Thermochemical equilibrium modeling of ash transformation during the thermal conversion of different biomass types with a focus on the speciation of P and K

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Abstract

With the emerging necessity to convert our current fossil fuel-based energy conversion systems into systems converting renewable energy resources comes the need for enhanced scientific research on biomass and anthropogenic waste fuels. Thermochemical calculations based on the properly evaluated thermodynamic data represent a potent precursor to estimate the potentials and risks of thermal conversion of biomass fuels in industrial plants.

For our purpose, thermochemical calculations are performed to analyze the chemical environment in the ash fraction of different biomass fuels. As biomass fuels display a wider range of ash-forming elements, both qualitatively and quantitatively, it is essential to obtain specific thermodynamic information for each fuel individually. The aim is to predict and possibly inhibit process-disrupting events, e.g., agglomeration, deposition, or corrosion, and instead improve the ash properties so that valuable ash fractions can alternatively be produced.

Within our projects, we analyze natural resources, such as agricultural crops and residues, and waste streams, such as animal manures and sewage sludge, but also mixtures of other wastes and natural resources. A recent focus was set on the speciation of P and K in the analyzed ashes since the fate of these elements determines the possibility of ash recycling as fertilizer or as fertilizer precursor. Our analysis methodology covers theoretical thermodynamic equilibrium calculations and lab-scale experiments.

This presentation aims to highlight our approach in the prediction of ash compositions and the characteristics of different biomass fuels using thermodynamic equilibrium calculations. The results obtained by these calculations help in the experimental design and in the interpretation of the experimental results. Essential limitations in the comparability with practical setups were identified, which have to be kept in mind and should be dealt with. One way of facilitating future approaches via thermodynamic equilibrium calculations could be a standardized methodology, e.g., a hierarchical structure in the parameter specification of the modeled practical system.

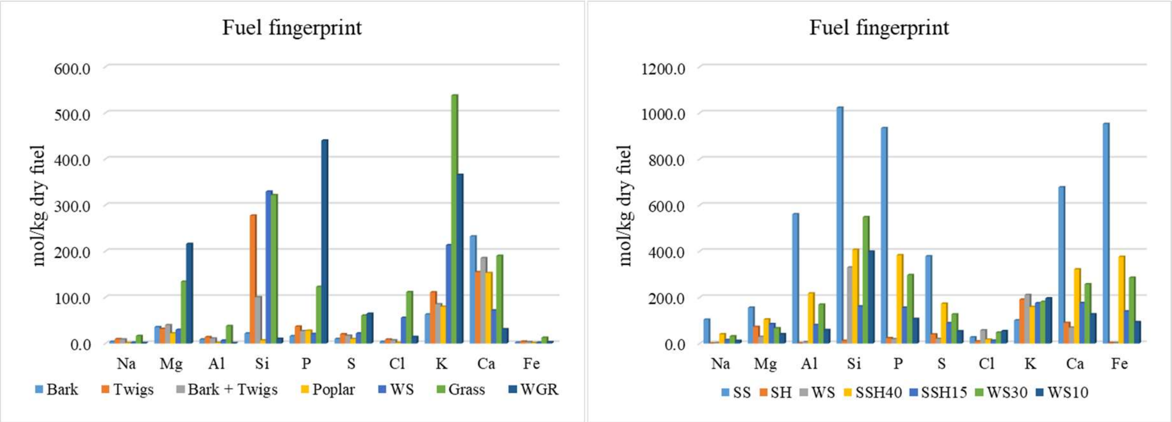

Figure 1: Fuel fingerprint of the fuels and fuel mixtures used in the thermochemical equilibrium calculations. Based on the individual fuel compositions and the gas conditions (combustion/gasification) the melting behavior, the ash speciation at the process temperature, and the phases formed by equilibrium precipitation were calculated.