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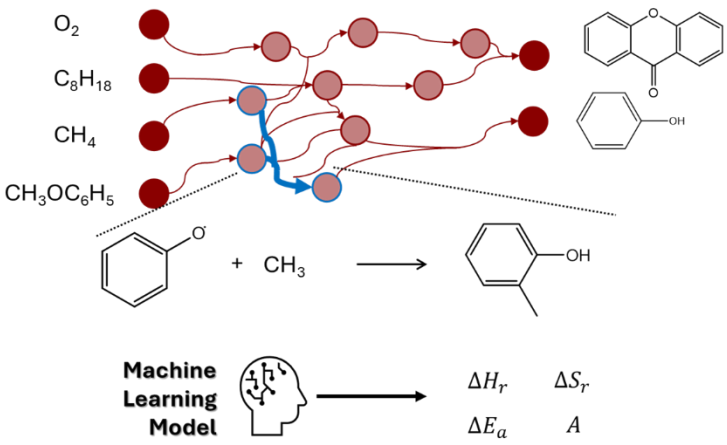
Kinetic Modeling of the Combustion of Lignin-based Biofuels: a Machine Learning Approach

Aim

The aim of this thesis is to develop a kinetic model for the combustion of lignin-based biofuels, by combining first-principle modeling with machine learning. This should lead to new insights into the formation of oxygenated aromatics during this process.

Justification



Recent studies show that around 80% of the worldwide energy production originates from the combustion of fossil fuels. To shift toward more environmentally friendly alternatives, researchers have been exploring the chemistry of renewable energy sources such as biofuels. Lignin, which is one of the main components of biomass, has been shown to be a valuable precursor of these biofuels. However, the combustion of lignin-based biofuels often leads to the formation of oxygenated aromatics. These species, and more specifically the oxygenated polycyclic aromatic hydrocarbons, are more toxic than their non-oxygenated counterparts. It is thus of great interest to understand the chemistry of this formation process.

First-principle kinetic models have shown their value in many combustion and pyrolysis applications. These types of kinetic models are based on the fundamental chemistry of the process and are therefore the ideal tool for identifying dominant reaction pathways. The development of such a model usually takes two major steps: the generation of the reaction network, and the assignment of thermochemical and kinetic properties to the molecules and reactions in the network. This second step often relies on the group additivity method. However, this method cannot describe longer-range interactions, which are present in aromatic species well. Over recent years, machine learning models have been shown to be a promising alternative to predict these properties.

In this thesis, a detailed kinetic model will be developed, and the effect of the implementation of machine learning in this modeling approach will be evaluated.

Program

- Literature survey on the combustion of lignin-based biofuels.
- Development of a reaction network for the combustion of lignin-based biofuels.
- Development of machine learning models predicting thermochemical/kinetic properties.
- Evaluation of the obtained kinetic model.

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