143y Kinetic Investigations of Propylene Epoxidation Using in Situ Generated H2o2 in CO2 Solvent Media

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A rising environmental awareness and increasingly stringent environmental laws demand alternative synthetic routes in the production of various commercially useful products. Current areas of research include the use of green oxidants, supercritical CO2 reaction media, the design of high performance catalysts, solvent-free routes, and the use of renewable resources. Our primary focus is the substitution of harsh organic solvents with more environmentally benign solvents; thereby, permitting greener chemical processing. Hydrogen peroxide is generally considered a benign oxidant that is a promising alternative to conventional oxidants. The typical method used to generate a majority of the world's H2O2 is the anthraquinone (AQ) process. This process is commercially successful because it not only prevents the direct contact of hydrogen and oxygen, but also produces H2O2 continuously at moderate conditions. Even so, the AQ process requires multiple unit operations, produces several significant waste streams, and is highly energy intensive. Thus, the relatively high cost of H2O2 production limits its use in commodity chemical processing. The most atom-efficient method for H2O2 production is the direct reaction of hydrogen and oxygen. However, this is also perhaps the most dangerous method for H2O2 production. The use of carbon dioxide as the organic solvent for this reaction has great potential. Carbon dioxide is non-flammable, relatively non-toxic, environmentally benign, naturally abundant, and cannot be further oxidized. Also, the safe operating range is broader for mixtures of H2/O2 when in carbon dioxide. Since H2 and O2 are completely miscible with CO2 at temperatures above 304 K—the critical temperature of CO2, carrying out the reaction in supercritical CO2 media allows for single phase operation. In so doing, the transport limitation barrier that exists in the conventional synthetic route of H2O2 is eliminated. In this poster, results from the kinetic investigations of propylene epoxidation using in situ generated H2O2 in CO2 solvent media are presented. The epoxidation of propylene was conducted in both batch and continuous mode reactors over a Pd/TS-1 catalyst. The conversion of propylene, the yield of propylene oxide, and the catalyst maintenance were measured. Also, reaction parameters such as temperature, pressure, and the H2/O2 ratio were varied in order to determine how these factors effect the conversions and yield of the reaction.