

## Challenges and Opportunities for Catalysis Research in Biofuels Refining

Although the last few decades have provided significant advances in ethanol biofuel production, much less effort has been directed toward the development of high-tech methods for converting biomass into "green" hydrocarbon fuels such as gasoline, diesel and jet fuel. These fuels are more attractive than ethanol because of their higher heat content and lower solubility in water. Moreover, they can be fully interchangeable with petroleum-derived fuels and can be directly incorporated into the existing infrastructure.

However, their production and refining involve numerous technological challenges. At the same time, these challenges represent excellent opportunities for research and development by the chemical engineering community.

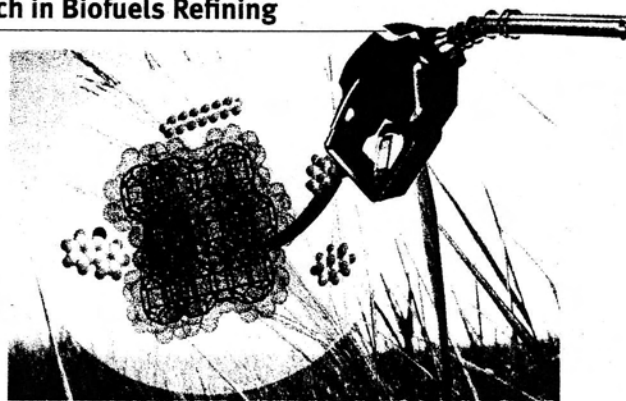
"An important body of fundamental knowledge already exists for catalytic processes involved in the upgrading of petroleum fuels," explains Prof. J. Dumesic of the Univ. of Wisconsin. "This knowledge, gained through efforts of researchers over many decades, can serve as the initial basis for biofuel refining. However, the complexity of new biorefining systems has only recently started to become apparent, requiring new and innovative approaches."

The complexity and instability of pyrolysis oils pose huge analytical challenges. Nonetheless, novel analytical techniques and modern instrumentation are making significant progress in this area and are now able to provide detailed information about chemical composition. This information will allow researchers to discriminate among the different chemical groups in the biofuels and could make the development of composition-property relationships possible.

The technological background gained in the area of fossil fuel refining has worked in the researchers' favor, while the extreme economic pressures to obtain something competitively priced in a minimum amount of time have not. A better understanding of the fundamental reactions occurring on the catalyst surface will help accelerate the development of effective catalytic strategies for the production of fuels with acceptable properties for the current infrastructure.

This is discussed in the May issue of *AICHE Journal*, in the Perspective article entitled "Molecular Engineering Approach in the Selection of Catalytic Strategies for Upgrading of Biofuels." The approach consists of utilizing model compounds and mixtures of model compounds that represent a more-complicated feedstock.

The main goal is to understand the fundamental chemistry involved in the reactions, and link this understanding to the practical impact of fuel composition on fuel prop-



erties. Some important relationships between the model compounds and their resulting fuel properties of interest are determined on the basis of their molecular structure. A linkage is proposed between the nature of catalyst active sites and the molecular structure of model compounds through the study of selected reactions and careful catalyst characterization. These two relationships can link the fuel properties of resulting products to specific catalysts and reaction conditions using the structure of model compounds.

Numerous properties influence the quality of a given fuel, including octane and cetane numbers, sooting tendency, water solubility, freezing point, viscosity, flash-point, cloud point, autoignition temperature, flammability limits, sulfur content, aromatic content, density, boiling point, vapor pressure, heat of vaporization, heating value, thermal and chemical stability, and storability. Catalytic upgrading can modify many of these properties. In designing a catalytic upgrading strategy, a refiner must know how each of these properties is affected by the structure of the molecule and how a given catalytic conversion of that structure in turn affects the properties.

The main complications of this method arise from the nonlinearities of blending effects. Studies based on a single model compound can be taken as a first approach to provide direction toward optimizing fuel properties, but not the ultimate solution. Surrogate blends are important for studying the effect of intermolecular interactions in solubility as well as adsorption competition among different molecules.

As one increases the complexity of the system, the picture of what is occurring on the surface becomes increasingly murky. However, fundamental studies are highly valuable in providing guidance for the development of rational refining strategies rather than purely empirical approaches.

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