



Prediction of the thermodynamics of biomass-derived mixtures for improved process engineering of renewable processes

Bio-thermo

Project Initiator(s)

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Project context

Having detailed knowledge of thermodynamic properties of the components in a reactor effluent is crucial for the design of efficient separation processes as well as for kinetic modelling of the involved reactions. Unfortunately, the thermodynamics of highly functionalized biomass derived components, which are gaining in industrial importance, have been insufficiently studied and are not adequately described by current models.

Innovation goal

Traditional thermodynamic models have the disadvantage that the binary interactions between all molecules in the mixture have to be known. This means that mixtures whose phase equilibria have not yet been experimentally investigated cannot be described using these methods. Group contribution methods can provide a solution, as they allow to predict the binary interactions based on the functionalities of the components. However, these methods were developed for petrochemicals. Hence, highly functionalized molecules are, typically, not well described by these group contribution methods. **The general objective of this project is to develop adequate thermodynamic models for biomass derivatives starting from first principles methods.** The models will be validated by a limited number of well-chosen experiments and, subsequently, used for separation process design purposes.

Requested expertise

1. Which type of molecules to be targeted, will be determined in consultation with the partners of the project. Therefore, INCAT is looking for a partner with vast expertise in an industrially relevant biomass conversion process.
2. Also a partner who is able to provide components at sufficient large quantities and purities for experimental model validation is requested.
3. Finally, a partner with experience in upscaling of a newly designed separation train would be a great added value.