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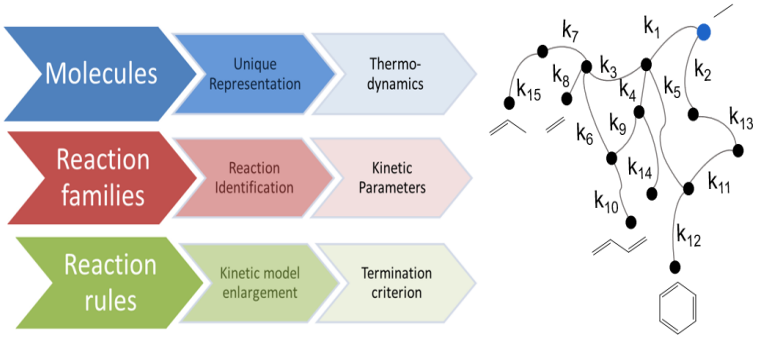
Genesys: Automatic generation of kinetic models for pyrolysis of hetero-atomic compounds in steam cracking

Aim

The aim of this thesis is to develop a kinetic model for the pyrolysis of hetero-atomic compounds, through combined theoretical calculations, kinetic modelling and experimental work.

Justification

Plastic waste recycling has become increasingly more popular in recent years. Classic methods such as incineration or landfilling are being replaced with more circular processes. One way to recycle plastic waste is by chemical recycling of plastic waste and employing it as a feedstock for steam cracking processes. Through this process, the plastic waste stream is recycled into new building blocks such as ethylene, propylene, ethane, acetylene, styrene and so on.



The downside of plastic waste recycling is that this stream does not contain pure hydrocarbons, but also hetero-atomic contaminants. Food waste, polymer additives and polymer structure will introduce impurities containing oxygen, nitrogen, chlorine and bromine among others. As these impurities can negatively influence the process, operability and quality of the product streams, having a mathematical model able to describe their influence is essential for the future integration of plastic waste as a feedstock.

In order to understand the influence of large hydrocarbon and hetero-atomic fuels for steam cracking, it is crucial to first have a detailed understanding of the pyrolysis kinetics of small and simple fuels. A study is done for the thermal decomposition of small fuels with hetero-atomic impurities. The result of this study will be used in the development of a kinetic model for the pyrolysis of these fuels. A kinetic model for small compounds will be constructed automatically with the use of Genesys, an in-house developed automatic network generator. On-the-fly fast estimation techniques for thermodynamic properties and kinetic parameters, such as group additivity, often lead to bigger errors when used for smaller molecules. For this reason, some thermodynamic and kinetic parameters will be determined with quantum mechanical techniques. Literature based or in-house developed experimental data will be used to extensively validate the developed kinetic model.

Program

- Literature survey regarding experimental and modelling studies for the pyrolysis of selected model compounds.
- Determination of thermodynamic properties and reaction rate coefficients with ab initio techniques.
- Generation of a kinetic model for the model compounds automatically with Genesys. Validation of the kinetic model with literature or new experimental datasets.

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