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Application of Nuclear Magnetic Resonance (1H-NMR) in the Analysis of Catalytic Aquathermolysis: Colombian Heavy Oil Case

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Abstract : The enhanced oil recovery by steam injection was considered a process that only generated physical recovery mechanisms. However, there is evidence of the occurrence of a series of chemical reactions, which are called aquathermolysis, which generates hydrogen sulfide, carbon dioxide, methane, and lower molecular weight hydrocarbons. These reactions can be favored by the addition of a catalyst during steam injection; in this way, it is possible to generate the original oil in situ upgrading through the production increase of molecules of lower molecular weight. This additional effect could increase the oil recovery factor and reduce costs in transport and refining stages. Therefore, this research has focused on the experimental evaluation of the catalytic aquathermolysis on a Colombian heavy oil with 12,8°API. The effects of three different catalysts, reaction time, and temperature were evaluated in a batch microreactor. The changes in the Colombian heavy oil were quantified through nuclear magnetic resonance 1H-NMR. The relaxation times interpretation and the absorption intensity allowed to identify the distribution of the functional groups in the base oil and upgraded oils. Additionally, the average number of aliphatic carbons in alkyl chains, the number of substituted rings, and the aromaticity factor were established as average structural parameters in order to simplify the samples' compositional analysis. The first experimental stage proved that each catalyst develops a different reaction mechanism. The aromaticity factor has an increasing order of the salts used: Mo > Fe > Ni. However, the upgraded oil obtained with iron naphthenate tends to form a higher content of mono-aromatic and lower content of poly-aromatic compounds. On the other hand, the results obtained from the second phase of experiments suggest that the upgraded oils have a smaller difference in the length of alkyl chains in the range of 240º to 270°C. This parameter has lower values at 300°C, which indicates that the alkylation or cleavage reactions of alkyl chains govern at higher reaction temperatures. The presence of condensation reactions is supported by the behavior of the aromaticity factor and the bridge carbons production between aromatic rings (RCH_2). Finally, it is observed that there is a greater dispersion in the aliphatic hydrogens, which indicates that the alkyl chains have a greater reactivity compared to the aromatic structures.

Keywords : catalyst, upgrading, aquathermolysis, steam
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