**Kinetic model development of special hydrocracking of sunflower oil and petroleum mixture**

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**Highlights**

* Sunflower oil and petroleum mixture special hydrocracking.
* 5-lump trickle bed reactor model development.
* Considering the change in hydrogen solubility along the reactor.

**1. Introduction**

Based on our previous work, a 5-lump kinetic and a simple reactor models were developed and validated against measurements in case of special hydrocracking of sunflower oil and petroleum mixture. In the model the effect of pressure has not considered and different parameter sets were determined for each pressure. The aim of that work was to characterize the catalyst fouling phenomena and its effect on the overall performance of the reactor. In this work the model is improved with the consideration of multiple phases and the mass transportation between these phases. Based on Korsten and Hoffmann reactor model [1]. Due to the reactions the composition of the reaction mixture changes along the reactor which has effect on the solubility of the hydrogen. The model of this effect is also built into the reactor model.

**2. Methods**

**Experiments**

A fixed-bed tubular reactor (diameter: 29 mm, length: 700 mm) was applied to perform the special hydrocracking reactions of the investigated oil mixture. The feedstock was the mixture of kerosene and sunflower oil in a mass ratio of 3:7. In the experimental system the temperature, the pressure and the LHSV can be controlled, so the hydrocracking experiments were performed at 533-613 K, 30-70 bar, 1.0-2.0 h-1 employing Pt/H-mordenite catalyst (Pt content: 0.45%, specific area, BET: 451 m2/g, micropore volume: 0.18 ml/g, Si/Al ratio from XRF: 19 mol/mol, acid sites by ammonia TPD: 0.82 mmol/g, particle diameter: 1.4 mm). The measurements were performed after reaching a steady state condition.

**Modeling**

The pseudo (lumped) components in the developed kinetic model was determined by their boiling point range. Since the experimental data contains 5 pseudo components (triglycerides, diesel, kerosene, gasoline, and gas fractions), the kinetic model was developed using these lumps. For further improvement, the mass transportation of hydrogen was built in the model through applying the Langmuir Hinshelwood mechanism and Henry’s law. The unknown parameters of the proposed reactpr model were estimated based on measurement data with the application non-linear global optimization algorithm.

**3. Results and discussion**

In Figure 1 the validation of our previously described kinetic model for the mentioned material system can be seen. As the processes take place in the reactor are described in more details in the improved model we think that catalyst fouling effect can characterized much more precisely. The more we know about catalyst fouling the higher production efficiency can be achieved in the reactor.



**Figure 1.** Parity plot for the previously described kinetic model at 30 bar

**4. Conclusions**

Our previous analysis of the investigated system revealed that there is a significant effect of catalyst fouling on the product composition. We consider the thermodynamic phases and the connections between each phase to improve the proposed reactor model. In the proposed model the effect of liquid composition on the hydrogen solubility was also considered. The performed model improvements support us to characterize the catalyst fouling phenomena.

**References**

1. Korsten H, Hoffmann U. AlChE J 1996; 42:1350–60.

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