MODELING FISHCER TROPSCH NON-CONVENTIONAL TREACTORS AND MEDIA

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Fischer Tropsch Synthesis (FTS) is an exothermic chemical reaction in which synthesis gas (or 'syngas'- a mixture of H_2 and CO) is converted into hydrocarbons or value-added chemicals. In this process, a catalyst (typically cobalt based or Iron based) is used in a Fixed Bed (FB) or Slurry Bed (SB) reactor for the conversion process. Qatar hosts both the technologies in its world's largest Gas to Liquid (GTL) facilities (Shell Pearl GTL and Sasol Oryx GTL). Although both the technologies have been commercially implemented in a large scale, further process intensification by radial scale-up has been a challenging task due to certain process limitation associated with transport characteristics of both the beds. In particular, the FB technology has issues related to hotspot formation owing to exothermicity of the FTS process which is significantly better in its SB counterpart. Our efforts in the current study are invested to understand the FB performance when it is radially scaled-up to a higher reactor geometry, and to possibly mitigate the effect of hotspot formation. In particular, the objective of this work is to utilize the merits of nonconventional Supercritical Fluids FTS (SCF-FTS) to consolidate the benefits of both the beds (FB and SB) to address the challenges related to hotspot formation. For this, we have developed a multi-dimensional computational fluid dynamics (CFD) model in COMSOL® to facilitate a high-resolution understanding of both the SCF-FTS and conventional Gas Phase (GP)-FTS from the perspective of bed thermal management. As an extension to our previous modeling efforts in development of 1-D and 2-D FB-FTS model [1-2], we are currently involved in development of a multiscale 2D model to investigate the pore characteristics using both the modes of operation. Comprehensive experimental investigations were carried out at different operating conditions to support the modeling efforts. A conventional cobalt catalyst with inferior thermal conductivity was investigated in both GP-FTS and SCF-FTS. Later, a novel Micro-fibrous Entrapped Cobalt Catalyst (MFECC) with superior thermal conductivity was investigated in both GP-FTS and SCF-FTS. Conventional catalyst operated SCF-FTS conditions gave a very high α value (0.90) than its GP-FTS. The MFECC catalytic bed on the other hand when operated in SCF-FTS conditions gave a slightly lower α value (0.86), but six-fold % CO conversion than in GP-FTS. MFECC catalytic bed also exhibited higher C_{5+} selectivity & higher catalyst activity in SCF-FTS. In order to closely understand the intricate difference in thermal performance shown by the MFECC bed compared to conventional FB, we have performed a detailed CFD calculation. Results of the MFECC bed have shown to provide orders of magnitude improvement in bed thermal conductivity and proved its capability to control hotspot formation. In particular, the results of $15\%\ \mathrm{Co}/\gamma-\mathrm{Al_2O_3}$ conventional FB at 20 bar and $245\ {}^{\mathrm{o}}\mathrm{C}$ at a gas hourly space velocity of 5000 1/h in a reactor tube of 0.59 inch ID shows hotspot formation of about $100\ {}^{\mathrm{o}}\mathrm{C}$ at the centerline. On the other hand, the temperature rise in MFECC bed for same operating condition was only $6\ {}^{\mathrm{o}}\mathrm{C}$. Further, a very recent outcome of this work enabled us to investigate the potential of scaling-up the radial geometry of the MFECC reactor to a 4" ID reactor to improve its throughput while maintaining temperature homogeneity in the reactor bed [2]. The proposed study is a part of a broader project involving both experimental and modeling studies, and is performed at multiple stages to enable mitigation of challenges related to reactor scale up, and runaway hotspot formation in a fixed bed FT reaction.

References

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