

Hydrocracking study of Asphaltene via reactive molecular dynamics

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Asphaltenes are molecular substances, which are composed of aromatic and saturate hydrocarbons consist of C, H, N, O, S atom and several metals in clued oil. Cracking of asphaltenes would be helpful in the oil industry by improving the low-grade heavy oil. Reactive molecular dynamics was employed to catch chemical reactions in cracking of a hypothetical asphaltene model with the bond-order-based energy calculation, which uses force field parameters derived from density functional theory implemented in LAMMPS. Chemical and physical parameters were found to be generally consistent with experimental data. In this initial work, during the pyrolysis of asphaltenes, some smaller units of aromatic compounds from the cracked S atom and many carobon radicals (impurities and high carbon content) were observed at high temperature from 1500K to 2000K. In order to assess the products, the hydrocracking of asphaltenes with the insertion of hydrogen gas was promoted and led to the production of the light cycling oil compounds (tetralin, decalin, coronene and so on..).