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Study of the Radical Chain Mechanism of Hydrocarbon Oxidation for in Situ Combustion Process

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Abstract

© 2017 Alexandra Ushakova et al. Despite the abundance of in situ combustion models of oil oxidation, many of the effects are still beyond consideration. For example, until now, initial stages of oxidation were not considered from a position of radical chain process. This is a serious difficulty for the simulation of oil recovery process that involves air injection. To investigate the initial stages of oxidation, the paper considers the sequence of chemical reactions, including intermediate short-living compounds and radicals. We have attempted to correlate the main stages of the reaction with areas of heat release observed in the experiments. The system of differential equations based on the equations of oxidation reactions was solved. Time dependence of peroxides formation and start of heat release is analytically derived for the initial stages. We have considered the inhibition of initial oxidation stages by aromatic oil compounds and have studied the induction time in dependence on temperature. Chain ignition criteria for paraffins and crude oil in presence of core samples were obtained. The calculation results are compared with the stages of oxidation that arise by high-pressure differential scanning calorimetry. According to experimental observations we have determined which reactions are important for the process and which can be omitted or combined into one as insignificant.

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