Energy and Economic Savings From Improved Catalysts

Executive Summary

November 1986

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FROM IMPROVED CATALYSTS

EXECUTIVE SUMMARY

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PREFACE

The Energy Conversion and Utilization Technologies Division of the U.S. Department of Energy (DOE) authorized two studies in support of developing a materials-by-design program. The first is a study by Universal Oil Products to assess the present and future potential for developing mathematical models of certain interatomic phenomena; these models are needed for the design and optimization of practical processes and materials. The second study, undertaken by the Pacific Northwest Laboratory (PNL), is to assess the energy and economic impacts of the ability to design improved catalysts. This document is the Executive Summary for the PNL study. The main reports for both studies are being published by the DOE.

ENERGY AND ECONOMIC SAVINGS FROM IMPROVED CATALYSTS

EXECUTIVE SUMMARY

The Pacific Northwest Laboratory (PNL) conducted this study for the U.S. Department of Energy (DOE) to estimate the energy and economic benefits of applying the materials-by-design approach to catalysts.

The integration of theoretical modeling and computational capabilities with information from rapidly advancing experimental techniques provides the framework for a materials-by-design tool to resolve materials and interface problems. The tool would allow scientists to relate the desired properties and performance characteristics to the atomic structure and bonding taking place in the material (especially at non-bulk sites such as surfaces and interfaces) using a computer. As progress continues, it is possible to envision designing a whole new generation of energy-related materials such as catalysts using the materials-by-design approach to supplement conventional methods for developing materials. Improvements in the technology of catalytic materials could have a major impact on energy consumption in many areas, including the processing of fuels and chemicals. The key question is whether there is sufficient payoff to warrant the research investment necessary to commercialize the materials-by-design approach.

Dr. James Eberhardt, a program manager for the Energy Conversion and Utilization Technologies (ECUT) program of the DOE, initiated this study through PNL to determine the potential of this approach. The purpose of the study was to estimate the energy and economic costs and benefits of applying the materials-by-design concept to catalysts. Catalysts are of particular interest because of the competitive challenge from Japan, West Germany, and France. Initial estimates developed in this study reveal a potential capital cost savings of \$31 billion and an operating cost savings of \$69 billion for chemical and petroleum refining plants over a 15-year period. The findings of this study substantiate the claim that a major U.S. effort to enhance

materials-by-design technology is warranted, at least for catalyst materials. In addition, this technology would ensure pre-eminence by the U.S. industry.

BACKGROUND

The development of materials-by-design for catalysts would offer at least three substantial benefits. First, energy and capital savings would result, which would improve the viability of the domestic petroleum refining and chemicals industries. These savings were quantitatively determined in this study for the petroleum refining and chemicals industries. Second, pre-eminence in the manufacturing of catalysts would be ensured. Because countries like Japan, West Germany, and France have established institutional networks to promote the discovery of new catalysts, U.S. industries could be at a disadvantage in trying to maintain a leading role in product and process development. Third, the development of improved catalysts would enhance the technical and economic competitiveness of producing synthetic fuels from alternative feedstocks.

In addition to the energy and economic savings, two potential benefits of the materials-by-design capability, which are not specifically evaluated in this study, should be noted: 1) shorter time to develop catalysts, and 2) faster attainment of scientific breakthroughs. Less time would be required to develop catalysts because much of the work could be done on computers, eliminating the need for a large amount of empirical research. Research goals could thus be attained more quickly and with fewer resources. Although these savings are significant, no attempt was made in this study to quantify them.

Attaining scientific breakthroughs would mean new catalysts, which could eventually redefine the chemical processing market. An example of the dramatic market impact of scientific breakthroughs is the effect of semiconductors. Semiconductors were probably not designed with the intention of revolutionizing the electronics market. They were designed as small, lightweight replacements for bulky vacuum tubes; however, their small size suddenly reduced room-sized computers to portable, even pocket-sized versions, opening the door to a vast array of new applications for computer technology. The market impact of scientific breakthroughs is hard to predict (and therefore not included in the estimates of cost savings), but there is a high probability that these

breakthroughs may occur using the materials-by-design approach. Because this study did not attempt to predict these breakthroughs for catalysts, the analysis is rather conservative. Thus, the potential cost saving of around \$100 billion represents only a part of the benefits.

All of these benefits clearly would be in the national interest because they would promote increased international competitiveness and decreased reliance on foreign sources of energy. Therefore, the DOE is sponsoring a materials-by-design program for catalysts. The goal of this program is to design catalysts that will drastically improve the performance and efficiency of catalytic or potentially catalytic processes that either consume or produce fossil energy.

To reach this goal in a timely fashion, two things are needed: 1) proper planning and focusing of research efforts, and 2) adequate justification for the extensive research effort needed to make materials-by-design a reality. DOE's ECUT Division has recognized these needs and has authorized two studies to begin addressing these areas. The first is a study by Universal Oil Products to assess the present and future potential for developing mathematical models of certain interatomic phenomena, for the design and optimization of practical processes and materials. The second study, conducted by PNL and described in this summary, is designed to assess the energy and economic impacts of the ability to design improved catalysts.

The value of being able to design catalysts to specification is difficult to quantify precisely, although it is enormous. However, the economic impact of developing materials-by-design may be gauged by considering the example of a direct methanation catalyst developed by the Gas Research Institute. The direct methanation catalyst has been estimated to save 20% of the energy and 15% of the capital cost of a typical synthetic natural gas (SNG) plant (Meyer and Hill 1982; Meyer, Hill, and Flowers 1982). These percentages translate to a capital cost savings of \$150 million per plant, an annual operating cost saving of \$20 million per plant, and a potential total cost savings exceeding \$500 million over the life of a single SNG plant.

PNL used three case studies (fluid catalytic cracking, alkylation, and styrene production) to evaluate the potential energy and economic savings from improved catalysts in existing processing in the refining industry and the impacts of new catalytic processes for the chemicals industry. These cases were selected because they are typical of large-scale catalytic processing: they use large amounts of energy and, therefore, could maximize the benefit from the development of improved catalysts. The benefits were estimated by comparing current capital and operating costs and energy uses with processes using the optimally designed catalysts. Nationwide impacts were then estimated for these case-study industries. In addition to these quantitative estimates, improved catalysts may have significant impacts on feedstock flexibility and environmental control, which are qualitatively described below.

POTENTIAL ENERGY SAVINGS

Fluid catalytic cracking, alkylation, and styrene production are energy-intensive processes. In all of these cases, improved catalysts would provide savings in feedstock and process energy usage.

Fluid Catalytic Cracking (FCC)

Catalytic cracking breaks down high molecular weight hydrocarbons from heavy petroleum fractions to lighter compounds, such as gasoline. About one-third of the total input to a refinery is processed by catalytic cracking, making it second only to hydrotreating as the largest catalytic refining operation in terms of process volume (Cantrell 1982). Total energy consumption for state-of-the-art FCC, including feedstock energy and all utility requirements, is currently 2.8×10^6 Btu/barrel (bbl) feedstock, or 2.12×10^4 Btu/lb gasoline produced (Cantrell 1982).

The amount of energy that could be saved by using an ideal catalyst is estimated to be 1.3×10^3 Btu/lb of gasoline produced. The energy savings would result from reduced feedstock requirements, which would be cut in half while still yielding the same volume of gasoline. Process energy savings are not apparent, but feedstock energy savings would be significant. In 1984 total gasoline production was 6.5×10^6 bbl/d (Oil and Gas Journal 1984), of which

1.86×10^6 bbl/d were produced by FCC (Cantrell 1982; U.S. Department of Commerce 1983). Assuming 100% market penetration, 2.57×10^{14} Btu/yr of feedstock energy could be saved.

Alkylation

Alkylation reactions combine mixed butylenes and/or propylenes with isobutane to form highly branched, high-octane enhancers for gasoline. The process volume is small relative to other refining operations, but process energy consumption is relatively high. Total energy consumption for a state-of-the-art alkylation process is currently 2.052×10^4 Btu/lb alkylate produced (Meyer, Chapin and Muir 1983). This total includes feedstock and production energy, and all utility requirements.

The amount of energy that could be saved by using an ideal catalyst is estimated to be 950 Btu/lb alkylate produced. Feedstock requirements would be unchanged, but the process energy requirements would be reduced by 85%. In 1982 production of alkylate was 5.89×10^5 bbl/d (Meyer, Chapin and Muir 1983). Assuming 100% market penetration, 4.85×10^{13} Btu/yr of process energy could be saved.

Styrene Production

Styrene is currently produced by catalytic alkylation of benzene with ethylene to ethylbenzene, followed by catalytic dehydrogenation to styrene. The energy consumption of styrene production is the largest in the chemicals industry, accounting for about 10% of the feedstock energy and 1% of the process energy. If ideal catalysts were used in styrene production processes, total energy requirements could be reduced by about 21%. For current annual styrene production, this represents a potential savings of 4.8×10^{13} Btu/yr.

POTENTIAL SAVINGS IN CAPITAL AND OPERATING COSTS

The results of capital and operating cost savings estimates for ideal catalyst substitution for fluid catalytic cracking, alkylation, and styrene production are summarized below. In all three cases, over half of the capital costs of a new plant could be saved.

Fluid Catalytic Cracking

Capital cost for a new state-of-the-art FCC unit producing 19,950 bbl/d of gasoline is reported to be \$67 million in 1983 dollars (Hammershaime and Verson 1983). If an ideal catalyst were used, requirements for flue gas cleanup, fractionation, and regeneration would not be as rigorous, and therefore, capital costs could be dramatically lower. Capital costs for a new FCC unit incorporating an ideal catalyst would be only half those of the state-of-the-art FCC unit, or \$34 million in 1983 dollars.

Alkylation

The capital cost for a new state-of-the-art alkylation unit producing 3,500 barrels/stream day of alkylate is reported to be \$9.5 million in 1983 dollars (Meyer, Chapin, and Muir 1983; Phillips Petroleum Company 1984). Alkylation units are currently of two types, using either HF or H_2SO_4 as a catalyst. Capital costs are equivalent for each type. If an ideal catalyst were used, requirements for acid circulation and cleanup would be eliminated, refrigeration requirements would be greatly reduced, and heating requirements would be somewhat reduced. Capital costs for an alkylation unit that incorporated the ideal catalyst would be 44% of the state-of-the-art alkylation units, or \$4.2 million in 1983 dollars. There would be an operating cost savings of \$3.00/bbl alkylate.

Styrene Production

Capital costs for an ideal styrene process would be about 83% less than the costs of a conventional plant. Savings would result from the simplicity of the plant. The current process requires capital equipment for two reaction steps, with complex separation operations required for each step. The ideal process would require only equipment for one reaction step and by-product hydrogen separation.

Operating costs for a styrene plant using an ideal catalyst would be reduced by 18% compared with the costs for existing plants using conventional technology. Savings would result from reduced feedstock, labor, and maintenance costs. In addition, purchased fuels and electricity would no longer be

required because some of the hydrogen produced during the process would be used as fuel. Excess by-product hydrogen could be sold for a cost credit.

CUMULATIVE NATIONAL IMPACTS: 1985-2000

Data for Standard Industry Classifications (SICs) were used as a basis for estimating the cumulative impacts for ideal catalysts. The time frame for this assessment, 1985 to 2000, is illustrative because the actual research needed to provide catalyst design capability would take a significant portion of this time period.

Feedstock Energy Savings

For chemicals production, an estimated 1.2 quad (1 quad is 10^{15} Btu) could be saved and for petroleum refining, 7.9 quad could be saved. This is a total savings of 9 quad out of a total of 539 quad to be used.

Process Energy Savings

An estimated 9.8 quad would be saved in chemicals production, but an increase of 1.15 quad for petroleum refining would be realized.^(a) Total process energy savings would be 8.65 quad out of a potential total of 138.7 quad.

Capital Cost Savings

An estimated cumulative total of about \$275.6 billion will be invested between 1985 and 2000: \$118.2 billion for the chemicals industry and \$157.4 billion for the petroleum refining industry. If ideal catalysts were available, capital cost savings of \$22.1 billion for organic chemicals production and \$22.5 billion for petroleum refining could be realized.

Operating Cost Savings

An estimated cumulative total of \$3.759 trillion would be invested in operating costs between 1985 and 2000: \$2.380 trillion for petroleum refining and \$1,379 billion for petrochemicals manufacture. If ideal catalysts were

(a) This increase is due to the greater weight placed on petroleum refining by the methodology used in this study; process energy savings were forfeited to attain larger feedstock energy and capital cost savings.

available, operating cost savings of \$55.8 billion for the chemicals industry and \$12.8 billion for the petroleum refining industry would be possible.

ADDITIONAL BENEFITS OF IMPROVED CATALYSTS

Improvements in catalysts offer several potential benefits that were not addressed in the case-study calculations. These additional benefits further support the rationale for developing materials-by-design technology for catalysts.

Reduced Environmental Impacts

The volume and content of pollutant by-product streams could be minimized. Improved catalysts could reduce toxic waste production and emissions that contribute to problems such as acid rain.

Greater Use of Alternative Feedstocks

One of the most strategically significant benefits that could result from developing a catalyst design capability would be the use of less expensive, more abundant, domestic resources such as coal and biomass for fuel and petrochemical productions. A decrease in U.S. dependency on foreign imports of petroleum would be a highly desirable benefit.

Development of New Chemicals and Processes

The availability of ideal catalysts would spur the development of new processes. For example, improved catalysts could play a key role in the development of technology to produce hydrogen by the photolysis process. This technology would result in the widespread availability of a clean burning fuel that does not produce any air pollutants.

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