mkin - Routines for fitting kinetic models with one or more state variables to chemical degradation data

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Abstract

In the regulatory evaluation of chemical substances like plant protection products (pesticides), biocides and other chemicals, degradation data play an important role. For the evaluation of pesticide degradation experiments, detailed guidance has been developed, based on nonlinear optimisation. The R add-on package **mkin** implements fitting some of the models recommended in this guidance from within R and calculates some statistical measures for data series within one or more compartments, for parent and metabolites.

Contents

Key words: Kinetics, FOCUS, nonlinear optimisation

1 Introduction

Many approaches are possible regarding the evaluation of chemical degradation data. The **kinfit** package (Ranke, 2013a) in R (R Development Core Team, 2013) implements the approach recommended in the kinetics report provided by the FOrum for Co-ordination of pesticide fate models and their USe (FOCUS Work Group on Degradation Kinetics, 2006, 2011) for simple data series for one parent compound in one compartment.

The **mkin** package (Ranke, 2013b) extends this approach to data series with metabolites and more than one compartment and includes the possibility for back reactions.

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