Pyrolysis of hydrocarbons confined in porous solids

A. C. Buchanan, III, Michelle K. Kidder, and Phillip F. Britt

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

Abstract

Mass transport limitations can play an important role in the processing of hydrocarbons. We recently initiated a fundamental examination of the effects of pore confinement on high temperature, free-radical reactions for fuel model compounds. 1,3-Diphenylpropane (DPP) and benzyl phenyl ether (BPE) have now been covalently attached to high surface area, mesoporous silicas, SBA-15 and MCM-41, whose pore sizes are varied from 1.7 – 5.6 nm. The resulting hybrid materials have been characterized by BET surface analysis, elemental and chemical analysis, FTIR and C-13 NMR. Initial results indicate that pyrolysis rates and product selectivities can be impacted in unexpected ways. For example, the pyrolysis rate (375 °C) for pore-confined DPP was found to be faster than for DPP on nonporous silicas, and the rate increased with decreasing pore size. The origin of this effect will be discussed.

Research sponsored by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.