Molecular Modelling and Simulation of Gas Oil Hydrocracking

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Abstract

The increasing demand and tightened product specifications for gasoline and middle distillates have made hydrocracking one of the most important secondary refining processes due to its flexibility of converting a wide range of heavy fractions. Typical kinetic modelling methods of gas oil hydrocracking can be classified as traditional lumping, continuous lumping, and structure oriented lumping. Molecular-level models, compared to conventional lumping models, have advantages of describing the process in more reliable and realistic ways in terms of both molecular species and reaction pathways and mechanisms.

This study focuses on two key areas of hydrocracking processes: molecular characterization of petroleum feedstock and products; and reaction kinetic modelling based on molecular information. For the characterisation part, one major problem is to obtain the very complex molecular composition of petroleum feedstock and its products with limited bulk properties. By means of the molecular type homologous series (MTHS) method (Peng, 1999), the molecular composition of reaction feedstock is derived, covering the temperature range of up to 850K and 11 homologous series. The obtained 174 MTHS matrix entries of reaction feedstock and the hydrogen are then applied as the inlet to simulate the molecules transformations through the reactor. The reaction pathways and networks are generated according to the molecular entries while the initial kinetic parameters are estimated based on the quantitative structure/reactivity correlations. The kinetic parameters of developed model is tuned using experimental data obtained from a pilot-plant hydrocracking reactor. Simulation results indicate that the developed model is capable of predicting molecular composition as well as interested bulk properties (e.g., density, distillation curve) of product over a wide range of operating conditions. In addition, the model can discover the variation trend of some important parameters, such as hydrogen consumption and light gas generation (C_1-C_4), which could be further integrated with hydrogen network for reasonable use of hydrogen. A case study is carried out to illustrate the developed methodology.