A new approach to simplify degradation kinetics

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Abstract

Simultaneous evaluation of all degradation data available for one environmental compartment using non-linear hierarchical models (NLHM) is suggested as efficient way to derive more realistic endpoints.

Current evaluation practice

In order to obtain DT_{50} values and formation fractions, degradation data of chemicals in the environment are currently analysed following FOCUS degradation kinetic guidance [1]. Therefore, separate evaluations of each data set and for different regulatory purposes are performed. The resulting degradation parameters are subsequently averaged (modelling endpoints) or only the longest derived DT_{50} is used (persistence endpoints).
The selection of the degradation model to best represent the observed residue pattern of each data set is heavily based on expert judgement and is thus often unpredictable and time consuming.
Besides, an arbitrary default value of 1000 days is chosen, when no robust DT_{50} can be derived for one of the data sets.
The resulting degradation parameters on the other hand are used in the environmental exposure and risk assessment and are the basis for important regulatory decisions like PBT classification and risk management. They should therefore be as robust and precise as possible.

Non-linear hierarchical models (NLHM)

A simultaneous evaluation of all individual datasets of environmental degradation data is possible using NLHM [2], also termed non-linear mixed-effect models or multilevel models. NHLM incorporate different models for the distribution of the degradation parameters, the variation of the residuals and the distribution of the parameters over the population (Figure 1).

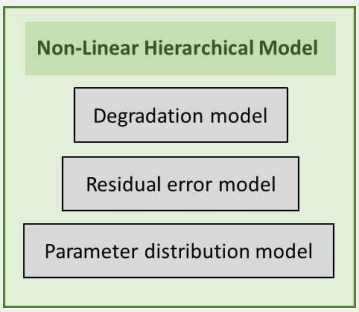

Figure 1: Components of NLHM

Degradation model:
SFO, DFOP, FOMC, HS

Residual error model:
e.g. constant variance, variance by variable, two-component error

Parameter distribution model:
Log-normal distribution for rate constants, normal distribution after logit or other suitable transformation for f.f.

An example of a kinetic assessment of a real data set evaluated with NLHM is shown in Figure 2. With NLHM, average degradation parameters over the complete available data set are derived. However, also degradation parameters for each individual data set will be obtained with NLHM, thus allowing for further analysis e.g the choice of differing endpoints for persistence assessment and/or for dependencies of the degradation on co-variables (e.g. pH of the soil), which can then be incorporated in the degradation model.

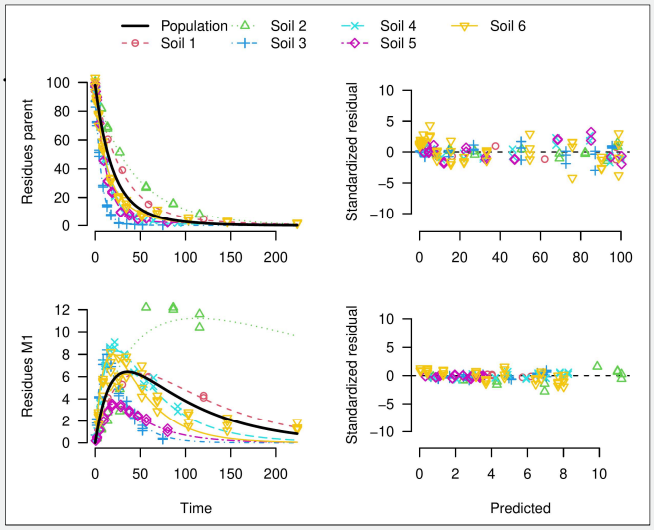

Figure 2: Kinetic evaluation of the degradation of an active substance with one metabolite in 6 soils applying NLHM (kinetic model: DFOP-SFO, residual model: constant variance)

Advantages of NLHM for kinetic assessment

Due to the simultaneous simulation, only one choice of the models best describing the residue data is required for the complete data set thus reducing decisions based on expert judgement.
The obtained degradation parameters are based on a synopsis of all available data and thus generally more robust. This makes the derivation of reliable degradation parameters also for slowly degrading compounds or for transformation products with an ill defined decline phase more likely. Since poor individual data sets are evaluated in context of the other available data, the use of arbitrary default values can be avoided.

Outlook

Further testing and refinements of the interface connecting NLHM software with currently used kinetic software are in progress [3]. The software will subsequently be simplified and made accessible to all kinetic experts for exploration and further testing.
Aspired future goal is the use of NHLM for kinetic evaluation of environmental degradation data in the regulatory context.

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