Addition Reactions of Model Compounds of Asphaltenes During Thermal Cracking

Amir H. Soleimanisalim¹, Murray R. Gray¹, Jeffrey M. Stryker², Rik R. Tykwinski³ ¹Department of Chemical and Materials Engineering, University of Alberta, Edmonton ²Department of Chemisry, University of Alberta, Edmonton, AB, Canada ³University of Erlangen-Nuremberg, Erlangen, Germany

In upgrading processes for bitumen and heavy oils, one of the most important issues is coke formation. Understanding of this process may help the industries to minimize coke, increase the liquid yield, and enhance operation. Coke formation is generally related to the asphaltene content of heavy oils, defined as the portion of crude oil insoluble in light n-alkanes, but soluble in aromatic solvents. Due to the complexity of asphaltenes, we can use model compounds to probe chemical and physical behavior. In this study, we investigate addition reactions of alkyl-bridged aromatic compounds to understand the molecular behaviour of asphaltenes during thermal cracking, especially the addition reactions which tend to form coke. In this research, 1,3,6,8tetrahexylpyrene (THP) was thermally cracked by itself and in mixtures with 2,6-bis[2-(phenanthren-9-yl)ethyl]pyridine (phenanthrene-(CH₂)₂-pyridine--(CH₂)₂-phenanthrene or PhPPh) in a batch stainless steel microreactor at different reaction conditions from 420°C to 450°C for 15 to 40min. The products where analysed with high performance liquid chromatography (HPLC), and matrix assisted laser desorption/ionization (MALDI). The results of THP pyrolysis showed significant formation of addition products at severe conditions, particularly at 450°C and 30min. The addition reactions started by cleavage of the weak C-C bond in alkyl chains, forming an olefin which can undergo to chain reactions and produce a range of addition products with mass larger than the starting compounds and with one or more pyrene groups in their structures.