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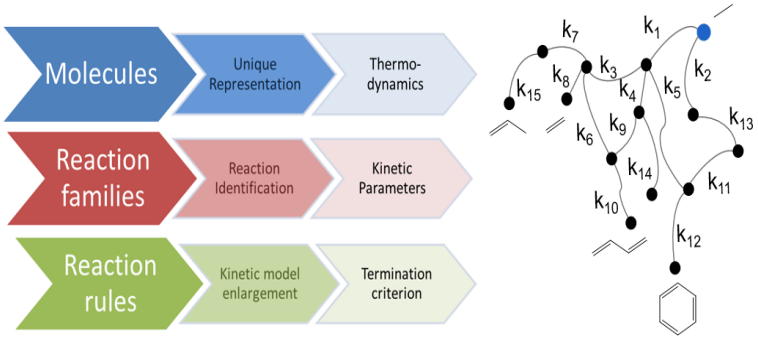
# Pyrolysis of chlorinated hydrocarbons in steam cracking: a combined modelling and experimental study

## Aim

The aim of this thesis is to develop a kinetic model for the pyrolysis of chlorinated hydrocarbons 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 heteroatomic 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 heteroatomic 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 chlorinated alkanes. The result of this study will be used in the development of a kinetic model for the pyrolysis of these molecules. 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. Based on earlier results, the model will be extended from chloroethane to chloropropane and possibly up to chloropentane. Literature based or in-house developed experimental data will be used to extensively validate the developed kinetic model.

## Program

- Literature survey on the composition of heteroatomic impurities in plastic pyrolysis oils and research regarding experimental and modelling studies for the pyrolysis of the selected chlorinated hydrocarbon model compounds.
- Extension of databases with thermodynamic and kinetic parameters for larger chlorinated hydrocarbons obtained from high-level quantum chemical calculations
- Generation of a kinetic model for chlorinated alkanes automatically with Genesys. Validation of the kinetic model with literature or new experimental datasets.

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