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Coach	**Supervisor(s)**	**Funding**
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Coke formation simulation during steam cracking

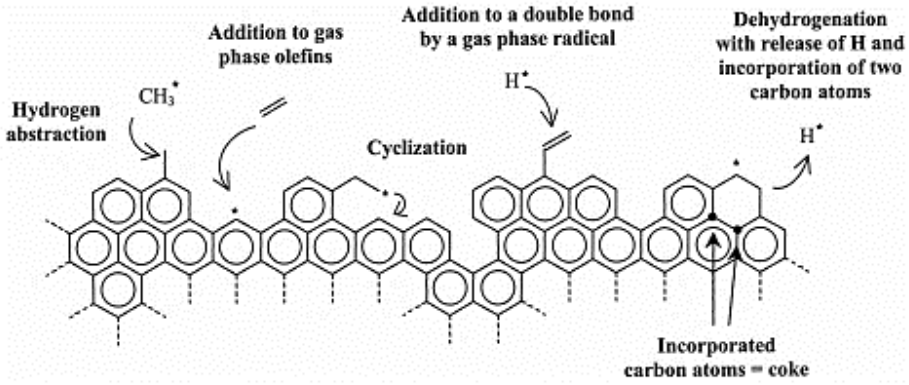
Aim

Understanding coke formation mechanism and constructing a semi-empirical kinetic model to simulate coke deposition during the steam cracking process.

Justification

Steam cracking is the major industrial process to produce olefins such as ethylene, propylene and butadiene. However, it is accompanied with coke formation on the inner wall of the tubular reactor. This coke formation has a deleterious influence on the energy efficiency and economic viability of the steam cracking process. The low thermal conductivity of the coke layer leads to a higher coil surface temperature to maintain the feed conversion. Simultaneously, the cross area in the reactor starts to decrease, leading to a higher pressure drop along the reactor coil. A higher feed inlet pressure is desired to satisfy the product specification. Once the coil surface temperature or inlet pressure exceeds the maximum material permissible value, the process has to be shout down to decoke the reactor.

At present, it is believed that carbon deposition occurs according to a combination of three main mechanisms, namely catalytic coke formation, free radical coke formation and condensation formation. Although extensive progress has been made in the fundamental modelling of the gas-phase chemistry, these existing models are not sufficient to simulate coke formation in different processes. Moreover, the surface reaction mechanism is not well studied among these models. The only general coke formation model is constructed for ethane steam cracking process and the involved reactions as shown below.



Program

1. Literature survey:
    - Investigation on coke depostion morphologies and carbon diffusion during the steam cracking process.
    - The influence of catalytic coke formation on the free radical coke formation.
2. Semi-empirical coke formation model construction based on existing experimental results, and the model validation with experimental results from the JSR and pilot setup.
3. Developing a kinetic model for the different types of coke formation with Genesys and modelling steam cracking reactors in Chemkin.

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