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Executive Summary

The Biomass Research and Development Board (Board) founded the Biomass Conversion Interagency Working Group (BCIWG) in the fall of 2007 to coordinate federally supported research, development, and deployment (RD&D) efforts aimed at the development of efficient and cost-effective conversion methods for the production of next-generation, plant-fiber based, cellulosic biofuels. It includes representation from the departments of Energy (DOE), Agriculture (USDA), Defense (DOD), and Interior (DOI); the National Science Foundation (NSF); and the Environmental Protection Agency (EPA). Its first task, completed in May 2008, was to conduct a Federal research inventory of biomass conversion research. With that input, along with several key government reports on biomass conversion science and technology, its second task was the preparation of this current document.

Many scientific and technological challenges need to be overcome in the next five to ten years to meet the ambitious RFS mandates for advanced biofuels supply through 2022. This report is designed to help the federal government maintain a well-coordinated and effective research portfolio to support biofuels conversion research.

The report focuses on the conversion of sustainably grown, nonfood, lignocellulosic (plant-fiber based) feedstocks into liquid transportation fuels. Examples of such feedstocks include agricultural and forest residue such as corn stover, wood chips, and portions of municipal solid waste, and dedicated energy crops such as switchgrass and short-rotation poplar trees. Although algae are a feedstock of great potential, the technical barriers associated with algae (production, processing, and conversion) are just beginning to be defined and addressed among federal agencies\(^1\). For many terrestrial oil crops, the technical barriers are dominated by production challenges rather than conversion. These and other conversion processes that impact near-term, mid-term, and long-term goals (see p. 18) will be the subject of future reports.

Significant scientific and technological challenges must be addressed to achieve efficient, cost-effective methods for converting lignocellulosic materials into liquid transportation fuels on a commercial scale. A major challenge is biomass recalcitrance, the inherent structural and chemical complexity that nature has built into plant fiber to protect plants from assault by both biological and non-biological forces. This recalcitrance makes it difficult to cost-effectively process plant fiber into usable intermediates that can be converted into liquid fuels. Processes that utilize whole biomass and circumvent recalcitrance face issues of catalyst activity, selectivity, and durability.

Another major challenge facing virtually all the processing methods is that the intermediates never emerge in pure form. Intermediates are always mixed with other chemicals (or in the case of bio-oils, are themselves a complex chemical mix). The extraneous chemicals in these mixtures, which come either from the plant itself or from the substances used in deconstruction, make subsequent processing of the intermediates more difficult. At the same time, science has achieved advances in recent years that may put solutions to this problem within reach.

The federal government has already committed substantial resources to both basic and applied research on biofuels. Members of the BCIWG will foster the interagency cooperation and coordination that is essential to help meet goals for the development of cost-competitive, next-generation, cellulosic biofuels.

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\(^1\) The National Algal Biofuels Technology Roadmap was published in May 2010.
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The Biomass Research and Development Board (Board) was originally created by Congress in the Biomass Research and Development Act of 2000, to “coordinate research and development activities relating to biofuels and biobased products between the Department of Agriculture and the Department of Energy, and with other departments and agencies of the Federal Government.” The Board is co-chaired by senior officials from the departments of Energy (DOE) and Agriculture (USDA) and includes senior officers from the U.S. Department of the Interior (DOI), U.S. Environmental Protection Agency (EPA), National Science Foundation (NSF), and the President’s Office of Science and Technology Policy (OSTP). Senior decision makers from other agencies and offices have also been invited by the Board to participate, including the U.S. Departments of Transportation, Defense, Commerce, and Treasury; the Office of the Federal Environmental Executive, and the Office of Management and Budget (as an ex officio member).

In October 2008 the Board released the National Biofuels Action Plan (NBAP). The NBAP outlines areas where interagency cooperation will help biobased fuel production technologies evolve from promising ideas to competitive solutions. The Board used a five-part supply-chain framework (Feedstock Production, Feedstock Logistics, Conversion, Distribution, and End Use) to identify Board action areas and develop interagency teams to better coordinate activities. In addition, the Board identified two crosscutting action areas—1) Sustainability and 2) Environment, and Health and Safety—into which the other working groups will provide future input.

For the purposes of this report, “conversion” is the transformation of nonfood plant fiber, or lignocellulose, from feedstocks to liquid fuels. Current technologies for accomplishing this are neither efficient nor sufficiently cost effective to compete effectively in the marketplace. The Renewable Fuel Standard (RFS) of the Energy Independence and Security Act (EISA) of 2007 mandates expanding the supply of renewable fuels to 36 billion gallons per year (BGY) by 2022, of which 21 billion gallons are expected to be “Advanced Biofuel.”

The NBAP calls for the creation of a Biomass Conversion Interagency Working Group (BCIWG), which will include members from DOE, USDA, EPA, DOD, NSF, and other agencies. This report satisfies the second deliverable from the BCIWG—an integrated, 10-year, federal research, development, and deployment (RD&D) biomass conversion survey that includes agency roles, goals, and key milestones; and identifies critical gaps.

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I. Introduction: Benefits and Challenges of Biofuels

The cars, trucks, buses, locomotives, barges, and airplanes that compose the nation’s transportation system operate almost exclusively on petroleum-based fuels. However, such reliance on a single fuel source has created challenges that the nation must address. As U.S. demand for oil increases and the production capability of domestic fuel sources decreases, dependence on foreign oil producers remains high. Further, concerns about climate change and other environmental impacts of burning fossil fuels, which releases greenhouse gases and pollutants into the atmosphere, have grown in concert with our understanding of the impacts.

Consumers in the U.S. currently have few practical alternatives to oil to meet their transportation fuel needs; however, sustainably produced biofuels have strong potential to address our nation’s energy security and climate change challenges in the near future. Corn ethanol has displaced some petroleum use, but greater promise lies in cellulosic or plant-fiber based biofuels.

In contrast to diminishing domestic petroleum reserves, the U.S. has the potential to use inedible plant fiber that—if cost-effective conversion technologies are developed—could be used as feedstock for biofuel production. The combustion of cellulosic biofuels in vehicle engines could substantially reduce net carbon dioxide (CO₂) emissions, because the CO₂ released while burning the fuel is reabsorbed by the next generation of feedstock plants as they grow.

There are significant scientific and technological challenges to achieving efficient and cost-effective methods to convert plant fiber, or lignocellulose, into liquid transportation fuels on a commercial scale. A chief challenge for several of the most significant conversion routes is biomass recalcitrance, the inherent strength and structural and chemical complexity that nature has built into plant fiber to protect plants from breakdown by both biological and nonbiological forces. This recalcitrance makes it difficult to move cost effectively from plant fiber to usable intermediates that can be converted to fuels. At the same time, advances in recent years may put solutions to these problems within reach.

First, genomics-based systems biology—much of it growing out the Human Genome Project—has provided an array of powerful new tools and techniques for understanding and manipulating biological systems and components—including plants, enzymes, and microorganisms—at the microscopic and nanoscale levels, to help overcome these challenges. Over the past several years, federally supported research, development, and deployment (RD&D) efforts have built a community of scientists who are aggressively applying systems biology tools to the problem of achieving cost-effective biofuels processing.

Second, RD&D efforts have made significant advances in chemical catalysis for biofuels conversion. Researchers are adapting a range of traditional thermochemical processes to overcome the challenge of cost-effective conversion, including gasification, Fischer-Tropsch synthesis, and pyrolysis, which are not constrained by the recalcitrance problem but have other issues, such as scalability and product
quality. Researchers are also developing promising new catalytic conversion methods that operate at lower temperatures and use sugars as intermediates.

The federal government has supported major efforts to develop detailed research roadmaps for both of these approaches. In 2006, DOE published *Breaking the Biological Barriers to Cellulosic Ethanol: A Joint Research Agenda*, the result of a scientific workshop jointly sponsored by DOE’s Office of Science and Office of Energy Efficiency and Renewable Energy. The workshop brought together leading scientists and researchers working in biological systems to map a detailed research agenda. In 2008, the National Science Foundation (NSF) published *Breaking the Chemical and Engineering Barriers to Lignocellulosic Biofuels: Next Generation Hydrocarbon Biorefineries*, based on a workshop jointly sponsored by NSF and DOE that brought together leading scientists and researchers in the chemical catalysis community.

The federal government has already committed substantial resources to both basic and applied research on biofuels. Since 2007, DOE has announced plans to commit over a five year period more than $1 billion to research, develop, and demonstrate cellulosic biofuels technology. Since 2006, USDA has invested almost $550 million for new biofuels technology RD&D. In addition, both DOE and NSF are offering substantial support to fundamental research efforts in genomics, metabolic engineering, catalysis, and chemistry that have potential applications in biofuels.

Scientific and technological challenges need to be overcome in the next five to ten years in order to meet the ambitious RFS mandates for advanced biofuels supply through 2022; this report outlines the scientific approaches to biofuels conversion research that are likely to overcome these challenges. The aim of the report is to assist the federal government in maintaining a well-coordinated and balanced research portfolio that supports the biofuels conversion research necessary to meet our national goals for the development and expansion of cellulosic biofuels over the next decade.
II. The Biomass Conversion Interagency Working Group

The Biomass Research and Development Board (Board) is the federal government’s multi-agency effort to coordinate RD&D activities relating to biobased fuels, biopower, and bioproducts. Created by the Biomass Research and Development Act of 2000 (as amended), the Board is co-chaired by the departments of Agriculture and Energy, and includes senior officers from the Department of Interior (DOI), Environmental Protection Agency (EPA), National Science Foundation (NSF) and Office of Science and Technology Policy (OSTP). At the discretion of the Board, other agencies are also invited to participate, and have included senior representatives of the Departments of Transportation, Defense, Commerce, and Treasury, as well as the Office of the Federal Environmental Executive and the Office of Management and Budget (as an ex officio member). The Board plays a central role in coordinating programs within and among departments and agencies of the federal government and bringing coherence to federal strategic planning.

The Energy Independence and Security Act (EISA) Renewable Fuel Standard (RFS), which the President signed into law in December 2007, requires the supply of 36 billion gallons per year (BGY) of biofuels by 2022. The RFS includes specific provisions for advanced biofuels that can be produced on a sustainable basis and that have lower lifecycle greenhouse gas emissions than conventional petroleum fuels. To coordinate the federally supported research needed to meet the challenging goals of the RFS and other biofuels initiatives, the Board’s major focus from 2007 to 2008 was the development of a National Biofuels Action Plan (NBAP). The NBAP outlines the interagency coordination of federally sponsored RD&D efforts that could enable biofuels to become a more prominent element of the national energy mix.

The Board created several interagency working groups, including Sustainability; Feedstock Production; Feedstock Logistics; Conversion Science and Technology; Distribution Infrastructure; and Environment, Health, and Safety. The groups were tasked with helping to coordinate research across the federal government to enable the creation of cost-effective and commercially viable biomass production and distribution technologies in the shortest possible time frame.

The NBAP also created the Biomass Conversion Interagency Working Group (BCIWG) to support the basic and applied research needed to develop cost-effective, commercially scalable processes to convert nonfood, lignocellulosic feedstocks into ethanol, higher alcohols, green gasoline, diesel, and aviation fuels. These conversion processes can help to reduce dependence on fossil fuels and foreign oil and achieve meaningful reductions in the volumes of greenhouse gases emitted by the transportation sector. With members including working-level representatives from DOE, USDA, EPA, DOD, DOI, and NSF, the BCIWG is engaged in two initiatives:

- Support accelerated RD&D through the development and implementation of mechanisms to improve interagency
coordination, promote interagency knowledge sharing, and track ongoing federal biomass conversion RD&D. This initiative has been fulfilled by the establishment of an interagency database featuring RD&D funding for the fiscal years (FY) 2006–2009 across DOE, USDA, EPA, DOD, DOI, and NSF. The initial version of this database was completed in May 2008 and is being used internally by the BCIWG.

- Develop a comprehensive, integrated, 10-year federal RD&D biomass conversion plan (this document) that includes agency roles, goals and key milestones, and identifies gaps.

The constituent programs of the BCIWG from DOE, USDA, NSF, EPA, DOD, and DOI and the research conducted in each program are shown in the Table 1, below.
### Table 1. Members of the Biomass Conversion Interagency Working Group

<table>
<thead>
<tr>
<th>Federal Agency</th>
<th>Program</th>
<th>Research</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Office of Science, Office of Biological and Environmental Research</td>
<td>DOE Bioenergy Research Centers</td>
<td>Advanced fundamental research on enzymatic-microbial conversion, with some additional research on chemical catalytic processing.</td>
</tr>
<tr>
<td>DOE Office of Science, Office of Biological and Environmental Research</td>
<td>DOE Genomics Science Research Program</td>
<td>Foundational systems biology research on plants and microbes with relevance to biomass conversion.</td>
</tr>
<tr>
<td>DOE Office of Science, Office of Biological and Environmental Research</td>
<td>DOE Joint Genome Institute</td>
<td>High-throughput genomic sequencing of biofuel-relevant plants and microbes.</td>
</tr>
<tr>
<td>DOE Office of Science, Office of Basic Energy Sciences</td>
<td>Catalysis Science and Physical Biosciences Programs</td>
<td>Fundamental, molecular-scale research on chemical catalytic processing and cell wall structure/recalcitrance.</td>
</tr>
<tr>
<td>DOE Office of Energy Efficiency and Renewable Energy, Office of Biomass Programs</td>
<td>Biochemical Conversion to Fuels</td>
<td>Innovative approaches to the production of advanced biofuels via basic and applied research in biochemical routes (ethanologens, enzymes, separations, etc.) to achieve biofuels cost targets.</td>
</tr>
<tr>
<td>DOE Office of Energy Efficiency and Renewable Energy, Office of Biomass Programs</td>
<td>Thermochemical Conversion to Fuels</td>
<td>Innovative approaches to the production of advanced biofuels via basic and applied research in thermochemical routes (gasification, pyrolysis, catalysis, upgrading, etc.) to achieve biofuels cost targets.</td>
</tr>
<tr>
<td>DOE Office of Energy Efficiency and Renewable Energy, Office of Biomass Programs</td>
<td>Demonstrations of Integrated Biorefineries</td>
<td>Large-scale demonstrations of biochemical and thermochemical processes to validate integrated biorefinery technologies with industrial partners.</td>
</tr>
<tr>
<td>USDA, Agricultural Research Service (ARS)</td>
<td>ARS National Program in Bioenergy Research</td>
<td>ARS bioenergy research enables new, commercially preferred biorefining technologies.</td>
</tr>
<tr>
<td>USDA National Institute of Food and Agriculture (formerly the Cooperative State Research Education and Extension Service)</td>
<td>Agriculture and Food Research Initiative Biobased Products and Bioenergy Production Research Program; Small Business Innovation Research Program; Agricultural Materials Program; and others.</td>
<td>Supports fundamental and applied extramural research on biofuels research, including: cellulosic ethanol, biodiesel, renewable hydrocarbons and novel catalytic processes, hydrogen fuel cells, algae, and biorefining and production of biobased products.</td>
</tr>
<tr>
<td>Department of Agriculture, Forest Service</td>
<td>R&amp;D Deputy Area and Forest Service Research Stations</td>
<td>Fundamental and applied biomass-utilization research in support of the agency mission to care for our forests. Specific areas in conversion to bioenergy and biobased products include: biomass deconstruction, biochemical conversion, thermal chemical conversion, and business case development.</td>
</tr>
<tr>
<td>National Science Foundation</td>
<td>Directorates of Engineering and Biology</td>
<td>Fundamental research in genomics, metabolic engineering, and thermal and catalytic chemistry.</td>
</tr>
<tr>
<td>Environmental Protection Agency</td>
<td>Office of Research and Development</td>
<td>Development of membrane technology for ethanol/water separation.</td>
</tr>
<tr>
<td>Department of the Interior</td>
<td>Biomass and Forest Health Program</td>
<td>Works collaboratively with DOE and USDA to encourage the utilization of woody biomass byproducts from restoration and fuels treatment projects.</td>
</tr>
<tr>
<td>Department of Defense</td>
<td>Air Force for Installations, Environment and Logistics</td>
<td>Development of processes for alternative jet and diesel fuel.</td>
</tr>
</tbody>
</table>
III. Pathways to Liquid Transportation Fuels

Significant challenges remain to achieving cost-effective production of lignocellulosic biofuels on a commercial scale. Chief among these are the low energy density of cellulosic biomass and biomass recalcitrance. There are two major routes for the conversion of cellulosic biomass to biofuels: enzymatic/microbial (“biological processing”) and thermal/chemical-catalytic (“thermal/chemical processing”). A hybrid approach that would combine the two methods may also prove effective.

Biological processing is currently most associated with cellulosic ethanol, and thermal/chemical processing is most associated with hydrocarbon biofuels such as diesel. However, both paradigms are developing pathways to make both alcohols and alkanes. As second-generation biofuels are being developed, the advantages of hydrocarbon biofuels are being given due consideration. One advantage is their higher energy density and correspondingly, higher vehicle miles per gallon: 115,000 Btu/gal for gasoline, 126,000 Btu/gal for jet fuel, and 139,000 Btu/gal for diesel; compared to 76,000 Btu/gal for ethanol and 105,000 Btu/gal for butanol. Additionally, these fuels are compatible with the existing infrastructure of refineries, pipelines, storage tanks, and engines, and constitute green, drop-in replacements to the petroleum-based fuels in use today.

Both types of processing begin with some form of grinding of the plant matter to reduce size and maximize surface area for processing. Barriers in this area are to be found in the Board’s Feedstock Logistics Interagency Working Group report.

For both processing methods, conversion proceeds in two major phases: (1) deconstruction of biomass and (2) fuel synthesis. Deconstruction is the process of breaking down plant fiber and reducing it to substances—called intermediates—that can then be converted into fuels. The desired intermediates vary according to the type of processing. In the case of biological processing and some of the newer types of chemical processing, the desired intermediates are simple sugars which form the building blocks of the cellulose and hemicellulose in plant fiber. In gasification, the desired intermediate is synthesis gas (syngas), which is a combination of carbon monoxide (CO) and hydrogen (H₂) that results from heating plant matter to extremely high temperatures. In pyrolysis, the intermediates are bio-oils (liquefied plant matter) and charcoal.

One of the major challenges facing virtually all the processing methods is that the intermediates never emerge in pure form. They are always mixed in with other chemicals, or, in the case of bio-oils, are themselves a complex chemical mix. The extraneous chemicals in these mixtures, which come either from the plant itself or from the substances used in deconstruction, make subsequent processing of the intermediates more difficult. In the case of biological processing, the extraneous chemicals typically have an inhibitory effect on the enzymes and microbes subsequently used in conversion. In the case of new chemical processing methods mentioned above, the extraneous chemicals can prevent the catalytic reactions needed for fuel synthesis from taking place.
The environmental impact and sustainability of the conversion process must also be addressed to facilitate commercialization of the new conversion technologies that grow out of today’s research. Issues such as water use, waste disposal, containment of any toxins, energy use, and other potential environmental impacts will necessarily be part of the calculus in designing commercial conversion plants. While it is probably too early to predict these environmental challenges with any specificity, issues of environmental impact and sustainability will need to be kept clearly in mind as conversion technologies move toward commercial development.

**Biological Processing**

Cellulose, hemicellulose, and lignin are assembled into a complex, nanoscale composite not unlike reinforced concrete, but with the capability to flex and grow much like a liquid crystal. Lignin shields the cellulose from attack by enzymes or other agents of degradation. In biological or enzymatic-microbial processing, deconstruction typically takes place in two separate steps: (1) chemical pretreatment, followed by (2) breakdown of plant fiber using enzymes (enzymatic hydrolysis).

Enzymes need access at a molecular scale to the plant fiber material in order to split the cellulose and hemicellulose into simple sugars. The main function of pretreatment is to separate the cellulose and, if possible, the hemicellulose, from the lignin, making both accessible to processing by enzymes. Pretreatment exposes the cellulose and hemicellulose to the enzymes. Without pretreatment, using enzymes alone releases only about 20 percent of the sugar. With pretreatment, sugar capture can rise as high as 90 percent. A second goal of pretreatment is to decrystallize the tightly wound cellulose, wholly or partially, in order to create more sites for enzymes to attack the cellulose. Cellulose is not water soluble (a cotton shirt does not dissolve in the washing machine because cotton is pure cellulose). Also, the tight, crystalline structure of cellulose inhibits reaction with enzymes; decrystallized or amorphous cellulose is far more amenable to enzymatic hydrolysis. The most common pretreatment methods applied today use either liquid hot water, steam explosion (with or without acid addition), diluted or concentrated acid solutions (e.g., sulphuric acid), alkaline solutions, or ammonia with heat and pressure [e.g., ammonia fiber explosion treatment (AFEX)].

Following pretreatment, there is usually some type of (imperfect) separation method to attempt to separate out the cellulose and hemicelluloses from the rest of the mixture. The separated substance is then treated with an enzyme-containing solution to break the cellulose and hemicelluloses down into sugars; this reaction is called hydrolysis or saccharification.

Finally, when the sugars are available, they are “fed,” in a solution, to microbes for microbial processing for synthesis of fuel. The simplest form of microbial processing is the age-old method of fermentation, or conversion of sugars by microbes (typically yeast) into ethanol.

Through biological reengineering, it has become possible to develop microbes that process simple sugars into higher alcohols and even hydrocarbon molecules that could be blended to produce green gasoline, diesel, and jet fuel. However, synthetic biology research is needed to enable these pathways and allow for commercialization of these technologies.

Each step in this process offers opportunities for modern genomics-based systems biology to effect decisive improvements that could lead to
cost-effective and commercially competitive biorefineries for production of cellulosic biofuels. Genomics-based techniques permit the rapid discovery of new microbes and enzymes through bioprospecting and metagenomics—sequencing communities of organisms from promising environments such as rain forests, hot pools, and compost heaps—where nature effects the rapid degradation of lignocellulose.

Genomics and the allied tools of systems biology provide the basis for new understanding of the actual operation of enzymes so as to maximize their effectiveness. Genomic-based techniques also provide powerful tools for reengineering microbes to resist inhibitory chemicals and high product concentrations, to improve the performance of fuel-synthesizing microorganisms, and to enable the synthesis of hydrocarbon fuels beyond ethanol. Additional technical tools that can offer improvements in the conversion of cellulosic biomass to fuels include metabolic and protein engineering, bioreactor engineering, advanced imaging techniques, and advanced process engineering.

**Thermal/Chemical Processing**

There are three main pathways for the thermal/chemical processing of lignocellulose: gasification, pyrolysis, and aqueous phase reforming. Both gasification and pyrolysis overcome the recalcitrance problem noted in the previous section and both convert the lignin portion of biomass into liquid fuels.

**Gasification**

Gasification, the oldest and most developed alternative, partially burns carbonaceous materials at high temperatures (600°C–900°C) using controlled amounts of air or oxygen, and/or steam. The product gas, syngas, consists mostly of CO and H₂.

Recent work has dealt with the incorporation of catalysts in the gasifier (catalytic gasification), so that multiple thermal and chemical processes occur in the same reactor, potentially eliminating process steps.

There are two main strategies for producing liquid fuels (or blending components for fuels) from syngas. The first is the fermentation or catalytic conversion of syngas to ethanol or higher alcohols. The second is the catalytic conversion to produce alcohols or alkanes, which can be catalytically upgraded to yield specified ranges of distillation cuts for gasoline, diesel, jet fuels such as Jet-A and JP-8, and kerosene. The liquid fuel that is produced depends on the type of catalyst used and the process parameters.

The fermentation of syngas offers an interesting alternative for the production of fuels such as ethanol or hydrogen. One advantage is that it is less sensitive than inorganic catalysts to syngas contaminants such as tar, alkali metals, and chlorides. As a result, the gas cleaning and conditioning requirements for syngas may be less stringent than the requirements for conventional catalytic conversions of syngas to fuels and meeting these requirements may be less costly.

**Pyrolysis**

Pyrolysis produces a sort of “biocrude” or bio-oil intermediate through a moderately high temperature reaction in the absence of oxygen. Bio-oils contain hundreds of oxygenated, organic molecules and must be further processed to produce green diesel or gasoline fuels. A potential advantage of pyrolysis is the production of a higher energy density bio-oil
intermediate, which could be transported from small, modular pyrolysis units at remote sites to a centralized refining site.

Current approaches to bio-oil production include:

**Slow Pyrolysis**

Slow pyrolysis is characterized by slower heating of 450°C–500°C and longer contact times at ambient pressure (compared to fast pyrolysis) to produce bio-oil, gases, and char. The biomass feedstock for slow pyrolysis must be dried.

**Fast Pyrolysis**

Fast pyrolysis is characterized by more rapid heating rates of 450°C–500°C and shorter contact times (1–2 seconds) at ambient pressure to produce bio-oil, gases, and char. The biomass feedstock for fast pyrolysis must also be dried.

**Liquefaction**

Bio-oils can also be produced by utilizing water at higher pressures (120–200 standard atmosphere [atm]) and relatively lower temperatures (300°C–400°C) in the absence of oxygen. The biomass feedstock does not need to be dried for liquefaction. The bio-oil produced from liquefaction has a lower oxygen content compared to the bio-oil derived from fast pyrolysis and is water insoluble.

Catalysts are being used more frequently in the pyrolysis stage to increase reaction selectivity and produce a bio-oil that contains less oxygen, has a lower tar content, and is easier to upgrade into a marketable fuel.

**Aqueous Phase Reforming**

Aqueous phase reforming produces hydrocarbon fuels from concentrated sugar-in-water solutions via chemical catalysis. Once lignocellulose has been deconstructed into sugars or sugar-like monomers, those intermediates are reacted over an inorganic catalyst in the liquid phase to form hydrocarbons. Thus, it is possible to produce green gasoline, diesel, and jet fuel directly from sugar cane, via chemical conversion of the sugar intermediates from the hydrolysis processes reviewed under “Biological Processing.” A hybrid, overall process might consist of enzymatic dissolution to sugar intermediates followed by reforming to hydrocarbons over inorganic catalysts.

In the next section, the technical challenges and barriers associated with both types of processing—biological and thermal/chemical—are described.
IV. Barrier Identification

Cost is the overarching barrier in all process steps, regardless of conversion method; a summary of other basic and applied research barriers for the biochemical and chemical processes is shown in Table 2. The greatest technical barrier to the biological conversion of lignocellulosic biomass and to the aqueous phase reforming route of chemical conversion is the intrinsic recalcitrance of the lignocellulose. Therefore, many of the postulated routes, either fermentation to ethanol, enzymatic or synthetic biological conversion to hydrocarbons, or aqueous phase reforming to hydrocarbons, face new fundamental challenges that require innovative, long-term RD&D efforts.

Table 2: Key Barriers for Biochemical and Chemical Conversion Processes

<table>
<thead>
<tr>
<th>Biochemical Platform: Enzymatic-Microbial Conversion</th>
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<tbody>
<tr>
<td>Pretreatment:</td>
</tr>
<tr>
<td>• Lack of complete access to the cellulose</td>
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<tr>
<td>• Generation of inhibitors that reduce the yield of fermentable sugars and that make downstream processing more difficult</td>
</tr>
<tr>
<td>Hydrolysis:</td>
</tr>
<tr>
<td>• Slow rate of reaction and inadequate yield of product hydrolyzed by current enzymes</td>
</tr>
<tr>
<td>Biochemical Fuel Synthesis:</td>
</tr>
<tr>
<td>• Toxicity of pretreatment byproducts and fuel synthesis products to the microbes used for synthesizing fuel</td>
</tr>
<tr>
<td>• Inability of existing microbes to process all the sugars in lignocelluloses efficiently</td>
</tr>
<tr>
<td>• Lack of natural processes to produce hydrocarbon fuels (green gasoline, diesel, jet fuel)</td>
</tr>
<tr>
<td>• Lack of value-added coproducts</td>
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</table>

<table>
<thead>
<tr>
<th>Thermochemical Platform: Thermal and Inorganic Catalytic Conversion</th>
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</thead>
<tbody>
<tr>
<td>Gasification:</td>
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<tr>
<td>• Lack of low-cost production of syngas from a broad range of feedstocks (within different regions)</td>
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<td>• Insufficiently scalable gasification facilities (small, medium, large)</td>
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<td>• Insufficient lifetime of clean-up catalysts at high conversion efficiencies</td>
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<td>• High cost of catalysts and ash accumulation in catalyst bed (for catalytic gasification)</td>
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<td>• Low conversion capacities of syngas fermentation microbes</td>
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<td>• Low syngas bioreactor efficiencies</td>
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<td>• Low catalyst selectivity, first-pass yield, and lifetimes</td>
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<td>• Lack of cost-effective, small-scale, catalytic facilities</td>
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<td>Pyrolysis:</td>
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<tr>
<td>• High oxygen and acid content of product bio-oil</td>
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<td>• Instability of product bio-oil</td>
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<tr>
<td>• Expense of construction materials</td>
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<td>• Lack of low-cost hydrogen reactant for hydrotreating</td>
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<td>• Lack of low-cost, corrosion-resistant, construction materials</td>
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<tr>
<td>• Inadequate yield, selectivity, and stability of catalysts</td>
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<tr>
<td>Aqueous Phase Reforming:</td>
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<td>• Not yet proven for cellulosic biomass</td>
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<td>• Inadequate catalyst activity, selectivity, and stability</td>
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February 2011
Biochemical Platform: Enzymatic-Microbial Conversion

The current pathways for the biochemical conversion of lignocellulosic biomass into biofuels are outlined in Figure 1 below. The pathways involve pretreating and then enzymatically breaking the biomass into five and six carbon (C5 and C6) sugars, which can then be fermented into ethanol and other alcohols or converted by microbes into hydrocarbons. The intermediate product of gasification, syngas, which is a mixture of carbon monoxide and hydrogen gas, can also be fermented into alcohols. A shortcut for the production of biofuels from lignocellulose is consolidated bioprocessing, in which the production of intermediates and the synthesis of fuel are combined in a single step.

Technical Barriers in Pretreatment

The major shortcomings of current pretreatment technologies include:

- Incomplete access to the material
- Generation of inhibitors that reduce the yield of fermentable sugars and make downstream processing more difficult.

Current pretreatment methods are also compromised by high cost, and pretreatment can produce chemical byproducts that reduce sugar yields and inhibit (i.e., are toxic to) the microbes used for fuel synthesis. The nature and amount of these byproducts depend on the type of pretreatment process and the feedstock.

Technical Barriers in Enzymatic Hydrolysis

Current enzymes are less than optimal for hydrolysis due to:

- Slow rate of reaction
- Inadequate yield of material hydrolyzed by current enzymes

Millions of years of evolution have made plant fiber an amazingly resilient material—likened even to flexible concrete—but there are many environments in nature where plant fiber is readily degraded. The handful of enzymes currently being used is a tiny subset of the cellulases—or cellulose degrading enzymes—that exist in nature. There is a widespread conviction among scientists that more effective enzymes and enzyme “cocktails” can be found

Figure 1. Overview of Biochemical Biomass Conversion Pathways and Products
in the natural environment, while some enzyme manufacturers are using genomic tools to develop new enzymes with improved characteristics. Also, plants can be genetically engineered to contain enzymes to assist in conversion. Discovering novel enzymes and/or reengineering enzymes could significantly improve the effectiveness and lower the cost of hydrolysis.

**Technical Barriers in Biochemical Fuel Synthesis**

Biochemical fuel synthesis poses several challenges, including:

- Toxicity of pretreatment byproducts and fuel synthesis products to the microbes used for synthesizing fuel
- Inability of existing microbes to process all the sugars in lignocelluloses efficiently
- Lack of natural processes to produce hydrocarbon fuels (green gasoline, diesel, jet fuel)
- Lack of value-added coproducts

First, as mentioned above, traditional pretreatment processes produce chemical byproducts that inhibit or poison the microbes or chemical catalysts used for synthesizing fuel. Second, intertwined with the hemicellulose are other chemicals that may also have an inhibitory effect. As the hemicellulose is degraded, these chemicals are released into the solution. A third challenge is the toxicity of the fuel itself above certain concentrations. Fourth, cellulose degrades into glucose, a six-carbon sugar that is readily processed by a wide range of microbes. However, hemicellulose degrades into both six-carbon and five-carbon sugars, and finding or engineering a microbe or community of microbes that can efficiently process both types of sugars poses a challenge. The composition of the particular feedstock is especially pertinent to this discussion. Woody biomass has a very different compositional profile than that of herbaceous plants such as corn stover and switchgrass, and it is possible that microbial strains will need to be tailored that can process the different sugar contents that result when these feedstocks are deconstructed. Fifth, current biocatalytic-based biorefineries lack processes for converting byproducts such as cell solids, lignin, and CO, into value-added products that both minimize waste streams from and improve the profitability of cellulosic biorefineries.

Both the individual components of biochemical conversion, such as the hydrolysis stage, and the overall pathway from feedstocks to fuel present a well-defined scientific endeavor promising remarkable success from dedicated research programs. Advances can come from the agencies that support biofuel research as well as from other sources, such as the medical and pharmaceutical sectors.

**Thermochemical Platform**

Thermochemical pathways for the production of biofuels from lignocellulosic biomass include the following methods: (1) gasification to syngas, which can then be fermented to alcohol or reacted via the catalytic Fischer-Tropsch synthesis reaction to hydrocarbons; (2) intermediate five- and six-carbon sugars, which can be produced from either catalytic or enzymatic deconstruction of biomass, can be converted into hydrocarbons via aqueous phase reforming and other associated catalytic processes; and (3) biomass can be pyrolyzed into bio-oil, which can then be converted into hydrocarbons via catalytic hydrotreating reactions. The same types of reactions are used to convert oily plant and animal feedstocks into hydrocarbons. Like consolidated bioprocessing, a catalytic version of pyrolysis exists in which
biomass is converted into biofuels, in this case hydrocarbons, in a single step.

**Technical Barriers to Gasification**

*Syngas production and cleanup* poses several challenges, including:

- Lack of low-cost production of syngas, especially at small scale
- Insufficient lifetime of clean-up catalysts at high conversion efficiencies
- High cost of catalysts and ash accumulation in catalyst bed (for catalytic gasification)

The syngas resulting from gasification is composed mostly of CO and H$_2$; however, the syngas from biomass gasification can contain other contaminants. These contaminants must be minimized or removed to enable the efficient conversion of syngas to fuels or power and to limit undesirable emissions. Contaminants such as hydrogen sulfide (H$_2$S), ammonia (NH$_3$), and tar can be corrosive and can foul and/or poison catalysts. The composition of the gaseous products from the gasification of biomass is dependent on gasifier design, the process parameters, the gasifying agent (water [H$_2$O] or air), the use of catalysts (in situ or separate catalyst bed), and the feedstock composition, which can vary with location, harvest, and season. There is a clear need for broad research on numerous biomass streams and reactor designs to assure cost-effective solutions for specific U.S. locations.

Advanced analytic research tools are required to examine the impurities in the syngas; the reaction with clean-up catalysts; competitive reactions with other components of the syngas stream; and the effectiveness impurities removal from the gaseous product.

There is a critical need to maintain the quality of syngas while minimizing capital and operational costs. Closely tied to this barrier is the need to understand and mitigate deactivation that is due to transient concentrations of impurities and accumulation of trace impurities, which can be done through long-term studies of catalysts with...
syngas derived from a variety of different biomass streams.

Catalytic gasification (gasification over a catalyst bed), can produce a tar-free syngas of a desired CO/H₂ ratio via a “water-gas shift” reaction. The main barriers to this approach are the high cost and limited lifetime of the catalysts as well as ash accumulation in the catalyst bed.

*Fuel synthesis via fermentation* poses several challenges, including:

- Low conversion capacities of syngas fermentation microbes
- Low syngas bioreactor efficiencies

Currently available microbes for syngas fermentation are product-inhibited, and therefore produce ethanol only at concentrations up to a few percent. This limitation results in higher ethanol-recovery costs. The development of strains that can tolerate higher ethanol concentrations would increase this technology’s commercial viability.

In addition, because CO and H₂ have very low solubilities in water, fermentation rates with syngas are low. Although elevated pressures in syngas fermentors would increase mass transfer rates and reduce reactor size, maintaining microbial productivity and minimizing equipment and operating costs are challenges in any high-pressure process, including fermentation.

*Fuel synthesis via inorganic catalysis* poses several challenges, including:

- Low catalyst selectivity, first-pass yield, and lifetime
- Lack of cost-effective, small-scale, Fischer-Tropsch facilities

Fischer-Tropsch synthesis is highly exothermic and often carried out in a fluidized bed configuration. Both of these characteristics can impact the deactivation and/or physical attrition of the catalyst. Additionally, there can be significant coke formation or clogging of catalytic active sites with wax byproducts during Fischer-Tropsch synthesis.

For ease of logistics, small-scale syngas production at remote sites is being examined. This effort also creates a need for complementary, small-scale, Fischer-Tropsch processes.

In addition to Fischer-Tropsch synthesis, there are other catalytic routes to hydrocarbons such as methanol synthesis, followed by methanol to gasoline (a commercial process). However, like conventional processes, they are viable only on a very large scale.

**Technical Barriers in Pyrolysis**

*The production of stable bio-oil* poses several challenges, including:

- High oxygen and acid content of product bio-oil
- Instability of product bio-oil
- High cost of construction materials
- Catalyst instability

Bio-oils contain higher concentrations of oxygen-containing molecules than petroleum. Oxygenated hydrocarbons are more chemically reactive than non-oxygenated hydrocarbons, and this contributes to the poor stability of bio-oils relative to petroleum or petroleum-derived products. High oxygen content also correlates with high acidity and, therefore, corrosiveness. Cost-effective and environmentally benign methods for inhibiting acid formation or
neutralizing acids would enable technology readiness.

Biomass can contain a significant amount of minerals, which likely act as heterogeneous catalysts. Detailed understanding of those minerals and the reactions of which they are capable would help to identify an optimal process.

Although numerous reaction pathways are involved in pyrolysis or liquefaction processes, fundamental understanding of these reactions and their dependence on chemical and physical conditions is lacking. In addition, detail of the mechanical and chemical breakdown of the biomass building blocks at sub-micron-length scales is lacking. Research in this area would aid the use of homogeneous or heterogeneous catalysts.

Fuel synthesis from bio-oils poses several challenges, including:

- High cost of hydrogen reactant for hydrotreating
- High cost of corrosion-resistant materials of construction
- Inadequate yield, selectivity, and stability of catalysts

Converting bio-oils into hydrocarbon fuels will likely involve three catalytic processes: (1) hydroprocessing to remove oxygen as water, (2) decarboxylation to remove oxygen as CO₂, and (3) catalytic cracking of longer-chain hydrocarbons. While using catalysts optimized for the hydroprocessing and catalytic cracking of petroleum products is a good starting point, the optimal catalysts for processing bio-oils will likely be very different.

Once catalysts have been refined for the conversion of bio-oils to fuel, long-term or accelerated aging studies will be required to probe deactivation processes. Without a detailed knowledge of the catalyst lifetimes once they are exposed to bio-oils, a viable process for the production of fuels with appropriate cost estimates cannot be constructed.

In order to facilitate the use of bio-oil in existing petroleum refineries, research on construction material requirements for hydrotreatment should consider the effect of switching back and forth between bio-oil streams and crude oil streams.

**Technical Barriers to Aqueous Phase Reforming**

*Homogeneous catalytic dissolution and aqueous phase reforming* poses several challenges, including:

- Not yet proven for cellulosic biomass
- Inadequate catalyst activity, selectivity, and stability

The production of biogasoline via aqueous phase reforming has been demonstrated for cane sugar feedstocks and efforts are underway to utilize this technology for the conversion of hydrolyzed cellulose. Issues of durability and poisoning of catalysts in the liquid phase are as yet unresolved. These fundamental issues are in addition to the reaction engineering, heat integration, and other process design issues that accompany the scale-up from benchtop research to commercial operation. Research and development efforts are needed in multiphase reactors design.
V. Conclusion

Significant scientific and technological challenges face the large-scale development of truly efficient, commercially viable, conversion methods for converting nonfood plant fiber into liquid transportation fuels. Nonetheless, the federally sponsored research portfolio described in these pages—comprising both transformational basic and applied research—is both aggressive and sufficiently diverse. With the increased resources provided by the federal Government since FY 2007, multiple investigators and teams of scientists are now pursuing a wide range of potential paths to a solution.

Progress has been notable. As recently as 2005, attention focused almost solely on the possibility of cellulosic ethanol. While cost-effective cellulosic ethanol remains the subject of much current research, within a few short years we have expanded our goals to include the development of cost-effective hydrocarbon biofuels—green gasoline, diesel, jet fuel—by both biobased and thermal/chemical means.

At this stage in the research effort, a diversity of approaches is appropriate. It is impossible to predict whether the key breakthroughs will come from biobased or thermal/chemical conversion methods, or whether we may find the greatest advantage in a hybrid approach that combines the two. To meet the ambitious goals for biofuels supply set forth in the EISA RFS, it is critical that we pursue the range of promising scientific and technological opportunities at hand.

History teaches that the pace and direction of scientific and technological progress are notoriously difficult to predict. It is in the very nature of scientific discovery to transform and surprise. Nonetheless, working back from the 2022 EISA goals for advanced biofuels, we can analyze where we will need to be, in terms of biofuels conversion science and technology, five and ten years hence in order to achieve the EISA RFS objectives. These milestones, summarized in Figure 3, are presented not as a prediction, but as a framework and a set of broad objectives to help gauge our progress as the federal government continues to support, provide oversight, and plan research in this field.

Continued coordination among the federal agencies and offices sponsoring this research is the other indispensable ingredient for success. The Board in general and the BCIWG in particular have provided a valuable forum for federal officials and program managers from different agencies and offices to keep apprised of other agencies’ activities and to help ensure a balanced and effective federal biofuels research portfolio. This portfolio will contribute to the scientific and technological foundation of a new cellulosic biofuels economy to enhance our nation’s energy and economic security; and to help protect our global environment in the years ahead.
**Figure 3. Key Milestones for Biofuels Conversion Science and Technology**

<table>
<thead>
<tr>
<th>CURRENT SITUATION</th>
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<tr>
<td>12.5 billion gallon per year operating production capacity from corn grain</td>
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<td>Concerns over oil price volatility &amp; energy security</td>
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<tr>
<td>Progressive production mandated by the Energy Independence and Security Act (EISA) to promote biofuel use</td>
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<tr>
<td>No commercial cellulosic biofuel plants</td>
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<tr>
<td>Inadequate conversion technology &amp; need for technology development</td>
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<tr>
<td>Concerns over climate change &amp; promise of cellulosic biofuel benefits</td>
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<tr>
<td>Concerns over biofuel sustainability &amp; potential market impacts</td>
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**INPUTS PLANNED AND UNDERWAY**

- Over $100 M committed and planned for three DOE Bioenergy Research Centers
- More than $1 B in DOE funds to 29 integrated biorefinery projects at the R&D, pilot, demonstration, and commercial scale
- Additional millions for related research
- Mobilization of world-class scientists and engineers at national laboratories and universities in both basic & applied biofuels research
- Strong support from the executive & legislative branches
- USDA and DOE loan guarantees funds for biorefinery development
- Cellulosic ethanol production tax credit
- USDA biomass crop assistance program
- Results from Intergency Biomass R&D Initiative projects

**NEAR TERM MILESTONES**

- Cost-competitive cellulosic ethanol
- Scientific breakthroughs toward cellulosic biofuels production cost parity with gasoline
- Commercial and demonstration scale cellulosic biofuels and hydrocarbon biorefineries with up to 100 million gallons per year total production capacity by 2014
- Next generation biofuel & synthetic biology R&D moves toward demonstration
- Additional pilot and demonstration scale biorefineries for cellulosic ethanol, and hydrocarbon biofuels

**MID TERM MILESTONES**

- Widespread adoption and deployment of new conversion technologies
- EPA’s RFS target of 5.5 billion gallons per year of cellulosic biofuels domestically produced and consumed by 2017
- Cellulosic biofuel production cost competitive with petroleum production
- Pre-commercial demonstration of cellulosic hydrocarbon biofuel production
- Private investment in flux in cellulosic biofuel facilities
- Significant emerging market for valuable bioproducts produced by integrated biorefineries
- Sustainability R&D completed to adequately address concerns

**LONG TERM MILESTONES**

- 36 billion gallons of renewable biofuels to be in use by 2022, including 71 billion gallons of advanced biofuels produced annually from which 16 billion gallons must come from cellulosic sources
- Advanced biofuels demonstrate lifecycle greenhouse gas emissions that are at least 50% lower than baseline lifecycle greenhouse gas emissions, preferably 80% lower than the baseline
- A significant portion of advanced biofuels are readily compatible with existing infrastructure such as refineries and distribution networks and modes of transportation
- Advanced biofuels are produced in a verifiable sustainable manner
- Continued investment and growth in the advanced biofuels sector
- Distribution infrastructure for 36 billion gallons per year of biofuels firmly established

**OUTCOMES BENEFITS TO SCIENCE AND SOCIETY**

- Long-term EISA mandated biofuel use targets achieved
- Biofuels, in combination with other transportation technologies significantly reduce demand for organization of the petroleum exporting countries (OPEC) petroleum
- Domestic biofuel production significantly invigorates U.S. manufacturing and economy
- Overall U.S. transportation CO2 footprint reduced
- Biofuel technologies enable creation of new, robust, biobased industries

* Subject to congressional appropriations
Appendix A.1 Research Tools—Biological Platform

Genomics-based systems biology has provided an array of powerful new tools and techniques for understanding and manipulating biological systems and components, including plants, enzymes, and microbes, at the microscopic and nanoscale levels. These tools will help overcome the challenges of developing microbes and enzymes that are effective in deconstructing lignocellulosic material into intermediate products and synthesizing those products into liquid fuels.

Rapid Genomic Sequencing

- Modern, high-throughput genomic sequencing provides unprecedented capabilities for understanding and modifying organisms (both plants and microbes).
- Many microbes and plants important to developing new feedstocks have been sequenced.
- Genomic sequencing is the foundation of systems biology and the typical first step in attempting to understand and modify organisms.
- High-throughput genomic sequencing technologies are rapidly improving. DOE’s Joint Genome Institute currently sequences more than 15 billion base pairs per month.

Bioprospecting/Metagenomics

- Innumerable microorganisms can degrade lignocellulose. Bioprospecting entails sampling environments that are rich in these microbes—such as tropical rainforests or compost heaps—and then sequencing them en masse (metagenomics), to identify new, more powerful enzymes.

Synthetic Biology

- Federally supported scientists have reengineered microbes to produce long-chain alcohols and hydrocarbon molecules, a first step toward potential large-scale microbial production of gasoline, diesel, and jet fuel.
- Scientists are seeking to reduce the costs of conversion through the reengineering of single microbes or microbial communities to perform the deconstruction and fuel synthesis steps.
Advanced Imaging (Nuclear Magnetic Resonance [NMR], High-Intensity Light Sources)

- Scientists are taking advantage of a host of powerful new imaging technologies that enable the study of the conversion process to the nanoscale level, helping to discover and develop improved enzymes.

High-End Computational Modeling

- Scientists are in the early stages of using advanced computer modeling to understand aspects of the conversion process that are difficult to observe by experiment. This modeling, often used to generate hypotheses later tested in the laboratory, leads to insights regarding biocatalytic mechanisms.

- In addition, there have been important advances on the applied side of the biofuels research effort:

Bioreactor Engineering

- Most bioreactors have been optimized for making pharmaceuticals and other bioproducts from liquid cell cultures. Few have been explicitly engineered to handle high-solids precursors, such as those from lignocellulosic feedstocks, to make fuel. To develop pretreatment and hydrolysis bioreactors that efficiently process biomass in this manner, and to do so at a commercial scale, would mean significantly reducing overall process costs.

Metabolic Engineering

- With the wealth of the genomic information being generated, scientists are modifying existing or designing entirely novel metabolic pathways within microorganisms to optimize the fuel synthesis rate and yield, or to improve tolerance to inhibitor compounds, which in turn will decrease the cost of producing biofuels.

Protein Engineering

- In addition to identifying new enzymes, scientists are using protein engineering and genetics-based technologies that exist today to improve the catalytic rates and the production costs of known hydrolytic enzymes. Capturing these improvements in the near term may mean significant cost-savings for the cellulosic ethanol biorefineries being built today.

Process Interface Engineering

- Conversion processes as part of an integrated biorefinery must take into account the type(s) of feedstock that can be sustainably produced in a given geographic location. With that in mind, modeling and demonstrations are being pursued to tailor and integrate downstream conversion process steps to arrive at the most optimal and cost-effective biorefinery design. One goal of interface engineering is to define the optimal pretreatment parameters for a given feedstock or downstream hydrolysis process. Another goal is to implement cost-effective separative technologies for a given feedstock or a given fuel-producing microbe to best utilize the solubilized sugars and residual biomass/chemicals.
Techno-Economic Analysis

- Engineers are designing and testing techno-economic models by integrating various technology breakthroughs to assess the financial impact these technologies bring to the overall process. These studies are critical to the mitigation of risk in building a commercial-scale biofuels refinery and to the evaluation and identification of process areas that need further research and development.
Appendix A.2 Research Tools—Thermochemical Platform

The fine chemicals and petrochemical fields have spent significant resources and time developing expansive chemistry and chemical engineering toolsets to establish more efficient and selective processes. Techniques for understanding and controlling chemical systems and components from the molecule- through the micro- and macro-length scales are all needed. These tools are being refined and redesigned for the specific application to resolve the challenges of deconstructing the lignocellulosic material into intermediate products and synthesizing those products into liquid fuels.

Computational Modeling

- Scientists are in the early stages of using advanced computer modeling to further understand the chemical and engineering aspects of the conversion process that are often difficult to observe through experimentation. Ideally, chemical and engineering modeling is used to reduce the number of negative outcome experiments by projecting or guiding the next set of experiments to accelerate progress towards the market. Additionally, this modeling can lead to insights regarding the mechanisms of catalysts in order to accelerate the optimization of reactants, enhance process control, and optimize energy usage. Computational modeling will enhance high-throughput experimentation by guiding discovery and in situ or process analytical tools through the initial validation stages and, subsequently, onto a pathway to process optimization.

High-Throughput Experimentation

- Automated and parallel processing systems that rapidly prepare, test, and analyze catalysts will accelerate catalyst design and subsequent optimization on a small scale. The number, and sometimes the quality, of measurable quantities are typically balanced against the number of experiments executed in a parallel. Significant focus is required to ensure that the results used to rank the next generation of catalysts at this scale readily transfer to validation reactions on a larger scale.

- Federally supported researchers and industrial partners have been developing new, high-throughput experimentation technologies and reactor configurations for the accelerated development and study of catalysts.

In situ Tools

- To better understand the dynamics of a catalytically active site, in situ tools are needed to probe biomass-derived streams. In situ tools have been developed to examine primarily gas-solid interfaces, particularly with controlled synthetic reactions streams, with great success. Further development to examine complex gas, liquid, and solid interfaces at demanding temperatures and pressures will facilitate enhanced understanding of catalysts in biomass-derived streams.
Advanced Process Analytical Tools

- In the pharmaceuticals and food industries, significant advances in the development of process analytical tools of complex reactant and product streams utilize multivariate analysis and/or chemometrics in combination with spectroscopic tools. These are beginning to be used to examine the complex matrices of feedstocks and reaction streams derived from biomass. Further advancement in this area is required in order to facilitate tighter closed-loop control and enable greater efficiency and selectivity of desired products.

Process Technology and Optimization

- Few commercial-scale reactors have been explicitly engineered to handle the high-solids, biomass-derived precursors needed to make biofuels. Developing gasification, pyrolysis, and intermediate upgrading and fuel synthesis reactors that efficiently process biomass-derived streams presents many challenges. Optimal usage of resources and minimization of unproductive side streams is critical to developing large-scale competitive processes.

Techno-Economic Analysis

- Engineers are designing and testing techno-economic models by integrating various technology breakthroughs to assess the financial impact these technologies have on the overall process. These studies are critical to the mitigation of risk in building a commercial-scale biofuels refinery and to the evaluation and identification of process areas that need further research and development.