Enhancing the catalytic properties of Mo/ZSM-5 catalysts for methane dehydroaromatization by ex situ formation of metal carbides

Abstract: Finding new uses for methane as a fuel and chemical feedstock in the manufacturing industry is of increasing interest since methane is the main constituent of natural gas, of which vast natural reserves are being exploited. Large quantities of this natural resource are being flared due to lack of infrastructure and high transportation costs. Among the different direct processing reactions that exist to convert methane to value-added products, there has been a growing interest in the heterogeneous catalytic conversion of methane to a mixture of benzene and hydrogen, by the non-oxidative methane aromatization reaction (6 CH₄(g) → C₆H₆(g) + 9H₂(g)), which happens in one step. Our group is carrying out a fundamental and systematic study of this catalytic process with the goal to answer some fundamental questions, which can mitigate the technological challenges of this process.

Zeolite-supported molybdenum catalysts have so far been the most widely studied catalysts for the methane aromatization reaction, however, they do not fulfill the conversion and stability requirements for commercialization. It is agreed that Mo carbide species, originated by exposure of the Mo oxide species to the reactant methane, are responsible for methane activation, however, the nature and amount of carbide phases formed in the induction period of the reaction are not controlled. Our group has recently discovered the importance of the conditions at which the zeolite-supported molybdenum carbides are formed on the catalyst stability. We have tested different preparation conditions and contrasted the structure of the fresh and spent catalysts to explain the difference in catalytic behavior. Our results have resulted in obtaining Mo/ZSM-5 catalysts that maintain remarkably stable benzene yields over long periods of time in reaction.

Dr. Sheima J. Khatib joined the Department of Chemical Engineering at Texas Tech University as tenure-track Assistant Professor in Spring 2015. She received her PhD in Chemistry under the guidance of Miguel Angel Bañares from the Autonomous University of Madrid and the Institute of Catalysis and Petrochemistry (CSIC) (Spain) in 2007. She continued her research from 2008-2010 in the Institute of Physical Chemistry “Rocasolano” also in Madrid, with Jose Maria Guil, and then moved to Virginia Tech to work in the group of Ted Oyama. Her expertise is in studying structure-activity relationships, adsorption microcalorimetry and membrane technology applied to heterogeneous catalysis. Her main areas of interest are natural gas conversion, dehydroaromatization, bio-inspired catalysts for heterogeneous chemical conversion, catalyst stability, determination of deactivation and regeneration pathways. Recently she received the 2019 NSF CAREER Award for a project combining methane dehydroaromatization with membrane technology. She is also passionate about exploring new engineering education methods in her classes and places much emphasis on teaching, having received five teaching awards including the 2019 Texas Tech Alumni Association Award, 2017 George T. and Gladys Abell-Hanger Faculty Award at Texas Tech University and the 2017 and 2018 AIChE student chapter awards, also at Texas Tech. She has given 12 invited lectures, published 22 peer-reviewed articles, serves as Director of the Southwest Catalysis Society; the Fuels and Petrochemicals Division (F&PD) and the Catalysis and Reaction Engineering Division (CRE) of the AIChE.