reaction DESIGN

CHEMKIN-PRO
Hydrocracking for Petroleum Processing

Hydrocracking is commonly used to process feedstocks that are unsuitable for catalytic cracking or reforming, due to high concentrations of either polycyclic aromatics (PAH), or of sulfur or nitrogen compounds, which act as catalyst poisons.

In hydrocracking, both the feedstock and relative rates of two competing reactions, hydrogenation and cracking, affect the outcome. Converting heavy aromatic feedstock to lighter products occurs under pressures of 1,000-2,000 psi and high temperatures (750-1,500 F) under the influence of hydrogen and specific catalysts. Other roles for hydrogen include helping to reduce tar formation, preventing coke build-up on the catalyst, and converting sulfur and nitrogen to hydrogen sulfide and ammonia.

The groundwork for optimizing hydrocracking and other high-dimensional simulations can be carried out with low-dimensional simulations, to assess the chemistry and obtain the trends for optimizing the process for desired selectivity. The CHEMKIN-PRO Honeycomb Monolith Reactor provides a method for modeling flow in the catalyst bed of hydrocracking reactors.

Setting Up in CHEMKIN-PRO

This process for hydrocracking using a bi-functional catalyst operates at conditions of high pressure (80 atm) and lower temperature (350 °C). The feed in this example is *n*-heptane and hydrogen at a ratio of 10/90 mol%. The bi-functional catalyst is platinum with silica-alumina (Pt/SiO_2-Al_2O_3).

The simulation uses input definitions of:

- **Gas-phase reactions:** Reversible elementary reactions of *n*-heptane applicable for pyrolysis as well as combustion. The gas-phase reactions describe decomposition of hydrocarbons as well as hydrogenation. At the conditions of the hydrocracker, the gas-phase chemistry is insignificant relative to the catalytic chemistry.
- **Surface reactions:** 40 surface reactions, which include the chemistry for *n*-heptane cracking on acidic sites of silica-alumina and hydrogenation of unsaturated hydrocarbons on metallic sites of platinum. The surface reactions used in this example are for illustrative purpose and they have not been calibrated for any particular experimental data. This example simulation is presented only for demonstration purposes. If you are interested in development and validation of reaction mechanisms for specific systems, Reaction Design may work with you through a services arrangement.

Results

Over 90% of *n*-heptane is converted to products by hydrocracking. Major products are propane and *n*-butane, and minor unsaturated products are olefins, including propene, butene, and heptane. Profiles of various products are shown in Figure 1. The impact of diverse parameters such as operating conditions, feed composition, and catalyst types can easily be investigated. In this example, we varied the loading of metallic sites while keeping the acidic sites constant on the bi-functional catalysts. Increasing the metallic sites has significant impact on selectivity. Higher platinum content in the catalyst results in higher selectivity of saturated products compared to the unsaturated products, as seen in Figure 2.

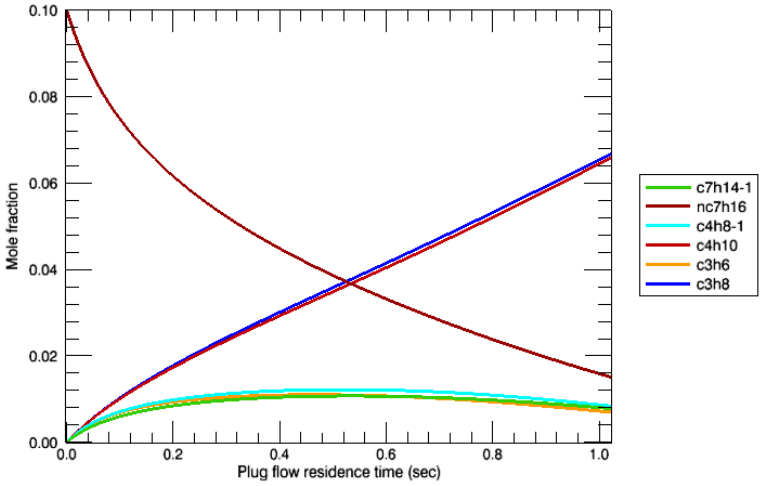

Figure 1. Hydrocracking of n-heptane - Mole fractions of feed and products at nominal temperature of 350 °C and 80 atm.

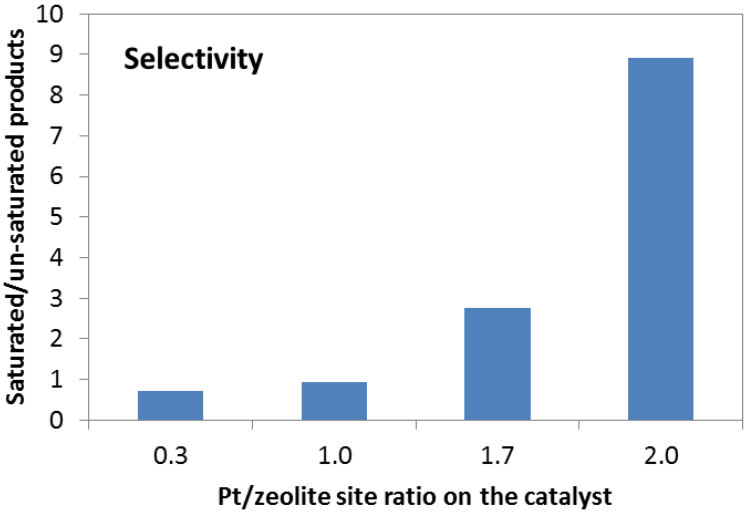

Figure 2. Hydrocracking of n-heptane - Selectivity of saturated to unsaturated products at various loadings of metallic to acidic sites on the catalyst.