Oral Presentations

Thermo-oxidative decomposition of quinolin-65 as an asphaltene model molecule

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Abstract

Asphaltenes is considered the heaviest, most aromatic and most surface-active fraction of crude oil. Because of their complex chemical structures, amphiphilic behavior, and polarizability asphaltenes exhibit a self–associating feature that promotes aggregation and subsequently increases the viscosity of crude oil. NPs have unique properties which allow them to be promising solutions to problems involving asphaltenes.

However, because of the complexity of asphaltenes, the understanding of their properties, in particular the structural factors ruling their self-association and subsequent adsorption and cracking tendencies are difficult. Hence, a model molecule, Quinolin-65 (Q65), which mimics the properties of asphaltenes, has been proposed to improve our understanding of asphaltene chemical behavior in the presence of NiO nanoparticles. The model molecule chemistry is studied using high-level of computational modeling. Thermo-oxidative behavior of O65, in the presence and absence of nanoparticles, is investigated experimentally and theoretically. Thermogravimetric analysis (TGA) was carried out using a simultaneous thermogravimetric analysis/differential scanning calorimetry (TGA/DSC) analyzer to probe the product gases during the thermo-oxidative process. Density functional theory (DFT) and the second-order Møller–Plesset (MP2) perturbation theory were employed to explore the reactions involved in the thermal decompositions as well as the interactions between the model molecule and singlet atomic (O ^{1}D) and molecular (O$_2$ $^1\Delta$) oxygen.

Both, the theoretical study and the thermogravimetric analysis, concluded that the thermo-oxidative decomposition of Quinolin-65 is a complex multi-step reaction process, which involves different reaction pathways. The thermodynamic parameters obtained in this study showed that the reaction process should start with the loss of the olefin chain in the Quinolin-65 molecule, followed by the oxidation of the aromatic chain, to produce mainly, H_2O, CO_2, and SO_2.

The significance of this work lies in the fact that the thermodynamic parameters obtained, ΔG in particular, are highly endogenic, including those involved in the formation of singlet oxygen. In addition, and because of the complexity and size of the Q65 molecule, its oxidation reaction mechanism suggests slow and tough reaction pathways, which strongly suggests the need for a catalyst.