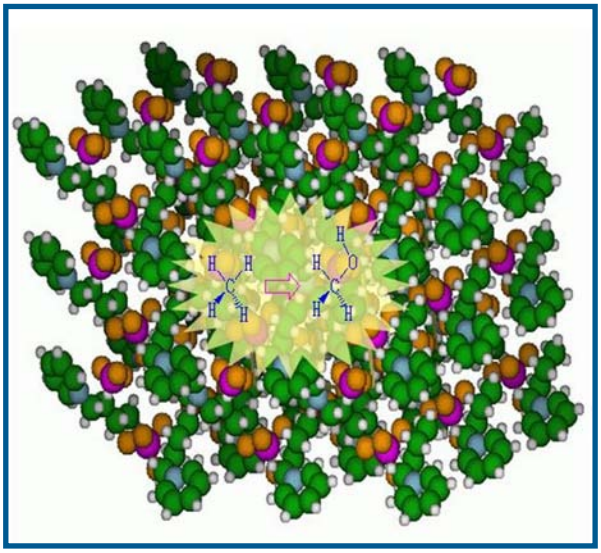
Using Ionic Liquids in Selected Hydrocarbon Conversion Processes

Ionic Liquids Promise Elimination of Hazardous and Environmentally Unfriendly Solvents

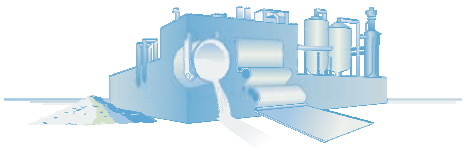
Current methanol production relies on expensive and energy intensive technology that initially coverts methane to syn-gas (CO/H_2) at a high temperature (>500ºC). Catalytic systems have recently been developed to directly convert methane to methanol. However, this new method uses highly concentrated sulfuric acid as the reaction media, which increases production costs by requiring separation of the methanol from sulfuric acid.

In the last 20 years, ionic liquids have emerged as a promising new solvent for selective hydrocarbon conversion. These solvents consist entirely of ionic species and are characterized by unique properties, such as low melting point, low vapor pressure, no toxicity, and thermal stability. Such properties make ionic liquids an ideal reaction media for a number of chemical processes.

This project seeks to replace all or part of the sulfuric acid reaction media with ionic liquids in the direct conversion of methane to methanol. The project team will combine novel experimental and theoretical methods to develop a fast-screening method to identify the best ionic liquids for an optimized catalyst/oxidant/solvent system. Ionic liquids promise to eliminate hazardous and environmentally unfriendly solvents while lowering the cost and energy consumption of methanol production.



Iillustration of an ionic liquid responsible for reducing the barrier for the catalysis of CH_4 to CH_3OH



Benefits for Our Industry and Our Nation

Ionic liquids have the potential to eliminate the use of today's hazardous and environmentally unfriendly solvents in the petrochemical industries. They also may enable the development of low-temperature, cost-effective, high-selectivity, direct oxidative methane-to-methanol conversion. By 2020, the energy savings for this technology could be as high as 30 trillion Btu per year for liquid acid alkylation alone.

Applications in Our Nation's Industry

Ionic liquids have the potential to become an ideal reaction media for many chemical processes. If successful, this research effort will have a significant impact on domestic petrochemical industries.

Project Description

The focus of the project is to improve the catalyzed system for methane selective oxidation by using ionic liquids as the reaction media. The project team also seeks to gain a fundamental understanding of ionic liquids for selective hydrocarbon conversion to enable the creation of new process systems.

Barriers

Major barriers to be overcome include:

- Ionic liquid materials are not typically synthesized on a large scale, which makes them relatively expensive. However, the cost of ionic liquids is expected to drop as more applications are identified.
- The chemical behavior of ionic liquids is not well understood.
- Most ionic liquids currently available are not suitable for C-H activation catalysis.

Pathways

The objectives of this project will be achieved through (1) developing a reliable model for solvent effects on the reactions in ionic liquids, based on increased fundamental understanding of the roles of ionic liquids in catalyzed chemical processes at the molecular level; (2) developing a rapid screening method for identifying the most promising ionic liquids for alkylation and arene reactions, utilizing strong collaboration between theory and experiment; and (3) developing new chemical processes for direct methane-to-methanol conversion that are cost-effective, highly selective, low-temperature, and environmentally friendly.

Progress and Milestones

- Conduct compatibility tests to determine stability of ionic liquids containing sulfuric acid and methanol (completed)
- Design low and high pressure reactors for testing methane conversion and conduct quantitative analyses (completed)
- Develop a database of the molecular structural information of ionic liquid prototypes (completed)
- Evaluate the utility of ionic liquids as a solvent for methane conversion (completed)
- Develop a rapid screening method for optimizing performance of candidate ionic liquid/catalyst systems (completed)
- Optimize and demonstrate the selected solvent/acid/catalyst system

Commercialization

The project has various partners that will participate in developing and commercializing the technology. Caltech's Power, Energy, and Environmental Research Center (PEER) will use novel experimental methods to screen new ionic liquid/catalyst test designs and will further develop those that seem promising. This experimental work will also serve to provide test data to tune and test theoretical predictive tools that will be developed at Caltech's Materials and Process Simulation Center (MSC). The Loker Hydrocarbon Research Institute at USC will provide their expertise in catalysis and reaction mechanisms for the particular hydrocarbon conversion processes. ChevronTexaco Corp. will provide inputs from an oil/chemical company perspective of selected hydrocarbon conversion processes, including insights about commercial catalyst technology. Sachem, Inc. has expertise in the development and the industrial application of ionic liquids and will offer guidance on the commercial application of viable ionic liquid candidate systems.

Project Partners

Material and Process Simulation Center (MSC)
California Institute of Technology (Caltech)
Principal Investigator:
William A. Goddard III (wag@wag.caltech.edu)

Power, Energy, and Environmental Research Center (PEER)
California Institute of Technology (Caltech)

Loker Hydrocarbon Institute
University of Southern California

ChevronTexaco Corp.
Richmond, CA

Salchem, Inc.

A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy
Bringing you a prosperous future where energy is clean, abundant, reliable and affordable

February 2009