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Impact of Catalysis on the Production of the Top 50 U. S. Commodity Chemicals

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Preface

The purpose of this report is to address the impact of catalysis on the production energy of the top 50 U. S. commodity chemicals and assess the limitations of the production routes. The report intends to present this information in a form which aids readers who may be unfamiliar with catalysis to make informed decisions. The author has endeavored to faithfully adhere to these criteria.

Summary

The impact of catalysis is evaluated for the production of the top 50 U.S. commodity chemicals. Information on each chemical is stored in an accompanying Excel™ 4.0 spreadsheet ("top50chem.xls"). This analysis tool allows the user to make assumptions about process yield improvements and evaluate the corresponding impact on the process and feedstock energy. Many scenarios have been investigated and are reported in the text. If all of the catalytic processes associated with the top 50 chemicals were raised to their maximum process yields, the corresponding process and feedstock energy savings would exceed 0.47 quads per year. More realistic process yield improvements of 1%, 5%, and 10% where possible, would save 0.03, 0.14, and 0.23 quads per year.

Many of the commodity chemicals face limitations from both the current catalyst and process. Catalysis is vital, but catalysis alone is not the answer to maximizing energy savings. Integration of catalysis development with process engineering research can lead to significant energy savings during the production of the top 50 chemicals.

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1.0 Introduction

Catalysis plays a major role in the production of 30 of the top 50 U.S. commodity chemicals.¹ The remainder are produced through primarily non-catalytic processes;² alternative catalytic routes are sought for several of these. Of the 20 non-catalytically produced chemicals, 6 are made from raw materials that are on the top 50 list and produced catalytically.³ The true scope of influence is 36 chemicals.

The total production of the top 50 chemicals surpassed 650 billion pounds in 1992, and represents an energy use exceeding 5 quads per year.⁴ The total energy expended in the catalytic production routes exceeds 3 quads per year.

Economic competitiveness and energy conservation in the chemicals and petrochemicals industries, along with a heightened environmental consciousness, drives the study of catalysis. The use of catalysts to speed the rate of the desired reaction is critical for profitability, environmental regulatory compliance, and even chemical production sustainability. This study addresses and attempts to quantify the effect of catalysis on the production routes of the top 50 chemicals. The effect of catalytic improvements on the production energy consumption is investigated, and a range of realistic energy savings goals are put forth. In addition, the true process limitations, whether catalytic or not, are qualitatively addressed.

¹ The following chemicals are produced in catalytic processes:

Sulfuric acid, Ammonia, Propylene, Nitric acid, Ethylene dichloride, Vinyl chloride, Benzene, Ethylbenzene, MTBE, Styrene, Methanol, Formaldehyde, Xylene, Toluene, p-xylene, Terephthalic acid, Ethylene oxide, Ethylene glycol, Cumene, Phenol, Acetic acid, Butadiene, Acrylonitrile, Propylene oxide, Vinyl acetate, Acetone, Cyclohexane, Adipic acid, Caprolactam, and Isobutylene.

² The following chemicals are produced via non-catalytic processes:

Nitrogen, Oxygen, Ethylene, Lime, Phosphoric acid, Sodium hydroxide, Sodium carbonate, Chlorine, Ammonium nitrate, Urea, Carbon dioxide, Hydrochloric acid, Ammonium sulfate, Potash, Carbon black, Titanium dioxide, Aluminum sulfate, Sodium silicate, Calcium chloride, and Sodium sulfate.

³ The following non-catalytic chemicals are produced from a catalytically produced top 50 chemical: Phosphoric acid, Urea, Ammonium Nitrate, Ammonium sulfate, Aluminum sulfate, and Sodium sulfate

⁴ Ingham, J., "Industrial Processes for High-Volume Chemicals", report submitted in fulfillment of NREL subcontract DR-2-12212-2, 1994.

1.1 Problem Statement

Production of a commodity chemical through a catalytic route requires several operations. These include raw materials recovery and purification, chemical reactor(s) to convert raw materials to saleable products, and ensuing chemical separation schemes. Unreacted material is separated from products and recycled to the reactor when economically feasible. Products may be further purified to saleable form. The reaction and subsequent separation steps are considered to be the most energy intensive operations of a chemical plant.

Energy efficiency and abatement of byproduct generation in the chemicals industry are strongly affected by the reaction and separation steps. Efficient reactors and separators equate to more economic processes, lower energy requirements, and reduced waste generation. Process efficiency is increased through higher product yields, lower reactor temperatures or smaller reactor sizes, optimal control of existing processes, and less energy intensive separation schemes. Catalysis plays a crucial role in the first two and indirectly plays a role in the latter.

- **Higher process yields:**

Improving process yields, and especially per pass yields, parallels energy and environmental savings. The process yield is calculated as the overall reactant conversion multiplied by the desired product selectivity. Higher conversions per pass equate to a less energy-intensive separation and recycle load. Higher product selectivities lead to efficient resource use and less production of low or no-value byproducts, that must be disposed of or vented to the environment.

Catalysis strongly affects both parameters.

- **Lower reactor temperature or smaller reactor size:**

A reduction in the reactor temperature and size, while achieving the same production rate, equates to lower energy use. The input energy required by the reactor furnace, heating jacket or other will be lowered by reducing the operating temperature. This may also permit alternative and less expensive materials of construction. A smaller volume but more efficient reactor will also require less energy to operate.

Catalysis significantly affects both of these parameters; it improves product yields, which in turn permits more efficient reactor operation and sizing.

- **Optimal process control of existing processes:**

A reaction and separation scheme with tight process control along an optimal pathway will require less input energy.

- **Less energy intensive separation schemes:**

New energy-efficient schemes for separating products from reactants may result from efficient chemical reactors. For example, the replacement of an energy-intensive distillation tower with a lower temperature membrane separation would result in process energy savings. However, this replacement may only be feasible if the volume of material to be separated is reduced through higher product yields.

Another process possibility for saving energy is the combination of reaction and separation in a single process step. The elimination of one operation reduces the number of pumps, valves and heaters needed; it may also result in synergistic process enhancements. For example, some industrial reactions are limited by equilibrium constraints, where, at a given temperature and pressure, only a small fraction of the reactants convert to products in a single pass. The *in situ* removal of products from reactants as they are formed prevents local equilibration. Disruption of thermodynamic equilibrium keeps the reaction rate higher; thus increasing the product yield per pass.

Catalysis plays a significant role in the entire production process and has many implications for downstream operations.

1.2 Background -- Role of Catalysis

In a "perfect world", reactions would be driven to completion in a single pass with perfect selectivity. In the real world, there are limits to attainable yields per pass. Thermodynamics, which embodies the energetic and entropic changes for given

molecules to adsorb on catalytic surfaces and react, dictates maximums in conversion and selectivity. Kinetics, which details the rate of adsorption and reaction, dictates when thermodynamic maximums can be achieved. Both of these phenomena play a significant role in the design and optimization of a chemical reactor, and thus the production of a commodity chemical.

Kinetics plays a strong and manipulatable role, while thermodynamics does not. A chemical reaction occurs by breaking a chemical bond between two atoms, rearranging atoms, and forming new bonds. Energy must be added to break the initial bond and to move atoms; this energy is then partially or fully recouped by the formation of a new bond. The total energetic change from reactants to products is thermodynamically controlled and constant. The initial energy expenditure, also known as the activation energy, is kinetically controlled and variable. It is precisely this point where catalysis plays a role. Activation energy barriers are lowered with the aid of a catalyst. Reactions with lower energy barriers require less input energy, i.e., heat, to proceed. For example, cyclohexene must be taken to 800°C without the aid of a catalyst before undergoing a chemical reaction (Pearce and Patterson, p. 2, 1981). In the presence of a palladium catalyst and temperatures exceeding 300°C, cyclohexene will dehydrogenate to benzene. At temperatures below 300°C, both benzene and cyclohexane will be formed in the presence of a palladium catalyst.

An understanding of why catalysts lower the reaction activation energy is historically important to industrial development cycles; it also shows the need and the pathway of future catalysis research.

As a molecule adsorbs on a catalytic surface, a quasi-bond is formed between surface atoms and the adsorbing reactant molecule. The formation of this bond pulls energy away from exposed atoms. Either surface adsorbed molecules or bulk phase gas/liquid molecules may break the bond of the exposed atom using less energy, i.e., a lower activation energy barrier. The reduction in energy needed to break the bond is related to the bond strength of the surface and adsorbed atom. Quantification of this energy would allow the user to predict energetic reaction changes for different catalytic surfaces, and thus potentially tailor materials/catalysts for specific applications. This quantification, however, is a non-trivial undertaking and has been the goal of theorists and experimentalists for decades.

The development and optimization of catalysts for use in production chemical reactors occurs through laboratory intensive and expensive trial and error. Catalysts are synthesized, tested, and revised. Previous experience often provides input on types of materials that may work, but there is no substitute for experimental development. The

development time scale may be prohibitively expensive. If the physical phenomena surrounding the interaction between catalyst and reactants were well characterized, then the overall time and expense of catalyst development and scale-up may be reduced.

An understanding of the physical phenomena is not an easy undertaking. Catalysis typically involves heterogeneous surfaces, which by themselves are often not well nor easily characterized, particularly under real-world conditions. The surface atoms and their arrangement determine the strength of the quasi-bond formed with the reactant molecules. This bond strength, in turn, dictates the ease at which a bond in the reactant molecule may be broken and thus the input energy required. Characterization of the surface structures and thus the energetics of the reaction is difficult. Many catalysts are comprised of multiple materials and form many different surface structures, which may differ from bulk compositions and structures.

The cornerstone of process improvement is understanding the governing principles, setting a target outcome, and then engineering the process based upon the governing principles to accomplish the goals. Catalysis plays such a major role in the production of the top 50 chemicals, and yet little is known from the governing principles about predicting outcomes. The ability to predict reaction parameters would allow the user to explore many possible catalytic scenarios. In essence, the user could engineer a catalyst to achieve a high conversion to the desired product and inhibit the production of side products. This ability will only be attained through concurrent experimental and theoretical investigations.

1.3 Integrated Problem Overview

Implementation of a new catalytic process from conception of an idea to commercialization requires many steps. Figure 1 summarizes these steps. Initially the catalyst development stage involves the synthesis and characterization of materials. Through concurrent experimental and theoretical investigations catalysts are understood and subsequently improved. The understanding gleaned from these steps is often mechanistic in nature and fundamental. For example, a noble metal catalyst may be studied in a planar configuration under ultra-high vacuum. This simple arrangement facilitates the study of the desired reaction on a well-characterized surface. Surfaces must be well-characterized to validate concurrent theoretical investigations. As theories are developed and validated, they provide an important tool for investigating many surfaces and catalytic scenarios, thus reducing expensive experimental time.

Figure 1. Process Development Cycle

The next phase of operation is the development of a catalyst into a process. Characterization of a planar surface or a fine powder is important for a fundamental mechanistic understanding, but is not readily scaleable to real-world applications. A catalyst that proves to be excellent from the initial research may then be pressed into pellets, or dispersed onto support materials. These new catalyst forms are tested on a laboratory-scale process. Experimental validation and macroscopic mass and energy balances developed from this stage will allow these catalysts to be scaled to a pilot-plant operation.

The final stage before commercialization is the deployment of a catalyst in a pilot plant. From this larger unit operation, the necessary parameters are developed to guide the plant process design. A pilot plant is often less expensive by less than a factor of ten than a full-production plant, and can find and eliminate potential devastating problems.

Concurrent interaction between all phases of catalyst research and development will reduce the time for scale-up. Problems encountered at each stage can be alleviated with interactions by researchers at all levels in the picture. Often choices are made with serious "downstream" implications. Early involvement of those downstream researchers can drive the entire process more quickly, and can provide input on avoiding potential downstream pitfalls.

2.0 Catalysis Analysis Project

2.1 Project Goal

The goal of this project is to ascertain potential energy savings through process efficiency improvements. The primary goal is the evaluation of the direct impact of catalysis on the energy consumption during the production of the top 50 chemicals. The quantitative parameter is the determination of energy savings associated with potential process improvements, which may or may not rise from catalyst developments. The secondary goal is the identification of the true process limitations, and the discussion of the role of catalysis as the sole or partial alleviator of these limitations.

The initial research sponsored by the DOE-EE-OIT-BCTR focuses on understanding and quantifying catalytic surface structures and associated energetics. An improved understanding of the physical phenomena surrounding catalytic surfaces and reaction kinetics will aid researchers to ultimately improve catalysts. Increased process efficiency will result from this research provided that the fundamental findings can be transferred to practical applications. This study does not attempt to quantify the path by which these improvements might occur, rather it identifies probable outcomes based on the assumption that these improvements have occurred.

2.2 Project Approach -- Analysis Tool

Information on each of the top 50 chemicals has been compiled in an Excel spreadsheet ("top50chem.xls"). The development of this analysis tool allows the user to update information as necessary, make assumptions about potential catalysts or processes, and evaluate the impact of these assumptions. Information on the following issues are included in the spreadsheet:

- Top 50 chemicals
- Annual production rate
- Catalyst
- Production route
- Reactants
- End uses
- Possible process limitations, catalytic or other

- Catalytic selectivity
- Process conversion
- Type of catalyst (i.e., metal, metal oxide, acidic)
- Current Catalysis-By-Design (CBD) project, which evaluates similar catalysts
- Process and feedstock energy required for production
- Current process yield
- Maximum yields and possible improvements from current yields
- Energy impact based on process yield improvements
- Use of other top 50 chemicals as a precursor
- Effect of overall increases in process efficiency
- Effect of specific types of catalysts (metals, metal oxides, acidic)
- Effect of yield improvements on individual chemicals (process energy only)
- Effect of yield improvements on chemicals (feedstock and process energy)
- Response factor between yield improvement and process energy savings.

The user is allowed to make assumptions about potential catalyst improvements, and evaluate the impact on the process energy use and on the sum of the process and the feedstock energy. For example, the effect of a certain process yield improvement can be investigated on the following:

- all chemicals
- all catalytically produced chemicals
- all catalytically produced chemicals made from a catalyst type currently under investigation
- all chemicals produced by a certain type of catalyst
- an individual chemical.

The program does not allow improvements beyond current process limits. For example, if the catalytic process yield were currently 98%, then the query of a 10% yield improvement would return the effect of a 2% increase. This program evaluates process yields and not yields per pass, and are thus somewhat conservative. For example, during the production of propylene oxide, the per pass yield has been reported as 10%, and the process yields are estimated at 90% (Pearce and Patterson, p. 149, 1981). The program allows the impact of a maximum 10% increase in process efficiency. In reality, much higher process energy savings might be realized from substantive improvements in the

per pass conversions and selectivities. No higher energy savings would be possible, though, from the feedstock energy.

Several assumptions have been made. A linear scale between process yield improvements and energy savings is used. The program allows the user to input a different scale if desired. The assumption of linearity clearly breaks down for large improvements in yields where little or no input energy would be predicted. However, for small or moderate process yield increases, the assumption of linearity seems reasonable. A linear scale is used in each evaluation because only moderate process yield improvements are possible for most chemicals.

2.3 Program Information

The following information is included with the accompanying Excel program ("top50chem.xls"). The numbers used in this program can be updated, as appropriate. The program can also be used for further investigations of interest to the user.

- **Top 50 chemical:**

The list of top 50 chemicals leads each page within the program.

- **Annual production rate:**

The 1992 production rate of each chemical is given in billions of pounds. These values were obtained from the 1993 Chemical and Engineering News annual report.

- **Catalyst:**

The catalyst(s) used in production of each commodity chemical is listed. Several catalysts are cited for many of the chemicals. In some cases, varied production routes are used by industry, and in others a multi-component catalyst is required.

- **Production route:**

The chief production route is briefly outlined. Some chemicals are manufactured by several catalytic routes. Important operating conditions and parameters are outlined.

- **Reactants:**
The raw material(s) for each chemical is listed. Several of the top 50 chemicals are made from a different top 50 commodity chemical.
- **End uses:**
The primary use(s) of each chemical is outlined. In some cases, the chemicals are used in a specific industry, while others are a precursor for many different products and industries.
- **Process limitations:**
There are many limitations that affect the overall chemical production efficiency. These include low catalytic activity and specificity, equilibrium constraints, high separation intensity, inefficient reactor design, and the like.
- **Current process yields:**
The catalytic selectivity and conversion of each production process is outlined. These numbers reflect the process yields and are not the yields per pass. Per pass yield data is more informative to determine the potential energy savings, but was not usually available. An energy-intensive reactant separation and recycle step is usually included such that process yields are considerably higher than per pass yields.
- **Catalyst type:**
Each catalyst is subdivided into three categories: metal, metal oxide, and acid/zeolite. These were included to correlate with ongoing research efforts in these three areas.
- **Applicable research project:**
The current CBD research projects are investigating metal, metal oxide, and zeolite catalysts. It is difficult to quantify the direct effect of any individual study, therefore, studies have been grouped by catalyst type.

- **Energy use:**

Two entries focus on the current production energy consumption.⁵ The first entry gives the process energy in Btu/lb, while the second entry gives the process and the feedstock energy, also in Btu/lb.

- **Use of other top 50 chemicals as a precursor:**

Many chemicals are produced using other top 50 chemicals as the reactant. The percentage that each reactant is used in the production of this chemical is also included.

- **Response factor between yield improvement and process energy savings:**

A linear response between yield improvements and process energy savings has been assumed in all analyses. For example, a process that experiences a 10% improvement in yield is assumed to require 10% less energy.

⁵ Ingham, J., "Industrial Processes for High-Volume Chemicals", report submitted in fulfillment of NREL subcontract DR-2-12212-2, 1994.

3.0 Results

Several scenarios are created involving catalytic improvements and potential energy savings associated with the production of the top 50 chemicals. The production energy arising from both the feedstock and process have been reported. The analyses done in this report evaluate the effect of process improvements on the process energy alone and on the sum of the process and feedstock energy. Many chemicals are produced from another top 50 commodity chemical; in these cases the feedstock energy is not counted twice. Appendix VI presents a sample calculation for determining the feedstock energy.

The true effect of current catalysis research efforts is difficult to accurately assess. The approach of this study is to hypothesize about potential process improvements and quantify, to the extent possible, the resulting energy savings. These process improvements may result from an improved catalyst, process, or synergistic combination of the two.

The first hypothesis (1a) is presented in Appendix I and investigates the impact of overall % yield improvements in all catalytic production routes. The second scenario (1b) evaluates the same overall % yield improvements, but includes only those chemicals produced using catalyst types (metals, metal oxides, and acids) currently under investigation. In both scenarios, the savings resulting from the process energy, both with and without the feedstock energy, has been calculated. Double counting of the feedstock energy has been eliminated from those chemicals that are produced using another top 50 chemical. For example, ethylbenzene is produced from benzene. Summation of the effect over every chemical requires that the benzene feedstock energy be included, while the ethylbenzene feedstock energy not be included. A sample calculation is presented at the end of Appendix VI.

The second hypothesis (2a), given in Appendix II, evaluates the effect of % yield improvements on the process and feedstock energy use for the different types of catalysts. These are subdivided into metals, metal oxides, and acids; the three types of catalysts under investigation in current catalysis research efforts. Process yield improvements of 1%, 2%, 5%, 10%, 15%, 20%, and 25% are evaluated for each type of catalyst. Chemicals are not allowed to exceed their maximum process improvement.

Scenario 2b further subdivides the metal catalyst group into noble metals, metal chlorides, metal acetates, and metal salts. Scenario 2c breaks down the acid catalyst category into zeolitic catalysts and other acids.

These analyses attempt to quantify which type of catalysis research could potentially have the greatest effect on the production of commodity chemicals. Some chemicals

have several production routes, and may use catalysts of different types. In those cases, the chemicals are included in several categories. This, in effect, double counts some chemicals, and the reader is cautioned not to sum the results to get the overall improvement reported in Scenario 1a.

The third investigation, tabulated in Scenarios 3a and 3b and presented in Appendix III, evaluates the energy impact on each of the top 50 chemicals individually. The analysis presented in Scenario 3a investigates the effect on the process energy only. Scenario 3b includes both the process and feedstock energy. Because the energy effects are not summed over many chemicals, no feedstock energy is subtracted if the chemical is made from another top 50 chemical. The approach of this analysis is to evaluate the individual impact of a chemical. Again the reader is cautioned not to sum the savings to get the total reported in Scenario 1a. The sum will appear artificially high because chemical feedstock energy will be double counted for many chemicals.

The fourth hypothesis, shown in Appendix IV, investigates the effect of overall process improvements not related to yield improvements. This quantifies potential savings resulting from other process improvements. All chemicals are included in this scenario, and not just those produced by catalytic routes. It should be noted that the production energies of some chemicals were not available. Fortunately, these were all non-catalytically produced and do not impact the earlier catalysis analyses.

4.0 Discussion

4.1 Catalysis Effects

Catalysis plays an important role in the production of the top 50 U.S. commodity chemicals. The four scenarios attempt to quantify this impact under different circumstances. The first scenario evaluates the effect of an overall yield improvement in all catalytic processes. This report addresses neither the feasibility nor the time line for potential yield increases, rather it assesses the effect if these improvements were achieved. Quantification of this effect emphasizes the need for continued research, which will ultimately lead to the overall reduction of industrial energy consumption.

Catalytic process improvements ranging between 1% and 25% are evaluated; for these increases, the sum of process and feedstock energy savings ranges between 0.03 and 0.39 quads. A slight decrease is observed when including only those catalytic processes whose catalyst type is under current CBD investigation. This decrease is not significant. Most of the important catalyst types are addressed under current CBD research activities.

If a 10% process yield improvement is held out as a realistic potential for research efforts, this would result in an energy savings of 0.23 quads per year.

The second scenario (2a) breaks down the catalytic processes into those currently made with the three main types of catalysts: metals, metal oxides, and acid catalysts. Of these, metal catalysts play the most significant role, followed by acid catalysts and metal oxides. An average increase of 10% would result in a savings of 0.201, 0.066, and 0.026 quads per year, respectively. This, however, neither addresses nor assesses the potential for replacement of a catalyst with a more efficient one of a different type. In addition, several of the top 50 chemicals are produced through different routes and may use more than one type of catalyst. In these cases, the effect has been included in each total.

Scenario 2b and 2c subdivide the metal and acid catalyst categories. Scenario 2b breaks the metals into noble metals, metal chlorides, metal acetates, and metal salts. Of these, noble metal catalysts play the most significant role, followed by metal chlorides, metal acetates, and metal salts. For a process yield improvement of 10%, savings of 0.18, 0.01, 0.006, and 0.003 quads per year, respectively, would be achieved. Scenario 2c breaks the acidic catalyst category into zeolite catalysts and other acids. Zeolites dominate this category. For a process yield improvement of 10%, 0.06 and 0.006 quads per year would be saved, respectively, for zeolites and other acid catalysts.

Scenarios 3a and 3b evaluate each chemical individually. In the first case, only the effect on process energy is included. In the latter scenario, both the process and feedstock energy are included. Savings resulting from improvements of 1%, 5%, and 10% are listed, as is the maximum process yield improvement and the corresponding savings. The greatest potential process improvements are associated with ammonia, benzene, styrene, butadiene, toluene, and the xylenes.

Summing the improvements of all catalytic chemicals at their maximum improvements (without double counting feedstock energy as appropriate) shows a maximum of 0.47 quads per year savings. This number could be improved through simultaneous process and catalyst improvements.

A linear assumption between process yield improvement and energy savings is appropriate for consideration of the feedstock energy. It may or may not be appropriate for the process energy. This assumption will clearly break down in the limit of large yield improvements, where the process energy would be predicted to drop to negligible levels. However, for more modest yield improvements, this assumption is considered valid.

A potential savings that is not included in these analyses is the effect of dramatic yield per pass improvements. For example, a process may now have an overall process yield of 90%, but a yield per pass of 5%. The program will only allow a process energy savings of 10%. In reality, if a suitable catalyst or catalyst/process combination were developed that elevated per pass yields to 90%, then process energy savings could significantly exceed 10%.

The final scenario (4) addresses the magnitude of overall process improvements, whether catalytic or not, to return certain energy savings. An overall efficiency increase of 10% in the production of each of the top 50 commodity chemicals would save 0.29 quads per year in process energy alone and upto 0.57 quads per year in process plus feedstock energy.

4.2 Integrated Catalysis and Process Effects

The previous analyses take the role of providing a first cut in identifying problem chemicals and defining the maximum effect of catalytic improvements. The current processes, for the most part, are fairly efficient (>90% yields). Catalytic improvements alone can at best make an incremental influence on energy consumption. Substantial gains in process efficiency can be gained, though, by taking a holistic approach.

Optimization of a chemical production route includes the development of an efficient catalyst, but is not limited to this. New production routes are needed to overcome the true process limitations. Accompanying these new production routes are the catalysts that will make them possible.

The production of ammonia is an example. Per pass yields range from 7% (Gonzalez 1991) to 20%, while the overall process yields are 85% to 90% (Chenier, p. 72, 1986). The high process yields are obtained by separating the unreacted material from the effluent stream and recycling it to the reactor. The real gain in process efficiency will be gained by raising per pass yields. Catalysis alone cannot achieve this goal. The reaction is exothermic and equilibrium limited. The per pass conversion is dictated by thermodynamics and is highest at high pressures and low temperatures. Catalysis can make the reaction proceed faster, but it cannot allow the conversion to exceed a thermodynamic maximum. Fortunately, the story does not end here. Thermodynamic maximums are a function of the temperature, pressure, and the local composition. Alteration of these parameters *in situ* permits process gains. For example, the optimal reactor design for this process would not allow the reactants and products to equilibrate. Ammonia would be separated from the nitrogen and hydrogen as it is produced and the reverse reaction quenched, possibly through temperature or pressure changes. The concept of an equilibrium shift reactor has been presented for other reactions (Ray et al. 1990). Development of a production reactor based on these novel reactor designs requires an appropriate active and specific catalyst for implementation. The coordination of both research efforts could lead to real energy savings.

Another example of an energy intensive commodity chemical is propylene oxide. Current propylene oxide yields are estimated at 10% per pass (Pearce and Patterson, p. 259, 1981), while the overall process yields are 90% (Pearce and Patterson, p. 256, 1981). Tremendous gains might be realized if a production route could achieve a 90% yield per pass. Current production routes use either chlorine or a hydroperoxide as an oxidant (Pearce and Patterson, p. 149, 1981), and are inefficient in terms of both energy and resource use. Direct oxidation of propylene to propylene oxide is one potential new production reaction pathway, but a suitable catalyst is required. Even if a direct oxidation catalyst were found, additional savings could materialize through process integration. Partial oxidation reactions of hydrocarbons are inherently unselective because of competing combustion reactions. Yields per pass during the direct oxidation route would still have to be kept low to maintain a high propylene oxide selectivity. Novel reactor design, and its corresponding catalyst development, could potentially return high per pass

yields and significant energy savings. Enhanced yields have been reported for partial oxidation reactions based on reactor design (Tonkovich et al. 1993).

A final chemical spotlight will be placed on styrene. Most styrene produced within the U.S. involves the direct dehydrogenation of ethylbenzene at elevated temperatures (Chenier, p. 160, 1986). Dehydrogenation reactions are notoriously equilibrium sensitive. The endothermic reaction requires elevated temperatures to achieve reasonable conversions per pass. Higher yields per pass at lower reaction temperatures could be achieved through incorporation of a reaction and separation scheme. Direct removal of hydrogen from the styrene product will shift the reaction towards the products. One possible design would incorporate a hydrogen permselective membrane (palladium, platinum, and other metallic alloys) for *in situ* hydrogen removal. Similar reaction types have demonstrated yields nearing unity on a laboratory scale (Armor 1989; Champagnie et al. 1990). Higher yields would permit lower reaction temperatures and tremendous energy savings from the reduction of temperature and recycle load.

Many of the production routes of the other top commodity chemicals can be affected by integrating process design and catalyst development. Simultaneous incorporation of these two research efforts will return high-energy savings.

5.0 Conclusions

Catalysis plays a vital role in the current production processes of the top 50 U.S. commodity chemicals and can create potential new production routes. The yields of 30 of these chemicals are determined by the catalyst and can be upgraded through catalytic improvements. The magnitude of current process yields reveal which chemicals are most strongly affected. The effect of process yield improvements is quantified in this study by making several assumptions. Using previously reported production energy values, cited process yields, and a linear response factor between yield and energy, the maximum allowable energy savings from current processes approaches 0.47 quads per year.

The development of new catalysts and the improvement of existing catalysts alone will not achieve the maximum possible energy savings from the production of the top 50 chemicals. Many of these chemicals are limited by process constraints that must be solved in conjunction with catalyst development. Potential energy savings from the production of the top 50 chemicals exist and can be realized through continued research and development into both catalysts and their integration into optimal processes.

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Appendix I

Scenario 1a:

The effect in process energy alone and process plus feedstock energy for improvements in all catalysts of ξ %.

ξ % Improvement	Process Energy Savings (quads/yr)	Process+Feedstock Energy Savings (quads/yr)
1	0.012	0.029
2	0.023	0.057
5	0.053	0.135
10	0.089	0.226
15	0.111	0.293
20	0.123	0.341
25	0.136	0.390

Scenario 1b:

The energy effect of an overall process yield improvement (in catalytic processes whose catalyst type is under investigation in the CBD program) of ξ %. Assuming a linear scale between energy consumption and yield.

ξ % Improvement	Process Energy Savings (quads/yr)	Process + Feedstock Energy Savings (quads/yr)
1	0.010	0.027
2	0.020	0.054
5	0.047	0.129
10	0.081	0.218
15	0.103	0.285
20	0.115	0.333
25	0.128	0.382

Appendix II

Scenario 2a:

The energy effect of yield improvements of ξ % in different catalyst types.

ξ % Improvement	Process + Feedstock Energy Savings -- Metal catalysts (quads/yr)	Process + Feedstock Energy Savings -- Metal oxide catalysts (quads/yr)	Process + Feedstock Energy Savings -- Acid catalysts (quads/yr)
1	0.024	0.004	0.011
2	0.048	0.008	0.020
5	0.119	0.014	0.049
10	0.201	0.026	0.066
15	0.258	0.039	0.081
20	0.296	0.054	0.097
25	0.333	0.071	0.113

Note: Summing across the rows in Scenario 2a will not give the results in Appendix I because some catalysts are counted twice. Some chemicals are made with several types of catalysts; in those instances, the energy savings is added to each category.

Scenario 2b:

The metal catalysts are evaluated by the type of metal (noble, metal chloride, metal acetate, or metal salt catalyst)

ξ % Improvement	Noble Metals -- P + F energy savings (quads)	Metal Chlorides -- P + F energy savings (quads)	Metal Acetates -- P + F energy savings (quads)	Metal Salts -- P + F energy savings (quads)
1	0.0212	0.0017	0.0006	0.0003
2	0.0425	0.0033	0.0012	0.0006
5	0.1064	0.0083	0.0029	0.0015
10	0.1809	0.0106	0.0063	0.0030
15	0.2387	0.0106	0.0063	0.0032
20	0.2761	0.0106	0.0064	0.0032
25	0.3127	0.0106	0.0064	0.0032

Scenario 2c:

Zeolitic catalysts are further evaluated within the category of acidic catalysts.

% Improvement	Acidic Zeolites -- P + F energy savings (quads)	Other Acidic Catalysts -- P + F energy savings (quads)
1	0.0092	0.0013
2	0.0184	0.0021
5	0.0456	0.0035
10	0.0595	0.0063
15	0.0741	0.0074
20	0.0895	0.0074
25	0.1058	0.0074

Appendix III

Scenario 3a:

The process energy effect of a ξ % yield increase for each chemical.

Chemical	Average P. Energy Savings - 1% (quads/yr)	Average P. Energy Savings - 5% (quads/yr)	Average P. Energy Savings - 10% (quads/yr)	Max. Process Yield % Increase	Average Energy Savings at Max. (quads)
Sulfuric Acid	0.0006	0.0006	0.0006	0.7985	0.0006
Nitrogen	0.0000	0.0000	0.0000	N/A	0.0000
Oxygen	0.0000	0.0000	0.0000	N/A	0.0000
Ethylene	0.0000	0.0000	0.0000	N/A	0.0000
Ammonia	0.0029	0.0144	0.0288	12.88	0.0370
Lime	0.0000	0.0000	0.0000	N/A	0.0000
Phosphoric Acid	0.0000	0.0000	0.0000	N/A	0.0000
Sodium Hydroxide	0.0000	0.0000	0.0000	N/A	0.0000
Propylene	0.0017	0.0085	0.0085	5.0	0.0085
Chlorine	0.0000	0.0000	0.0000	N/A	0.0000
Sodium Carbonate	0.0000	0.0000	0.0000	N/A	0.0000
Urea	0.0000	0.0000	0.0000	N/A	0.0000
Nitric Acid	0.0002	0.0009	0.0011	5.95	0.0011
Ethylene Dichloride	0.0003	0.0014	0.0016	5.95	0.0016
Ammonium Nitrate	0.0000	0.0000	0.0000	N/A	0.0000
Vinyl Chloride	0.0010	0.0050	0.0068	6.9	0.0068
Benzene	0.0001	0.0006	0.0012	28.0	0.0034
Ethylbenzene	0.0001	0.0001	0.0001	1.99	0.0001
MTBE	0.0006	0.0006	0.0006	1.0	0.0006
Carbon Dioxide	0.0000	0.0000	0.0000	N/A	0.0000
Styrene	0.0005	0.0025	0.0049	37.0	0.0182
Methanol	0.0004	0.0007	0.0007	1.99	0.0007
Formaldehyde	0.0000	0.0000	0.0000	9.0	0.0000
Xylene	0.0003	0.0014	0.0028	28.0	0.0079
Toluene	0.0003	0.0013	0.0027	28.75	0.0076

Scenario 3a (contd.):

Process energy effect for the top 26-50 chemicals.

Chemical	Average P. Energy Savings -- 1% (quads/yr)	Average P. Energy Savings -- 5% (quads/yr)	Average P. Energy Savings -- 10% (quads/yr)	Max. Process Yield % Increase	Average Energy Savings at Max (quads)
Hydrochloric Acid	0.0000	0.0000	0.0000	N/A	0.0000
p-Xylene	0.0005	0.0027	0.0054	80.0	0.0435
Terephthalic Acid	0.0003	0.0016	0.0031	10.36	0.0032
Ethylene Oxide	0.0000	0.0000	0.0001	24.0	0.0002
Ethylene Glycol	0.0003	0.0006	0.0006	1.99	0.0006
Ammonium Sulfate	0.0000	0.0000	0.0000	N/A	0.0000
Cumene	0.0000	0.0001	0.0001	2.98	0.0001
Potash	0.0000	0.0000	0.0000	N/A	0.0000
Phenol	0.0002	0.0012	0.0024	11.8	0.0028
Acetic Acid	0.0002	0.0008	0.0017	10.9	0.0018
Butadiene	0.0007	0.0035	0.0070	34.3	0.0240
Carbon Black	0.0000	0.0000	0.0000	N/A	0.0000
Acrylonitrile	0.0001	0.0004	0.0007	30.0	0.0022
Propylene Oxide	0.0002	0.0009	0.0019	10.0	0.0019
Vinyl Acetate	0.0002	0.0009	0.0018	10.0	0.0018
Titanium Dioxide	0.0000	0.0000	0.0000	N/A	0.0000
Acetone	0.0001	0.0007	0.0013	11.8	0.0016
Cyclohexane	0.0000	0.0000	0.0000	1.99	0.0000
Aluminum Sulfate	0.0000	0.0000	0.0000	N/A	0.0000
Sodium Silicate	0.0000	0.0000	0.0000	N/A	0.0000
Adipic Acid	0.0002	0.0011	0.0022	10.0	0.0022
Calcium Chloride	0.0000	0.0000	0.0000	N/A	0.0000
Caprolactam	0.0000	0.0002	0.0005	9.75	0.0005
Sodium Sulfate	0.0000	0.0000	0.0000	N/A	0.0000
Isobutylene	0.0000	0.0000	0.0000	1.99	0.0000

Scenario 3b

The process plus feedstock energy effect of a ξ % yield increase for each chemical.

Chemical	Average P+F Ener. Savings - 1% (quads/yr)	Average P+F Ener. Savings - 5% (quads/yr)	Average P+F Ener. Savings - 10% (quads/yr)	Max. Process Yield % increase	Average Ener. Savings at Max (quads/yr)	Catalyst Type
Sulfuric Acid	0.0006	0.0006	0.0006	0.7985	0.0006	MO
Nitrogen	0.0000	N/A	N/A	N/A	N/A	
Oxygen	0.0000	N/A	N/A	N/A	N/A	
Ethylene	0.0000	N/A	N/A	N/A	N/A	
Ammonia	0.0067	0.0333	0.0665	12.88	0.0857	M
Lime	0.0000	N/A	N/A	N/A	N/A	
Phosphoric Acid	0.0000	N/A	N/A	N/A	N/A	
Sodium Hydroxide	0.0000	N/A	N/A	N/A	N/A	
Propylene	0.0064	0.0322	0.0322	5.0	0.0322	M, Z
Chlorine	0.0000	N/A	N/A	N/A	N/A	
Sodium Carbonate	0.0000	N/A	N/A	N/A	N/A	
Urea	0.0000	N/A	N/A	N/A	N/A	
Nitric Acid	0.0002	0.0009	0.0011	5.95	0.0011	M
Ethylene Dichloride	0.0015	0.0076	0.0090	5.95	0.009	M
Ammonium Nitrate	0.0000	N/A	N/A	N/A	N/A	
Vinyl Chloride	0.0010	0.0050	0.0068	6.9	0.0068	charcoal
Benzene	0.0023	0.0114	0.0228	28.0	0.0639	M
Ethylbenzene	0.0020	0.0041	0.0041	1.99	0.0041	Z
MTBE	0.0029	0.0029	0.0029	1.0	0.0029	acid
Carbon Dioxide	0.0000	0.0000	0.0000	N/A	N/A	
Styrene	0.0021	0.0107	0.0215	37.0	0.0794	Z, MO
Methanol	0.0014	0.0029	0.0029	1.99	0.0029	MO
Formaldehyde	0.0008	0.0038	0.0069	9.0	0.0069	M
Xylene	0.0015	0.0073	0.0146	28.0	0.0409	M, Z
Toluene	0.0014	0.0068	0.0137	28.75	0.0393	M

Scenario 3b (contd).

Process plus feedstock energy savings for the top 26-50 chemicals.

Chemical	Average Energy Savings -- 1% (quads/yr)	Average Energy Savings -- 5% (quads/yr)	Average Energy Savings -- 10% (quads/yr)	Max. Process Yield % Increase	Average Energy Savings at Max	Catalyst Type
Hydrochloric Acid	0.0000	0.0000	0.0000	N/A	0.0000	
p-Xylene	0.0016	0.0080	0.0159	80.0	0.1272	Z
Terephthalic Acid	0.0014	0.0068	0.0135	10.36	0.0140	M
Ethylene Oxide	0.0009	0.0045	0.0090	24.0	0.0216	M
Ethylene Glycol	0.0008	0.0015	0.0015	1.99	0.0015	acid
Ammonium Sulfate	0.0000	0.0000	0.0000	N/A	0.0000	
Cumene	0.0010	0.0029	0.0029	2.98	0.0029	Z
Potash	0.0000	0.0000	0.0000	N/A	0.0000	
Phenol	0.0009	0.0047	0.0093	11.8	0.0110	M, acid
Acetic Acid	0.0005	0.0023	0.0046	10.9	0.0051	M
Butadiene	0.0015	0.0074	0.0149	34.3	0.0510	M, MO
Carbon Black	0.0000	0.0000	0.0000	N/A	0.0000	
Acrylonitrile	0.0009	0.0043	0.0087	30.0	0.0260	MO
Propylene Oxide	0.0008	0.0038	0.0076	10.0	0.0076	M
Vinyl Acetate	0.0005	0.0026	0.0052	10.0	0.0052	M
Titanium Dioxide	0.0000	0.0000	0.0000	N/A	0.0000	
Acetone	0.0005	0.0026	0.0051	11.8	0.0060	M, acid
Cyclohexane	0.0004	0.0008	0.0008	1.99	0.0008	M
Aluminum Sulfate	0.0000	0.0000	0.0000	N/A	0.0000	
Sodium Silicate	0.0000	0.0000	0.0000	N/A	0.0000	
Adipic Acid	0.0005	0.0025	0.0050	10.0	0.0050	M
Calcium Chloride	0.0000	0.0000	0.0000	N/A	0.0000	
Caprolactam	0.0003	0.0013	0.0026	9.75	0.0026	M, acid
Sodium Sulfate	0.0000	0.0000	0.0000	N/A	0.0000	
Isobutylene	0.0002	0.0003	0.0003	1.99	0.0003	MO, Z

Appendix IV

Scenario 4:

Effect of an overall ξ % improvement in each process (not based on yield improvements);
this includes all catalytically and non-catalytically produced chemicals.

ξ % Improvement	Process Energy Savings (quads/yr)	Process + Feedstock Energy Savings (quads/yr)
1	0.029	0.057
2	0.057	0.114
5	0.143	0.284
10	0.286	0.569
15	0.430	0.853
20	0.573	1.138
25	0.716	1.422

Appendix V: Catalytic Production of Top 50 Chemicals

Additional information is provided in the Excel program.

Catalytically Produced Chemical	Reactant	Catalyst	Production Route
Sulfuric Acid	Sulfur	VPO	Multi-stage process
Ammonia	H ₂ from syn gas, N ₂	Fe, Ni/Al ₂ O ₃	Low Y. per pass, recycle
Propylene	Propane -- nat gas /nap.	Catofin cats-metals; zeo.	Dehydrogenation
Nitric Acid	Ammonia	Pt, Rh	Ammonia oxidation
Ethylene Dichloride	Ethylene, chlorine	Metallic Cl's; Fe, Cu, An	Direct- or ox-chlor.
Vinyl Chloride	Ethylene dichloride	Charcoal	Thermal dehydrochlor.
Benzene	Naphtha	Pt	Cat. reforming
Ethylbenzene	Ethylene, benzene	Al-Cl's; zeolites	Alkylation
MTBE	Methanol, isobutylene	Acidic ion ex. resin	Alkylation
Styrene	Ethylbenzene	Zeolites; metal ox.	Dehydrogenation
Methanol	Syn gas	Cu-ZnO, Cr-Zn -oxides	Low Y. per pass, recycle
Formaldehyde	Methanol	Ag	Oxidative dehydrog.
Xylene	Naphtha	Pt, zeolites	Cat. reforming
Toluene	Naphtha	Pt	Cat. reforming
p-Xylene	Xylene	zeolites	Isomer equilibration
Terephthalic Acid	p-Xylene	Co-Mn	Oxidation
Ethylene Oxide	Ethylene	Ag	Direct ox.; low Yields
Ethylene Glycol	Ethylene oxide	Acids; Te-ox; Rh(R&D)	Hydration
Cumene	Propylene, benzene	Phosphoric acid; zeolites	Alkylation
Phenol	Cumene	Cu-ZnO; acids	Oxidation then cleav.
Acetic Acid	Methanol	Rh	Methanol carbonylation
Butadiene	Butanes/butenes	Fe ₂ O ₃ , or metals	Catalytic dehydrog.
Acrylonitrile	Ammonia, propylene	Bi-Mo-Fe oxides	Oxidation
Propylene Oxide	Propylene	Metal acetyls	Propylene oxidation
Vinyl Acetate	Acetic acid, ethylene	Metal chlorides or acet.	Oxidation
Acetone	Cumene	Cu-ZnO; acids	Oxidation then cleav.
Cyclohexane	Benzene	Ni, Pd, Pt	Dehydrogenation
Adipic Acid	Cyclohexane, nitric acid	Co napthenate or acet.	Oxidation
Caprolactam	Cyclohexane or phenol	Pd; acids	C. to cyclohexanone 1 st
Isobutylene	Butane	Zeolites; metal oxides	Dehydrogenation/ isom.

Appendix VI: Production Energy

Catalytically Produced Chemical	Process Energy (Btu/lb)	Process + Feedstock Energy (Btu/lb)	Max Yield Improvement (%)
Sulfuric Acid	840	840	0.80
Ammonia	8000	18500	12.88
Propylene	7500	28500	5.0
Nitric Acid	1120	1120	5.95
Ethylene Dichloride	1700	7800	5.95
Vinyl Chloride	7500	7500	6.9
Benzene	1000	19000	28.0
Ethylbenzene	600	18600	1.99
MTBE	5600	26600	1.0
Styrene	5500	24000	37.0
Methanol	4250	16450	1.99
Formaldehyde	0	11000	9.0
Xylene	4400	22900	28.0
Toluene	4400	22650	28.75
p-Xylene	9600	28100	80.0
Terephthalic Acid	5500	24000	10.36
Ethylene Oxide	170	16170	24.0
Ethylene Glycol	5600	14700	1.99
Cumene	1025	21085	2.98
Phenol	6500	25200	11.8
Acetic Acid	4600	12900	10.9
Butadiene	22000	46750	34.3
Acrylonitrile	2600	30600	30.0
Propylene Oxide	7000	28000	10.0
Vinyl Acetate	6650	19480	10.0
Acetone	5630	21430	11.8
Cyclohexane	340	17440	1.99
Adipic Acid	12500	28500	10.0
Caprolactam	3400	19400	9.75
Isobutylene		12000	1.99

Sample calculations

The following are sample calculations to avoid double counting feedstock energy for chemicals produced from a top 50 commodity chemical.

If allowable reactant yield improvement higher than allowable product yield increase:

$$\text{Total Energy} = \{\text{Process} + \text{Feedstock}\}_{\text{product}} - (\text{Feedstock Energy})_{\text{product}}$$

Example: The energy savings from a 10% yield increase in ethylbenzene (benzene).

$$\{\text{Process} + \text{Feedstock}\}_{\text{product}} = 18600 \text{ Btu/lb product}$$

$$(\text{Feedstock Energy})_{\text{product}} = 18000 \text{ Btu/lb product}$$

$$\text{Total Energy (use when summing processes)} = 600 \text{ Btu/lb product (w/o double counting)}$$

$$\text{Total Energy (when only ethylbenzene evaluated)} = 18600 \text{ Btu/lb product}$$

$$\text{Energy savings (when summing processes)} = 0.1(600) = 60 \text{ Btu/lb (w/o double counting)}$$

$$\text{Energy savings (when ethbenz. evaluated)} = 0.1(18600) = 1860 \text{ Btu/lb}$$

If allowable reactant yield improvement lower than allowable product yield increase:

$$\begin{aligned} \text{Total Energy} = & \{\text{Process} + \text{Feedstock}\}_{\text{product}} - \\ & (1 + Y_{\text{reactant}} - Y_{\text{product}}) \times (\text{Feedstock Energy})_{\text{product}} \end{aligned}$$

Example: The total energy savings from a 10% yield increase in propylene oxide (made from propylene). Only a 5% process improvement for propylene is possible.

$$\{\text{Process} + \text{Feedstock}\}_{\text{product}} = 28000 \text{ Btu/lb}$$

$$(\text{Feedstock Energy})_{\text{product}} = 7000 \text{ Btu/lb}$$

$$\text{Total Energy (use when summing processes)} = 28000 - (1 + 0.05 - 0.10) \times 7000 = 21350 \text{ Btu/lb}$$

$$\text{Total Energy (when only prop. oxide evaluated)} = 28000 \text{ Btu/lb product}$$

$$\text{Energy savings (when summing processes)} = 0.05(21350) = 1067.5 \text{ Btu/lb} \times \{\text{prod. rate}\}$$

$$\text{Energy savings (only prop. oxide evaluated)} = 0.05(28000) = 1400 \text{ Btu/lb} \times \{\text{prod. rate}\}$$

Appendix VII: Current Catalytic Process Yield Data

For some chemicals a range of conversion, selectivity, or yield values are reported. Preference is given to the citation that is most recent, has the most sources, or is viewed to be the most credible; the symbol (†) indicates the values that are used in the program.

Chemical	Selectivity	Conversion	Proc. Yield	Citation
Sulfuric Acid [†]	99.5	99.7	99.2	A1.1
<i>Sulfuric Acid</i>	99.5	62.5 (1st pass)	*	A1.1a
Ammonia [†]	99	88	87.1	A1.2
<i>Ammonia</i>	99	21 (per pass)	*	A1.2a
Propylene [†]	95	100	95	A1.3
Propylene	95	95	90.25	A1.3a
<i>Propylene</i>	95	60 (per pass)	*	A1.3a
Nitric Acid [†]	95	99	94.05	A1.4
Ethylene Dichloride [†]	99	95	94.05	A1.5
<i>Ethylene Dichloride</i>	99	55 (per pass)	*	A1.5a
Vinyl Chloride [†]	98	95	93.1	A1.6
<i>Vinyl Chloride</i>	98	50 (per pass)	*	A1.6a
Benzene [†]	80	90	72	A1.7
Benzene	76	99	75.2	A1.7a
Ethylbenzene [†]	99	99	98.01	A1.8
MTBE [†]	100	99	99	A1.9
Styrene	90	50	45	A1.10
Styrene [†]	90	70	63	A1.10a
Methanol [†]	99	99	98.01	A1.11
<i>Methanol</i>	99	7 (per pass)	*	A1.11a
<i>Methanol</i>	99	60 (per pass)	59.4	A1.11b
Formaldehyde [†]	91	100	91	A1.12
Xylene [†]	90	80	72	A1.13
Toluene [†]	95	75	71.25	A1.14
p-Xylene [†]	20	100	20	A1.15
Terephthalic Acid [†]	99.6	90	89.64	A1.16
Terephthalic Acid	90	95	85.5	A1.16a

Current Catalytic Process Yield Data (contd.)

Chemical	Selectivity	Conversion	Proc. Yield	Citation
Ethylene Oxide	70	90	63	A1.17
Ethylene Oxide [†]	80	95	76	A1.17a
<i>Ethylene Oxide</i>	70	9 (per pass)	*	A1.17b
<i>Ethylene Oxide</i>	60	35 (per pass)	*	A1.17c
Ethylene Glycol [†]	99	99	98.01	A1.18
Ethylene Glycol	*	90	*	A1.18a
Cumene [†]	99	98	97.02	A1.19
<i>Cumene</i>	*	40 (per pass)	*	A1.19a
Phenol [†]	90	98	88.2	A1.20
Acetic Acid [†]	99	90	89.1	A1.21
Butadiene [†]	90	73	65.7	A1.22
Butadiene	80	75	60	A1.22a
Butadiene			80	A1.22b
Butadiene			65	A1.22c
Acrylonitrile [†]	70	100	70	A1.23
Propylene Oxide [†]	90	100	90	A1.24
<i>Propylene Oxide</i>	90	10 (per pass)	9	A1.24a
Vinyl Acetate [†]	90	100	90	A1.25
Vinyl Acetate	*	*	95	A1.25a
Acetone [†]	90	98	88.2	A1.26
Acetone			96.7	A1.26a
Cyclohexane [†]	99	99	98.01	A1.27
Adipic Acid [†]	90	100	90	A1.28
Adipic Acid	80	5 (per pass)	3.2	A1.28a
Caprolactam [†]	95	95	90.25	A1.29
Isobutylene [†]	99	99	98.01	A1.30
Isobutylene			92	A1.30a

Citations

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Appendix VIII

Use of the Excel ("top50chem.xls") spreadsheet

User input variables are marked in blue.

Output results are color coded in either red, green, or yellow.

Each page begins with a listing of the top 50 chemicals.

Page 1 (columns A-E):

Lists the 1992 production levels, the catalyst(s) used during production, process notes on the production route(s), and the catalytic value (1 = catalytic, 0 = non-catalytic).

Page 2 (columns F-H):

Lists the reactants required for production and the end uses of the product chemical.

Page 3 (columns I-J):

Lists the chief process limitations.

Page 4 (columns K-P):

Lists the process conversion and selectivity, the catalyst(s) used, the type of catalyst employed, and the applicable current CBD project.

Page 5 (columns Q-Z):

Lists the process energy per pound required, the process and feedstock energy per pound, the 1992 process energy in billion BTU, the 1992 process plus feedstock energy required in billion BTU, the estimated process yield (a function of the user input query --cell AV2), the current process yield, the process energy savings in billions BTU, and the total energy savings (process and feedstock energy) in billions BTU.

Page 6 (columns AA-AK):

Lists the process energy savings including downstream effects from the use of a top 50 reactant, if applicable. Also listed are the appropriate top 50

reactant(s), the approximate amount of each top 50 reactant used for production of this chemical, and the applicable CBD project.

Page 7 (*columns AM-AS*):

Lists the total 1992 process energy use, the 1992 process plus feedstock energy value (without double counting feedstock energy), other process improvements, the energy savings from process and total energy arising from a process improvement not solely related to catalytic improvements. Cell AS2 asks the user to input a process improvement value. Cells AS4 and AS6 return the process energy and feedstock plus process energy savings values reported in Scenario 4, respectively.

Page 8 (*columns AT-BB*):

User inputs the impact (or improvement) to be evaluated in cell AV2. The effect on each type of catalyst is returned in cells AX2, AX3, and AX4 for all metals, metal oxides, and all acid catalysts (Scenario 2a). Cells AW5, AX5, AY5, and AZ5 return the effect on noble metals, metal chlorides, metal acetates, and metal salts, respectively (Scenario 2b). Cells AW8 and AX8 return the effect on zeolites and other acid catalysts, respectively (Scenario 2c). The process and the feedstock plus process impact on all catalysts is returned in cells AY2, AZ2, AY4, and AY6 (Scenarios 1a and 1b). Columns BA and BB return the individual effect on each chemical (Scenario 3a and 3b).

Page 9 (*columns BC - BI*):

This is a calculation only page. The maximum allowable process yield is listed, along with the proposed yield improvement, the hypothesized yields, and the effects per chemical from both energy calculations.

Page 10 (*columns BJ-BQ*):

The user can enter a response factor in cell BK2. All analyses done in this report used a response factor of 1.0 between yield improvement and energy savings. The final two columns show the total energy in all catalytic processes.

Page 11 (*columns BR-BZ*):

This page contains data only. Included is the process, the feedstock, the total energy, the excess feedstock energy, and the sum of process plus feedstock energy without double counting the feedstock energy.

Page 12 (*columns CA-CK*):

Lists the energy values and the potential energy savings resulting from the current CBD projects; also listed is the savings from the different types of catalysts.

Page 13 (*columns CM-CS*):

This page subdivides the metal catalyst category into four subcategories (noble metals, metal chlorides, metal acetates, and metal salts).

Page 14 (*columns CT-CX*):

This page subdivides the acid catalyst category into two groups (zeolites and other acids).

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