Data from degradation experiments in various environmental media are routinely evaluated using different software packages to derive parameters that can be used for the purpose of fate modelling or for comparison with regulatory trigger values in the environmental risk assessment. Especially parameter estimation for degradation models including formation and decline of transformation products or phase transfer processes, while possible in almost any programming language or mathematical software toolkit, is greatly simplified by software tools that have been tailored to this task.

The software packages ModelMaker and KinGUI v.1 that were frequently used for this purpose have not received any updates since many years. Meanwhile, some new, actively maintained tools have been published that specialise in fitting solutions of systems of differential equations to experimental data.

This poster reports the results of a multicriteria evaluation of these software tools on behalf of the German Federal Environment Agency (UBA), including a validity check using a number of example datasets.

The system of evaluation criteria established for this purpose includes the areas of functionality, performance, user interface and user friendliness, extensibility and documentation. The weighting of the criteria, which was agreed with UBA, is different for two user groups A and B. For user group A, which should represent 80% of the use cases, the focus is on usability. For user group B, the flexibility in the model definition is most important. After the screening of at first 15 candidate tools the software tools KinGUII, gmkin, CAKE and OpenModel were selected for the further check of validity and final rating.

A validity check was performed by comparing the results for a suite of partly newly generated test datasets. Generally, good agreement between the tools was observed for datasets with up to three metabolites. For the different tools, user options were identified that should be taken care of in order to obtain results that are as reliable as possible.

KinGUII and gmkin obtained the highest scores in the final evaluation for user groups A and B. CAKE was found to be a valid alternative for user group A, provided the degradation scheme is sufficient for the dataset at hand. Subject to some caveats, the flexible OpenModel software package that is built using a different technical basis was found to be a possible independent alternative for user group B.