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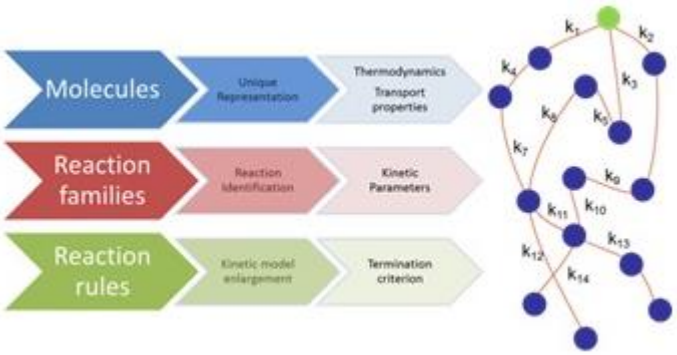
Genesys: Automatic generation of kinetic models for hetero-atomic compounds

Aim

The aim of this master thesis is to develop ab initio kinetic models for the pyrolysis of hetero-atom (nitrogen, oxygen and sulphur) containing compounds via newly calculated group additive values.

Justification

In the European chemical industry, there is a strong drive to shift to renewable and alternative feedstocks in the pursuit of sustainability and increased profitability.These feeds entail a wide variety of hetero-atomic species, which have a different chemical behavior compared to hydrocarbon molecules. As these compounds can negatively influence the process, operability and quality of the products streams, having a mathematical model able to describe their influence is essential for the future development and integration of renewable and alternative process streams.



Accurate chemical kinetic models are extremely powerful and valuable. Many significant public policy and business decisions are and have been made on the basis of predictions using detailed kinetic models. However, for most technologically important systems constructing a reliable and sizable kinetic model remains to be very difficult and time consuming. Recent advancements in chemistry and informatics have enabled a new kinetic modelling approach of tracking each molecule and intermediate throughout the reaction process using fundamental kinetics information. Several tools have been developed to automatically build large kinetic models, such as the in-house developed automatic network generator Genesys. When constructing such large reaction networks, the availability of accurate thermodynamic data for all species and rate coefficients for all possible reactions is a prerequisite. For hetero-atomic compounds, lack of this type of information is in most cases the limiting factor of these network generation tools. A systematic approach to address this problem of data scarcity consists of the development of group additivity models based on high-level computational methods.

Program

- Evaluating the existing group additivity values from literature and collaborators in Genesys.
- Determining new thermodynamic and kinetic group additivity values from ab initio calculations and implementing them in Genesys.
- Building kinetic models for the pyrolysis of hetero-atomic species and validating them to experimental data.

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