Effects of Pore Confinement on Hydrocarbon Pyrolysis

A. C. Buchanan, III, Michelle K. Kidder, Phillip F. Britt, Edward W. Hagaman, Zongtao Zhang, and Sheng Dai

Chemical Sciences Division
Oak Ridge National Laboratory
Bethel Valley Road
P.O. Box 2008, MS-6197
Oak Ridge, Tennessee 37831-6197

Abstract

Mass transport limitations impact the thermochemical and catalytic processing of hydrocarbon resources into desirable products. Our previous studies of the fundamental aspects of restricted mass transport on high temperature, free-radical reactions for hydrocarbon resources employed model compounds that were covalently attached to the external surface of nonporous silica nanoparticles (Cabosil). We are now examining the impact of pore confinement on the pyrolysis (375°C) kinetics and product distribution for the probe molecule, 1,3-diphenylpropane (DPP). This molecule has been attached to the surface of high surface area, mesoporous silicas, SBA-15 and MCM-41, whose pore sizes can be controlled. Reaction of the surface silanols of the mesoporous silicas with *p*-(3-phenylpropyl)phenol gave the corresponding surface-attached (Si-O-C_{aryl} linkage) DPP, which has been characterized by BET surface analysis, elemental and chemical analysis, FTIR and NMR. Initial pyrolysis results indicate that the rate and product distribution depend on the pore size of the mesoporous silica (1.9-5.6 nm). The DPP pyrolysis behavior will also be compared with that in the gas phase and on the nonporous silica.

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