Molecular Structure of heavy Oils and Coal Liquefaction Products

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Challenges of Modeling Steam Cracking of Heavy Feedstocks

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Definition of the problem
Steam cracking of hydrocarbons is one of the most important processes of the petrochemical industry. In this process hydrocarbons are cracked into commercially more important products such as light olefins and aromatics. Feedstocks ranging from light alkanes such as ethane and propane up to complex mixtures such as naphthas are converted at temperatures ranging from 900-1200 K in tubular reactors suspended in large gas-fired furnaces. A recent tendency is to use heavier feedstocks such as heavy gas oils, vacuum gas oils (VGO) or gas condensates. This is because the demand for heavy gas oils and VGO's as fuel is becoming less and less important, resulting in large remains of these low cost fuels. Therefore they become more and more interesting as alternative for naphtha from an economic point of view. One problem is, that the cracking behavior differs significantly of that of lighter fractions, and hence, that the reaction network used to simulate the cracking behavior of these heavy fractions needs several fundamental changes. On the other hand characterizing or reconstruction of these complex feedstocks inevitable results in challenges.

Contribution
A single event microkinetic model (SEMK) for steam cracking of hydrocarbon fractions is developed and applied. The constructed reaction network is the most extensive reaction network ever generated for steam cracking. The number of reactions considered in the reaction network is more than doubled. Also the number of molecules considered in the microkinetic model is extended from 218 to 478. Di-, tri-, poly- and naphtheno-aromatic compounds are now considered and the maximum carbon number of the molecules is increased to 33. The introduction of these aromatic compounds is on the one hand necessary to be able to simulate VGO fractions. On the other hand these molecules form also an important part of the pyrolysis fuel oil fraction. The complexity of modeling heavy feedstocks inevitable results in some lumping of feedstock molecules. How and why components are lumped and how model components can be easily "de-lumped" will be extensively discussed. Special attention will also be paid to the feedstock characterization/reconstruction problem related to using these complex feedstocks in a simulation model. Comparison of results obtained in a pilot plant and simulated results show how uncertainties on the characterization of these heavy feedstocks propagate to the simulation results.

Significance
For the first time a SEMK reaction network is developed which is able to simulate steam cracking of very heavy fractions such as gas oils, gas condensates and vacuum gas oils. Modeling the cracking behavior of these heavy feedstocks results in some challenges such as necessity of lumping, feedstock reconstruction, etc. The simulation model for steam cracking allows to address these challenges and illustrate and understand how more molecular detail in the model and in the feedstock characterization/reconstruction model can benefit the model predictions.

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