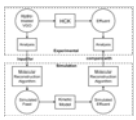


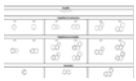
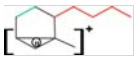
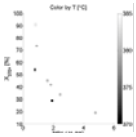

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Full Length Article

A single events microkinetic model for hydrocracking of vacuum gas oil

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Highlights

- Extension of Hydrocracking Single Events Model from paraffins to cyclic species.
- Sucessful application to HCK of a real VGO feed.
- Model is shown to be useful for an industrial process with real feed.
- Detailed analysis of reaction kinetic of individual molecular families is presented.

Abstract

The single events microkinetic modelling approach is extended to include saturated and unsaturated cyclic molecules, in addition to paraffins. The model is successfully applied to hydrocracking (HCK) of an hydrotreated Vacuum Gas Oil (VGO) residue in a pilot plant, under industrial operating conditions, on a commercial bi-functional catalyst. The molecular composition of the VGO feed is obtained by reconstruction based on a combination of analytical data (SIMDIS, GCxGC, mass spectrometryspectrometry). The necessary extensions to the single events methodology, which has previously only been applied to much simpler reacting systems (i.e. HCK of paraffins) are detailed in this work. Feeds typically used in the petrochemical industry typically contain a far more complex mixture of hydrocarbons, including cyclic species (i.e. naphthenes & aromatics). A more complex reaction network is therefore required in order to apply a single events model to such feeds. Hydrogenation, as well as endo- and exo-cyclic reactions have been added to the well-known acyclic β-scission and PCP-isomerization reactions. A model for aromatic ring hydrogenation was included in order to be able to simulate the reduction in aromatic rings, which is an important feature of HCK units. The model was then applied to 8 mass balances with a wide range of residue conversion (20–90%). The single events model is shown to be capable of correctly simulating the macroscopic effluent characteristics, such as residue conversion, yield structure, and weight distribution of paraffinic, naphthenic, and aromatic compounds in the standard cuts. This validates the overall model. The single events model provides far more detail about the fundamental chemistry of the system. This is shown in a detailed analysis of the reaction kinetics. The

evolution of molecule size (i.e. carbon number), number of saturated/unsaturated rings, or the ratio of branched and un-branched species can be followed along the reactor. This demonstrates the explanatory power of this type of model. Calculations are performed on the IFPEN high performance computing cluster, with parallelization via MPI (message passing interface). This was very useful in order to reduce time consuming problems especially for the parameter fitting step

Keywords

Hydrocracking; Single events; Microkinetic modelling; Catalysis

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