consists at least of six samples. According to SETAC 1995, data is based at least of eight data points.

Guidance for water sediment studies is, for example, provided by OECD (in Test Guideline No. 308) and SETAC (1995). Both state that a minimum of 6 sampling points should be included.

In accordance with the EC Guidance Document on Persistence in Soil (DG VI - 9188/VI/97 - Rev 8 of 12.07.2000), number of data points should not be smaller than five.

FOCUS 2006 replicate values are used individually for each sampling interval. The degradation model is then fitted to all individual data points at the same time.

Suggested weights by FOCUS 2006 are related to the observed value $\frac{1}{o^2}$, $\frac{1}{o}$ or to the measured variance $\frac{1}{\sigma}$.

All samples after the first non-detect (< LOD) should be omitted unless positive detections above LOQ are made later in the experiment.

3.2 Initial values

Parameter fitting is nothing else than solving a nonlinear optimization problem. Due to the non-linearity of the problem it is possible that there are several combinations of parameters leading in a similar objective function value (local optima). However, we are interested in a single combination of parameters that results in the smallest possible value for the merit function (global optimum). Therefore were are repeating the fitting procedure several times and take the best solution (minimal objective function value).

Here, we present an idea on how to get suitable initial values. We suggest to fit the single linear differential equations separately. The resulting parameter values are used as initial values for the fit of the total system.

FOCUS 2006 (p.79)/ 2014 (p.82) recommends the following on the choice of initial values:

- Set M_{wat_0} equal to the measured value of parent in water at time point zero (as it is expected to be closed to the measured initial concentration)
- Degradation rate constant of parent in sediment ln(2)/measured interpolated time until 50% of the initial concentration has disappeared
- Degradation rate constant of metabolite and the formation of metabolite can be calculated from the degradation rate of parent, the time to maximum formation of the metabolite and the maximum amount formed in study

Table 6: Suggestions for initial values

No	Model	Ordinary Differential Equation	Analytical Solution	Parameters
1	Parent without metabolites	$\frac{d}{dt}M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t)$ $\frac{d}{dt}M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t)$	$M_{wat}(t) = M_{wat_0} \cdot \exp\left(\left(-k_{degwat} - k_{sorp}\right) \cdot t\right)$ $M_{sed}(t) = M_{sed_0} \cdot \exp\left(\left(-k_{degsed} - k_{des}\right) \cdot t\right)$	k_{degwat}, k_{sorp}, M_{wat_0} k_{degsed}, k_{des}, M_{sed_0}
2	Parent with a single metabolite (Water)	$\frac{d}{dt}M_{met}(t) = f_{wat} - k_{degmet} \cdot M_{met}(t)$	$M_{met}(t) = \frac{f_{wat}}{k_{degmet}} + \left(M_{met_0} - \frac{f_{wat}}{k_{degmet}}\right) \cdot \exp\left(-k_{degmet} \cdot t\right)$	f_{wat}, k_{degmet}, M_{met_0}
3	Parent with a single metabolite (Sediment)	$\frac{d}{dt}M_{met}(t) = f_{sed} - k_{degmet} \cdot M_{met}(t)$	$M_{met}(t) = \frac{f_{sed}}{k_{degmet}} + \left(M_{met_0} - \frac{f_{sed}}{k_{degmet}}\right) \cdot \exp\left(-k_{degmet} \cdot t\right)$	f_{sed}, k_{degmet}, M_{met_0}
4	Parent with a single metabolite	$\frac{d}{dt}M_{met}(t) = (f_{wat} + f_{sed}) - k_{degmet} \cdot M_{met}(t)$	$M_{met}(t) = \frac{f_{wat}}{k_{degmet}} + \frac{f_{sed}}{k_{degmet}} + \left(M_{met_0} - \frac{f_{wat}}{k_{degmet}} - \frac{f_{sed}}{k_{degmet}}\right) \cdot \exp\left(-k_{degmet} \cdot t\right)$	f_{sed}, f_{wat}, k_{degmet}, M_{met_0}

3.3 Solver

As objective function we minimize the sum of squares (quadratic deviation between observed and predicted data). The optimization problem is non-linear, as objective function is quadratic and constraints are non-linear (composition of exponential functions).

As solver, the DegKinManager 2.0 uses the NelderMeadSolver Class by Microsoft Solver Foundation. The solver is suitable to find a local minimum or maximum for a box-constrained nonlinear function.

The implementation is based on the method described in Nelder, J.A. and Mead, R., "A Simplex Method for Function Minimization", Computer Journal 7 (4): 308-313 (Jan., 1965) with the modifications described in Lee, D. and Wiswall, M., "A Parallel Implementation of the Simplex Function Minimization Routine".

4 Evaluation

The program DegKinManager 2.0 provides a statistical and visual evaluation of the output data. Visual assessment is the main tool for assessing goodness of fit (FOCUS 2006). The following criteria are recommended for a standard assessment by FOCUS 2006 to give additional information.

Procedure (following FOCUS 2006/2014)

1. Check the visual result
2. Avoid over-parametrization
3. Use realistic initial values
4. Constrain parameter ranges
5. Carry out stepwise fitting if necessary

The χ^2 statistics shall be used to assess the quality of the fit and the t-test shall be used to evaluate the confidence in the parameter estimates (FOCUS 2006).

4.1 Visual assessment

According to FOCUS 2006/2014, measured and fitted data must always be presented graphically. It is suggested to plot measured concentrations and the calculated curve versus time. Furthermore, for revealing patterns of over- or under-predictions, a second plot should be made of the residuals (predicted values minus observed values). Optionally and not required for a standard assessment, a plot of measured versus calculated values can be presented. If transformed data is used, also the residuals shall be calculated based on the transformed data.

4.2 Statistical assessment

For the statistical assessment of goodness of fit, we present several criteria. In general, the statistical calculation can be done for the total data set, and separately for the single compartments. For the calculation of the degree of freedom for the χ^2statistics for the single compartments we consider the following maximal number of model parameters (Table 7).

Table 7: Number of parameters for each compartment and all model variants

No	Model	Water	Sediment	Metabolite	Model parameter
1	Parent without Met.	3	3	0	6
2	Parent with Met. (Water)	3	3	3	9
3	Parent with Met. (Sediment)	3	3	3	9
4	Parent with Met.	3	3	4	10

According to FOCUS 2006, the goodness of fit should be performed for each compartment separately. Thus, only the parameters specific to that compartment are considered in the χ^2calculation. The χ^2statistics should be calculated using all data within a compartment used in the fit. Furthermore, the error value should be below 15% and the fit must be visually acceptable (FOCUS 2006).

Thus considering the compartments separately and following the recommendations of fixing the initial residue in sediment and the initial residue for the metabolite in optimization, we have 3 active parameters for water (model variant 1-4), 2 active parameters for sediment (model variant 1-4) and 2 active parameters (model variant 2-3) respectively 3 active parameters for the metabolite (model variant 4).

Note: in Table 7 the maximal possible number of parameters for each model variant is given, in case all parameters are variable in optimization.

However the statistical assessment is a guidance and not absolute cut-off criterion (FOCUS 2006). Please find in Table 8, an overview of the applied statistical measurements.

Let $N \in \mathbb{N}$ be the total number of data, $O \in \mathbb{R}_+^N$ the experimental observation and $C \in \mathbb{R}_+^N$ the corresponding calculated model prediction. The means of the data are represented by $\bar{O} \in \mathbb{R}_+^N$ respectively $\bar{C} \in \mathbb{R}_+^N$.

Table 8: Statistical measurements to compare the correspondence of model prediction and experimental data

Statistics	Formula
Model error	The number $m \in \mathbb{N}$ denotes the degrees of freedom (number of measurements minus number of model parameters) and let be $\alpha \in (0,1)$. Let χ^2_{tab} be the tabulated $\chi^2_{m,\alpha}$. Usually a value of $\alpha = 0.05$ is chosen. $$\epsilon = 100 \cdot \frac{1}{\bar{O}} \cdot \sqrt{\frac{1}{\chi^2_{\text{tab}}} \cdot \sum_{i=1}^{N} (C_i - O_i)^2}$$
Coefficient of Determination	$$r^2 = \left(\frac{\sum_{i=1}^{N} (O_i - \bar{O})(C_i - \bar{C})}{\sqrt{\sum_{i=1}^{N} (O_i - \bar{O})^2 \cdot \sum_{i=1}^{N} (C_i - \bar{C})^2}} \right)^2$$
Model efficiency	$$EF = 1 - \frac{\sum_{i=1}^{N} (C_i - O_i)^2}{\sum_{i=1}^{N} (O_i - \bar{O})^2}$$
Absolute Residuals	$$AR = \sum_{i=1}^{N} \lvert C_i - O_i \rvert$$
Squared Residuals	$$SR = \sum_{i=1}^{N} (C_i - O_i)^2$$
Scaled Root Mean Squared Error	$$SRMSE = \frac{1}{\bar{O}} \sqrt{\frac{1}{N} \sum_{i=1}^{N} (C_i - O_i)^2}$$
Scaled Total Error	$$STE = \frac{\sum_{i=1}^{N} \lvert C_i - O_i \rvert}{\sum_{i=1}^{N} O_i}$$

For the t-test (single-sided) a significance level of 10 percent ($p < 0.1$) is considered appropriate (FOCUS 2006). For the calculation of t-test, we need to calculate the standard error of the single parameters first.

Calculation of standard error of the single parameters

The standard error of a parameter p_i is the ith diagonal entry of the covariance-variance matrix. The covariance-variance matrix is the inverse of the Hessian containing the second derivative of the least square

objective with respect to the parameters. The Hessian can be calculated approximately by the Jacobian (J, derivatives first order): and mean squared error (MSE)

$$H \approx (J^T \cdot J)^{-1} \cdot MSE$$

The Hessian is also called covariance-variance matrix. Our estimation is done equivalently as in Matlab (http://de.mathworks.com/help/stats/nlinfit.html#btk7ign-3).

In general, t-test can be carried out to assess whether a parameter differs from zero at the chosen significance level. A parameter value that is not significantly different from zero is uncertain due to the variability in data or the model is not adequate (FOCUS 2006).

If the parameters are normally distributed, then

$$t = \frac{\hat{a_i}}{\sigma_i}$$

is t-distributed.
$\hat{a}_i$estimate of parameter i
$\sigma_i$standard error of parameter i

The probability (p-value) corresponding to the calculated t-value is read from statistical tables or calculated with Excel (TDIST) or statistical packages (single-sided; degrees of freedom equals the number of observations minus the total number of estimated model parameters).

FOCUS2006: "Note that to calculate the t-test for the individual parameter, the total degrees of freedom are used, which depend on the total number of parameters estimated in the fit, as opposed to the compartment parameters only as used for the Chi square calculation."

The number of observations includes replicates. The parameter is considered significantly different from zero if the probability is smaller than 0.1, i.e. considering a 10 percent significance level for water-sediment studies.

If the probability is between 0.05 and 0.1, the parameter may still be considered acceptable. Significance levels above 10 percent are not considered acceptable.

4.3 Regulatory endpoints

Regulatory endpoints for parent compounds and metabolites include DT50 and DT90 values (FOCUS 2006/2014). These values are used as triggers for higher-tier experiments e.g. fish life cycle test is required when DT90 in water or sediment is greater than 100 days (Annex II to Dir. 91/414/EEC).

Calculation of degradation time (FOCUS 2006, p. 51, Box 5-1/ FOCUS 2014, p. 54, Box 5-1):

$$DT_x = \frac{\ln\left(\frac{100}{100 - x}\right)}{k_{deg}}$$

$$DT_{50} = \frac{\ln(2)}{k_{deg}} \text{ and } \quad DT_{90} = \frac{\ln(10)}{k_{deg}}.$$

5 Working with DegKinManager 2.0

5.1 Installing DegKinManager 2.0

The program DegKinManager 2.0 is currently available at the software website of the Fraunhofer Institute for Molecular Biology and Applied Ecology IME. Permanently, the program and associated material is linked to the download area http://software.ime.fraunhofer.de/DegKinManager/.

Please download the installer "DegKin_setup_xxxxxxxx.exe" and follow the instructions. After installing DegKinManager successfully, the start form of the program appears.

5.2 DegKinManager 2.0

Procedure:

1. Select a model
   a. Parent without metabolites
   b. Parent with a single metabolite in water
   c. Parent with a single metabolite in sediment
   d. Parent with a single metabolite
2. Enter experimental data
3. Select settings for each parameter value (initial value, lower bound, upper bound)
   It is often useful to let the system propose reasonable initial parameters
4. Start the optimisation
5. Assess the quality of the results (statistical and graphical evaluation)

By starting the program DegKinManager 2.0, a start screen appears (Figure 5). Clicking at start the proper program is started.

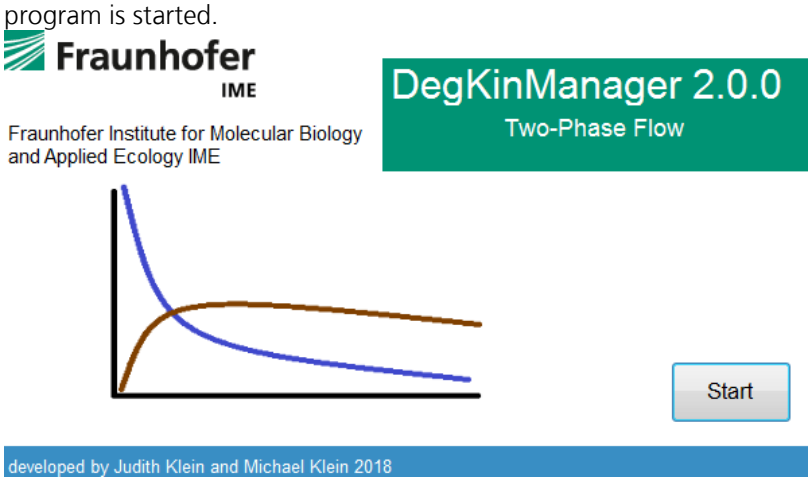

Figure 5: Start screen of the program DegKinManager 2.0

In the main form the user has to decide on the type of optimisation:

1. Parent without metabolites
2. Parent with a single metabolite in water
3. Parent with a single metabolite in sediment
4. Parent with a single metabolite

The model variants are presented graphically (Figure 6).

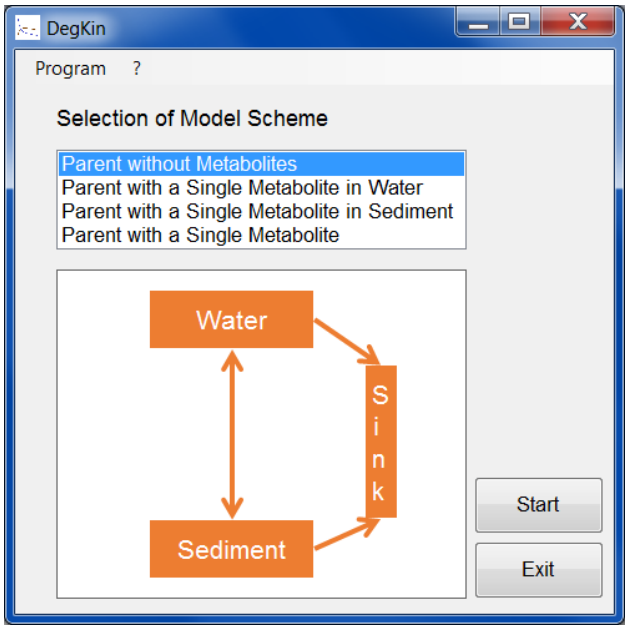

Figure 6: Main form of the DegKinManager 2.0

Clicking at "Start" opens the experimental data (tab page "Environmental Residues") form where the user has to enter the experimental data on residues as well as information on the parameters (tab page "Parameters")

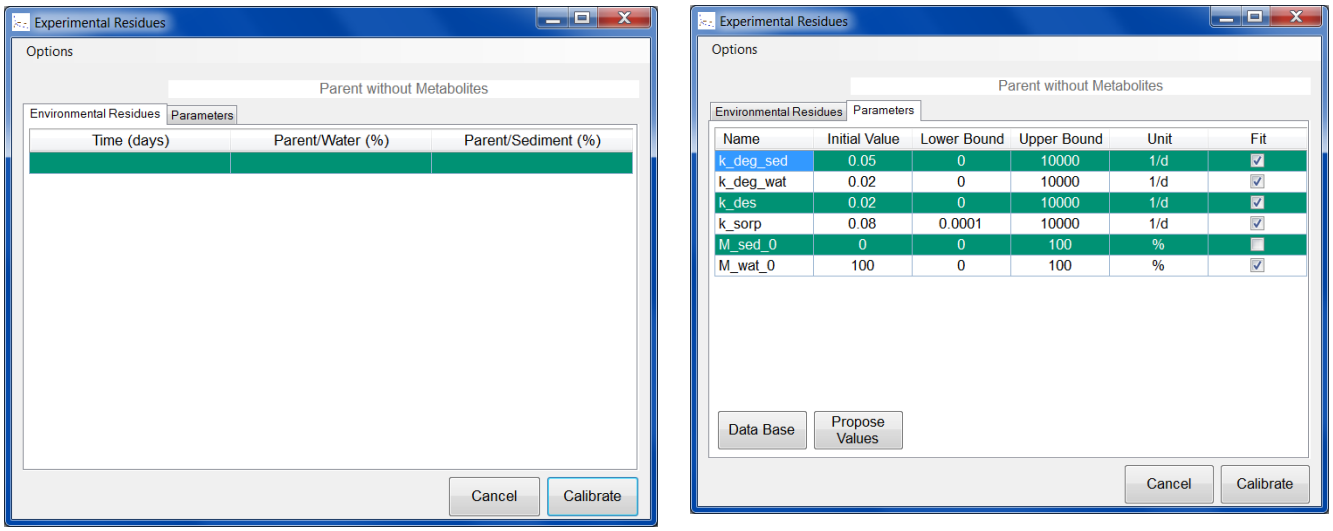

Figure 7: Experimental residues form

Experimental data (Figure 8) can be entered manually or by copy paste (CTRL-C,CTRL-V) from EXCEL. Fitting is only possible if experimental data is entered.

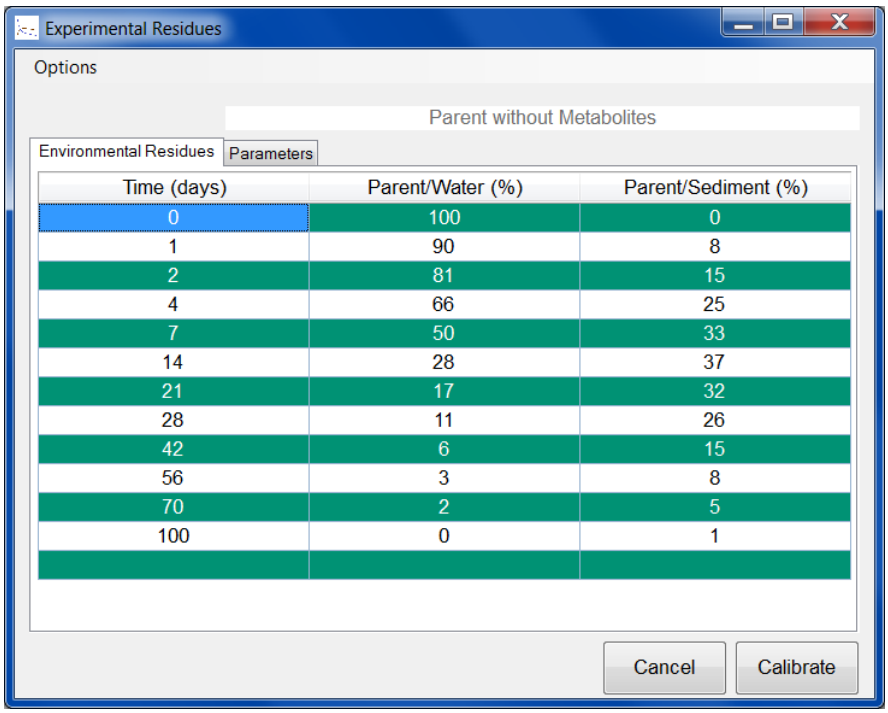

Figure 8: Experimental data in environmental residues tab page

With respect to the model parameters, the user can decide on the initial values (or click at propose values or choose values from data base), on the lower and upper bound of model parameters. Additionally, the user can decide which parameter should be considered in the fitting routine. This enables the user to fit model parameters separately. It is often useful to let the system propose reasonable initial parameters.

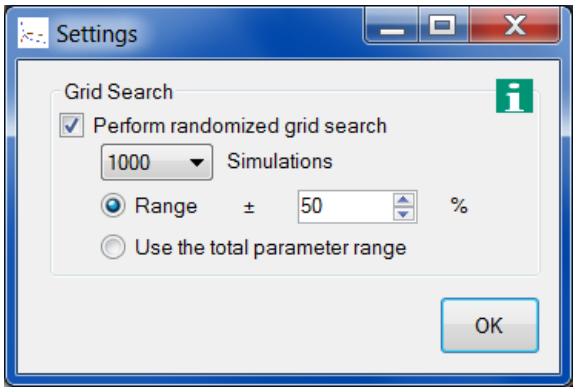

Figure 9: Settings of solver

By clicking at "Options", it is possible to change the settings of the used solver (Figure 9), namely if the optimization routine of finding the initial values as well as the proper optimization routine should be performed several times.
Fitting is solving a nonlinear optimization problem. Repeating the procedure several times could lead to a better optimum (grid search). The user can specify the number of simulation as well as the range of initial values of parameters. The initial values are generated uniformly distributed in the chosen range.

Experimental data: Sampling points below LOD or LOQ that are included as ½ LOD or ½ (LOQ+LOD).
Experimental data should be handled in terms of mass or equivalent, e.g. % applied radioactivity, remaining in each compartment.

Due to its non-linearity various initial values lead to different local optima. To increase the possibility of finding the best parameter values, it is possible to perform a grid search. The grid search is based on Monte-Carlo simulations. Instead of solving the non-linear optimization problem only one time, the routine is repeated several times using in each simulation random pseudo numbers similar to the initial values (in Figure 9, 1000 simulations). The higher the number of simulations, the higher the possibility to find a suitable parameters. However an increasing number of simulations, also increases the calculation time. The (pseudo-) random numbers follow a uniform distribution. The user can specify a percentage range or the respective total parameter range (lower bound, upper bound) given in the parameter data table is used.

The result of the optimization is represented as

1. Calibration Chart (Figure 10): Visual representation of the change of residue of parent in water and sediment in time (and for model variant 2-4 the metabolite)
2. Predicted-Measured Chart (Figure 11): Plot of predicted and measured data
3. Residual Chart (Figure 12): Relationship between predicted data and residual (predicted minus observed values)
4. Report (Figure 13): Text file containing experimental input data, model parameters (initial value, lower bound, and upper bound), result of optimization, and the equations representing the analytical solution functions, evaluation (DT50 and DT90 of degradation rates), statistical assessment of all data and all compartments separately.

The program enables the user to save, copy into clipboard and print the results by clicking at the menu items “Save”, “Save All”, “Print” and “Copy”.

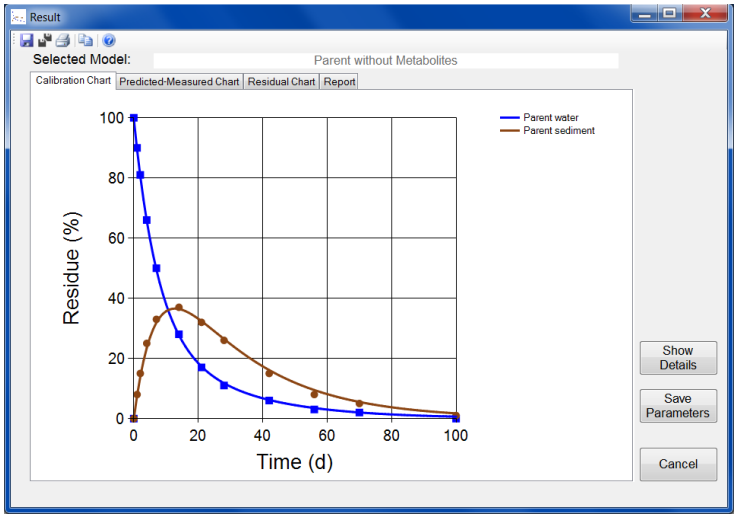

Figure 10: Graphical result of fitting, change of residue (%) in time

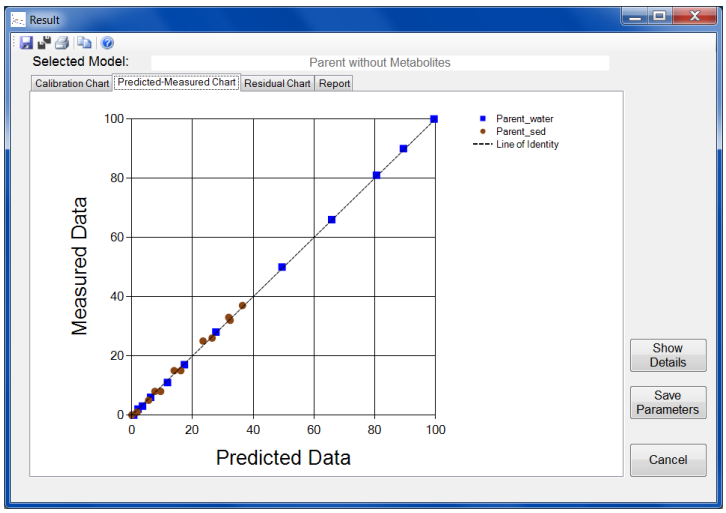

Figure 11: Predicted data versus measured data

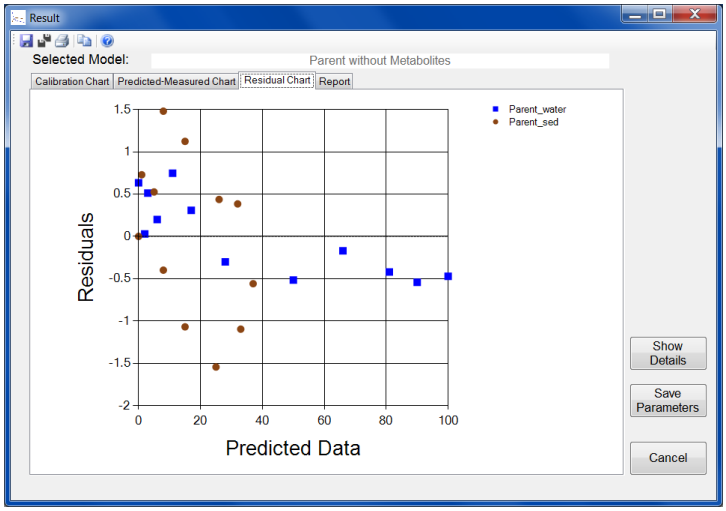

Figure 12: Predicted data versus residuals (predicted minus observed data)

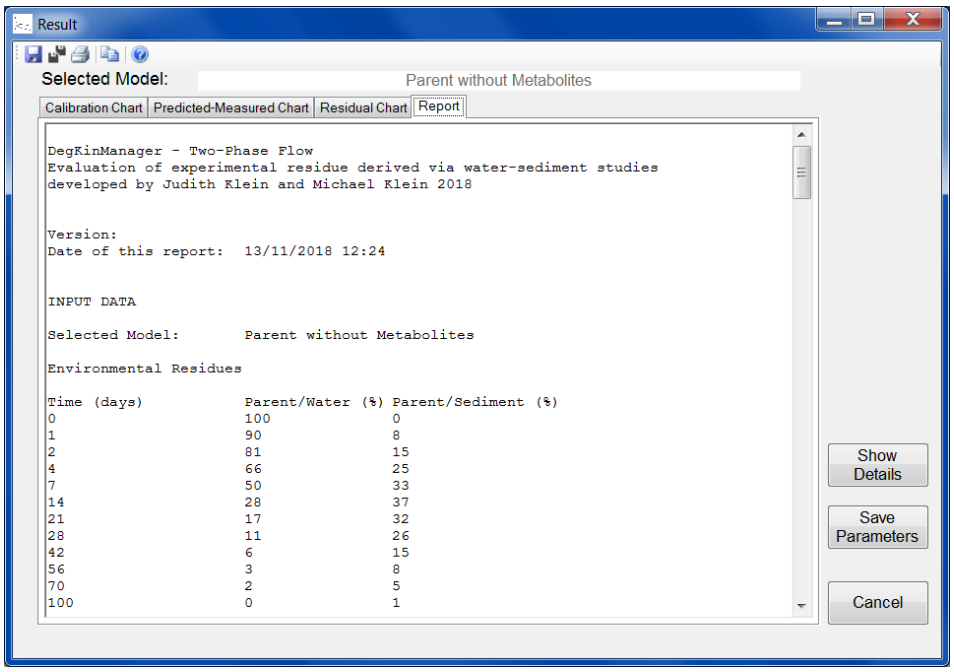

Figure 13: Text report file

By clicking at the button "Calibration Details", the program provides more information on the single run (Figure 14).
Furthermore, it is possible to save the parameter values in a local data base on your computer.

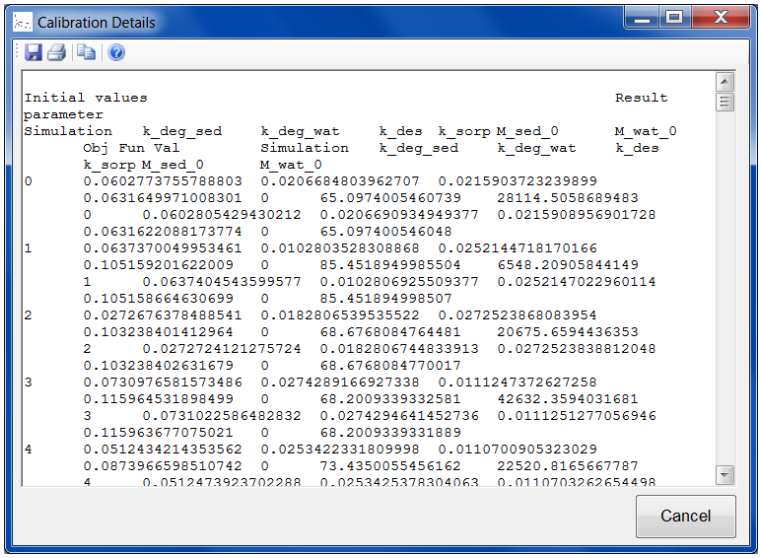

Figure 14: Fitting details

6 Plausibility check of analytical solution of DegKinManager 2.0

In contrast to DegKinManager 1.0/ ModelMaker 4.0 in DegKinManager 2.0 the differential equation system representing the single models are solved analytically and thus they are solved exactly. We compare the results of discretized solution (EXCEL) and the analytical results obtained by DegKinManager 2.0. Therefore we create hypothetical data in EXCEL which is then used for validating the analytical solution. For this, all parameters are kept constant.

6.1 Input data

The test data set is obtained by solving each model variant stepwise using Euler method with step size 1. We use the same parameter data set given for water sediment study in Klein (2010) in chapter 4.3. Experimental residues can be seen in Table 10.

Table 9: True parameter values used for generating the hypothetical data sets

Parameter name	True values			
	No formation	Formation in water	Formation in sediment	Formation in water and sediment
f_sed (-)	-	-	0.8	0.8
f_wat (-)	-	0.2	-	0.2
k_deg_met(time^{-1})	-	0.01	0.01	0.01
k_deg_sed (time^{-1})	0.05	0.05	0.05	0.05
k_deg_wat (time^{-1})	0.02	0.02	0.02	0.02
k_des (time^{-1})	0.02	0.02	0.02	0.02
k_sorp (time^{-1})	0.08	0.08	0.08	0.08
M_wat_0 (%)	100	100	100	100

6.2 Calculation result

Figure 15 to Figure 18 show the calculation result for each model variant of DegKinManager 2.0. As visual assessment, we consider the change of residues in time as well as a residual plot between analytical solution (predicted data) and approximate solution (measured data) for each model variant.

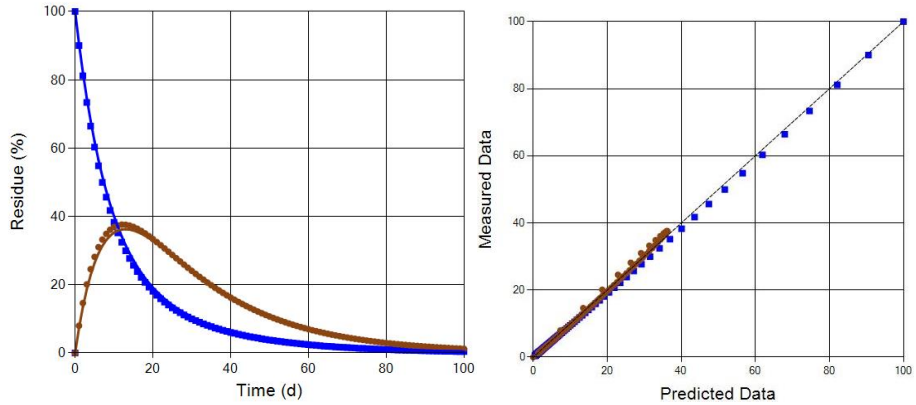

Figure 15: Model variant 1: Parent without metabolites. Change of residues in time as well as a plot showing analytical data (predicted data) versus approximate data (measured data): Residue of parent in water (blue) and residue of parent in sediment (brown).

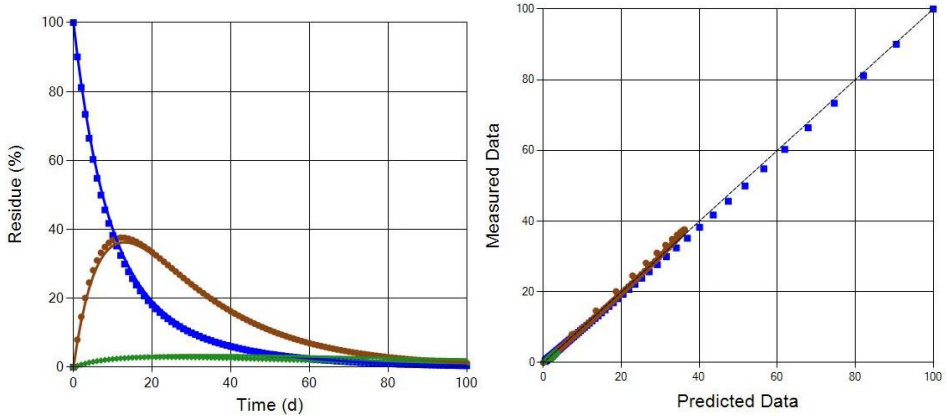

Figure 16: Model variant 2: Parent with a single metabolite in water. Change of residues in time as well as a plot showing analytical data (predicted data) versus approximate data (measured data): Residue of parent in water (blue), residue of parent in sediment (brown), residue of metabolite (green).

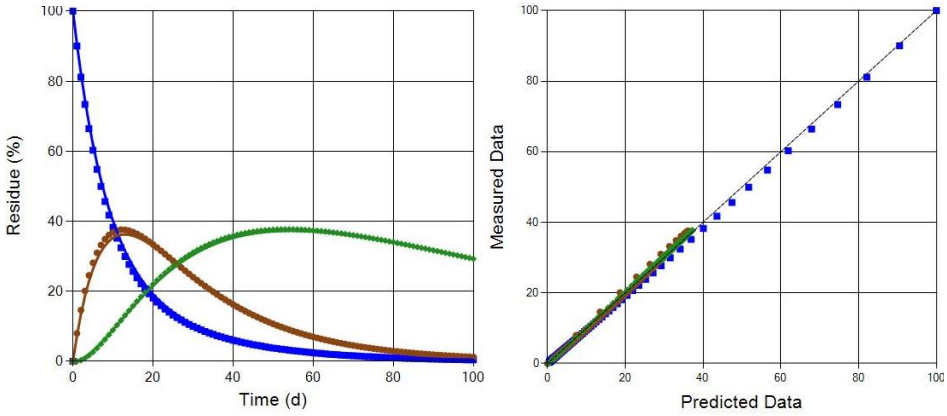

Figure 17: Model variant 3: Parent with a single metabolite in sediment. Change of residues in time as well as a plot showing analytical data (predicted data) versus approximate data (measured data): Residue of parent in water (blue), residue of parent in sediment (brown), residue of metabolite (green).

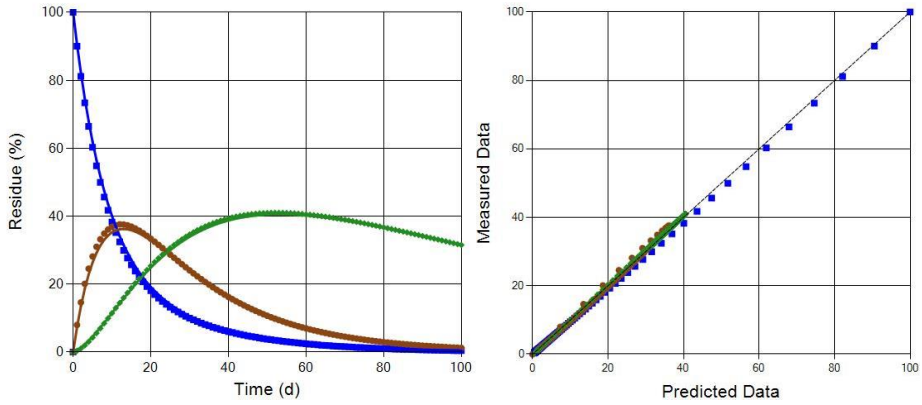

Figure 18: Model variant 4: Parent with a single metabolite. Change of residues in time as well as a plot showing analytical data (predicted data) versus approximate data (measured data): Residue of parent in water (blue), residue of parent in sediment (brown), residue of metabolite (green).

The figures (Figure 15-Figure 18) show a good correspondence between approximate and analytical solution. Using for the discretization a smaller step size than 1 would further decrease the deviation of approximate and analytical solution.

7 Result of test simulations using DegKinManager 2.0

The aim of this chapter is to show the performance of the software DegKinManager 2.0. For testing, we use hypothetical test data set and chosen initial values. Furthermore we compare the performance of DegKinManager 2.0 to the performance of DegKinManager 1.0 which was based on ModelMaker 4.0 (shell). It is not possible to review the results with KinGUI as it is not possible to model both compartments, water and sediment, separately.
Again, we test all four predefined models separately:

1. Parent without metabolites
2. Parent with a single metabolite in water
3. Parent with a single metabolite in sediment
4. Parent with a single metabolite

We prove the plausibility of the result of DegKinManager 2.0 similarly as in Klein (2010). Namely, by assessing the goodness of fit by visual as well as statistical assessment. In addition to that, we compare the regulatory endpoints of DegT50 and DegT90 "true" and fitted values.

7.1 Input data

As test data set, we use the similar data set used in Klein (2010) in chapter 4.3. Experimental residues can be seen in Table 10, which correspond to the Table 11 in Klein (2010).

Table 10: Experimental residues (hypothetical test data set)

Model variant	1 - 4	1 - 4	2	3	4
Time (d)	Parent water (%)	Parent sediment (%)	Metabolite (%)	Metabolite (%)	Metabolite (%)
0	100	0	0	0	0
1	90	8	0	0	0
2	81	15	1	0	1
4	66	25	1	2	3
7	50	33	2	5	7
14	28	37	3	14	17
21	17	32	3	22	27
28	11	26	4	28	33
42	6	15	4	35	40
56	3	8	4	36	41
70	2	5	3	34	39
100	0	1	3	28	32

The data is hypothetical test data set to check the fitting routine which was obtained by using the parameter values given in Table 11.

Table 11: True parameter values used for generating the hypothetical data sets

Parameter name	"True values"			
	No formation	Formation in water	Formation in sediment	Formation in water and sediment
f_sed (-)	-	-	0.8	0.8
f_wat (-)	-	0.2	-	0.2
k_deg_met(time^{-1})	-	0.01	0.01	0.01
k_deg_sed (time^{-1})	0.05	0.05	0.05	0.05
k_deg_wat (time^{-1})	0.02	0.02	0.02	0.02
k_des (time^{-1})	0.02	0.02	0.02	0.02
k_sorp (time^{-1})	0.08	0.08	0.08	0.08
M_wat_0 (%)	100	100	100	100

The initial parameter setting are presented in Table 12. For all model variants the same lower and upper bounds are used (Table 13).

Table 12: Initial parameter setting for DegKinManager 2.0 and ModelMaker 4.0 in optimization

Parameter name	Initial values			
	No formation	Formation in water	Formation in sediment	Formation in water and sediment
f_sed (-)	-	-	0.5	0.5
f_wat (-)	-	0.5	-	0.5
k_deg_met(time^{-1})	-	0.001	0.001	0.001
k_deg_sed (time^{-1})	0.01	0.01	0.01	0.01
k_deg_wat (time^{-1})	0.01	0.01	0.01	0.01
k_des (time^{-1})	0.5	0.5	0.5	0.5
k_sorp (time^{-1})	0.5	0.5	0.5	0.5
M_wat_0 (%)	100	100	100	100

Table 13: Lower and upper bounds of model parameters used in optimization for DegKinManager 2.0 as well as ModelMaker 4.0

Name	Lower Bound	Upper Bound
f_sed (-)	0	1
f_wat (-)	0	1
k_deg_met(time^{-1})	0	10000
k_deg_sed (time^{-1})	0	10000
k_deg_wat (time^{-1})	0	10000
k_des (time^{-1})	0	10000
k_sorp (time^{-1})	0.0001	10000
M_met_0 (%)	0	10000
M_sed_0 (%)	0	10000
M_wat_0 (%)	0	10000

7.2 Optimization results

The main results of the optimization are presented in Table 14 (parent, model variant 1-4) and Table 16 (metabolite, model variant 2-4). The output file of the DegKinManager 2.0 is documented in section A.4.

Table 14: Optimization result - actual parameter values as well as result obtained for each model variant

Parameter name	Actual values*	Result values			
		No formation	Formation in water	Formation in sediment	Formation in water and sediment
f_sed (-)	0.8	-	-	0.762	0.823
f_wat (-)	0.2	-	0.213	-	0.104
k_deg_met(time^{-1})	0.01	-	0.008	0.01	0.01
k_deg_sed (time^{-1})	0.05	0.051	0.052	0.052	0.051
k_deg_wat (time^{-1})	0.02	0.019	0.019	0.019	0.019
k_des (time^{-1})	0.02	0.024	0.032	0.032	0.024
k_sorp (time^{-1})	0.08	0.088	0.088	0.087	0.088
M_wat_0 (%)	100	100.025	99.935	99.899	100.024

The fitted model parameters of parent are very similar to the actual ones (Table 14). This results also in very similar regulatory endpoints for fitted model parameters as well as "true value" (Table 15).

Table 15: Comparison of regulatory endpoints for the parent compound

Model type → Model parameter↓	"True value"*	No formation	Formation in water	Formation in sediment	Formation in water and sediment
chi² (water)	-	0.557	0.542	0.541	0.557
chi² (sediment)	-	1.216	1.508	1.54	1.217
EF (water)	-	1	1	1	1
EF (sediment)	-	1	0.999	0.999	1
DT50 (water)	34.66	35.94	36.832	36.568	36.064
DT50 (sediment)	13.86	13.533	13.273	13.345	13.509
DT90 (water)	115.13	119.39	122.354	121.477	119.801
DT90 (sediment)	46.05	44.957	44.091	44.332	44.874

* Formation in water and sediment

In Table 16, the comparison of "true" and calibrated values with respect to regulatory endpoints for the metabolite is presented (model variant 2-4). As statistical measurement, in Table 15 and Table 16, the chi² values as well as the model efficiency (EF) is presented for each compartment and the metabolite separately. For all model variants, the statistical criteria show a good correspondence between model prediction and experimental data.

Table 16: Comparison of regulatory endpoints for the metabolite

Model type → Model parameter↓	"True value"*	Formation in water	Formation in sediment	Formation in water and sediment
chi²	-	9.81	1.727	0.963
EF	-	0.961	0.999	1
DT50	69.31	88.046	71.461	69.615
DT90	230.26	292.482	237.389	231.255

* Formation in water and sediment

In Figure 19 to Figure 22, the visual assessment of optimization results of DegKinManager 2.0 is presented. As visual assessment, we consider the change of residues in time as well as a residual plot between predicted data and residuals for each model variant.

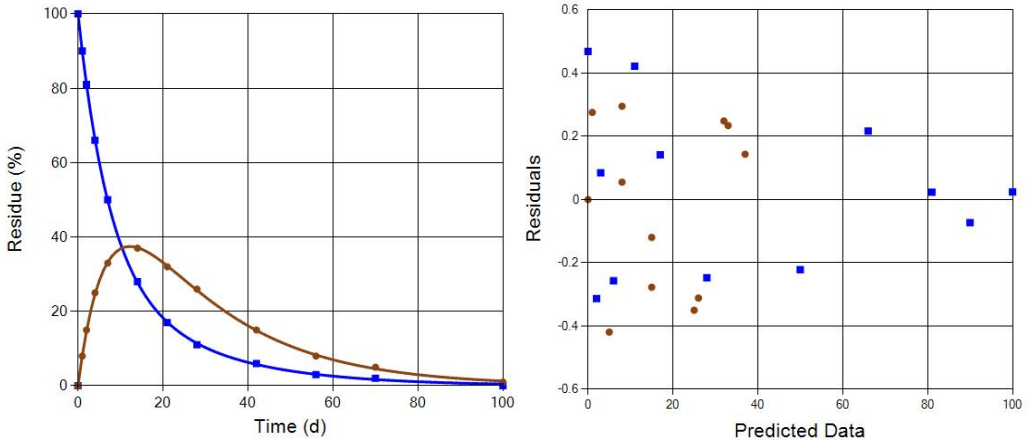

Figure 19: Model variant 1: Parent without metabolites. Change of residues in time as well as residual plot: Residue of parent in water (blue) and residue of parent in sediment (brown).

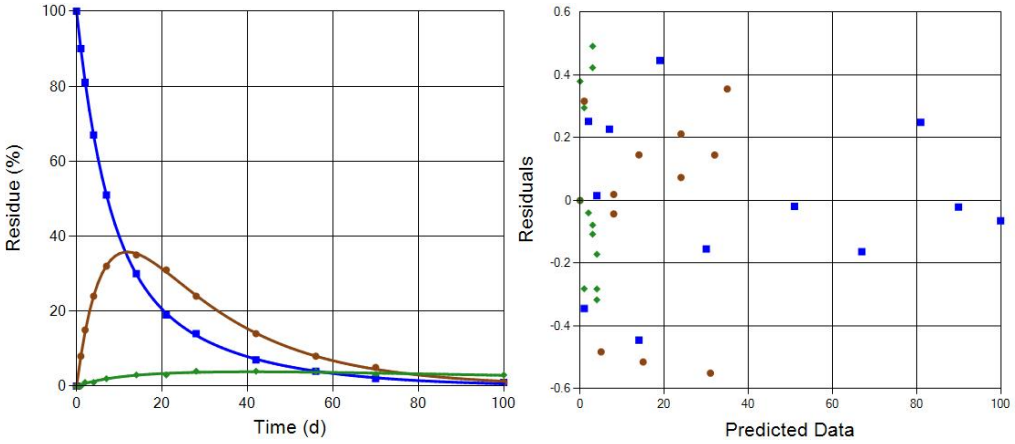

Figure 20: Model variant 2: Parent with a single metabolite in water. Change of residues in time as well as residual plot: Residue of parent in water (blue), residue of parent in sediment (brown) and residue of metabolite (green).

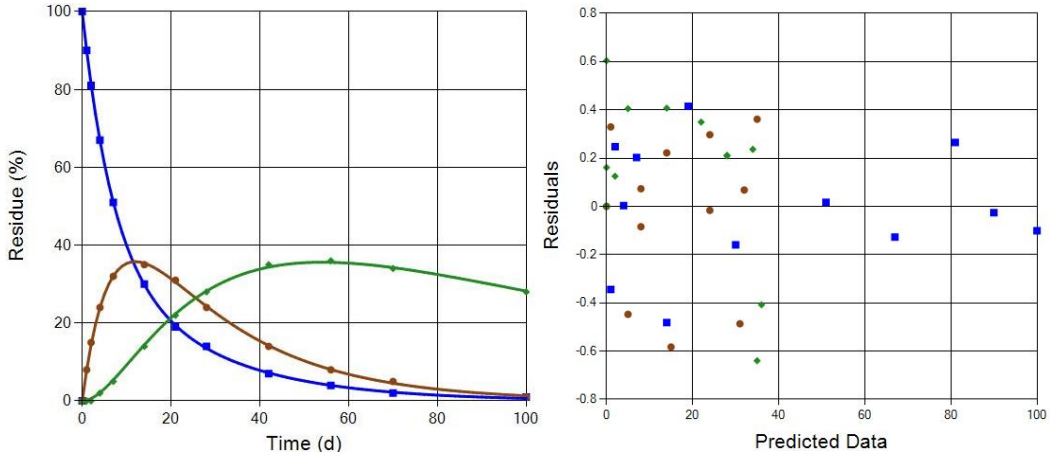

Figure 21: Model variant 3: Parent with a single metabolite in sediment. Change of residues in time as well as residual plot: Residue of parent in water (blue), residue of parent in sediment (brown) and residue of metabolite (green).

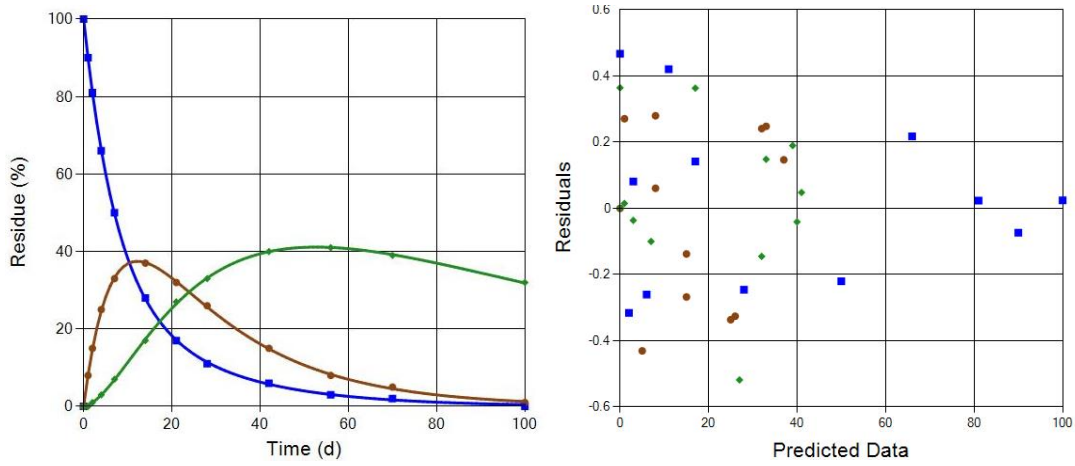

Figure 22: Model variant 4: Parent with a single metabolite. Change of residues in time as well as residual plot: Residue of parent in water (blue), residue of parent in sediment (brown) and residue of metabolite (green).

7.3 Comparison to DegKinManager 1.0/ModelMaker 4.0

In this section, we compare the results obtained using the program DegKinManager 2.0 to the results derived by using DegKinManager 1.0 respectively ModelMaker 4.0 (Klein M (2010)). The text report of DegKinManager 1.0 is presented in section A.5.

The parameter values of ModelMaker 4.0 (Table 17) are very similar to the optimization results obtained by DegKinManager 2.0 (Table 14).

Table 17: ModelMaker 4.0: Comparison of true and fitted parameters for the parent compound

Parameter name	Actual values*	Result values			
		No formation	Formation in water	Formation in sediment	Formation in water and sediment
f_sed (-)	0.8	-	-	0.762	0.823
		-	-	*0.7638*	*0.8214*
f_wat (-)	0.2	-	0.213	-	0.104
		-	*0.2121*	-	*0.1096*
k_deg_met(time^{-1})	0.01	-	0.008	0.01	0.01
		-	*0.0079*	*0.0097*	*0.0099*
k_deg_sed (time^{-1})	0.05	0.051	0.052	0.052	0.051
		0.0511	*0.052*	*0.0518*	*0.0512*
k_deg_wat (time^{-1})	0.02	0.019	0.019	0.019	0.019
		0.0194	*0.0189*	*0.019*	*0.0192*
k_des (time^{-1})	0.02	0.024	0.032	0.032	0.024
		0.0238	*0.0326*	*0.0322*	*0.0238*
k_sorp (time^{-1})	0.08	0.088	0.088	0.087	0.088
		0.0879	*0.0873*	*0.0869*	*0.088*
M_wat_0 (%)	100	100.025	99.935	99.899	100.024
		100.02	*99.93*	*99.9*	*100.01*

DegKinManager 2.0, *ModelMaker 4.0/ DegKinManager 1.0*
* Formation in water and sediment

Table 18: ModelMaker 4.0: Comparison of true and fitted parameters for the metabolite

Model type → Model parameter↓	"True value"*	No formation	Formation in water	Formation in sediment	Formation in water and sediment
chi² (water)	-	0.557	0.542	0.541	0.557
		0.58525	*0.56339*	*0.55749*	*0.58197*
chi² (sediment)	-	1.216	1.508	1.54	1.217
		1.2309	*1.52881*	*1.52245*	*1.24679*
DT50 (water)	34.66	35.94	36.832	36.568	36.064
		35.82	*36.67*	*36.44*	*36.08*
DT50 (sediment)	13.86	13.533	13.273	13.345	13.509
		13.57	*13.32*	*13.39*	*13.53*
DT90 (water)	115.13	119.39	122.354	121.477	119.801
		118.98	*121.83*	*121.05*	*119.86*
DT90 (sediment)	46.05	44.957	44.091	44.332	44.874
		45.09	*44.25*	*44.47*	*44.96*

DegKinManager 2.0, *ModelMaker 4.0/ DegKinManager 1.0*
* Formation in water and sediment

Table 19: ModelMaker 4.0: Comparison of regulatory endpoints for the metabolite

Model type → Model parameter↓	"True value"*	Formation in water	Formation in sediment	Formation in water and sediment
chi²	-	9.81 *9.81708*	1.727 *1.67558*	0.963 *0.95683*
DT50	69.31	88.046 *87.95*	71.461 *71.32*	69.615 *69.67*
DT90	230.26	292.482 *292.15*	237.389 *236.93*	231.255 *231.44*

DegKinManager 2.0, *ModelMaker 4.0/ DegKinManager 1.0*

* Formation in water and sediment

7.4 Discussion and Conclusions

We presented the performance of the software DegKinManager 2.0 using a hypothetical test data set testing all four model variants. In Klein M (2010) the same data set was used to test the model performance DegKinManager 1.0 which in fact uses the program ModelMaker 4.0.

The example simulations show that the software DegKinManager 2.0 works sufficiently well for all four model variants. It is possible even without using the option "propose initial values" to obtain a very good optimization result (visual assessment and statistical assessment).

Additional, we presented in Table 17 the optimization result of ModelMaker 4.0 using the same data set. The same initial values in ModelMaker 4.0 and DegKinManager 2.0 are used. The statistical assessment indicate for both software tools a good correspondence between the hypothetical data and predicted data. Furthermore, the results of both software tools are very similar.

A Supplementary Material

A.1 Description of analytical model solution

In this section we consider a mathematical sketch on how to solve the models analytically.

A.1.1 Parent without metabolites

Mathematically, we consider an ordinary differential equation system.

$$\frac{d}{dt}M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$

$$\frac{d}{dt}M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$

$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$

As both equations are linear differential equations with constant coefficients, we can reformulate the two equations to one equation $y' = A \cdot y$ with state variable $y = (M_{wat}, M_{sed})^T$ and the two dimensional matrix $A \in \mathbb{R}^{2x2}$.

$$\begin{pmatrix} M_{wat} \\ M_{sed} \end{pmatrix}' = \begin{pmatrix} -k_{degwat} - k_{sorp} & k_{des} \\ k_{sorp} & -k_{degsed} - k_{des} \end{pmatrix} \cdot \begin{pmatrix} M_{wat} \\ M_{sed} \end{pmatrix}$$

The system is a homogenous differential equation system. The idea is to find functions $M_{wat},\ M_{sed}: [0, t_n] \rightarrow [0{,}100]$ solving the system. We consider finite many time points $t \in [0, t_n]$. For the analytical solution of this system, we have to calculate the eigenvalues of the matrix A. The characteristic polynomial of the equation is.

$$\begin{aligned} &\det(\lambda \cdot I - A) \\ &= \det\begin{pmatrix} \lambda + k_{degwat} + k_{sorp} & -k_{des} \\ -k_{sorp} & \lambda + k_{degsed} + k_{des} \end{pmatrix} \\ &= \left(\lambda + k_{degwat} + k_{sorp}\right) \cdot \left(\lambda + k_{degsed} + k_{des}\right) - k_{des} \cdot k_{sorp} \\ &= \lambda^2 + \left(k_{degwat} + k_{sorp} + k_{des} + k_{degsed}\right) \cdot \lambda + k_{degwat} \cdot k_{des} + k_{degwat} \cdot k_{degsed} + k_{sorp} \cdot k_{degsed} \end{aligned}$$

Setting this equation to zero we obtain the eigenvalues of the system (assumption real eigenvalues $\lambda_1, \lambda_2 \in \mathbb{R}$ with $\lambda_1 \neq \lambda_2$).

$$\begin{aligned} &\lambda_{1,2} \\ &= -\frac{1}{2} \\ &\cdot \Bigg(k_{degwat} + k_{sorp} + k_{des} + k_{degsed} \\ &\pm \sqrt{\left(k_{degwat} + k_{sorp} + k_{des} + k_{degsed}\right)^2 - 4 \cdot \left(k_{degwat} \cdot k_{des} + k_{degwat} \cdot k_{degsed} + k_{sorp} \cdot k_{degsed}\right)} \Bigg) \end{aligned}$$

Having found the eigenvalues of the system, we can calculate the eigenvectors $v_1 = (v_{11}, v_{12})^T$ and $v_2 = (v_{21}, v_{22})^T$.

$$v_{1,2} = \left(-\frac{1}{2 \cdot k_{sorp}} \cdot \left(k_{degwat} + k_{sorp} - k_{des} - k_{degsed} \pm \sqrt{\left(k_{degwat} + k_{sorp} + k_{des} + k_{degsed}\right)^2 - 4 \cdot \left(k_{degwat} \cdot k_{des} + k_{degwat} \cdot k_{degsed} + k_{sorp} \cdot k_{degsed}\right)} \right), 1 \right)^T$$

The analytical solution of the system is

$$\begin{pmatrix} M_{wat} \\ M_{sed} \end{pmatrix} = c_1 \cdot \exp(\lambda_1 \cdot t) \cdot \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix} + c_2 \cdot \exp(\lambda_2 \cdot t) \cdot \begin{pmatrix} v_{21} \\ v_{22} \end{pmatrix}$$

where the coefficients $c_i, i = 1,2$ can be determined using the value of M_{wat} and M_{sed} at the initial time point.

$$\begin{pmatrix} M_{wat}(0) \\ M_{sed}(0) \end{pmatrix} = c_1 \cdot \begin{pmatrix} v_{11} \\ v_{12} \end{pmatrix} + c_2 \cdot \begin{pmatrix} v_{21} \\ v_{22} \end{pmatrix}$$

$$\Leftrightarrow \begin{pmatrix} M_{wat}(0) \\ M_{sed}(0) \end{pmatrix} = \begin{pmatrix} v_{11} & v_{21} \\ v_{12} & v_{22} \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\Leftrightarrow \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} v_{11} & v_{21} \\ v_{12} & v_{22} \end{pmatrix}^{-1} \cdot \begin{pmatrix} M_{wat}(0) \\ M_{sed}(0) \end{pmatrix}$$

$$\Leftrightarrow \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{1}{v_{11} \cdot v_{22} - v_{12} \cdot v_{21}} \cdot \begin{pmatrix} v_{22} & -v_{21} \\ -v_{12} & v_{11} \end{pmatrix} \cdot \begin{pmatrix} M_{wat}(0) \\ M_{sed}(0) \end{pmatrix}$$

$$c_1 = \frac{1}{v_{11} \cdot v_{22} - v_{12} \cdot v_{21}} \cdot (v_{22} \cdot M_{wat}(0) - v_{21} \cdot M_{sed}(0))$$

$$c_2 = \frac{1}{v_{11} \cdot v_{22} - v_{12} \cdot v_{21}} \cdot (-v_{12} \cdot M_{wat}(0) + v_{11} \cdot M_{sed}(0))$$

All together, we obtain for the change of residues in water

$$M_{wat}(t) = c_1 \cdot \exp(\lambda_1 \cdot t) \cdot v_{11} + c_2 \cdot \exp(\lambda_2 \cdot t) \cdot v_{21}$$

and for the change of residues in sediment

$M_{sed}(t) = c_1 \cdot \exp(\lambda_1 \cdot t) \cdot v_{12} + c_2 \cdot \exp(\lambda_2 \cdot t) \cdot v_{22}$.

A.1.2 Parent with a single metabolite in water

We are interested in the solution function of above linear system, namely the residue of parent in water and sediment as well as the residue of the metabolite in water in time $M_{wat},\ M_{sed}, M_{met}: [0, t_n] \rightarrow [0,100]$.

$$\frac{d}{dt} M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$

$$\frac{d}{dt} M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$

$$\frac{d}{dt} M_{met}(t) = k_{degwat} \cdot f_{wat} \cdot M_{wat}(t) - k_{degmet} \cdot M_{met}(t)$$

$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$
$$M_{met}(0) = M_{met_0} \in \mathbb{R}_+$$

Mathematically, we consider an ordinary differential equation system. As all equations are linear differential equations with constant coefficients, we can reformulate the three equations to one equation $y' = B \cdot y$ with state variable $y = (M_{wat}, M_{sed}, M_{met})^T$ and the three dimensional matrix $B \in \mathbb{R}^{3x3}$.

$$\begin{pmatrix} M_{wat} \\ M_{sed} \\ M_{met} \end{pmatrix}' = \begin{pmatrix} -k_{degwat} - k_{sorp} & k_{des} & 0 \\ k_{sorp} & -k_{degsed} - k_{des} & 0 \\ k_{degwat} \cdot f_{wat} & 0 & -k_{degmet} \end{pmatrix}$$

For the analytical solution of this system, we have to calculate the eigenvalues of the matrix B. This can be done easily applying the Laplace's formula on the last column. We obtain one additional eigenvalue in comparison to model without metabolites, namely $\lambda_3 = -k_{degmet}$. The other eigenvalues are the same as above concerning the first model variant.

The characteristic polynomial of the system is $\det(\lambda \cdot I - B) = \left(\lambda + k_{degmet}\right) \cdot \det(\lambda \cdot I - A)$.

Having found the eigenvalues of the system, we can calculate the eigenvectors $v_1 = (v_{11}, v_{12}, v_{13})^T$, $v_2 = (v_{21}, v_{22}, v_{23})^T$ and $v_3 = (v_{31}, v_{32}, v_{33})^T$.

$$v_{11} = \frac{\lambda_1 - \lambda_3}{k_{degwat} \cdot f_{wat}}, \qquad v_{12} = \frac{k_{degwat} + k_{sorp} + \lambda_1}{k_{des}} \cdot \frac{\lambda_1 - \lambda_3}{k_{degwat} \cdot f_{wat}}, \qquad v_{13} = 1$$
$$v_{21} = \frac{\lambda_2 - \lambda_3}{k_{degwat} \cdot f_{wat}}, \qquad v_{22} = \frac{k_{degwat} + k_{sorp} + \lambda_2}{k_{des}} \cdot \frac{\lambda_2 - \lambda_3}{k_{degwat} \cdot f_{wat}}, \qquad v_{23} = 1$$

$$v_{31} = 0, \qquad v_{32} = 0, \qquad v_{33} = 1$$

The analytical solution of the system is

$$\begin{pmatrix} M_{wat} \\ M_{sed} \\ M_{met} \end{pmatrix} = c_1 \cdot \exp(\lambda_1 \cdot t) \cdot \begin{pmatrix} v_{11} \\ v_{12} \\ v_{13} \end{pmatrix} + c_2 \cdot \exp(\lambda_2 \cdot t) \cdot \begin{pmatrix} v_{21} \\ v_{22} \\ v_{23} \end{pmatrix} + c_3 \cdot \exp(\lambda_3 \cdot t) \cdot \begin{pmatrix} v_{31} \\ v_{32} \\ v_{33} \end{pmatrix}$$

where the coefficients c_i , $i = 1,2,3$ can be determined using the value of M_{wat}, M_{sed} and M_{met} at the initial time point.

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} v_{11} & v_{21} & v_{31} \\ v_{12} & v_{22} & v_{32} \\ v_{13} & v_{23} & v_{33} \end{pmatrix}^{-1} \cdot \begin{pmatrix} M_{wat}(0) \\ M_{sed}(0) \\ M_{met}(0) \end{pmatrix}$$

As $v_{13} = v_{23} = v_{33} = 1$ and $v_{31} = v_{32} = 0$, we obtain:

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \frac{1}{v_{11} \cdot v_{22} - v_{12} \cdot v_{21}} \cdot \begin{pmatrix} v_{22} & -v_{21} & 0 \\ -v_{12} & v_{11} & 0 \\ v_{22} - v_{12} & v_{21} - v_{11} & v_{11} \cdot v_{22} - v_{12} \cdot v_{21} \end{pmatrix} \cdot \begin{pmatrix} M_{wat}(0) \\ M_{sed}(0) \\ M_{met}(0) \end{pmatrix}$$

Thus, the first two coefficients are calculated equivalently as above for the residue of parent in water and sediment without a metabolite.

$$c_1 = \frac{1}{v_{11} \cdot v_{22} - v_{12} \cdot v_{21}} \cdot (v_{22} \cdot M_{wat}(0) - v_{21} \cdot M_{sed}(0))$$
$$c_2 = \frac{1}{v_{11} \cdot v_{22} - v_{12} \cdot v_{21}} \cdot (-v_{12} \cdot M_{wat}(0) + v_{11} \cdot M_{sed}(0))$$
$$c_3 = \frac{1}{v_{11} \cdot v_{22} - v_{12} \cdot v_{21}} \cdot \left((v_{22} - v_{12}) \cdot M_{wat}(0) + (v_{21} - v_{11}) \cdot M_{sed}(0) + (v_{11} \cdot v_{22} - v_{12} \cdot v_{21}) \cdot M_{met}(0)\right)$$

All together, we obtain for the change of residues in water

$$M_{wat}(t) = c_1 \cdot \exp(\lambda_1 \cdot t) \cdot v_{11} + c_2 \cdot \exp(\lambda_2 \cdot t) \cdot v_{21} ,$$

for the change of residues in sediment

$$M_{sed}(t) = c_1 \cdot \exp(\lambda_1 \cdot t) \cdot v_{12} + c_2 \cdot \exp(\lambda_2 \cdot t) \cdot v_{22}$$

and for the change of residue of the metabolite

$$M_{met}(t) = c_1 \cdot \exp(\lambda_1 \cdot t) \cdot v_{13} + c_2 \cdot \exp(\lambda_2 \cdot t) \cdot v_{23} + c_3 \cdot \exp(\lambda_3 \cdot t) \cdot v_{33}$$

In total, this yields to:

$$M_{wat}(t) = \frac{k_{degwat} + k_{sorp} + \lambda_2 \cdot M_{wat}(0) - k_{des} \cdot M_{sed}(0)}{\lambda_2 - \lambda_1} \cdot \exp(\lambda_1 \cdot t)$$
$$+ \frac{k_{des} \cdot M_{sed}(0) - \left(k_{degwat} + k_{sorp} + \lambda_1\right) \cdot M_{wat}(0)}{\lambda_2 - \lambda_1} \cdot \exp(\lambda_2 \cdot t),$$

$$M_{sed}(t) = \frac{k_{degwat} + k_{sorp} + \lambda_1}{\lambda_2 - \lambda_1} \cdot \left(\frac{k_{degwat} + k_{sorp} + \lambda_2}{k_{des}} \cdot M_{wat}(0) - M_{sed}(0) \right) \cdot \exp(\lambda_1 \cdot t)$$
$$+ \frac{k_{degwat} + k_{sorp} + \lambda_2}{k_{des}} \cdot \left(\frac{k_{des} \cdot M_{sed}(0) - \left(k_{degwat} + k_{sorp} + \lambda_1\right) \cdot M_{wat}(0)}{\lambda_2 - \lambda_1} \right) \cdot \exp(\lambda_2 \cdot t)$$
$$M_{met}(t) = c_1 \cdot \exp(\lambda_1 \cdot t) + c_2 \cdot \exp(\lambda_2 \cdot t) + c_3 \cdot \exp(\lambda_3 \cdot t).$$

A.1.3 Parent with a single metabolite in sediment

$$\frac{d}{dt} M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$
$$\frac{d}{dt} M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$
$$\frac{d}{dt} M_{met}(t) = k_{degsed} \cdot f_{sed} \cdot M_{sed}(t) - k_{degmet} \cdot M_{met}(t)$$

$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$
$$M_{met}(0) = M_{met_0} \in \mathbb{R}_+$$

Mathematically, we have an ordinary differential equation system. As all equations are linear differential equations with constant coefficients, we can reformulate the three equations to one equation $y' = C \cdot y$ with state variable $y = (M_{wat}, M_{sed}, M_{met})^T$ and the three dimensional matrix $C \in \mathbb{R}^{3x3}$.

We obtain the following linear system:

$$\begin{pmatrix} M_{wat} \\ M_{sed} \\ M_{met} \end{pmatrix}' = \begin{pmatrix} -k_{degwat} - k_{sorp} & k_{des} & 0 \\ k_{sorp} & -k_{degsed} - k_{des} & 0 \\ 0 & k_{degsed} \cdot f_{sed} & -k_{degmet} \end{pmatrix}$$

For the solution of this system, we have to calculate the eigenvalues of the matrix C. This can be done easily applying the Laplace's formula on the last column. We obtain one additional eigenvalue than in the model without metabolites, namely $\lambda_3 = -k_{degmet}$. The other eigenvalues are the same as above. The characteristic polynomial is calculated by $\det(\lambda \cdot I - C) = \left(\lambda + k_{degmet}\right) \cdot \det(\lambda \cdot I - A)$.

A.1.4 Parent with a single metabolite

$$\frac{d}{dt} M_{wat}(t) = -k_{degwat} \cdot M_{wat}(t) - k_{sorp} \cdot M_{wat}(t) + k_{des} \cdot M_{sed}(t)$$
$$\frac{d}{dt} M_{sed}(t) = -k_{degsed} \cdot M_{sed}(t) - k_{des} \cdot M_{sed}(t) + k_{sorp} \cdot M_{wat}(t)$$
$$\frac{d}{dt} M_{met}(t) = k_{degwat} \cdot f_{wat} \cdot M_{wat}(t) + k_{degsed} \cdot f_{sed} \cdot M_{sed}(t) - k_{degmet} \cdot M_{met}(t)$$

$$M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+$$
$$M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+$$
$$M_{met}(0) = M_{met_0} \in \mathbb{R}_+$$

Mathematically, we have an ordinary differential equation system. As all equations are linear differential equations with constant coefficients, we can reformulate the three equations to one equation $y' = D \cdot y$ with the state variable $y = (M_{wat}, M_{sed}, M_{met})^T$ and the three dimensional matrix $D \in \mathbb{R}^{3x3}$.

The linear system to solve is:

$$\begin{pmatrix} M_{wat} \\ M_{sed} \\ M_{met} \end{pmatrix}' = \begin{pmatrix} -k_{degwat} - k_{sorp} & k_{des} & 0 \\ k_{sorp} & -k_{degsed} - k_{des} & 0 \\ k_{degwat} \cdot f_{wat} & k_{degsed} \cdot f_{sed} & -k_{degmet} \end{pmatrix}.$$

For the analytical solution of this system, we have to calculate the eigenvalues of the matrix D. This can be done easily applying the Laplace's formula on the last column. We obtain one additional eigenvalue than in the model without metabolites, namely $\lambda_3 = -k_{degmet}$. The other eigenvalues are the same as above.

The characteristic polynomial can be calculated using $\det(\lambda \cdot I - D) = \left(\lambda + k_{degmet}\right) \cdot \det(\lambda \cdot I - A)$.

Remark: We obtain the same eigenvalues for the matrices B, C, and D. Thus for all model variants, we obtain the same eigenvalues. However, their eigenvectors differ.

A.2 Checking the statistical assessment: χ^2

In this section, we check the calculation of χ^2 error. We compare the obtained statistical result of fitting the parameter to model 3: Parent with a single metabolite. In total we have eight active parameters.

Table 20: Number of active parameters for model variant 4 (parent with a single metabolite)

Compartment	Parameters	Number of active parameters
Water	k_{degwat}, k_{sorp}, M_{wat_0}	3
Sediment	k_{degsed}, k_{des}	3
Metabolite	f_{sed}, f_{wat}, k_{degmet}	3

The statistical assessment of the model optimization run can be seen in Table 21, whereas the result of statistical assessment of the EXCEL spreadsheet FOCUS_DEGKIN v2 can be seen in Figure 23. The statistical assessments coincide.

Table 21: Statistical result of DegKinManager 2.0

	Parent/Water	Parent/Sediment	Metabolite
Number of observations	12	12	12
Number of active parameter	3	2	3
Deg. of Freedom	9	10	9
Model error (Chi²)	0.557	1.217	0.963
Coefficient of Determination (R²)	1	1	1
Model efficiency	1	1	1
Absolute deviation	2.491	2.745	1.969
Quadratic deviation	0.752	0.792	0.628
SRMSE	0.007	0.015	0.011
STE	0.005	0.013	0.008

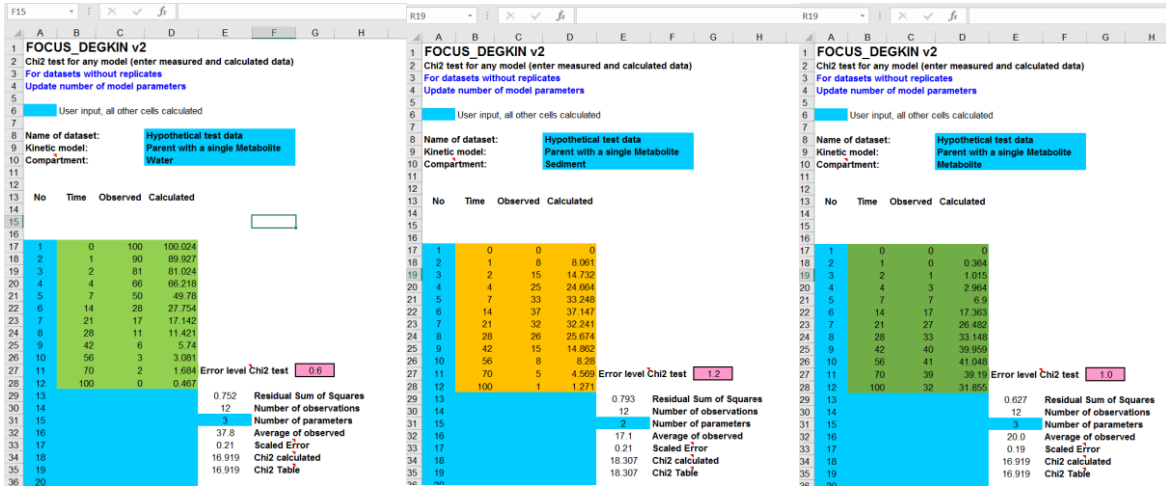

Figure 23: Statistical assessment using the EXCEL sheet FOCUS_DEGKIN v2

A.3 Documentation of checking the plausibility of analytical model solution

Table 22: Experimental residues (hypothetical test data set)

Model variant	01-Apr	01-Apr	2	3	4
Time (d)	Parent water (%)	Parent sediment (%)	Metabolite (%)	Metabolite (%)	Metabolite (%)
0	100	0	0	0	0
1	90	8	0.4	4	0.4
2	81.16	14.64	0.752	3.6	1.076
3	73.3368	20.108	1.0616	6.8104	1.97548
4	66.40528	24.567384	1.3337152	9.675768	3.0533924
5	60.2560997	28.1600895	1.57266202	12.2352215	4.27117496
6	54.7936915	31.0093712	1.78223317	14.5231133	5.59589119
7	49.9345098	33.2222106	1.96576328	16.5696298	6.99948189
8	45.605503	34.8914166	2.12618605	18.4013139	8.45811353
9	41.742781	36.0974577	2.26608434	20.0415209	9.95161107
10	38.2904521	36.9100581	2.38773378	21.5108169	11.4629644
11	35.199608	37.3895902	2.49314091	22.8273268	12.9778989
12	32.427439	37.5882876	2.58407653	24.0070379	14.4845019
13	29.9364609	37.5513025	2.66210475	25.0640651	15.9728982
14	27.6938409	37.3176282	2.7286085	26.0108829	17.4349671
15	25.6708093	36.9209015	2.78481169	26.8585277	18.864098

16	23.8421464	36.3901032	2.8317987	27.6167748	20.2549763
17	22.1857339	35.7501677	2.87053131	28.2942929	21.6033992
18	20.6821638	35.0225146	2.90186362	28.8987793	22.9061149
19	19.3143977	34.2255117	2.926555	29.4370781	24.160683
20	18.0674682	33.3748777	2.94528149	29.9152832	25.3653542
21	16.9282189	32.4840337	2.95864573	30.3388291	26.5189656
22	15.8850777	31.5644089	2.9671857	30.7125695	27.6208502
23	14.9278581	30.6257065	2.97138229	31.040847	28.6707584
24	14.0475864	29.6761357	2.97166608	31.3275528	29.6687905
25	13.2363505	28.7226131	2.9684231	31.5761807	30.6153383
26	12.4871677	27.7709382	2.96200004	31.789873	31.5110349
27	11.7938697	26.825946	2.95270871	31.9714609	32.3567107
28	11.1510017	25.8916393	2.94083002	32.1235011	33.153357
29	10.5537343	24.9713047	2.92661742	32.2483062	33.902093
30	9.99778694	24.0676121	2.91030001	32.3479725	34.6041392
31	9.47936049	23.1827022	2.89208516	32.4244042	35.2607934
32	8.99507849	22.3182619	2.8721609	32.4793346	35.873411
33	8.54193588	21.4755898	2.85069799	32.5143444	36.4433877
34	8.11725409	20.6556534	2.82785178	32.5308784	36.9721451
35	7.71864175	19.859138	2.80376376	32.5302598	37.4611188
36	7.34396033	19.0864897	2.77856305	32.5137028	37.9117477
37	6.99129409	18.3379522	2.75236763	32.4823242	38.3254657
38	6.65892373	17.6135991	2.72528546	32.4371528	38.7036943
39	6.34530334	16.9133611	2.69741544	32.3791382	39.047837
40	6.04904022	16.2370501	2.66884835	32.3091589	39.3592743
41	5.7688772	15.5843798	2.63966754	32.2280289	39.6393597
42	5.50367708	14.9549834	2.6099497	32.1365037	39.8894168
43	5.25240904	14.3484287	2.57976541	32.0352858	40.1107367
44	5.01413671	13.7642314	2.54917974	31.9250293	40.3045761
45	4.78800767	13.2018662	2.51825269	31.8063445	40.4721562
46	4.57324422	12.6607761	2.48703967	31.6798013	40.6146613
47	4.36913532	12.1403813	2.45559185	31.5459331	40.7332387
48	4.17502942	11.6400855	2.42395656	31.4052392	40.8289981
49	3.99032819	11.1592818	2.39217754	31.258188	40.9030116
50	3.814481	10.6973584	2.3602953	31.1052192	40.9563141
51	3.64698007	10.2537018	2.32834732	30.9467463	40.9899032
52	3.4873561	9.82770105	2.2963683	30.783158	41.0047402
53	3.33517451	9.41875046	2.26439035	30.6148207	41.0017503
54	3.19003207	9.02625189	2.23244325	30.4420794	40.9818235
55	3.0515539	8.64961682	2.20055451	30.2652599	40.9458154
56	2.91939085	8.28826796	2.16874963	30.0846695	40.8945482
57	2.79321712	7.94164047	2.13705221	29.9005984	40.828811
58	2.67272822	7.60918301	2.10548403	29.7133211	40.7493614
59	2.55763906	7.29035845	2.07406526	29.523097	40.656926
60	2.44768232	6.98464448	2.04281451	29.3301716	40.5522016
61	2.34260698	6.69153396	2.01174895	29.1347772	40.4358561
62	2.24217696	6.41053514	1.9808844	28.9371337	40.3085293

63	2.14616997	6.14117183	1.95023542	28.7374494	40.1708341
64	2.05437641	5.8829834	1.91981539	28.5359218	40.0233574
65	1.96659843	5.63552468	1.88963659	28.3327376	39.8666606
66	1.88264908	5.39836582	1.85971025	28.1280742	39.7012814
67	1.80235149	5.17109214	1.83004664	27.9220994	39.5277338
68	1.72553819	4.95330381	1.80065512	27.7149724	39.3465096
69	1.65205044	4.7446156	1.77154417	27.5068442	39.1580788
70	1.58173771	4.54465654	1.74272149	27.2978578	38.9628908
71	1.51445707	4.3530696	1.71419401	27.0881487	38.7613751
72	1.45007276	4.1695113	1.68596795	26.8778455	38.553942
73	1.38845571	3.99365133	1.65804889	26.66707	38.3409833
74	1.32948316	3.82517219	1.63044173	26.4559375	38.1228733
75	1.27303829	3.66376879	1.60315083	26.2445575	37.8999694
76	1.21900984	3.50914804	1.57617997	26.0330334	37.6726126
77	1.16729181	3.36102846	1.54953241	25.8214635	37.4411285
78	1.1177832	3.21913981	1.52321093	25.6099405	37.2058275
79	1.07038768	3.08322268	1.49721784	25.3985525	36.9670059
80	1.02501336	2.95302811	1.47155503	25.1873824	36.7249463
81	0.98157259	2.82831721	1.44622399	24.9765091	36.4799181
82	0.93998167	2.70886081	1.4212258	24.766007	36.2321779
83	0.90016072	2.59443909	1.39656121	24.5559462	35.9819704
84	0.86203343	2.48484121	1.37223063	24.3463931	35.7295289
85	0.82552691	2.379865	1.34823415	24.1374105	35.4750754
86	0.79057152	2.2793166	1.32457157	23.9290575	35.2188214
87	0.7571007	2.18301016	1.30124243	23.7213898	34.9609681
88	0.72505084	2.09076751	1.27824598	23.5144599	34.7017073
89	0.6943611	2.00241785	1.25558126	23.3083174	34.4412211
90	0.66497335	1.91779749	1.23324708	23.1030086	34.179683
91	0.63683196	1.83674953	1.21124204	22.8985775	33.917258
92	0.60988376	1.75912362	1.18956452	22.695065	33.6541027
93	0.58407785	1.68477567	1.16821277	22.4925097	33.3903662
94	0.55936558	1.6135676	1.14718482	22.2909477	33.1261899
95	0.53570038	1.54536712	1.12647859	22.0904128	32.8617081
96	0.51303768	1.48004745	1.10609182	21.8909367	32.5970485
97	0.49133486	1.41748714	1.08602213	21.6925489	32.3323321
98	0.47055112	1.35756983	1.06626703	21.4952768	32.0676736
99	0.4506474	1.30018403	1.04682389	21.299146	31.8031819
100	0.43158634	1.24522294	1.02769001	21.1041805	31.53896

A.4 Documentation of model output: DegKinManager 2.0

A.4.1 Model variant 1: Parent without metabolites

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DegKinManager - Two-Phase Flow
Evaluation of experimental residue derived via water-sediment studies
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developed by Judith Klein and Michael Klein 2018

Version:
Date of this report: 05/12/2018 11:31

INPUT DATA

Selected Model: Parent without Metabolites

Environmental Residues

Time (days)	Parent/Water (%)	Parent/Sediment (%)
0	100	0
1	90	8
2	81	15
4	66	25
7	50	33
14	28	37
21	17	32
28	11	26
42	6	15
56	3	8
70	2	5
100	0	1

Parameters

Name	Initial Value	Lower Bound	Upper Bound	Unit	Fit
k_deg_sed	0.01	0	10000	1/d	True
k_deg_wat	0.01	0	10000	1/d	True
k_des	0.5	0	10000	1/d	True
k_sorp	0.5	0.0001	10000	1/d	True
M_sed_0	0	0	10000	%	False
M_wat_0	100	0	10000	%	True

OUTPUT DATA

Result of parameter fitting (objective function value: 1.542)

Parameter	Value	Standard Error	Prob > t
k_deg_sed	0.051	0.0034382	5.5793e-16
k_deg_wat	0.019	0.0015781	1.0842e-13
k_des	0.024	0.0024795	4.2499e-11
k_sorp	0.088	0.0011407	1.4081e-19
M_sed_0	0.000	-	-
M_wat_0	100.025	0.2059903	1.4081e-19

Time (days)	Parent/Water (%)	Parent/Sediment (%)
0.000	100.025	0.000
1.000	89.927	8.055
2.000	81.024	14.723
3.000	73.164	20.198
4.000	66.217	24.650
5.000	60.068	28.225
6.000	54.617	31.050
7.000	49.778	33.234
8.000	45.475	34.873
9.000	41.642	36.049
10.000	38.222	36.832
11.000	35.164	37.284
12.000	32.424	37.457
13.000	29.965	37.397
14.000	27.752	37.144

15.000	25.758	36.730
16.000	23.956	36.185
17.000	22.324	35.534
18.000	20.842	34.798
19.000	19.494	33.995
20.000	18.265	33.141
21.000	17.141	32.249
22.000	16.112	31.330
23.000	15.166	30.393
24.000	14.296	29.447
25.000	13.492	28.499
26.000	12.750	27.553
27.000	12.061	26.615
28.000	11.422	25.689
29.000	10.827	24.777
30.000	10.273	23.882
31.000	9.754	23.006
32.000	9.270	22.151
33.000	8.815	21.318
34.000	8.389	20.508
35.000	7.987	19.721
36.000	7.610	18.958
37.000	7.253	18.219
38.000	6.917	17.504
39.000	6.599	16.813
40.000	6.298	16.146
41.000	6.013	15.502
42.000	5.743	14.880
43.000	5.487	14.282
44.000	5.243	13.705
45.000	5.012	13.150
46.000	4.792	12.616
47.000	4.582	12.102
48.000	4.382	11.608
49.000	4.192	11.134
50.000	4.011	10.677
51.000	3.838	10.239
52.000	3.673	9.818
53.000	3.516	9.414
54.000	3.365	9.026
55.000	3.222	8.653
56.000	3.085	8.295
57.000	2.953	7.952
58.000	2.828	7.623
59.000	2.708	7.307
60.000	2.594	7.004
61.000	2.484	6.714
62.000	2.379	6.435
63.000	2.279	6.168
64.000	2.183	5.911
65.000	2.091	5.666
66.000	2.003	5.430
67.000	1.919	5.204
68.000	1.838	4.988
69.000	1.761	4.780
70.000	1.687	4.581
71.000	1.616	4.390
72.000	1.549	4.207
73.000	1.484	4.032
74.000	1.421	3.864
75.000	1.362	3.703
76.000	1.305	3.549
77.000	1.250	3.401
78.000	1.198	3.259
79.000	1.148	3.123
80.000	1.100	2.993

81.000	1.054	2.868
82.000	1.010	2.748
83.000	0.968	2.634
84.000	0.927	2.524
85.000	0.888	2.418
86.000	0.851	2.317
87.000	0.816	2.221
88.000	0.782	2.128
89.000	0.749	2.039
90.000	0.718	1.954
91.000	0.688	1.873
92.000	0.659	1.794
93.000	0.631	1.720
94.000	0.605	1.648
95.000	0.580	1.579
96.000	0.556	1.513
97.000	0.532	1.450
98.000	0.510	1.389
99.000	0.489	1.331
100.000	0.468	1.276

Analytic solution function
M_wat(t) = 66.715 * Exp(-0.140 * t) + 33.310 * Exp(-0.043 * t)
M_sed(t) = -90.750 * Exp(-0.140 * t) + 90.750 * Exp(-0.043 * t)

EVALUATION

	k_deg_wat	k_deg_sed
DT50	35.940	13.533
DT90	119.390	44.957

MEASURED VERSUS PREDICTED VALUES (%)

Compound: Parent
Compartment: Water

Time	Measured	Predicted
0.000	100.000	100.025
1.000	90.000	89.927
2.000	81.000	81.024
4.000	66.000	66.217
7.000	50.000	49.778
14.000	28.000	27.752
21.000	17.000	17.141
28.000	11.000	11.422
42.000	6.000	5.743
56.000	3.000	3.085
70.000	2.000	1.687
100.000	0.000	0.468

Compound: Parent
Compartment: Sediment

Time	Measured	Predicted
0.000	0.000	0.000
1.000	8.000	8.055
2.000	15.000	14.723
4.000	25.000	24.650
7.000	33.000	33.234
14.000	37.000	37.144
21.000	32.000	32.249
28.000	26.000	25.689
42.000	15.000	14.880
56.000	8.000	8.295
70.000	5.000	4.581

100.000 1.000 1.276

STATISTICS

	Complete Data Set
No obs.	24
No act. param.	5
Deg. of Freedom	31
Model error (Chi²)	0.674
Coeff. of Det. (R²)	1.000
Model efficiency	1.000
Abs. deviation	5.224
Quadr. deviation	1.542
SRMSE	0.009
STE	0.008

	Parent/Water	Parent/Sediment
No obs.	12	12
No act. param.	3	2
Deg. of Freedom	9	10
Model error (Chi²)	0.557	1.216
Coeff. of Det. (R²)	1.000	1.000
Model efficiency	1.000	1.000
Abs. deviation	2.494	2.730
Quadr. deviation	0.753	0.790
SRMSE	0.007	0.015
STE	0.005	0.013

The calibration was done using the Nelder Mead solver by Microsoft Solver Foundation. The implementation of the solver implements the method described in Nelder, J.A. and Mead, R., "A Simplex Method for Function Minimization", Computer Journal 7 (4): 308-313 (Jan., 1965) with the modifications described in Lee, D. and Wiswall, M., "A Parallel Implementation of the Simplex Function Minimization Routine".

A.4.2 Model variant 2: Parent with a single metabolite in water

DegKinManager - Two-Phase Flow
Evaluation of experimental residue derived via water-sediment studies
developed by Judith Klein and Michael Klein 2018

Version:
Date of this report: 05/12/2018 11:37

INPUT DATA

Selected Model: Parent with a Single Metabolite in Water

Environmental Residues

Time (days)	Parent/Water (%)	Parent/Sediment (%)	Metabolite (%)
0	100	0	0
1	90	8	0
2	81	15	1
4	67	24	1
7	51	32	2

14	30	35	3
21	19	31	3
28	14	24	4
42	7	14	4
56	4	8	4
70	2	5	3
100	1	1	3

Parameters

Name	Initial Value	Lower Bound	Upper Bound	Unit	Fit
f_wat	0.5	0	1	-	True
k_deg_met	0.001	0	10000	1/d	True
k_deg_sed	0.01	0	10000	1/d	True
k_deg_wat	0.01	0	10000	1/d	True
k_des	0.5	0	10000	1/d	True
k_sorp	0.5	0.0001	10000	1/d	True
M_met_0	0	0	10000	%	False
M_sed_0	0	0	10000	%	False
M_wat_0	100	0	10000	%	True

OUTPUT DATA

Result of parameter fitting (objective function value: 2.829)

Parameter	Value	Standard Error	Prob > t
f_wat	0.213	0.3303416	2.6153e-01
k_deg_met	0.008	0.0349289	4.0899e-01
k_deg_sed	0.052	0.0355585	7.5538e-02
k_deg_wat	0.019	0.0330971	2.8797e-01
k_des	0.032	0.0085015	3.2690e-04
k_sorp	0.088	0.0338491	7.5011e-03
M_met_0	0.000	-	-
M_sed_0	0.000	-	-
M_wat_0	99.935	0.2051585	8.2091e-19

Time (days)	Parent/Water (%)	Parent/Sediment (%)	Metabolite (%)
0.000	99.935	0.000	0.000
1.000	89.979	7.957	0.380
2.000	81.249	14.485	0.719
3.000	73.582	19.797	1.023
4.000	66.836	24.073	1.295
5.000	60.889	27.471	1.540
6.000	55.634	30.123	1.761
7.000	50.981	32.145	1.960
8.000	46.852	33.635	2.141
9.000	43.178	34.677	2.304
10.000	39.901	35.343	2.452
11.000	36.970	35.695	2.586
12.000	34.341	35.785	2.709
13.000	31.977	35.659	2.820
14.000	29.845	35.355	2.922
15.000	27.916	34.906	3.014
16.000	26.166	34.338	3.099
17.000	24.574	33.677	3.176
18.000	23.121	32.942	3.246
19.000	21.791	32.150	3.311
20.000	20.570	31.315	3.369
21.000	19.446	30.450	3.423
22.000	18.408	29.564	3.472
23.000	17.448	28.667	3.516
24.000	16.556	27.765	3.557
25.000	15.727	26.864	3.593
26.000	14.954	25.969	3.627

27.000	14.232	25.084	3.657
28.000	13.555	24.212	3.684
29.000	12.920	23.356	3.708
30.000	12.323	22.518	3.729
31.000	11.760	21.699	3.748
32.000	11.230	20.901	3.765
33.000	10.729	20.124	3.779
34.000	10.254	19.370	3.791
35.000	9.805	18.638	3.802
36.000	9.379	17.929	3.810
37.000	8.974	17.243	3.817
38.000	8.590	16.579	3.822
39.000	8.224	15.938	3.826
40.000	7.875	15.319	3.828
41.000	7.543	14.721	3.829
42.000	7.227	14.145	3.829
43.000	6.925	13.590	3.827
44.000	6.637	13.055	3.824
45.000	6.361	12.540	3.820
46.000	6.098	12.044	3.815
47.000	5.846	11.567	3.809
48.000	5.606	11.108	3.802
49.000	5.375	10.666	3.794
50.000	5.155	10.242	3.785
51.000	4.944	9.834	3.776
52.000	4.742	9.441	3.766
53.000	4.549	9.064	3.755
54.000	4.363	8.702	3.743
55.000	4.186	8.354	3.731
56.000	4.015	8.019	3.718
57.000	3.852	7.698	3.705
58.000	3.696	7.389	3.691
59.000	3.546	7.093	3.676
60.000	3.402	6.808	3.661
61.000	3.265	6.535	3.646
62.000	3.132	6.273	3.630
63.000	3.006	6.021	3.614
64.000	2.884	5.779	3.597
65.000	2.768	5.547	3.580
66.000	2.656	5.324	3.563
67.000	2.548	5.109	3.546
68.000	2.446	4.904	3.528
69.000	2.347	4.707	3.510
70.000	2.252	4.517	3.491
71.000	2.161	4.336	3.473
72.000	2.074	4.161	3.454
73.000	1.990	3.994	3.435
74.000	1.910	3.833	3.416
75.000	1.833	3.679	3.397
76.000	1.759	3.531	3.377
77.000	1.688	3.388	3.358
78.000	1.620	3.252	3.338
79.000	1.555	3.121	3.318
80.000	1.492	2.995	3.298
81.000	1.432	2.875	3.278
82.000	1.374	2.759	3.258
83.000	1.319	2.648	3.238
84.000	1.266	2.541	3.218
85.000	1.215	2.439	3.198
86.000	1.166	2.341	3.177
87.000	1.119	2.246	3.157
88.000	1.074	2.156	3.136
89.000	1.030	2.069	3.116
90.000	0.989	1.986	3.096
91.000	0.949	1.906	3.075
92.000	0.911	1.829	3.055

93.000	0.874	1.755	3.035
94.000	0.839	1.685	3.014
95.000	0.805	1.617	2.994
96.000	0.773	1.552	2.973
97.000	0.741	1.489	2.953
98.000	0.712	1.429	2.933
99.000	0.683	1.372	2.913
100.000	0.655	1.316	2.893

Analytic solution function
M_wat(t) = 59.911 * Exp(-0.150 * t) + 40.024 * Exp(-0.041 * t)
M_sed(t) = -80.383 * Exp(-0.150 * t) + 80.383 * Exp(-0.041 * t)
M_met(t) = -1.694 * Exp(-0.150 * t) + -4.836 * Exp(-0.041 * t) + 6.530 * Exp(-0.008 * t)

EVALUATION

	k_deg_wat	k_deg_sed	k_deg_met
DT50	36.832	13.273	88.046
DT90	122.354	44.091	292.482

MEASURED VERSUS PREDICTED VALUES (%)

Compound: Parent
Compartment: Water

Time	Measured	Predicted
0.000	100.000	99.935
1.000	90.000	89.979
2.000	81.000	81.249
4.000	67.000	66.836
7.000	51.000	50.981
14.000	30.000	29.845
21.000	19.000	19.446
28.000	14.000	13.555
42.000	7.000	7.227
56.000	4.000	4.015
70.000	2.000	2.252
100.000	1.000	0.655

Compound: Parent
Compartment: Sediment

Time	Measured	Predicted
0.000	0.000	0.000
1.000	8.000	7.957
2.000	15.000	14.485
4.000	24.000	24.073
7.000	32.000	32.145
14.000	35.000	35.355
21.000	31.000	30.450
28.000	24.000	24.212
42.000	14.000	14.145
56.000	8.000	8.019
70.000	5.000	4.517
100.000	1.000	1.316

Compound: Metabolite
Compartment: Water

Time	Measured	Predicted
0.000	0.000	0.000
1.000	0.000	0.380
2.000	1.000	0.719
4.000	1.000	1.295
7.000	2.000	1.960

14.000	3.000	2.922
21.000	3.000	3.423
28.000	4.000	3.684
42.000	4.000	3.829
56.000	4.000	3.718
70.000	3.000	3.491
100.000	3.000	2.893

STATISTICS

	Complete Data Set
No obs.	36
No act. param.	7
Deg. of Freedom	29
Model error (Chi²)	1.343
Coeff. of Det. (R²)	1.000
Model efficiency	1.000
Abs. deviation	8.125
Quadr. deviation	2.829
SRMSE	0.015
STE	0.012

	Parent/Water	Parent/Sediment	Metabolite
No obs.	12	12	12
No act. param.	3	2	2
Deg. of Freedom	9	10	10
Model error (Chi²)	0.542	1.508	9.810
Coeff. of Det. (R²)	1.000	0.999	0.962
Model efficiency	1.000	0.999	0.961
Abs. deviation	2.402	2.856	2.866
Quadr. deviation	0.749	1.121	0.959
SRMSE	0.006	0.019	0.121
STE	0.005	0.014	0.102

The calibration was done using the Nelder Mead solver by Microsoft Solver Foundation. The implementation of the solver implements the method described in Nelder, J.A. and Mead, R., "A Simplex Method for Function Minimization", Computer Journal 7 (4): 308-313 (Jan., 1965) with the modifications described in Lee, D. and Wiswall, M., "A Parallel Implementation of the Simplex Function Minimization Routine".

A.4.3 Model variant 3: Parent with a single metabolite in sediment

DegKinManager - Two-Phase Flow
Evaluation of experimental residue derived via water-sediment studies
developed by Judith Klein and Michael Klein 2018

Version:
Date of this report: 05/12/2018 11:39

INPUT DATA

Selected Model: Parent with a Single Metabolite in Sediment

Environmental Residues

Time (days)	Parent/Water (%)	Parent/Sediment (%)	Metabolite (%)

0	100	0	0
1	90	8	0
2	81	15	0
4	67	24	2
7	51	32	5
14	30	35	14
21	19	31	22
28	14	24	28
42	7	14	35
56	4	8	36
70	2	5	34
100	1	1	28

Parameters

Name	Initial Value	Lower Bound	Upper Bound	Unit	Fit
f_sed	0.5	0	1	-	True
k_deg_met	0.001	0	10000	1/d	True
k_deg_sed	0.01	0	10000	1/d	True
k_deg_wat	0.01	0	10000	1/d	True
k_des	0.5	0	10000	1/d	True
k_sorp	0.5	0.0001	10000	1/d	True
M_met_0	0	0	10000	%	False
M_sed_0	0	0	10000	%	False
M_wat_0	100	0	10000	%	True

OUTPUT DATA

Result of parameter fitting (objective function value: 3.496)

Parameter	Value	Standard Error	Prob > t
f_sed	0.762	1.1763830	2.6152e-01
k_deg_met	0.010	0.0480983	4.2066e-01
k_deg_sed	0.052	0.0488685	1.4881e-01
k_deg_wat	0.019	0.0456011	3.3729e-01
k_des	0.032	0.0113867	4.4108e-03
k_sorp	0.087	0.0466356	3.5899e-02
M_met_0	0.000	-	-
M_sed_0	0.000	-	-
M_wat_0	99.899	0.1614987	8.2091e-19

Time (days)	Parent/Water (%)		Parent/Sediment (%)	Metabolite (%)
0.000	99.899	0.000	0.000	
1.000	89.974	7.916	0.161	
2.000	81.265	14.417	0.604	
3.000	73.611	19.713	1.274	
4.000	66.873	23.983	2.125	
5.000	60.928	27.381	3.118	
6.000	55.673	30.038	4.221	
7.000	51.017	32.068	5.405	
8.000	46.883	33.568	6.647	
9.000	43.204	34.622	7.927	
10.000	39.920	35.300	9.228	
11.000	36.983	35.665	10.537	
12.000	34.348	35.768	11.842	

13.000 31.978 35.654 13.135
14.000 29.841 35.361 14.407
15.000 27.907 34.922 15.652
16.000 26.152 34.365 16.865
17.000 24.556 33.713 18.043
18.000 23.099 32.986 19.182
19.000 21.765 32.201 20.281
20.000 20.541 31.373 21.337
21.000 19.415 30.514 22.349
22.000 18.376 29.633 23.318
23.000 17.414 28.740 24.242
24.000 16.521 27.841 25.122
25.000 15.692 26.943 25.958
26.000 14.918 26.050 26.751
27.000 14.195 25.167 27.501
28.000 13.518 24.297 28.209
29.000 12.884 23.442 28.877
30.000 12.287 22.604 29.505
31.000 11.725 21.786 30.094
32.000 11.195 20.988 30.645
33.000 10.695 20.211 31.160
34.000 10.221 19.456 31.640
35.000 9.773 18.724 32.087
36.000 9.348 18.014 32.500
37.000 8.944 17.326 32.882
38.000 8.561 16.661 33.234
39.000 8.196 16.019 33.556
40.000 7.848 15.398 33.851
41.000 7.518 14.800 34.119
42.000 7.202 14.222 34.361
43.000 6.901 13.665 34.578
44.000 6.614 13.129 34.772
45.000 6.339 12.612 34.943
46.000 6.077 12.114 35.092
47.000 5.827 11.636 35.221
48.000 5.587 11.175 35.330
49.000 5.358 10.732 35.420
50.000 5.138 10.305 35.492
51.000 4.928 9.895 35.547
52.000 4.727 9.501 35.586
53.000 4.534 9.123 35.609
54.000 4.350 8.759 35.617
55.000 4.173 8.409 35.612
56.000 4.003 8.073 35.592
57.000 3.841 7.750 35.560
58.000 3.685 7.440 35.516
59.000 3.536 7.142 35.460
60.000 3.393 6.856 35.393
61.000 3.256 6.582 35.316
62.000 3.124 6.318 35.229
63.000 2.998 6.064 35.133
64.000 2.877 5.821 35.028
65.000 2.761 5.588 34.914
66.000 2.649 5.363 34.793
67.000 2.542 5.148 34.664
68.000 2.440 4.941 34.528

```
69.000 2.341  4.743  34.385
70.000 2.247  4.553  34.236
71.000 2.157  4.370  34.082
72.000 2.070  4.194  33.921
73.000 1.986  4.026  33.756
74.000 1.906  3.864  33.585
75.000 1.830  3.709  33.410
76.000 1.756  3.560  33.230
77.000 1.685  3.417  33.047
78.000 1.617  3.279  32.860
79.000 1.552  3.147  32.669
80.000 1.490  3.021  32.475
81.000 1.430  2.899  32.278
82.000 1.372  2.783  32.079
83.000 1.317  2.671  31.876
84.000 1.264  2.564  31.672
85.000 1.213  2.461  31.465
86.000 1.164  2.362  31.256
87.000 1.118  2.267  31.045
88.000 1.073  2.176  30.833
89.000 1.029  2.088  30.620
90.000 0.988  2.004  30.404
91.000 0.948  1.923  30.188
92.000 0.910  1.846  29.971
93.000 0.874  1.772  29.753
94.000 0.838  1.701  29.534
95.000 0.805  1.632  29.315
96.000 0.772  1.567  29.095
97.000 0.741  1.504  28.874
98.000 0.711  1.443  28.654
99.000 0.683  1.385  28.433
100.000       0.655  1.329  28.212

Analytic solution function
M_wat(t) = 60.162 * Exp(-0.149 * t) + 39.737 * Exp(-0.041 * t)
M_sed(t) = -80.612 * Exp(-0.149 * t) + 80.612 * Exp(-0.041 * t)
M_met(t) = 22.901 * Exp(-0.149 * t) + -101.746 * Exp(-0.041 * t) + 78.844 * Exp(-
0.010 * t)

EVALUATION

       k_deg_wat    k_deg_sed    k_deg_met
DT50   36.568 13.345 71.461
DT90   121.477      44.332 237.389

MEASURED VERSUS PREDICTED VALUES (%)

Compound:    Parent
Compartment: Water

Time   Measured     Predicted
0.000  100.000      99.899
1.000  90.000 89.974
2.000  81.000 81.265
4.000  67.000 66.873
7.000  51.000 51.017
```

14.000 30.000 29.841
21.000 19.000 19.415
28.000 14.000 13.518
42.000 7.000 7.202
56.000 4.000 4.003
70.000 2.000 2.247
100.000   1.000 0.655

Compound: Parent
Compartment: Sediment

Time   Measured   Predicted
0.000 0.000 0.000
1.000 8.000 7.916
2.000 15.000 14.417
4.000 24.000 23.983
7.000 32.000 32.068
14.000 35.000 35.361
21.000 31.000 30.514
28.000 24.000 24.297
42.000 14.000 14.222
56.000 8.000 8.073
70.000 5.000 4.553
100.000   1.000 1.329

Compound: Metabolite
Compartment: Sediment

Time   Measured   Predicted
0.000 0.000 0.000
1.000 0.000 0.161
2.000 0.000 0.604
4.000 2.000 2.125
7.000 5.000 5.405
14.000 14.000 14.407
21.000 22.000 22.349
28.000 28.000 28.209
42.000 35.000 34.361
56.000 36.000 35.592
70.000 34.000 34.236
100.000   28.000 28.212

STATISTICS

       Complete Data Set
No obs.   36
No act. param.   7
Deg. of Freedom   29
Model error (Chi²) 1.190
Coeff. of Det. (R²) 1.000
Model efficiency   1.000
Abs. deviation   9.114
Quadr. deviation   3.496
SRMSE 0.013
STE   0.011

	Parent/Water	Parent/Sediment	Metabolite
No obs.	12	12	12
No act. param.		3	2	2
Deg. of Freedom		9	10	10
Model error (Chi²)		0.541	1.540	1.727
Coeff. of Det. (R^2)		1.000	0.999	1.000
Model efficiency		1.000	0.999	0.999
Abs. deviation		2.390	2.968	3.756
Quadr. deviation		0.748	1.170	1.577
SRMSE	0.006	0.019	0.021	
STE	0.005	0.015	0.018	

The calibration was done using the Nelder Mead solver by Microsoft Solver Foundation. The implementation of the solver implements the method described in Nelder, J.A. and Mead, R., "A Simplex Method for Function Minimization", Computer Journal 7 (4): 308-313 (Jan., 1965) with the modifications described in Lee, D. and Wiswall, M., "A Parallel Implementation of the Simplex Function Minimization Routine".

A.4.4 Model variant 4: Parent with a single metabolite

DegKinManager - Two-Phase Flow
Evaluation of experimental residue derived via water-sediment studies
developed by Judith Klein and Michael Klein 2018

Version:
Date of this report: 05/12/2018 11:41

INPUT DATA

Selected Model: Parent with a Single Metabolite

Environmental Residues

Time (days)	Parent/Water (%)	Parent/Sediment (%)	Metabolite (%)
0	100	0	0
1	90	8	0
2	81	15	1
4	66	25	3
7	50	33	7
14	28	37	17
21	17	32	27
28	11	26	33
42	6	15	40
56	3	8	41
70	2	5	39
100	0	1	32

Parameters

Name	Initial Value	Lower Bound	Upper Bound	Unit	Fit
f_sed	0.5	0	1	-	True
f_wat	0.5	0	1	-	True
k_deg_met	0.001	0	10000	1/d	True
k_deg_sed	0.01	0	10000	1/d	True
k_deg_wat	0.01	0	10000	1/d	True
k_des	0.5	0	10000	1/d	True
k_sorp	0.5	0.0001	10000	1/d	True
M_met_0	0	0	10000	%	False
M_sed_0	0	0	10000	%	False
M_wat_0	100	0	10000	%	True

OUTPUT DATA

Result of parameter fitting (objective function value: 2.172)

Parameter	Value	Standard Error	Prob > t
f_sed	0.823	1.2017676	2.5202e-01
f_wat	0.104	0.2861216	3.5574e-01
k_deg_met	0.010	0.0452127	4.1289e-01
k_deg_sed	0.051	0.0423635	1.1780e-01
k_deg_wat	0.019	0.0429042	3.2650e-01
k_des	0.024	0.0077955	2.4778e-03
k_sorp	0.088	0.0436678	2.6511e-02
M_met_0	0.000	-	-
M_sed_0	0.000	-	-
M_wat_0	100.024	0.2032202	2.0283e-18

Time (days)	Parent/Water (%)	Parent/Sediment (%)	Metabolite (%)
0.000	100.024	0.000	0.000
1.000	89.927	8.061	0.364
2.000	81.024	14.732	1.015
3.000	73.164	20.210	1.897
4.000	66.218	24.664	2.964
5.000	60.069	28.239	4.175
6.000	54.619	31.064	5.497
7.000	49.780	33.248	6.900
8.000	45.477	34.886	8.360
9.000	41.644	36.060	9.857
10.000	38.224	36.842	11.372
11.000	35.166	37.292	12.891
12.000	32.426	37.463	14.403
13.000	29.967	37.402	15.896
14.000	27.754	37.147	17.363
15.000	25.760	36.731	18.798
16.000	23.957	36.185	20.194
17.000	22.325	35.532	21.547
18.000	20.843	34.795	22.855
19.000	19.495	33.990	24.114
20.000	18.266	33.135	25.323
21.000	17.142	32.241	26.482
22.000	16.112	31.321	27.588
23.000	15.166	30.383	28.643
24.000	14.295	29.436	29.645

25.000 13.492 28.487 30.596
26.000 12.749 27.540 31.497
27.000 12.060 26.601 32.347
28.000 11.421 25.674 33.148
29.000 10.826 24.762 33.902
30.000 10.271 23.866 34.609
31.000 9.753 22.990 35.270
32.000 9.268 22.135 35.888
33.000 8.813 21.301 36.463
34.000 8.386 20.491 36.997
35.000 7.985 19.704 37.491
36.000 7.607 18.940 37.947
37.000 7.251 18.201 38.366
38.000 6.914 17.486 38.750
39.000 6.596 16.795 39.100
40.000 6.295 16.127 39.417
41.000 6.010 15.483 39.703
42.000 5.740 14.862 39.959
43.000 5.483 14.264 40.186
44.000 5.240 13.687 40.386
45.000 5.008 13.132 40.560
46.000 4.788 12.598 40.708
47.000 4.578 12.085 40.833
48.000 4.379 11.591 40.935
49.000 4.189 11.116 41.015
50.000 4.007 10.660 41.074
51.000 3.834 10.222 41.114
52.000 3.669 9.801 41.135
53.000 3.512 9.397 41.137
54.000 3.362 9.010 41.123
55.000 3.218 8.637 41.093
56.000 3.081 8.280 41.048
57.000 2.950 7.937 40.988
58.000 2.824 7.608 40.914
59.000 2.705 7.293 40.827
60.000 2.590 6.990 40.728
61.000 2.481 6.700 40.617
62.000 2.376 6.421 40.496
63.000 2.275 6.154 40.363
64.000 2.179 5.898 40.221
65.000 2.088 5.653 40.069
66.000 2.000 5.417 39.909
67.000 1.916 5.192 39.740
68.000 1.835 4.976 39.564
69.000 1.758 4.768 39.380
70.000 1.684 4.569 39.190
71.000 1.613 4.379 38.993
72.000 1.546 4.196 38.790
73.000 1.481 4.021 38.581
74.000 1.419 3.853 38.367
75.000 1.359 3.693 38.148
76.000 1.302 3.539 37.925
77.000 1.248 3.391 37.697
78.000 1.195 3.249 37.466
79.000 1.145 3.114 37.231
80.000 1.097 2.984 36.992

```
81.000 1.051  2.859  36.751
82.000 1.007  2.740  36.506
83.000 0.965  2.625  36.259
84.000 0.925  2.516  36.010
85.000 0.886  2.411  35.758
86.000 0.849  2.310  35.505
87.000 0.814  2.213  35.250
88.000 0.780  2.121  34.993
89.000 0.747  2.032  34.735
90.000 0.716  1.947  34.476
91.000 0.686  1.866  34.216
92.000 0.657  1.788  33.955
93.000 0.630  1.713  33.694
94.000 0.603  1.642  33.432
95.000 0.578  1.573  33.169
96.000 0.554  1.507  32.906
97.000 0.531  1.445  32.644
98.000 0.509  1.384  32.381
99.000 0.487  1.326  32.118
100.000       0.467  1.271  31.855

Analytic solution function
M_wat(t) = 66.666 * Exp(-0.140 * t) + 33.358 * Exp(-0.043 * t)
M_sed(t) = -90.817 * Exp(-0.140 * t) + 90.817 * Exp(-0.043 * t)
M_met(t) = 28.489 * Exp(-0.140 * t) + -119.224 * Exp(-0.043 * t) + 90.735 * Exp(-
0.010 * t)

EVALUATION

       k_deg_wat     k_deg_sed     k_deg_met
DT50   36.064 13.509 69.615
DT90   119.801       44.874 231.255

MEASURED VERSUS PREDICTED VALUES (%)

Compound:     Parent
Compartment: Water

Time   Measured      Predicted
0.000  100.000       100.024
1.000  90.000 89.927
2.000  81.000 81.024
4.000  66.000 66.218
7.000  50.000 49.780
14.000 28.000 27.754
21.000 17.000 17.142
28.000 11.000 11.421
42.000 6.000  5.740
56.000 3.000  3.081
70.000 2.000  1.684
100.000       0.000  0.467

Compound:     Parent
Compartment: Sediment

Time   Measured      Predicted
```

0.000	0.000	0.000
1.000	8.000	8.061
2.000	15.000	14.732
4.000	25.000	24.664
7.000	33.000	33.248
14.000	37.000	37.147
21.000	32.000	32.241
28.000	26.000	25.674
42.000	15.000	14.862
56.000	8.000	8.280
70.000	5.000	4.569
100.000		1.000 1.271

Compound: Metabolite
Compartment: Water and Sediment

Time	Measured	Predicted
0.000	0.000	0.000
1.000	0.000	0.364
2.000	1.000	1.015
4.000	3.000	2.964
7.000	7.000	6.900
14.000	17.000	17.363
21.000	27.000	26.482
28.000	33.000	33.148
42.000	40.000	39.959
56.000	41.000	41.048
70.000	39.000	39.190
100.000		32.000 31.855

STATISTICS

	Complete Data Set
No obs.	36
No act. param.	8
Deg. of Freedom	28
Model error (Chi²)	0.918
Coeff. of Det. (R²)	1.000
Model efficiency	1.000
Abs. deviation	7.206
Quadr. deviation	2.172
SRMSE	0.010
STE	0.008

	Parent/Water	Parent/Sediment		Metabolite
No obs.	12	12	12	
No act. param.	3	2	3	
Deg. of Freedom	9	10	9	
Model error (Chi²)	0.557	1.217	0.963	
Coeff. of Det. (R²)	1.000	1.000	1.000	
Model efficiency	1.000	1.000	1.000	
Abs. deviation	2.491	2.745	1.969	
Quadr. deviation	0.752	0.792	0.628	

```
SRMSE  0.007  0.015  0.011
STE    0.005  0.013  0.008
```

The calibration was done using the Nelder Mead solver by Microsoft Solver Foundation. The implementation of the solver implements the method described in Nelder, J.A. and Mead, R., "A Simplex Method for Function Minimization", Computer Journal 7 (4): 308-313 (Jan., 1965) with the modifications described in Lee, D. and Wiswall, M., "A Parallel Implementation of the Simplex Function Minimization Routine".

A.5 Documentation of model output: DegKinManager 1.0/ ModelMaker 4.0

A.5.1 Model variant 1: Parent without metabolites

```
D E G K I N
Evaluation of experimental residues based on ModelMaker 4.0

developed by Michael Klein


Program version:                        1.0 (25 November 2014)
Date of this report    :                05.12.2018, 09:02:19
Project:                                Validation_Model1.prj



INPUT DATA CONSIDERED FOR THE FITTING

Kinetic model:          Water sediment - without metabolites

Experimental residues (%)

       Time            Parent  Water    Parent Sediment
        0.00                  100.00              0.00
        1.00                   90.00              8.00
        2.00                   81.00             15.00
        4.00                   66.00             25.00
        7.00                   50.00             33.00
       14.00                   28.00             37.00
       21.00                   17.00             32.00
       28.00                   11.00             26.00
       42.00                    6.00             15.00
       56.00                    3.00              8.00
       70.00                    2.00              5.00
      100.00                    0.00              1.00



RESULTS OF THE FITTING

R²:                     0.99992 (complete data set, n =24)


Parameter                    Value              Error     Prop > t
       M0                  100.0200             1.8390    4.54E-09
k_deg_wat                    0.0194             0.0078    0.017649
k_deg_sed                    0.0511             0.0076    0.000026
   k_sorp                    0.0879             0.0060    6.73E-08
    k_des                    0.0238             0.0080    0.006907
```

MINIMUM ERROR FOR PASSING CHI²-TEST (%)

Compound	Value	Degrees of Freedom	DT50
	DT90	Compartment	
Parent	0.58525	9	35.82 118.98
	Water		
Parent	1.23090	10	13.57 45.09
	Sediment		

MEASURED VERSUS PREDICTED VALUES (%)

Compound: Parent

Time	Measured	Predicted	Residuals
Compartment: Water			
0.00	100.00	100.02	0.02
1.00	90.00	89.88	-0.12
2.00	81.00	80.94	-0.06
4.00	66.00	66.10	0.10
7.00	50.00	49.65	-0.35
14.00	28.00	27.66	-0.34
21.00	17.00	17.10	0.10
28.00	11.00	11.41	0.41
42.00	6.00	5.75	-0.25
56.00	3.00	3.09	0.09
70.00	2.00	1.69	-0.31
100.00	0.00	0.47	0.47
Compartment: Sediment			
0.00	0.00	0.00	0.00
1.00	8.00	8.10	0.10
2.00	15.00	14.81	-0.19
4.00	25.00	24.77	-0.23
7.00	33.00	33.36	0.36
14.00	37.00	37.22	0.22
21.00	32.00	32.27	0.27
28.00	26.00	25.69	-0.31
42.00	15.00	14.87	-0.13
56.00	8.00	8.29	0.29
70.00	5.00	4.58	-0.42
100.00	1.00	1.28	0.28

A.5.2 Model variant 2: Parent with a single metabolite in water

D E G K I N
Evaluation of experimental residues based on ModelMaker 4.0

developed by Michael Klein

Program version: 1.0 (25 November 2014)

Date of this report : 05.12.2018, 15:33:43
Project: Validation_Model2.prj

INPUT DATA CONSIDERED FOR THE FITTING

Kinetic model: Water sediment - Metabolite formed in water only

Experimental residues (%)

Time	Parent Water	Parent Sediment	Met. 1
0.00	100.00	0.00	0.00
1.00	90.00	8.00	0.00
2.00	81.00	15.00	1.00
4.00	67.00	24.00	1.00
7.00	51.00	32.00	2.00
14.00	30.00	35.00	3.00
21.00	19.00	31.00	3.00
28.00	14.00	24.00	4.00
42.00	7.00	14.00	4.00
56.00	4.00	8.00	4.00
70.00	2.00	5.00	3.00
100.00	1.00	1.00	3.00

RESULTS OF THE FITTING

R^2: 0.99988 (complete data set, n =36)

Parameter	Value	Error	Prop > t
M0	99.9300	1.8656	4.54E-09
k_deg_M1	0.0079	0.0124	0.269426
k_deg_wat	0.0189	0.0083	0.024573
k_deg_sed	0.0520	0.0091	0.000096
k_sorp	0.0873	0.0062	1.04E-07
k_des	0.0326	0.0095	0.003142
f_wat	0.2121	0.1339	0.071931

MINIMUM ERROR FOR PASSING CHI^2-TEST (%)

Compound	Value DT90	Degrees of Freedom Compartment	DT50
Parent	0.56339	9	36.67 121.83
	Water		
Parent	1.52881	10	13.32 44.25
	Sediment		
Metabolite 1	9.81708	10	87.95 292.15

MEASURED VERSUS PREDICTED VALUES (%)

Compound: Parent

Time	Measured	Predicted	Residuals
Compartment: Water			
0.00	100.00	99.93	-0.07
1.00	90.00	89.93	-0.07
2.00	81.00	81.17	0.17
4.00	67.00	66.72	-0.28
7.00	51.00	50.85	-0.15
14.00	30.00	29.76	-0.24
21.00	19.00	19.41	0.41
28.00	14.00	13.55	-0.45
42.00	7.00	7.23	0.23
56.00	4.00	4.02	0.02
70.00	2.00	2.26	0.26
100.00	1.00	0.66	-0.34
Compartment: Sediment			
0.00	0.00	0.00	0.00
1.00	8.00	8.01	0.01
2.00	15.00	14.57	-0.43
4.00	24.00	24.19	0.19
7.00	32.00	32.27	0.27
14.00	35.00	35.42	0.42
21.00	31.00	30.47	-0.53
28.00	24.00	24.21	0.21
42.00	14.00	14.14	0.14
56.00	8.00	8.02	0.02
70.00	5.00	4.52	-0.48
100.00	1.00	1.32	0.32

Compound: Metabolite 1

Time	Measured	Predicted	Residuals
0.00	0.00	0.00	0.00
1.00	0.00	0.38	0.38
2.00	1.00	0.72	-0.28
4.00	1.00	1.30	0.30
7.00	2.00	1.96	-0.04
14.00	3.00	2.92	-0.08
21.00	3.00	3.42	0.42
28.00	4.00	3.68	-0.32
42.00	4.00	3.83	-0.17
56.00	4.00	3.72	-0.28
70.00	3.00	3.49	0.49
100.00	3.00	2.89	-0.11

A.5.3 Model variant 3: Parent with a single metabolite in sediment

D E G K I N

Evaluation of experimental residues based on ModelMaker 4.0

developed by Michael Klein

Program version: 1.0 (25 November 2014)
Date of this report : 05.12.2018, 15:33:47
Project: Validation_Model3.prj

INPUT DATA CONSIDERED FOR THE FITTING

Kinetic model: Water sediment - Metabolite formed in sediment only

Experimental residues (%)

Time	Parent Water	Parent Sediment	Met. 1
0.00	100.00	0.00	0.00
1.00	90.00	8.00	0.00
2.00	81.00	15.00	0.00
4.00	67.00	24.00	2.00
7.00	51.00	32.00	5.00
14.00	30.00	35.00	14.00
21.00	19.00	31.00	22.00
28.00	14.00	24.00	28.00
42.00	7.00	14.00	35.00
56.00	4.00	8.00	36.00
70.00	2.00	5.00	34.00
100.00	1.00	1.00	28.00

RESULTS OF THE FITTING

R^2: 0.99986 (complete data set, n =36)

Parameter	Value	Error	Prop > t
M0	99.9000	1.8758	4.54E-09
k_deg_M1	0.0097	0.0022	0.000718
k_deg_wat	0.0190	0.0087	0.028036
k_deg_sed	0.0518	0.0097	0.000168
k_sorp	0.0869	0.0062	9.88E-08
k_des	0.0322	0.0096	0.003661
f_sed	0.7638	0.1648	0.000464

MINIMUM ERROR FOR PASSING CHI^2-TEST (%)

Compound	Value	Degrees of Freedom	DT50	DT90	Compartment
Parent	0.55749	9	36.44	121.05	Water
Parent	1.52245	10	13.39	44.47	Sediment

Metabolite 1 1.67558 10 71.32 236.93

MEASURED VERSUS PREDICTED VALUES (%)

Compound: Parent

Time	Measured	Predicted	Residuals
Compartment: Water			
0.00	100.00	99.90	-0.10
1.00	90.00	89.92	-0.08
2.00	81.00	81.18	0.18
4.00	67.00	66.75	-0.25
7.00	51.00	50.88	-0.12
14.00	30.00	29.76	-0.24
21.00	19.00	19.39	0.39
28.00	14.00	13.52	-0.48
42.00	7.00	7.21	0.21
56.00	4.00	4.01	0.01
70.00	2.00	2.25	0.25
100.00	1.00	0.66	-0.34
Compartment: Sediment			
0.00	0.00	0.00	0.00
1.00	8.00	7.97	-0.03
2.00	15.00	14.51	-0.49
4.00	24.00	24.11	0.11
7.00	32.00	32.20	0.20
14.00	35.00	35.43	0.43
21.00	31.00	30.53	-0.47
28.00	24.00	24.28	0.28
42.00	14.00	14.21	0.21
56.00	8.00	8.06	0.06
70.00	5.00	4.55	-0.45
100.00	1.00	1.33	0.33

Compound: Metabolite 1

Time	Measured	Predicted	Residuals
0.00	0.00	0.00	0.00
1.00	0.00	0.15	0.15
2.00	0.00	0.58	0.58
4.00	2.00	2.09	0.09
7.00	5.00	5.37	0.37
14.00	14.00	14.40	0.40
21.00	22.00	22.36	0.36
28.00	28.00	28.22	0.22
42.00	35.00	34.37	-0.63

56.00	36.00	35.60	-0.40
70.00	34.00	34.23	0.23
100.00	28.00	28.20	0.20

A.5.4 Model variant 4: Parent with a single metabolite

D E G K I N
Evaluation of experimental residues based on ModelMaker 4.0

developed by Michael Klein

Program version: 1.0 (25 November 2014)
Date of this report : 05.12.2018, 15:33:55
Project: Validation_Model4.prj

INPUT DATA CONSIDERED FOR THE FITTING

Kinetic model: Water sediment - Metabolite formed in water and sediment

Experimental residues (%)

Time	Parent Water	Parent Sediment	Met. 1
0.00	100.00	0.00	0.00
1.00	90.00	8.00	0.00
2.00	81.00	15.00	1.00
4.00	66.00	25.00	3.00
7.00	50.00	33.00	7.00
14.00	28.00	37.00	17.00
21.00	17.00	32.00	27.00
28.00	11.00	26.00	33.00
42.00	6.00	15.00	40.00
56.00	3.00	8.00	41.00
70.00	2.00	5.00	39.00
100.00	0.00	1.00	32.00

RESULTS OF THE FITTING

R^2: 0.99991 (complete data set, n =36)

Parameter	Value	Error	Prop > t
M0	100.0100	1.8438	4.54E-09
k_deg_M1	0.0099	0.0022	0.000772
k_deg_wat	0.0192	0.0080	0.019492
k_deg_sed	0.0512	0.0078	0.000033
k_sorp	0.0880	0.0060	6.46E-08
k_des	0.0238	0.0081	0.007401
f_sed	0.8214	0.1856	0.000830
f_wat	0.1096	0.2442	0.333596

MINIMUM ERROR FOR PASSING CHI²-TEST (%)

Compound	Value	Degrees of Freedom	DT50	DT90	Compartment
Parent	0.58197	9	36.08	119.86	Water
Parent	1.24679	10	13.53	44.96	Sediment
Metabolite 1	0.95683	9	69.67	231.44	

MEASURED VERSUS PREDICTED VALUES (%)

Compound: Parent

Time	Measured	Predicted	Residuals
Compartment: Water			
0.00	100.00	100.01	0.01
1.00	90.00	89.87	-0.13
2.00	81.00	80.94	-0.06
4.00	66.00	66.11	0.11
7.00	50.00	49.66	-0.34
14.00	28.00	27.67	-0.33
21.00	17.00	17.10	0.10
28.00	11.00	11.41	0.41
42.00	6.00	5.74	-0.26
56.00	3.00	3.08	0.08
70.00	2.00	1.69	-0.31
100.00	0.00	0.47	0.47
Compartment: Sediment			
0.00	0.00	0.00	0.00
1.00	8.00	8.11	0.11
2.00	15.00	14.82	-0.18
4.00	25.00	24.79	-0.21
7.00	33.00	33.39	0.39
14.00	37.00	37.23	0.23
21.00	32.00	32.27	0.27
28.00	26.00	25.68	-0.32
42.00	15.00	14.85	-0.15
56.00	8.00	8.27	0.27
70.00	5.00	4.56	-0.44
100.00	1.00	1.27	0.27

Compound: Metabolite 1

Time	Measured	Predicted	Residuals
0.00	0.00	0.00	0.00
1.00	0.00	0.36	0.36
2.00	1.00	1.01	0.01
4.00	3.00	2.95	-0.05
7.00	7.00	6.89	-0.11
14.00	17.00	17.37	0.37
21.00	27.00	26.50	-0.50
28.00	33.00	33.16	0.16
42.00	40.00	39.96	-0.04
56.00	41.00	41.04	0.04
70.00	39.00	39.18	0.18
100.00	32.00	31.85	-0.15

References

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List of abbreviations

Abbreviation	Description
DegT50	half-life in a medium due to degradation (transformation) processes
DT50	half-life in a medium due to degradation (transformation) and other processes such as volatilisation and leaching
FOCUS	FOrum for the Co-ordination of pesticide fate models and their USe
LOD	limit of detection
LOQ	limit of quantification
SFO	single first order kinetics
UBA	Umweltbundesamt