A fundamental study of the Deep Injection-Floating Catalyst Chemical Vapor Deposition reactor via 3D reactive simulations

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Catalytic methane pyrolysis offers an alternative pathway from high-emission processes to sustainable technologies, yielding hydrogen and solid carbon with no CO_x emissions. By adjusting operating conditions and catalytic materials, it is possible to control the synthesis of high-quality carbon products, including carbon nanotubes (CNTs). A promising method for CNT synthesis is thermo-catalytic cracking in Floating Catalyst Chemical Vapor Deposition (FCCVD), where carbon feedstock is injected along a carrier gas in a tubular reactor and decomposes on metal nanoparticles, formed *in situ*, serving as catalyst and template for CNT growth. Achieving successful CNT growth requires precise synchronization between catalyst particle formation and feedstock activation to avoid issues like overgrowth or early deactivation. In this work, the ferrocene precursor and homogeneous pyrolysis chemistry, catalyst nanoparticle dynamics and the and the complex fluid dynamic patterns using reactive CFD 3D simulations providing guidelines for reactor design.

This study presents a multiscale CFD model within the catalyticFOAM framework to simulate iron nanoparticle formation and homogeneous methane pyrolysis in an FCCVD reactor. The approach employs a semi-detailed kinetic scheme for ferrocene decomposition and iron nananoparticle (FINs) formation and a homogenoues methane pyrolysis scheme to predict soot formation, coupled to momentum and energy transport, in which radiative heat transfer is accounted for using the DOM model. As an example, the main results of CFD simulations are reported in Figure 1 for in the case of inlet gas mixture composed of 61% He, 36.5 % H_2, 2.5% CH_4 and 100 ppm of ferrocene, fed at 433 K with a flowrate of 4663 sccm.

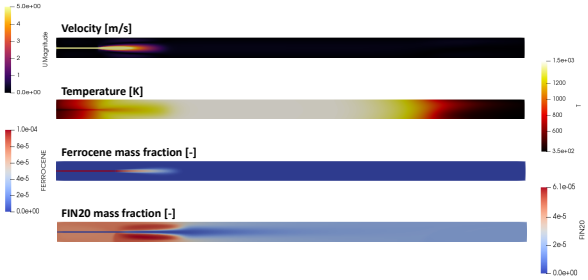

Figure 1: Velocity, temperature, ferrocene and FIN20 species mass fraction maps for DI-FCCVD reactor fed with 61% He, 36.5 % H_2, 2.5% CH_4 and 100 ppm of ferrocene, fed at 433 K with a flowrate of 4663 sccm

These simulations describe the conversion of the catalytic precursor and methane within the unit, providing insights into the spatial distribution of iron nanoparticles, as well as predicting the soot formation. This allows the proper tuning of the operating conditions in order to obtain favorable nanoparticle diameters for high-quality CNT synthesis and limit soot formation.

Keywords: *Turquoise hydrogen, carbon nanotubes, CFD simulations, ferrocene, iron nanoparticles*