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Research of Geometric and Electronic Structure of Heavy Oil Components and its Influence on the Preparation for Transportation and Processing

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Abstract

It is expected that the extraction of light oils will decrease in the next 10-15 years. In this regard, companies are increasingly paying attention to the so-called abnormal oil: high-viscous and heavy. High-viscous and heavy oils are specified by increased content of high-molecular components (asphaltenes, resins, paraffins), which complicate such hydrocarbon raw materials processing. In addition, it is known that in some temperature ranges, as well as while mixing highly viscous and heavy oils upon income to the oil refinery, sharp rheological properties deteriorate, indicating a change in the structure of the oil dispersed system.

The physico-chemical and structural-rheological properties of the oil dispersion system are determined by the structure, size and composition of complex structural units resulting from the association of paraffins, asphaltene-resinous components. Therefore, in order to choose the stimulation technique in the preparation and processing of heavy oils, it is necessary to gather information about hydrocarbon composition, especially structure of paraffins, resins and asphaltenes. Molecular weight of various asphaltenes is 700-6000 c.u., for resins it is lower - from 300 to 700 c.u. Also, resins and asphaltenes contain the micro-quantities of Fe, Ca, Mg, Cu, Ni, and V.

To study the structure, as a model of high-viscosity and heavy oils, we selected molecules of paraffins C_{19+}, resins and asphaltenes, containing aromatic and heterocyclic fragments. Calculations of geometric and electronic structures of the molecules were carried out using the density functional method DFT with B3LYP/6-31G (d,p) in the GAMESS and GAUSSIAN programs. Analysis of the bond length and order, valence and dihedral angles, charges, ionization potential, formation energy, energies of the boundary molecular orbitals, oil dispersed system components makes it possible to determine the possibilities for interaction and formation of a new structural unit of the disperse system. Moreover, it will be possible to determine the energy of possible physic-chemical effect while treatment of heavy hydrocarbon feedstock to provide necessary rheological properties, as well as to determine thermodynamic properties of complex organic systems which are important for modeling its processing processes.