Catalysis for Alternative Energy Generation

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Editors

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Preface

Chemistry without catalysis is like a bell without sound, or a warrior without blade.

Alwin Mittasch

In the twenty-first century, human beings face the exhaustion of fossil energy feedstock. The amount of high quality and easily accessible feedstocks is decreasing, hence the use of heavy and dirty feedstocks must perforce be explored. Poisoned crudes need to be treated in order to remove contaminants such as Nitrogen- and Sulfur-containing molecules and metals. Thus it is imperative to consider alternative sources of energy – such as biomass – for chemicals and for transportation fuels. To underline its importance let me refer to President Bush: *President Bush launches the Hydrogen Fuel Initiative. "Tonight I am proposing $1.2 billion in research funding so that America can lead the world in developing clean, hydrogen-powered automobiles. With a new national commitment, our scientists and engineers will overcome obstacles to taking these cars from laboratory to showroom so that the first car driven by a child born today could be powered by hydrogen, and pollution-free."*

Alternative feedstocks, such as biomass and renewables, are being investigated in biorefineries for the production of biofuels and (bio)chemicals. These feedstocks contain many oxygen-containing molecules, hence they are more or less polar. This poses special problems for the development of catalytic technology to treat such new feedstocks.

Very pure and simple natural feedstocks, such as methane and light alkanes, can also be used as the basis for production of fuels and chemicals. The fundamental problems here are the selective activation of the C–H bond without the formation of excessive amounts of CO_2, hydrogenation of CO_2, or its conversion into other useful materials.

Looking through the possible technologies, it becomes clear that catalysis is the key technology to help solve the problems associated with the use of alternative feedstocks. Traditional catalysts are extremely efficient for pure, apolar oil feedstocks. Heavy and dirty feedstocks require catalysts for removal and decomposition of poisonous molecules and for removal of heavy metals. Can these processes be combined in one catalyst? This "ideal" catalyst fixes the heavy metals in such a way that they serve as catalytic sites for decomposition and removal of the poisonous molecules. In addition, the catalyst contains the acid sites necessary for cracking and isomerization of long-chain hydrocarbons.

In the case of biomass and renewables, poisoning of the catalyst surface by polar molecules must be avoided. The "ideal" catalyst takes oxygen atoms out of the polar molecules and stores them in its structure in such a way that the catalyst becomes ready to do its job, the conversion of biomass into fuels and basic chemicals.

For methane conversion, catalytic research boils down to "selectivity": selective activation of the C–H bond while avoiding complete burning of methane into carbon dioxide and water.

The ideal catalysts, as described above, do not exist, except for the enzymes that activate methane by insertion of an oxygen atom in the C–H bond. We must rely on

1. The design and construction of improved catalyst materials, which are designed by either combinatorial methods or rational catalyst design, based on theory and advanced characterization methods
2. The intelligent combination of different types of catalysts, making use of the respective strengths of these catalytic materials; all combinations should be allowed: enzyme plus heterogeneous catalyst, homogeneous plus heterogeneous catalyst; and so on;. In this respect, photocatalysis also comes into the picture; and
3. Alternative reaction media in which catalytic and separation technologies are combined. Examples include catalysis in ionic liquids, supercritical conditions. In this way, nonreactive aggregates of molecules can be disentangled into monomolecular entities, which are more susceptible to catalytic attack.

Finally, irrespective of the catalytic process developed, questions will be raised about the sustainability of the catalyst, its impact on the environment, and its impact on climate. The economic, environmental, and social impacts of a process must be evaluated before production can start. Scientists must take these considerations into account in multidisciplinary studies.

Readers of this book will learn about the importance of catalysis in these processes. Introductory chapters discuss catalysis and catalytic processes to handle the broad variety of alternative feedstocks (biomass, methane, very heavy crude, and bitumen) that one can use for the production of transportation fuels and chemicals. The start of the discussion is knowledge of the performance of the catalysts currently on the market and the performance of catalysts in development. Further chapters explore the effect of impurities and poisons in these alternative feedstocks on the performance of existing catalyst materials and propose new challenges for improving these materials. In addition, several routes are designed to approach the "ideal" multifunctional catalyst or the "most appropriate" combination of "ideal" catalytic materials to handle these new feedstocks.

The role of new tools of investigation, in situ spectroscopic observation of catalysts in action, and theory in this process of catalyst development is highlighted. Finally, the socioeconomic implications in using these alternative feedstocks are briefly covered.

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