PyKineMod: A Software Tool for Automated Modeling of Reaction Systems from Data

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Highlights

- Software for automated modelling of complex homogeneous reaction systems
- Includes data preprocessing, automated raw law generation modules
- Incremental and simultaneous methods for identifying rate laws and parameter estimates

1. Introduction

Kinetic modeling of reaction systems is an important step for model-based scale-up, optimization and control of chemical reactors. Typically, kinetic modeling is performed in a stepwise manner. First, a set of experiments is designed based on a priori knowledge of the system and experimental data are generated by performing the experiments. The human modeler uses the experimental data and a priori knowledge of reaction systems to postulate candidate stoichiometries and possible kinetic models for each reaction. Then, an optimization problem is formulated to identify a reliable kinetic model from data [1,2]. Here, all combinations of stoichiometries and reaction kinetic candidates are tested to find a reliable kinetic model from data. This is a time-consuming and costly exercise [1]. Furthermore, some of the sub problems may not converge. This approach for kinetic modeling is called "simultaneous identification approach" and it leads to optimal parameter estimates from data. Alternatively, the "incremental model identification" approach decomposes the model identification task into a set of subtasks such as stoichiometry identification, computing contribution of individual reaction rate, a reaction-rate and corresponding parameter identification each reaction from a set of rate candidates, and refining the identified parameters for the final identified kinetic models [3,4]. In this manner, the combinatorial complexity of the simultaneous model identification is avoided. In this work, we present "PyKineMod", python-based software for rapid kinetic identification of reaction systems using concentration data.

2. Methods

The overview of the software framework of PyKineMod and submodules is given in Figure 1. The major submodules in PyKineMod are as follows: (i) Data preprocessing, (ii) datatools, (iii) ratelawgenerator, (iv) simulate, and (v) incremental. The functionality of different modules is given next. The objective of the data preprocessing module is to reduce noise in concentration data and obtain the filtered data. The datatools module handles different input types such as experimental conditions, stoichiometry, species molecular weights, reactor types ("batch", "semi-batch", "CSTR") that are supplied to the incremental model object. The ratelawgenerator module automatically generates different types of reaction-rate candidates using the stoichiometric information. The "simulate" module allows simulating reaction systems for the specified reaction systems under different conditions.

The "incremental" module performs the kinetic model identification task using the set of models generated by "ratelawgenerator" module and denoised concentration data from the data preprocessing module and the "simulate" module. In this software, two-types of the incremental model identification approaches, namely, the extent-based and the rate-based approaches are implemented. Statistically unbiased parameter estimates are generated using the simultaneous identification approach and the outputs obtained from the previous step in the incremental approach.

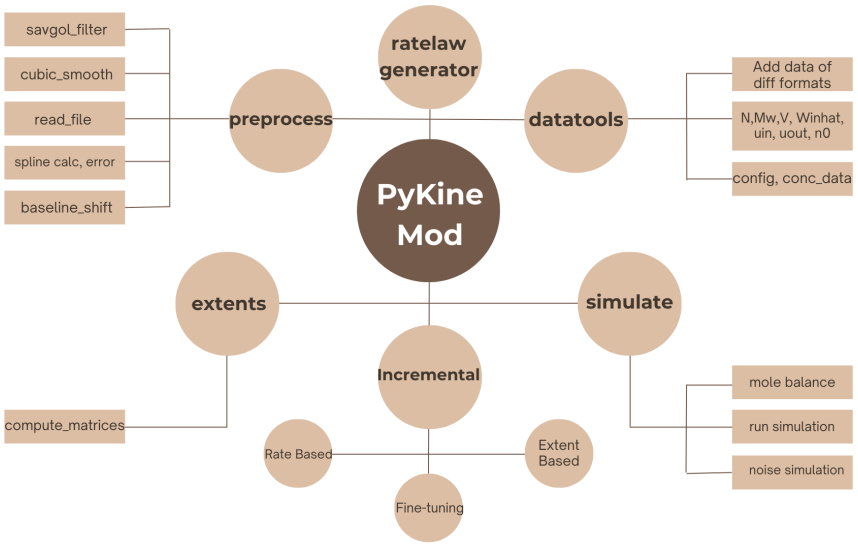

Figure 1: Overview of the PyKinMod and its modules and submodules for Kinetic modeling.

3. Results

PyKineMod has been tested on several complex reaction systems. Specifically, we present results from two reaction systems, namely, acetoacetylation of pyrrole, and ethanolysis of phthalyl chloride. Both reaction systems involve multiple reactions. It has been shown that the PyKineMod tool can identify reaction-rate expressions and corresponding parameters without any inputs from the human-modeller. It also provides the final summarized fitting for each reaction and the fine-tuned models. This summary can be used for gaining a better mechanistic understanding of the reaction systems.

4. Conclusions

An automated kinetic modelling software for homogeneous reaction systems from concentration data. is presented. It implements the incremental model identification approach for rapid discrimination of different rate expression candidates and obtaining an initial guess of parameters. It also fine-tunes the identified kinetic models for obtaining statistically optimal parameter estimates using the simultaneous model identification approach. In the future, PyKineMod will be extended to model heterogeneous reaction systems. Furthermore, it will be extended to handle spectral data in the plug flow reactors.

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Keywords

Automated Kinetic Modelling, Incremental Identification, Software Tool, Concentration Data