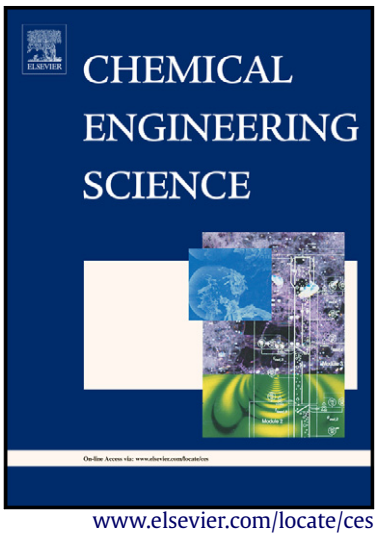

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Catalytic performance of cobalt-silica catalyst for Fischer-Tropsch synthesis: effects of reaction rates on efficiency of liquid synthesis

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Abstract

A one-dimensional pseudo-homogeneous mathematical model of a fixed bed reactor for Fischer-Tropsch (FT) synthesis was developed for the flow of simulated N_2-rich syngas over an in-house cobalt-silica catalyst. This study aims at improving the efficiency of FT synthesis by maximizing the liquid productivities and selectivity, as well as maximizing the syngas conversion and minimizing the methane formation. The developed model predicts the fraction of the reactants and products along the reactor bed length. The rate of syngas conversion and the rate of CO_2, H_2O, CH_4, C_2H_4, C_2H_6, C_3H_8, n-C_4H_{10}, i-C_4H_{10} and $C_{6.05}H_{12.36}$ (C_{5+}) formation were calculated by developing advanced codes in MATLAB. The reaction equations were proposed as a number of lumped chemical reactions (8 reactions, including water gas shift reaction) by means of the molar coefficients of reaction molecules (11 reactive species). The kinetic parameters were estimated by global optimization in MATLAB using the global search method. Optimum values were achieved during the search process. The results predicted by the model were in very good agreement with those measured experimentally at different operating conditions, with respect to conversion and the FT products' selectivity. The rates of production and consumption were derived from a modified power-law rate expression. This study shows that the adapted rate model can deliver a better prediction of final conversion and selectivity. The accuracy of the fitted model relative to the experimental data was determined by a quantitative analysis method using the mean absolute relative residual percentage (MARR %) for the total of 35 data points. It was found that the model based on the modified equation provided a better fit to the experimental data with a MARR of 6.57%, compared to the classic equation with a MARR of 12.24%.

The model predicts the influence of reaction rates on the performance of the fixed bed FT reactor using an unpromoted Co/SiO_2 catalyst at 503 K, 15 bar and 6 L g_{cat}^{-1} h^{-1}. As a result, the conversions of 91.57 and 97.26% were achieved for CO and H_2, respectively with the FT C_{5+} synthesis reaction rate of 7.81×10^{-5} mol g_{cat}^{-1} s^{-1}. The higher rate of C_{5+} formation was found by increasing FT reaction rates compared to the rate of lighter the hydrocarbons' formation. At the same condition, only 5.04 and 8.91% methane and C_2-C_4 selectivity respectively, were predicted; while the highest value of 86.05% liquid (C_{5+}) selectivity was obtained in this case. It was concluded that the higher rate of conversion of H_2 inside the pores filled with liquid products, compared to that of CO, caused an increase in the H_2/CO ratio in the catalyst pores; and thus, a shift towards the formation of lighter hydrocarbons.

Keywords: Fischer-Tropsch synthesis; fixed bed reactor; mathematical modelling; kinetic model