Aalborg Universitet

The Physical Chemistry of the CatLiq® Process

Nielsen, Rudi P.

Link to publication from Aalborg University

Abstract

The CatLiq® process is a thermochemical conversion process for wet biomass. It differs from other thermochemical conversions such as hydrothermal upgrading, gasification and pyrolysis in a number of ways including process conditions, catalysts and product. Possible reaction pathways have been investigated based on literature studies to give an overview of the reactions that may occur in the process. This includes the effect of both heterogeneous and homogeneous catalysts as well as acid/base related reactions.

At processing conditions the solubility of salts are very low due to a low dielectric constant, which means salts are likely to precipitate in the process. A model based on the extended Debye-Hückel equation has been developed to determine the solubility of salts at various pressures and temperatures. The method is based on calculating the saturation index which is the ratio between activities and solubility product. However for very soluble salts there is a significant deviance due to problems using the extended Debye-Hückel equation at high molalities. The model works at ambient conditions, however due to scarce solubility data at various pressures and temperatures it is difficult to validate the model without performing experimental determination of these solubilities for calculation of correction parameters.

Another model has also been developed for determination of phase distributions and compositions. This model is a multiphase flash routine which yields acceptable results compared with literature data of various mixtures, but some issues arise when using it on the CatLiq® system. Reasons for these include the lack of interaction parameters for the components, a very simplified composition used in the calculation and simple mixing rules. The composition and bubble point of the process stream has been measured experimentally, and based on the measured composition a model composition has been estimated. However, only a small fraction of the compounds in the process stream could be identified using GC/MS, meaning that the model composition is a very simplistic image of the actual composition.

A laboratory scale facility has been developed to perform fast screening experiments, and although being a batch reactor it does show comparable results with the measurement from the CatLiq® pilot plant.

Overall an overview of the CatLiq® process has been generated and models developed that although not perfect in their operation forms a solid base on which to perform further development.