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An investigation on the performance of a FTS fixed-bed reactor using CFD methods☆

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A B S T R A C T

In the present work, a numerical model was developed and validated in order to simulate and improve the conversion of synthesis gas ($CO+H_2$) to higher hydrocarbons in a Fischer–Tropsch Synthesis (FTS) fixed-bed reactor. The reactor was a 3.1 cm diameter and 2.75 m length steel tube in which saturated water was employed to control the peak temperature within the catalyst bed. A 2-D CFD model with an optimized mesh of 22,016 square cells was developed to model hydrodynamics, chemical reaction, non-ideality of the mixture, heat and mass transfer in the reactor. Good agreement was achieved between pilot experimental data and the model. The result showed that adjusting the boiling water flow rate in the range of 25–250 g.min^{-1} allows maintaining the FTS temperature at suitable values. An optimum value of 573 K was obtained for feed temperature.

1. Introduction

Fischer–Tropsch Synthesis (FTS) is a set of catalytic chemical reactions that convert a mixture of carbon monoxide and hydrogen (so-called synthesis gas) into liquid hydrocarbons. Fixed-bed is one of the most competing reactor technologies for FT [1]. Bi-functional catalysts are used to promote the yield and quality of the gasoline from FTS [2]. Although the reaction scheme has been studied and used for a long time, its study today is still of interest because of the high pressure on hydrocarbon prices all over the planet. Butt et al. [3] prepared and characterized Fe and FeCo catalysts on ZSM-5 support for FTS. Schulz et al. [4] studied the selective conversion of syngas to gasoline on iron/HZSM5 catalysts. Calleja et al. [5] carried out some experiments to investigate the effects of process variables including temperature, space velocity; CO/H_2 feed ratio and pressure on the activity of a Co/HZSM5 zeolite bifunctional catalyst. They reported that their catalyst exhibits higher selectivity and yield in comparison with conventional catalysts. Liu et al. [6] used a two-dimensional heterogeneous model to simulate steady and unsteady behavior of a fixed bed FTS reactor. They also reported the impact of feed temperature, flow rate and the wall temperature on the steady state behavior of the reactor [7]. Wang et al. [8] developed a one-dimensional heterogeneous model to predict the performance of fixed-bed Fischer–Tropsch reactors. Marvast et al. [9] simulated the behavior of the FT fixed-bed reactor using a two-dimensional heterogeneous model at steady state condition.

In the recent years the remarkable increases in computation speed made CFD a powerful and effective tool to model and understand complex processes [10–12]. Selma et al. [13,14] and Bannari et al. [15] developed advanced methods for describing gas–liquid hydrodynamics in bubble column reactors. Troshko and Zdravistch [16] employed an Eulerian multifluid formulation CFD method to model Fischer–Tropsch synthesis in bubble column reactors. They applied their experimentally validated model to an industrial scale bubble column reactor. Their model was qualitatively successful in predicting the hydrodynamic effects, but heat transfer effects were not considered. Arzamendi et al. [17] developed a three dimensional CFD model to model heat transfer in a low-temperature Fischer–Tropsch synthesis microchannel reactor. In their experiments, boiling water was used as coolant. Arzamendi et al. [18] formulated a kinetic model for describing the preferential oxidation of CO (CO-PrOx) in H_2 rich streams with CO_2 and H_2O in the feed. They studied the influence of the operating variables on the CO-PrOx in microchannels and microslits by implementing the rate equations in CFD codes.

In the present work, a CFD model was developed to model FTS in a fixed bed reactor. Adequate equation of state was employed to model the non-ideality of the gas mixture. A heat sink was defined to model the performance of boiling water which was used to establish isothermal condition in the reactor. The model predictions were validated with pilot experimental data.

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