

## **FAST PYROLYSIS OF CONTAMINATED BIOMASS: THE CHEMICAL AND THERMODYNAMIC DESCRIPTION OF THE INTERMEDIATE LIQUID COMPOUND**

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The fast pyrolysis of waste- and contaminated biomasses is an attractive process for the production of second-generation bio-energy and bio-chemical products. However, fundamental descriptions of the chemical and physical events of this process are challenging due to its multiphasic nature and the complexity of the contaminated biomass feedstocks (often containing heavy metals and inorganic salts). Furthermore, it is hypothesized that the presence of a biomass molten phase (the intermediate liquid compound (ILC)) can alter the speciation of these inorganics and results in substantial variations in product distributions. The aim of this study is to describe the ILC as partitioning platform for inorganics from both a chemical and thermodynamic perspective.

As a first step, a lumped kinetic reaction model was proposed to take into account the molten phase secondary reactions occurring in the ILC during pyrolysis. The model predictions were validated using experimental data obtained from fast pyrolysis in different micro-pyrolyzers (at 500-600 °C and heating rates of 27 and 110 °C/s, respectively). In general, the comparison of model outputs and experimental data were satisfactory and showed the importance of considering molten phase reactions in lumped kinetic schemes.

In a second step, model components (glucose, sucrose and water) were selected to represent the ILC and the effect of feedstock phase change on resulting pyrolysis volatile products was investigated in a micro-pyrolyzer at 400-500°C in two different ways: (1) by introducing a rapid melting stage of the solid sugar at 240°C prior to its pyrolysis and (2) by dissolving the sugar in water prior to pyrolysis. The product distribution for both cases were then compared to the results obtained when the sugar was pyrolyzed in its solid form. The results showed that for both cases the pre-pyrolysis phase change of the sugar significantly affected the yields of volatile products and the product distribution suggested that fragmentation reaction pathways were favoured when the sugar was pyrolyzed in its liquid form. Similar experiments will be performed to investigate the effect of phase change in the presence of inorganic salts (such as AAEMs and heavy metal complexes) in the ILC. These compounds will be added through impregnation and dissolution techniques.

Furthermore, the vapour-liquid equilibrium of the sugar/water systems was described by thermodynamic calculations using the NRTL model implemented in the ProsimPlus software, whereas the speciation of the inorganics in the system and their effect on evaporation was studied using the Mixed Solvent Electrolyte (MSE) model of the OLI System thermodynamic software. The results showed that the presence of salts can significantly modify the boiling point of the sugar-water mixture and demonstrated the important impact of salts on the thermodynamics of the ILC. Future work will focus on investigating the pyrolysis of the ILC through an intensification technique in a microfluidic reactor as well as integrating the results from experimental work and thermodynamic modelling tools to model the ILC and the effects of a wider range of inorganics.