TEXAS A&M UNIVERSITY at QATAR

Chemical Engineering Program

Thesis Defense

2-DIMENSTIONAL COMPUTATIONAL FLUID DYNAMIC MODELING ON COMSOL MULTIPHYSCIS OF A FISCHER TROPSCH FIXED BED REACTOR USING A NOVEL MICROFIBROUS CATALYST AND SUPERCRTICAL REACTION MEDIA

Aya Abusrafa

25^{th} September 2019, 5:30- 6:30 PM

LH 144

Fischer Tropsch synthesis (FT) is a highly exothermic catalyzed reaction to produce a variety of hydrocarbon products and value-added chemicals. To overcome the limitations associated with conventional FT reactors, utilizing high conductivity catalytic structures consisting of microfibrous entrapped cobalt catalyst (MFECC) has been proposed to enhance heat removal from the reactor bed. Additionally, utilization of supercritical fluids (SCF-FT) as a reaction media with liquid-like heat capacity and gas-like diffusivity have been employed to mitigate hot spot formation in FT reactors.

The objective of the present study is to investigate the performance of FT Fixed bed/PB reactors operating using SCF-FT as a reaction media and MFECC structures using a conventional cobalt-based catalyst in terms of thermal management, syngas conversion, and product selectivity. A 2-D Computational Fluid Dynamics (CFD) model of an FT reactor was developed in COMSOL® Multiphysics v5.3a for three systems; non-conventional MFECC bed and conventional PB both operating under gas phase conditions (GP-FT) and non-conventional PB in SCF-FT media. The potential of scaling-up a typical industrial 1.5" diameter reactor bed to a larger tube diameter (up to 4" ID) was studied as a first step towards process intensification of the FT technology. An advantage of increasing the tube diameter is that it allows for the use of higher gas flow rates, thus enabling higher reactor productivity, and a reduction in the number of tubes required to achieve a targeted capacity. The high fidelity 2-D model developed in this work was built on experimental data generated at a variety of FT operating conditions both in conventional GP-FT operation and in SCF-FT reactor bed.

Results showed that the MFECC bed provided excellent temperature control and low selectivity toward undesired methane (CH_4) and high selectivity toward the desired hydrocarbon cuts (C_{5+}). For the 4" diameter, the maximum temperature rise in the MFECC bed was always 2% below the inlet operational temperature. However, in PB the temperature can go up to 53% higher than the inlet temperature. This resulted in 100% selectivity toward methane and 0% selectivity toward the higher hydrocarbon cuts (C_{5+}). On the other hand, the CH_4 selectivity in the MFECC case was maintained below 24%, while the C_{5+} selectivity was higher than 70%. Similarly, the maximum temperature rise in SCF-FT for the 4" ID bed was just 15 K compared to ~800 K in the GP-FT bed. The enhancement in thermal performance in the SCF-FT reactor bed is attributed to the high thermal capacity of SCF media (~2500 J/kg/K) compared to GP media (~1300 J/kg/K), which resulted in the elimination of hotspot formation.

Aya Abusrafa

Aya is a Chemical Engineering graduate student at Texas A&M University. She obtained her undergraduate degree in Chemical Engineering from Qatar University in 2016. After her graduation she worked as a research assistant at the Center for Advanced Materials at Qatar University. Aya worked on her thesis under the supervision of Dr. Nimir Elbashir, Dr. Patrick Linke Dr. Ibrahim Hassan.

FOR MORE INFORMATION:
Cherine Hamed
cherine.hamed@qatar.tamu.edu

TEXAS A&M UNIVERSITY at QATAR