

Kinetic Parameters Estimation for a Tubular Fischer-Tropsch Synthesis Reactor

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Introduction

Fischer-Tropsch synthesis (FTS) reaction is known to produce hydrocarbons with a variety of chain length, and the temperature control of a reactor is significantly difficult due to the high exothermic reaction. Therefore, a lot of research effort has been made to develop an accurate kinetic model to predict the effect of operating conditions on the product distribution and dynamic behaviors of a reactor. In this paper, a mathematical model for Fischer-Tropsch synthesis (FTS) reaction has been developed by assuming (1) different active sites for FTS and water gas shift (WGS) reaction and (2) the re-adsorption of olefin to the active sites. Kinetic parameters are estimated to fit the experimental data under various conditions, and the simulation results on the basis of estimated parameters show that the developed model can describe the product distribution and the conversion satisfactorily.

Mathematical Model and Parameter Estimation

For simplicity, no radial concentration and temperature gradient along radial axis has been assumed, and then a one-dimensional fixed-bed reactor has been developed. The bulk gas density is calculated as a function of composition and the reaction rates are available in Wang *et al.* (2003) [1-3].

Experimental data under 14 different conditions are used to estimate kinetic parameters. The objective function is defined to minimize the CO conversion and number-/weight-averaged chain lengths of paraffins and olefins. The 'lsqcurvefit' in MATLAB is used, where the Levenberg-Marquardt method is utilized, and the initial values for estimation are specified using the values in the literature [1].

Results and Discussion

The estimated results are shown in Figures 1 and 2. The predicted values of CO conversion are in good agreement with experimental values except cases 5, 13 and 14 (*cf.* Figure 1a) while little deviation has been observed between the experimental and simulated values of the average chain lengths (*cf.* Figure 1b). As a result, the entire distributions of paraffin and olefin products are predicted significantly well as shown in Figure 2.

The developed model will be utilized to determine operating conditions for desired distribution of hydrocarbon products, and to optimize the catalytic loading of the reactor to prevent the thermal runaway.

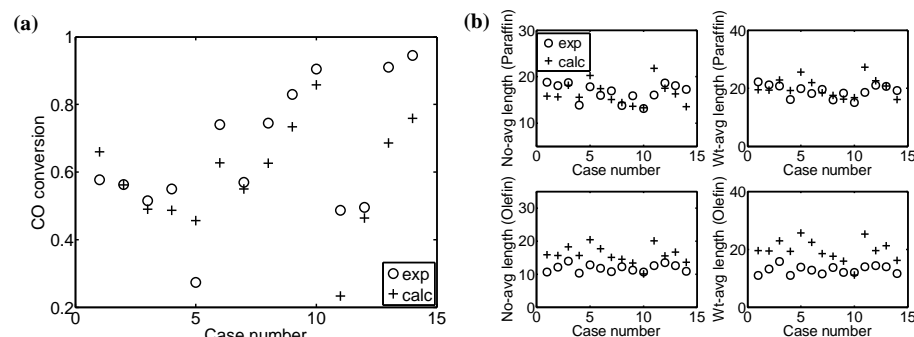


Figure 1. Experimental and estimated values of (a) CO conversion and (b) number- and weight-averaged length of paraffins and olefins for all experimental conditions.

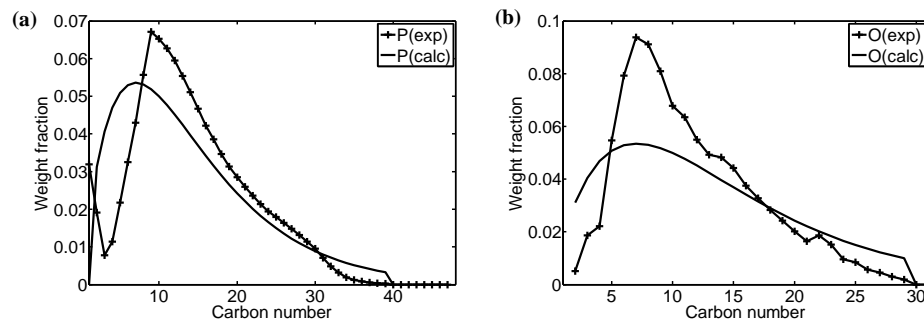


Figure 2. Product distribution of (a) paraffins and (b) olefins under the condition of the temperature of 513K, SV of 2300 h⁻¹, and H₂/CO ratio of 2, and the pressure of 10 bar.

References

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