LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 914, 9052 Gent, Belgium

Coaches	Supervisors	Funding
dr. ir. Ruben Van de Vijver	dr. ir. Ruben Van de Vijver, prof. dr. ir. Kevin M. Van Geem	-

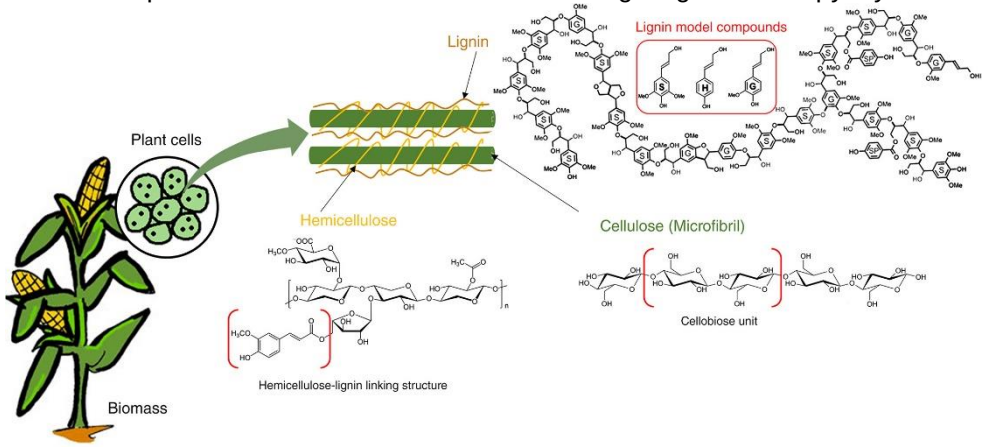
Theoretical and modelling study of biomass pyrolysis reactions

Aim

The aim is to a create kinetic models which describe the pyrolysis chemistry of selected biomass model compounds.

Justification

With depleting oil reserves and increasing concerns in terms of pollution and climate change, the chemical industry is shifting towards circular and sustainable processes. An important aspect is transitioning from the current dependence of fossil resources such as crude oil, shale oil and shale gas to alternative feedstocks. Biomass is one of the most promising replacements for fossil resources, especially the portion of agricultural plants which are not edible, to not compete with food production. These portions of plants mainly comprise cellulose, hemicellulose and lignin. These are large polymeric molecules, and to use these feedstocks to the chemical industry, they first need to be broken down to smaller compounds. The current route we are investigating is the fast pyrolysis of biomass to obtain bio-oil. Fast pyrolysis is a process during which the biomass is exposed to high temperatures during a short time which involves a radical mechanism to obtain the main products.



Having a detailed understanding of the underlying radical mechanism is key to develop, design and optimize pyrolysis reactors, both at the laboratory scale and industrial scale. For this, we use quantum chemistry to calculate the reaction rate coefficients and the thermodynamic parameters of all the molecules and radicals, and we use those in automatic kinetic model generation software to get the full kinetic models. These models are subsequently fed to reactor simulations, in the first step to validate the kinetic model, and later to make prediction aiding the development of adequate reactors.

Program

1. Ab initio calculations to obtain rate coefficients for the relevant reactions during the pyrolysis of selected model compounds.
2. Building of group additivity schemes to be implemented in the automatic kinetic model generator Genesys based on the ab initio calculations.
3. Using Genesys to build a kinetic model for the same selected model compounds, and validating the kinetic model against experimental data available at the LCT using reactor simulations.