Institute for Chemical Technology and Polymer Chemistry
Department Chemical Technology
Prof. Dr. Olaf Deutschmann

Bachelor-/ Vertiefer-/ Masterarbeit im Bereich Chemie /Chemieingenieurwesen /Verfahrenstechnik

Numerical simulation of natural gas and biogas pyrolysis

Numerische Simulation der Pyrolyse von Erdgas und Biogas

Background

Pyrolysis of methane is getting increased attention due to possibility to produce CO_2 free hydrogen and solid carbon. There are complex physio-chemical phenomena involved in this high-temperature multiphase process as shown in Figure-1. We have extensively studied pure methane pyrolysis in recent years using numerical simulations and experimental validation. In reality, however, the raw material is not pure methane, but rather natural gas or biogas. In this work, we want to study pyrolysis of natural gas and biogas, in which methane is major species along with other hydrocarbons and CO_2.

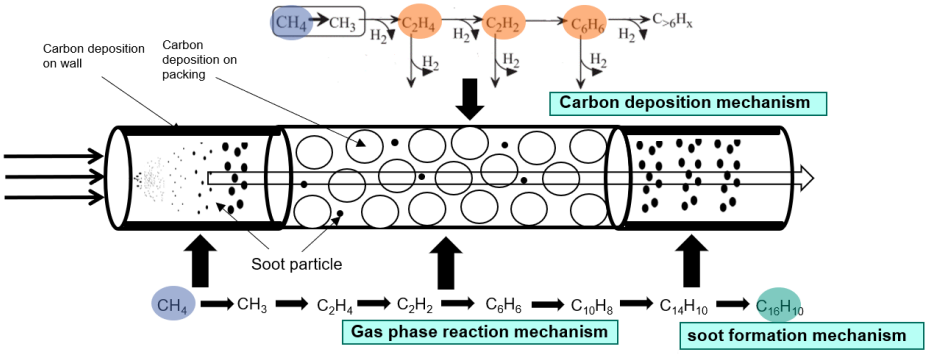

Figure 1: Schematic of the methane pyrolysis reaction

Work description

Scope of this work is numerical simulation of lab reactor for natural gas and biogas pyrolysis.

1. Thermodynamic analysis will be performed for various possible inlet compositions.

2. Kinetic simulations will be performed with detailed gas phase mechanisms. Impact of process parameters such as temperature, feed composition, residence time will be studied. The performed simulations will be compared to the experiments (not the part of this work) to validate the kinetics.

3. In the last part, coupling of gas phase mechanisms with surface reactions (eg. deposition, soot) will be evaluated.

Important outcome of the thesis should be validated kinetics useful for evaluating process in detail. If the topic has triggered interest in you then feel free to contact on email address below for further discussion.

Contact
Manas Mokashi
manas.mokashi@kit.edu