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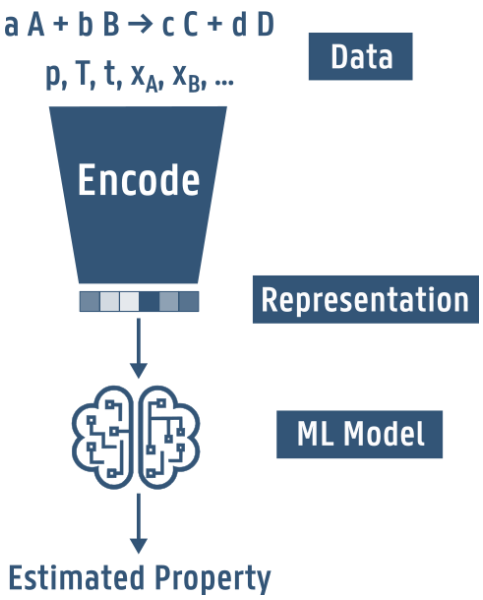
Machine Learning Meets Kinetic Modeling: Predicting Activation Energies and Pre-Exponential Factors

Aim

The aim of this master thesis is to generate machine learning models for estimating rate coefficients of free-radical reactions in pyrolysis and combustion processes. This model can be used in combination with a model for predicting thermochemical properties (enthalpies, entropies, heat capacities) for "learning" kinetic models.

Justification



Accurately estimating reaction properties is essential in several applications such as automatic kinetic model generation or planning synthesis routes for developing new drugs. Several methods are currently used for calculating rate coefficients: such as high-level *ab initio* methods and Benson group additivity schemes. *Ab initio* methods achieve high accuracy but are computationally very expensive. Automatic kinetic model generation tools, such as Genesys, make use of group additivity for making accurate predictions at a minimal computational cost. The main drawback of the latter method is its application range: group additive values must be available for all groups in each molecule. Moreover, extra correction factors for ring strain are required when dealing with cyclic species. Cyclic and – more specifically – polycyclic species are expected to play an important role in future pharmaceutical applications and in processes using renewable feedstocks (e.g. lignin, plastic waste, …). Since it is impossible to create corrections for all possible polycyclic combinations and group additivity schemes are not able to achieve high accuracy for polycyclic species, machine learning models are a promising alternative. This has been shown for molecular properties and can be extended to reaction properties. Because chemical reactions are different, more complex data structures than molecules, upgrading from a molecular property prediction method to a reaction property prediction method is not straightforward. Using machine learning for estimating kinetics parameters fits in the context of developing a self-learning kinetics estimator.

Program

- Literature survey on existing machine learning methods for reaction property prediction
- Data curation: generating clean datasets of reaction properties in pyrolysis and combustion processes
- Create the architecture of a machine learning model and train this model on the curated datasets
- Train the model on existing benchmarks and compare with literature results

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