Diffusion and Reaction in Fe-Based Catalyst for Fischer-Tropsch Synthesis Using Micro Kinetic Rate Expressions

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Abstract

Introduction: In the early 1920's, Gas-To-Liquids (GTL) and Coal-To-Liquids (CTL) technologies were developed to account for the depleting crude oil resources. During this period, Franz Fischer and Hans Tropsch developed a process to convert synthesis gas (syn gas), derived from coal gasification, to a wide range of high value-added products. This process later came to be known as Fischer-Tropsch (F-T) synthesis. F-T synthesis was an experimental success but its economic viability became a topic of concern as refining of crude oil was a more developed and an economically attractive option [1]. The syn gas used in F-T synthesis can be derived from various feed stocks like coal, natural gas, biomass, and waste. This indirect liquefaction process, also termed as feed-to-liquids, is often referred to as XTLs where X can be C=coal, G=natural gas, B=biomass or W=waste [2].

Multi-Tubular Fixed Bed Reactors (MTFBR) and Slurry Bubble Colum Reactors (SBCR) are widely employed for FTS. An MTFBR is similar to a shell and tube heat exchanger with a catalytic reaction taking place on the tube-side. A typical MTFBR contains about 10 to 50,000 tubes. A coolant flows on the shell-side to maintain isothermal conditions in the reactor. To model such a system, detailed knowledge about shell-side fluid solid interactions coupled with tube-side fluid-solid transport kinetics is required. In this study, attention is focused on modeling of diffusion and non-isothermal reaction in FT catalyst particles since this analysis is a fundamental underpinning for any reactor-scale model.

The primary objective of this study is three-fold: (1) to simulate an isothermal 1-D catalyst pellet model for spherical geometry; (2) use the isothermal pellet model results as a starting point for the non-isothermal case; and (3) use extrusion coupling in the COMSOL Multiphysics® software to link the catalyst pellet (2-D domain) to a single reactor tube (1-D domain). The later provides the starting point for developing a robust model for MTFBR.

Methods: A micro kinetic olefin readsorption model proposed by Wang et al. [3] for an iron-based catalyst is used to study the coupled diffusion, reaction and transport effects using COMSOL Multiphysics. Transport of diluted species is coupled to catalytic reaction in the catalyst particle. This model contains 43 species that participate in 40 independent reactions

which leads to 44 nonlinear coupled ODE's in the case of the 1-D non-isothermal model. COMSOL Multiphysics is used to determine the concentration profiles for all species across the particle spatial domain. Model parameters that are varied include particle diameter, bulk H2/CO ratio, bulk temperature, and bulk pressure.

Results and Discussion: The concentration profiles of the species in a typical Fe-based catalyst are shown in Figure 1. The Vapor-Liquid equilibrium (VLE) calculations using Soave-Redlich-Kwong (SRK) equation of state will also be presented to examine the phase behavior in the catalyst pores. It is shown that to properly model the FT system and to accurately describe the catalyst performance, detailed models for the transport-kinetic interactions that define the yield of each hydrocarbon products are required versus using a lumped approach.

Figures used in the abstract

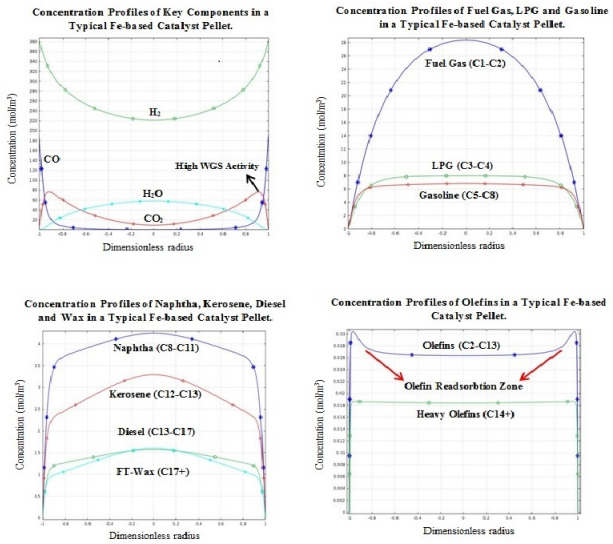

Figure 1: Concentration Profiles of Species in a Typical Fe-based Catalyst Pellet (Parameters: dp = 1.5 mm, Tb = 523 K, Pb = 25 bar, H2/CO = 2, pellet density, ρp (gm/m3) = 1.95 x 106, pellet porosity, εp = 0.51 and pellet tortuosity, τ = 2.6).