ABSTRACT

A three phase heterogeneous model was developed to simulate the performance of pilot plant and industrial trickle bed reactors employed for hydrodesulfurisation of diesel fractions. The model was based on two film theory and incorporated mass transfer phenomena at the gas-liquid and liquid-solid interfaces. All the major reactions taking place in hydrotreating of diesel fraction were modeled. The hydrodesulfurization reaction rates were described using Langmuir-Hinshelwood mechanism to take into account the inhibiting effects of hydrogen sulfide. The hydrodearomatization reactions were treated as irreversible and pseudo first order reactions with respect to the concentration of aromatics. The hydrodenitrogenation and olefin saturation reactions were assumed to be pseudo first order reactions. The mild hydrocracking reactions were modeled using three lumps of diesel, wild naphtha and light hydrocarbons.

Pilot plant experiments were carried out to evaluate the performance of four different catalysts using a feedstock collected from industrial diesel hydrodesulfurization unit. The reactor temperature was varied from 320 to 360°C and liquid hourly space velocity from 1.0 h⁻¹ to 2.5 h⁻¹ at a constant operating pressure of 40 kg/cm² and H₂/oil ratio of 200 lit/lit to study the influence of operating conditions on product quality. All the catalysts were evaluated under similar operating conditions using the same feed diesel oil.
The three phase heterogeneous model was solved to estimate kinetic parameters for various hydrotreating reactions using the data generated in pilot plant experiments. A partial wetting model was proposed to account for incomplete wetting of catalyst particles in pilot plant reactors.

The model comprises of a set of first order differential equations and non-linear algebraic equations. Runge-Kutta 4th order integration algorithm was used to solve differential equations. The algebraic equations were solved by using Newton-Raphson technique. Linear regression techniques were used to fit the experimental data with model equations. The programs to solve the model equations were coded in FORTRAN.

The model was applied to simulate the performance of pilot plant trickle bed reactor at varied operating conditions and verified with experimental data. The model simulations were found to agree well with experimental data.

The three phase non-isothermal heterogeneous model was applied to simulate the performance of industrial reactor at varied operating conditions using the kinetic parameters estimated from pilot plant experiments. Temperature profiles in the industrial diesel hydrodesulfurization unit were generated. The feed and product samples from the industrial reactor were analyzed and used to validate the model simulations. The model was found to simulate the performance of industrial reactor adequately. The model was also applied to study the influence of operating conditions such as reactor temperature and feed rate on product quality. The model was also applied to predict the performance of industrial reactor loaded with high activity new generation catalysts.