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Micro kinetic modelling of methane pyrolysis over a carbonaceous catalyst.

Aim

In this thesis, it is aimed to estimate the kinetic parameters of methane pyrolysis reaction over carbonaceous catalyst through a combined experimental and micro kinetic study.

Justification

The catalytic decomposition of methane (CDM) presents a pathway for producing clean hydrogen and obtaining value-added carbon, all while avoiding the release of greenhouse gases. Two advantages of carbonaceous catalysts for this purpose are their low cost and sulfur resistance.
Kinetic modeling for the pyrolysis of heavier hydrocarbons over a carbonaceous catalyst has already been presented in the literature [1,2]. In this context, the first step is the generation of vacant active sites through H-abstraction reactions from armchair and zigzag sites of carbonaceous catalysts, using one of the following methods:

- Hydrogen abstraction by a gas-phase radical.
- Hydrogen abstraction through the thermal cleavage of the C-H bond.

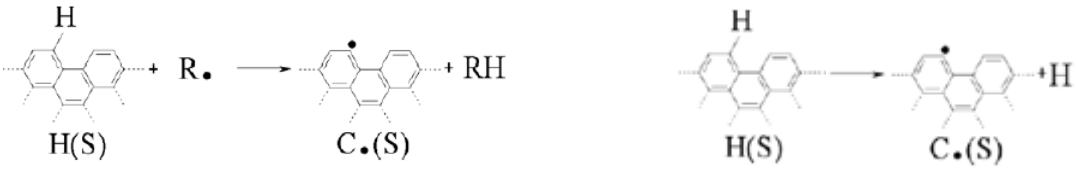

Fig.1 Initiation reaction of hydrocarbon pyrolysis on armchair site.
Left: initiation by gas phase radical, right: initiation by thermal cleavage f C-H bond

The existing kinetic models have not been introduced for pure methane. Since heavier hydrocarbons can be thermally decomposed to radicals at the reaction temperature, they initiate surface reactions by forming active sites through the reaction of produced radicals with H-C bonds. However, the significance of the second way of surface initiation has remained lost. Consequently, the simulation of methane pyrolysis reactions using these mechanisms leads to a negligible amount of conversion, contradicting the experimental data.
In this master thesis, we will develop a micro kinetic model for surface reactions of methane decomposition on carbonaceous catalyst, focusing on the initiation and coke formation reactions.

Program

- Literature study on kinetic modeling of methane decomposition and different carbonaceous catalyst.
- Conducting methane pyrolysis experiments in presence of carbon catalyst in a lab-scale reactor.
- Performing catalyst charectersation (XRD, N_2 adsorption, SEM) for fresh and spent catalyst.
- Micro kinetic modeling to estimate kinetic parameters of existing reaction path way.

References

[1] R. Lacroix, R. Fournet, I. Ziegler-Devin, and P. M. Marquaire, “Kinetic modeling of surface reactions involved in CVI of pyrocarbon obtained by propane pyrolysis,” *Carbon N Y*, vol. 48, no. 1, pp. 132–144, Jan. 2010.
[2]Wang, Q. Song, Y. Wu, X. Li, T. Li, and X. Zeng, “Modelling and numerical simulation of n-heptane pyrolysis coking characteristics in a millimetre-sized tube reactor,” *Combust Flame*, vol. 201, pp.4456,Mar.2019.