**289u Molecular Based Kinetic Modeling of Hds-Fcc Process**

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Heavy oil upgrading and ultra-clean fuel production are critical matters for petroleum industry. Processes must be engineered both to increase refinery efficiency and to protect the environment. One of the practical ways to achieve these goals is the flexible usage of the combination of hydrodesulfurization (HDS) and fluid catalytic cracking (FCC). The control and fine-tuned optimization of this process would be enhanced through the development of high-fidelity reaction models based on the molecular characters of feedstock. While this is to be developed for the combined process, as a first step, kinetic models of FCC were generated and examined. Software for the computer generation of kinetic models was exploited to generate an optimum set of elementary steps corresponding to a mechanistic kinetic model for the catalytic cracking of vacuum gas oils. The kinetics model building program uses graph theoretic concepts to represent the molecules as atomic connectivity matrices and the reactions as matrix operations. The rate constants for each reaction family were constrained to follow the Evans-Polyani relationship, which, for each reaction family, relates the rate constant to the enthalpy of reaction. This helped to reduce both the complexity of the reaction network and the number of rate parameters to be optimized. The comparison of model outputs and experimental measurements is favorable.