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KinOpt: A Python package for chemical kinetics analysis and optimization

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Software

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Summary

KinOpt is a Python package designed to streamline the process of kinetic data analysis and optimization with a suite of features tailored to meet the diverse needs of researchers.

Chemical reaction kinetics are a frequent research topic, and modeling them is becoming increasingly common (Corezzi et al., 2010; Dimier et al., 2004; Wang et al., 2022). Generally, this modeling is taken into account by means of temperature dependence $g(T)$ coupled to a model of reaction $f(\alpha)$:

$$\frac{d\alpha}{dt} = g(T) \times f(\alpha)$$

with $\frac{d\alpha}{dt}$ the rate of reaction, α the extent of reaction, and T the temperature.

In most cases, the temperature dependence is an Arrhenius law: $g(T) = A\exp^{(\frac{-E_a}{RT})}$, with A the pre-exponential factor, E_a the activation energy, and R the universal gas constant. But this temperature dependence is not always valid. To ensure its validity, isoconversional analysis can be performed. This isoconversional analysis consists of retrieving the reaction parameters (temperature and reaction rate) at a specific stage of the chemical reaction in order to obtain the parameters of certain kinetic models (such as the activation energy of the reaction). Isoconversional analysis is also a method that can be used to elucidate actual reaction mechanisms (thereby facilitating the selection of the appropriate $f(\alpha)$ reaction model).

The selection of a kinetic equation does not guarantee the optimization of the model to the experimental data, particularly in cases of a complex topology of the response surface (as seen in Adenson et al. (2018)). Consequently, the efficacy of multiple optimization strategies must be thoroughly evaluated.

Statement of need

The motivation behind the creation of this software stems from two primary factors: 1. There is currently no open-source software available for isoconversional analysis or kinetic model optimization. 2. The identification, implementation, and use of isoconversional methods or reaction models is a time-consuming process, necessitating the selection of an appropriate optimization method and cost function to find the parameters of the kinetic model. Furthermore, the risk of human error increases with each step in this process.

The Python programming language was selected due to its ubiquity and user-friendliness and on the basis that the optimizations required for isoconversional methods and for fitting the parameters of kinetic models do not necessitate exceptional computational performance.

Additionally, the connection between the code and the graphical interface is straightforward. Finally, given the prevalence of non-programmers within the field of chemical reaction kinetics, the adoption of a straightforward programming language such as Python facilitates enhanced contributions from this community (*for example, a reaction model not included in the program can be added simply by defining a function starting with* `rate_` *in the* `kinetic_models.py` file).

Key Features of KinOpt:

- **Isoconversional Analysis**: Uncover the conversion dependence of activation energies through rigorous isoconversional analysis. The current version of KinOpt supports three different methods: Friedman method (Sbirrazzuoli, 2007), Vyazovkin method (Vyazovkin, 1997) and Advanced Vyazovkin method (Vyazovkin, 2008).
- **Kinetic Rate Law Selection**: Select your reaction model using standard reaction law such as n-th order reaction, autocatalytic reaction, Kamal and Sourour model (Sourour & Kamal, 1976). You can also add a vitrification/diffusion term if necessary.
- **Kinetic Rate Law Optimization**: Fine-tune the parameters of the main kinetic rate law using global and local optimization algorithms (Virtanen et al., 2020), ensuring accurate modeling of reaction kinetics under various conditions.
- **User-Friendly Interface**: Navigate effortlessly through KinOpt's intuitive graphical user interface (GUI), making complex analyses accessible to users of all levels.
- **Easy Data Interpretation and Management**: Generate results files that are seamlessly readable within KinOpt, simplifying the process of analyzing and interpreting kinetic data. All data used for optimization can be found in a human-readable `.txt` file.

Documentation

The project's documentation is hosted on readthedocs at: KinOpt Documentation.

Tutorials are also available on **Youtube**.

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