Fischer-Tropsch Trickle-Fixed-Bed Reactor Model

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Introduction

In light of increasing fuel costs and concerns over dependence on foreign oil, application of Fischer-Tropsch (FT) technology is an important, economical option for production of synthetic fuel liquids from biomass, coal, and stranded natural gas. The objective of this work is the development of a robust, user-friendly mathematical model for simulation of FT synthesis on cobalt and iron catalysts in a trickle-fixed-bed recycle reactor. A 1D (pseudo-homogeneous 2D) reactor model has been developed in Visual Basic Applications (VBA) and gives insight into operating envelopes of reactor conditions for FT reactors and aids in understanding the critical factors in early stages of reactor design and optimization.

Methods

The reactor is modeled as a shell and tube heat exchanger with catalyst pellets on the tube side and high pressure boiling water on the shell side. Reactor design equations for mass, energy, and momentum given by Davis and Davis [1] and Froment and Bischoff [2] are solved numerically using a fourth order Runge-Kutta Method [3] with a step size of 0.003 meters. With final conversion specified, the VBA code determines the required length of reactor. All of the water is removed before recycling liquid and gaseous products. Liquid and gaseous effluents are recycled at user-specified recycle ratios. A general n^{th}-order Thiele modulus is used to account for diffusional resistance within catalyst particles. Selectivity is specified by the user as in Table 1. Light hydrocarbon products in the model are specified to have the molecular weight and physical properties of pentane (C_5H_{12}) while the heavy hydrocarbon products are modeled as $C_{25}H_{52}$ and $C_{20}H_{42}$ for Co and Fe respectively.

Table 1. Selectivity models for Co and Fe catalysts

Catalyst	CH_4	C_2-C_7	C_{8+}	CO_2
Co	5%	16%	79%	0%
Fe	4.9%	10.9%	54.2%	30%

The base case simulations model a 400 bbl per-day FT plant operating at 60% CO conversion to produce liquid hydrocarbons. Catalyst particles are 2.0 mm diameter trilobe pellets. The resulting relatively short diffusion length (0.25 mm) gives effectiveness factors of 0.4 to 0.8. Other catalyst geometries (spheres, cylinders, and hollow cylinders) and diameters were also investigated. Four kinetic models for each catalyst were studied.

Results and Discussion

The reactor model was partially validated using data from the Shell Bintulu and Sasol Arge full scale fixed bed reactors for Co and Fe respectively [4]. In each of the simulations, 9 parameters were fixed and T_{in}, T_W, and catalyst activity were adjusted resulting in tube lengths, catalyst charges, and catalyst productivities within 10% of reported values.

Temperature profiles for runs made as a function of recycle ratio (R) (Figure 1) suggest that temperature control without recycle (R = 0) is difficult due to large temperature rises and the presence of hot spots. As R increases, the temperature profiles become more flat indicating that moderate recycle ratios (R = 2-4) give more stable operation.

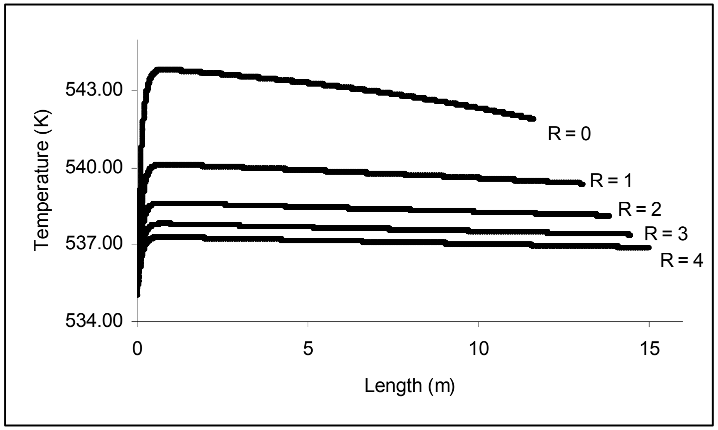

Figure 1. Temperature profiles as a function of recycle ratio for Fe catalysts

Parametric studies were conducted to determine effects of recycle ratio, pressure, inlet temperature, wall temperature, tube diameter, kinetic model, void fraction, and number of reactor tubes on predicted reactor length (i.e. mass of catalyst). Some observations include: (1) gas recycle facilitates good temperature control (2) lowering cooling water temperature (T_w) increases reactor length due to kinetic temperature dependence, and (3) catalyst geometry can have a significant effect on reactor length.

Significance

Modeling has the potential to reduce the cost of a reactor by a factor of 5 – 10 [4]. Improved reactor modeling can reduce the high cost of entry into the BTL, CTL, and GTL industries making FT technology more competitive and attractive as an alternative fuel source.

References

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