

Process Design and Costing of Bioethanol Technology: A Tool for Determining the Status and Direction of Research and Development

Robert Wooley,* Mark Ruth, David Glassner, and John Sheehan

Biotechnology Center for Fuels and Chemicals, National Renewable Energy Laboratory, Golden, Colorado 80401

Bioethanol is a fuel-grade ethanol made from trees, grasses, and waste materials. It represents a sustainable substitute for gasoline in today's passenger cars. Modeling and design of processes for making bioethanol are critical tools used in the U.S. Department of Energy's bioethanol research and development program. We use such analysis to guide new directions for research and to help us understand the level at which and the time when bioethanol will achieve commercial success. This paper provides an update on our latest estimates for current and projected costs of bioethanol. These estimates are the result of very sophisticated modeling and costing efforts undertaken in the program over the past few years. Bioethanol could cost anywhere from \$1.16 to \$1.44 per gallon, depending on the technology and the availability of low cost feedstocks for conversion to ethanol. While this cost range opens the door to fuel blending opportunities, in which ethanol can be used, for example, to improve the octane rating of gasoline, it is not currently competitive with gasoline as a bulk fuel. Research strategies and goals described in this paper have been translated into cost savings for ethanol. Our analysis of these goals shows that the cost of ethanol could drop by 40 cents per gallon over the next ten years by taking advantage of exciting new tools in biotechnology that will improve yield and performance in the conversion process.

Introduction

The U.S. Department of Energy's Biofuels Program. For roughly 20 years, the U.S. Department of Energy (DOE) has funded research on the development of renewable, domestically produced fuels for transportation. The program is driven by a number of important national issues: national security, economic competitiveness in the global market, rural economic development, climate change, air pollution, and others. For a more detailed discussion of these issues, see the related article in this journal issue by Sheehan and Himmel (1).

The Office of Fuels Development at DOE is responsible for managing the Biofuels Program, which specifically targets transportation fuels made from biomass. The Biofuels Program has two major components: a feedstock development program led by Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee, and a conversion technology development program led by the National Renewable Energy Laboratory (NREL) in Golden, Colorado.

Over the years, the program has worked on a varied portfolio of fuel products. Today, the Biofuels Program focuses the bulk of its resources on the development of fuel grade bioethanol made from the cellulose and hemicellulose components of trees, grasses, and many waste materials. The abundance of these biopolymers in nature makes them important resources for the production of bioethanol.

One simple, but difficult, hurdle faces bioethanol as a commercially viable fuel substitute-cost. When DOE first began its research on bioethanol, it set its goals for cost

competitiveness on the basis of skyrocketing projections for future petroleum prices. Dire projections for oil prices and availability, in the context of the harrowing experience of long lines at gas stations and fears of OPEC-driven supply shortages, seemed reasonable in the late 1970s (2). Today, we are faced with a very different reality: cheap oil. Petroleum prices are now at historically low levels, and DOE projects only slight increases over the next 20 years (3, 4).

Why We Conduct Rigorous Process Design Studies. The moving target for making cost competitive bioethanol has forced the Biofuels Program to constantly rethink its approach and to push the potential for technology improvements to its limit. With this increasing demand for cost competitiveness comes a demand for greater reliability and credibility in predicting the cost of bioethanol production. In today's fuel market, every penny in cost savings makes a difference. Thus, today more than ever, sound process design, modeling, and cost analysis are essential to the success of our research.

Our process design studies serve three purposes. The first one we have already alluded to. For a given feedstock cost, we need to be able to predict the absolute cost of bioethanol. We use this information to judge the potential for market penetration of bioethanol. The second purpose of such studies is to understand the economic impacts of proposed research strategies and consequently to guide process development. By translating research goals into process performance parameters that can be reflected in our process models, we can predict the impacts of these goals on the bottom line—the cost savings per gallon of bioethanol produced. Finally, we use current and projected technology costs as inputs to policy discussions.

* Corresponding Author.

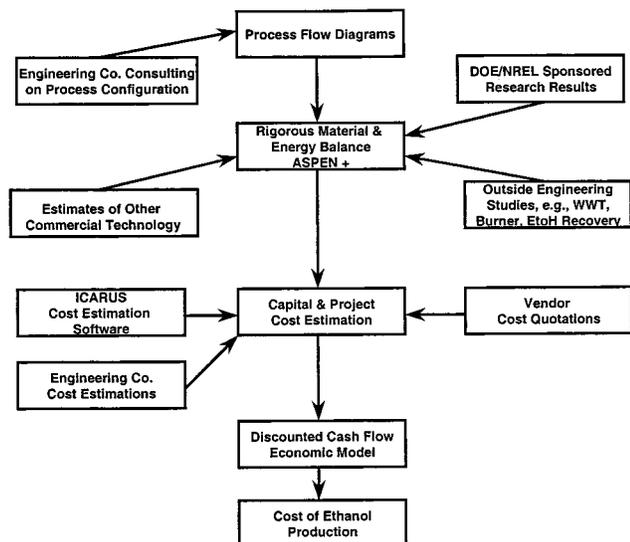


Figure 1. The biofuels program's approach to process design and costing using ASPEN PLUS.

Thus, process design and economics are an integral part of the planning process.

Methods

How We Conduct Process Design Studies. We have a long history of using process design to set direction for our research (5–8). Over the years, we have developed cost estimates using a variety of in-house modeling tools and spreadsheets. We have also relied on engineering firms to develop cost estimates. Unfortunately, these various studies were often hard to relate to each other, differing as they did in assumptions and approaches and the degree of explicit documentation. As a result, while these studies often answered specific questions posed at various times, they did not necessarily serve as consistent navigational tools for the program.

In the past two years, NREL has worked hard to upgrade its process analysis capability and to develop an approach to process design that ensures greater consistency and rigor. This approach is outlined schematically in Figure 1. The cornerstone of this effort is the use of Aspentech's ASPEN PLUS process simulator (9) to model bioethanol process technology. This process simulator is widely accepted and used in the chemical and petroleum industries. It offers a capability for carrying out thermodynamically rigorous material and energy balances for complex processes. The process model described in this paper consists of 144 unit operations, 668 streams (462 material and 206 heat or work), 57 components, and 70 control blocks. The model uses built in physical property data as well as property data developed at NREL (10). Thus, it addresses the need for both rigor and credibility in our analysis.

We recognize that there are tradeoffs between complexity and rigor and accessibility in the development of our process models. We have chosen a commercial simulation package to model the complete biomass to ethanol process because it builds much of the technical sophistication into the basic architecture of the software, avoiding the need to build this sophistication from scratch. While a complex process can certainly be modeled using a spreadsheet, a spreadsheet of this magnitude would require the developer and all users to be far too involved with the finest details to ensure that it was used correctly. So rather than spend considerable effort mak-

ing a complex spreadsheet comprehensible, we chose to use the ASPEN PLUS simulator, which already includes all of the management and convergence of hundreds of streams and blocks and frees up our engineers to concentrate on the process data and configuration. This approach greatly speeds our model development and simplifies our ability to transfer the model to others, but this does require that other users also have a license to ASPEN PLUS.

The ASPEN PLUS process simulator also serves as a central repository for all inputs to the process, whether they come from outside engineering firms used to provide design data on specific aspects of the process or they come from research results generated by the Biofuels Program. Thus, any changes to process flow diagrams or process design assumptions are made in one model. This eliminates inconsistencies in approach.

We utilize outside engineering expertise to further improve the integrity of our modeling. The results presented in this paper reflect a detailed review of the process model by Delta-T Corporation, an engineering firm with extensive experience in the design and construction of ethanol facilities. They provided invaluable input on current practices in the industry for many aspects of the process. Merrick Engineering provided similar input on the design of the wastewater treatment section (11). A comprehensive description of the process model and input from Delta-T Corporation is available elsewhere (12).

Process flow diagrams and ASPEN-generated material and energy balances are used to generate detailed equipment designs. Purchased and installed costs for equipment are obtained from vendor quotes, wherever necessary, particularly for highly specialized units. We obtained cost data on standard pieces of equipment (such as pumps and heat exchangers) from the ICARUS cost estimation software (13) and from cost databases maintained by Delta-T Corporation. As with ASPEN PLUS, ICARUS is commonly used by engineering and construction firms in the chemical industry, and it lends credibility to our cost estimates. All of the detailed cost data and assumptions are published in a report (12) that is available on our laboratory's website (http://www.ott.doe.gov/biofuels/process_engineering.html).

Overall Basis for the Process Design Study. Four overarching assumptions provide a fundamental framework for our process design:

- The choice of process technology and configuration
- The choice of feedstock
- The size of the proposed plant
- Dedicated ethanol/electricity production versus the biorefinery concept

We describe the basis for each of these assumptions in the following sections.

The Choice of Process Technology and Configuration. There are several processes possible for converting biomass to ethanol. For the purposes of this paper, we limit ourselves to processes that involve four basic steps:

- Conversion of carbohydrate biopolymers to sugar
- Fermentation of sugars to ethanol
- Ethanol recovery
- Residue utilization

There are a number of technology platforms available today that perform these steps by different means. The distinguishing feature among these platforms is the approach used to accomplish the first step, converting carbohydrate biopolymers to sugar. The Biofuels Program has established partnerships with entrepreneurs actively

engaged in exploiting some of these technologies in niche applications. Their efforts will lead to the establishment of "pioneer plants" that will demonstrate the commercial viability of producing ethanol from cellulose and/or hemicellulose. These companies are using processes that are based on concentrated acid hydrolysis (14) and two-stage dilute acid processes (15, 16) to produce fermentable sugars from biomass.

We have, since the late 1980s, focused on the development of a new generation of genetically engineered cellulase enzyme systems. This work initially involved the isolation of genes expressing enzyme components from different microbes for the purpose of producing artificial enzyme consortia that exhibit better synergism than natural enzyme systems (17). More recently we have turned our attention to protein engineering of the individual enzyme components (18). These enzymes can be used to release sugars from cellulose, in lieu of more established inorganic acid catalysts. By virtue of its "less trodden" nature and the potential for improvements offered by the explosion in innovations occurring in the field of biotechnology, enzyme technology, in our view, offers the greatest opportunity for future cost reduction (19). While it is our goal to model all of the technology platforms supported by the program, analysis to date shows that the enzymatic conversion technology has the lowest potential cost and it is our first priority for process design.

The process design presented here reflects the best available estimates for performance of an enzyme-based process, as it would look if it were to be designed and built soon. This design case reflects the current status of our research efforts. It is a benchmark for evaluating research progress. Performance parameters used in the design reflect current laboratory and pilot plant results and sometimes expected laboratory results over the course of the next year or two.

The Choice of Feedstock. A variety of feedstocks can be used to produce bioethanol. Our industrial partners are looking to waste materials that offer low-cost, niche opportunities. These include softwoods collected as part of forest health management activities, municipal solid waste, and agricultural residues (such as bagasse, rice straw, and corn stover). In the long run, we envision the use of energy crops such as hybrid poplar and switchgrass.

For purposes of convenience and continuity, we have selected yellow poplar sawdust as a "model" feedstock for use in our ongoing integrated process development work. A typical composition for yellow poplar used for this process analysis is typical yellow poplar (20). The composition is translated into components that are tracked in the ASPEN PLUS model. The values for each component are normalized to 100% as shown in Table 1. Even before the economics of the enzyme process have met the threshold of cost competitiveness, we expect to be working with industrial partners who are focused on specific feedstocks. Corn stover is one of the largest sources of available biomass for ethanol production and is a feedstock that we believe will be of commercial interest to future partners. Thus, we include data on its composition in Table 1, as well (21). Corn stover is very similar in composition to our model feedstock. It is worth noting, however, that lignin and acetate levels in stover are significantly lower. This may mean that pretreatment of stover could be easier and could result in a more readily digested feedstock for enzymes. The downside to this lower lignin content is that less fuel is available for steam and electricity production in the plant. The process (and

Table 1. Feedstock Composition (Hardwood Yellow Poplar)

component	hardwood yellow poplar	corn stover
cellulose	42.4	40.9
xylan	18.1	21.5
arabinan	0.5	0.2
mannan	2.9	0.0
galactan	0.0	1.0
acetate ^a	4.6	1.9
lignin	26.6	16.7
ash	1.0	6.8
other ^b	3.9	11.0

^a Acetate is the acetate groups present in the hemicellulose polymer. They are generally converted to acetic acid in the prehydrolysis reactor. ^b No quantification of the remaining unknown components is available.

our analysis of it) will have to be adapted to specific feedstocks to accommodate differences in composition.

Composition is not the only factor that will affect our process design. Differences in feedstocks will, for example, affect the nature of the feedstock handling systems. The biggest impact, however, is in feedstock cost. Oak Ridge National Laboratory has developed feedstock supply cost curves for a number of feedstocks (22). These costs can range from \$15 to \$40 per U.S. ton (dry) (from \$17.50 to \$44 per MT), depending on the level of demand and type of material. The ethanol cost results presented here use a fixed feedstock cost of \$25 per U.S. ton (dry) (\$27.50 per MT). We can (and have) disaggregated feedstock and conversion costs to allow more sophisticated analysis of market penetration for bioethanol based on biomass supply cost curves, fuel market demand data, and conversion costs.

The Size of the Plant. Plant size is important in the overall cost of production. We use the following scaling equation to adjust equipment costs for different sizes:

$$\text{New Cost} = \text{Original Cost} \left(\frac{\text{New Size}^*}{\text{Original Size}^*} \right)^{\text{exp}}$$

* size could be a characteristic linearly related to the size.

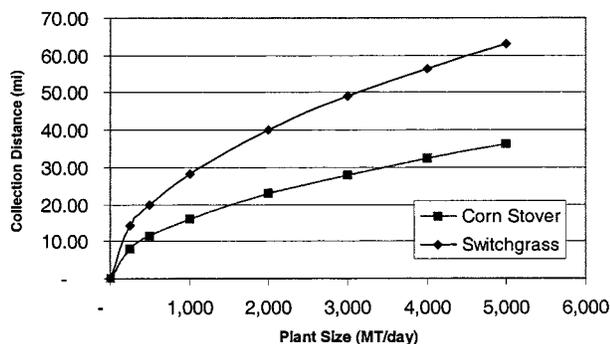
The size factor is adjusted using an exponential term, which allows for economies-of-scale when the exponent is less than 1. Generally, equipment costs scale with an exponent of about 0.7. An exponent of 1 would translate to linear scaling. The point at which this diminishes is when the equipment is as large as it can be built and multiple pieces of equipment are necessary. For a plant capacity of 2000 tons per day of dry feedstock, we find that, while some equipment (like the production fermentors and the pretreatment equipment) has reached their maximum size, there are still economies-of-scale available in many parts of the process.

Savings due to economies-of-scale are offset by increased costs for feedstock collection. Put quite simply, the more feedstock a plant demands, the farther out it must go to get it. Furthermore, increased collection activity could lead to higher prices for the feedstock. Collection distance for a plant is highly site specific. Still, we have done preliminary analyses to get a better understanding of this tradeoff between plant size and feedstock collection costs. The important assumptions for this analysis are shown in Figure 2 shows the effect of plant size on collection distance for two feedstocks: corn stover (the residue left in the field after harvest) and switchgrass. The results of the analysis suggest that a 2000 ton per day plant is reasonable for both corn stover (which has a collection radius of 23 miles) and switchgrass (which has a collection radius of 40 miles).

Table 2. Major Assumptions for Feedstock Collection Analysis

assumption	corn stover	switchgrass
yield (MT biomass per acre)	1.67 ^a	6.15 ^b
percent of surrounding acres participating in collection	50%	10%
percent of surrounding acreage available for crop production	75%	75%

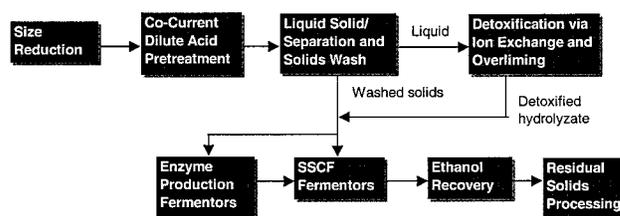
^a Corn stover yield based on reported yields from an ongoing corn stover collection demonstration project. This yield allows for quantities left behind to control soil erosion (23). ^b Switchgrass yield based on an analysis of the ORNL ORECL county level database for energy crops (24).

**Figure 2.** The effect of plant size on feedstock collection distance.

Estimates of the incremental transportation cost (not presented in detail here) of going from 1000 to 2000 MT per day are less than \$2 per MT of biomass (12, 23). Even the 4000 MT per day plant size may be workable, as long as economies-of-scale still apply. Thus, for the purposes of this study, we chose to stay with the 2000 MT per day capacity used in many of our previous studies.

Dedicated Ethanol/Electricity Production Versus the Biorefinery Concept. An implicit assumption we make in our design studies is that we limit the range of products made at the facility to ethanol and electricity. This assumption is not only unrealistic but also seriously limiting in the picture it paints for economic viability of bioethanol technology. The lessons of today's petroleum refineries and today's wet mill corn ethanol plants are clear. Coproducts are critical to carrying the bottom line for these facilities. Petroleum refiners, for example, may support the bulk of a large-scale plant's output by making fuels, but it enhances its profitability through the production and sale of higher-value petrochemical intermediates. Similarly, wet mill corn ethanol plants typically view ethanol as among the lowest-value products leaving the plant gate. However, introducing coproducts into our design opens up a myriad of possible products and process scenarios. Rather than tying our analysis to specific coproducts, we prefer to leave these choices up to the future entrepreneurs who will make this technology a commercial reality. In that way, we can use our analysis to identify key technical issues for the core technology components.

Details of the Design Basis for a Near-Term Bioethanol Plant Design. An early proposed process for using enzymes in the production of bioethanol assumed that the enzymatic hydrolysis of cellulose and the fermentation of glucose would be carried out in two sequential steps (25). Later, Gulf Oil Company and the University of Arkansas introduced the important concept of simultaneous saccharification and fermentation (SSF) (26, 27). In the SSF process scheme, cellulase enzyme and fermenting microbes are combined. Monomeric sug-

**Figure 3.** Process flow diagram for the enzymatic process evaluated in this study.

ars are continuously produced by the enzymes and converted by fermentative organisms to ethanol avoiding product inhibition of the enzymes. The SSF process has, more recently, been improved through the use of organisms capable of fermenting the glucose from cellulose and the hemicellulosic sugars together. This new variant of SSF, known as SSCF for Simultaneous Saccharification and CoFermentation, is shown schematically in Figure 3. It is the basis for our process design.

Overview of the SSCF Process. After size reduction, the biomass is pretreated using dilute acid at high temperature. This accomplishes two things: the hydrolysis of most of the hemicellulose to its constituent sugars and a loosening of the lignin-hemicellulose-cellulose complex. The latter renders the remaining cellulose more amenable to enzymatic attack. The heart of the pretreatment step is a reactor similar to pulp digesters that permits co-current contacting of biomass and acid at elevated temperatures. The unreacted solid phase is separated from the liquid hydrolysate, which contains acetic acid and other inhibitors in addition to the hemicellulose sugars. The acid and inhibitors are removed using "overliming" and ion exchange before the liquid and solid biomass can be recombined and sent to subsequent biological processing steps. Some combinations of feedstock and microorganisms allow elimination of these "conditioning" steps.

A small portion of the biomass slurry is diverted to the cellulase production fermentors, while the bulk of the material is sent on to the SSCF vessels. The product stream from the SSCF reactors contains a relatively low concentration of ethanol as well as unreacted lignin residue. A traditional two-column distillation brings the ethanol concentration up to the azeotrope level. A vapor phase molecular sieve system is used to remove the remaining water. Solids from the bottoms of the first distillation column are dewatered and sent on to residue processing. In this case, the lignin is combusted to produce steam for use in the plant.

We assume an on-line time of 96%, which allows a little over two weeks per year for downtime, based on input from Delta-T Corporation. The design also reflects costs and performance associated with an "nth" plant. In other words, we do not account for cost of engineering guarantees and other costs related to reducing the risk of introducing new technology.

The plant design is broken down into nine process areas. Highlights of the design issues in each area are discussed briefly in the following sections. Readers interested in a more detailed discussion of the design can request copies of our published report (12).

Area 100: Feed Handling and Storage. The plant is designed to accommodate 136 trucks per day, each carrying around 47 MT of wet material. The handling area includes weigh stations, solids conveyor systems, and washers designed to handle an average of 176 MT

Table 3. Key Design Inputs for Pretreatment Reactor

acid concentration	0.5%
residence time	10 min
temperature	190 °C
solids in reactor	22%
hemicellulose sugar yields	75%
furfural yield from xylan and arabinan	10%
HMF yield from mannan and galactan	15%

per hour (wet basis). Bulldozers maintain 40-foot piles in an area designed to hold 7 days of material.

Area 200: Pretreatment and Hydrolyzate Conditioning. The pretreatment reactor is one of the most unique pieces of equipment in this plant. Its design was done with input from a manufacturer of digester equipment for the pulp and paper industry. Conditions and yields for the pretreatment reactor are shown in Table 3. These design inputs are based on experiments conducted on yellow poplar hardwood in NREL's pilot scale Sunds reactor with adjustments made for expected near-term improvements (20). Other conditions or equipment may yield similar or superior results. We assume that the results of the Sunds pilot unit will scale directly to the production-scale reactor. The cost of the reactor turns out to be one of the biggest uncertainties in the process. Our design assumes that the reactor is built from Hastelloy C, based on corrosion experiments conducted by the Tennessee Valley Authority (28). Reliable vendor quotes for this unit are not available, due to the lack of experience in fabricating these units for our operating conditions. A preliminary quote, for example, showed a factor of 3 or more difference in cost between stainless steel and Hastelloy C construction. This cost differential most likely reflects a high degree of risk that would not exist for an "nth" plant (29). On the basis of input from Delta-T Corporation, we settled on a cost for the Hastelloy C reactor that is 50% higher than the cost for the 304 stainless reactor.

Material exiting the pretreatment reactor is flash-cooled from 12.2 to 1 atm in a vessel made of Carpenter 20. This flash step removes much of the furfural and hydroxymethyl furfural (HMF) and a portion of the acetic acid. Removal of these heterocyclic aldehydes is beneficial since these compounds can be detrimental in the fermentation step. Modeling of this flash vaporization in ASPEN PLUS using an equation of state specific for acetic acid allowed us to more accurately account for acetic acid losses in the vapor phase due to dimerization. A continuous belt filter is used to separate the liquid hydrolyzate prior to removal of acetic acid, a known inhibitor in the fermentation (30). The continuous ion exchange system removes 88% of the acetic acid and 100% of the sulfuric acid in the hydrolyzate and minimizes dilution with no loss of sugars. Overliming requires reducing the pH of the ion exchanged material to pH 2 with sulfuric acid, followed by addition of lime to a pH of 10. The hydrolyzate is then adjusted to pH 4.5 for the fermentation step and filtered to remove gypsum. No accounting for reactions that may occur in the overliming step is done in the process model. We are still studying this step to better understand what is happening (31). A better understanding may allow us to identify more efficient alternatives.

Area 300: Simultaneous Saccharification and CoFermentation. The fermentation step includes two seed trains with five stages for building up the inoculum to the production fermentors. A 10% volume of inoculum is added to subsequent fermentors in each stage until

Table 4. Key Design Inputs for SSCF Production Fermentors (32)

temperature	30 °C
initial solids level (soluble and insoluble)	20%
residence time	7 days
cellulase level	15 FPU/g of cellulose
corn steep liquor	0.25%
theoretical yield of ethanol from glucose	92%
theoretical yield of ethanol from xylose	85%

Table 5: Key Design Inputs for Cellulase Production

cellulase requirement for SSCF	15 FPU/g of cellulose
yield of enzyme	200 FPU/(g of cellulose + xylose)
productivity	75 FPU/liter·h
initial cellulose concentration	4%

an adequate volume is built up to feed the three continuous trains of 3600000-L (950000-gal) production vessels. There are six vessels in each train, for a total of 18 production vessels. The vessels are costed as stirred 304 stainless steel reactors. They are not pressure-rated for steam sterilization. This design is consistent with current practice in the corn ethanol industry. Specifications for the production fermentors are shown in Table 4. The design is based on bench scale performance data (32) for NREL's genetically engineered *Zymomonas mobilis* (33), which is capable of fermenting glucose and xylose only.

Area 400: Cellulase Production. This area includes eleven 1000000-L (264000-gal) aerated fermentors operated in batch mode (eight are operating at all times). Three trains of three seed fermentors each are used to provide inoculum to the production vessels. They are sized to provide 5% inoculum to each subsequent fermentor in the train. The large vessels are costed as stirred 304 stainless steel reactors. They are not pressure-rated for steam sterilization. A requirement for steam sterilization would significantly increase the capital cost of this area.

Design inputs for this part of the process are summarized in Table 5. The design is based on bench scale data for the production of enzyme (34) by one of the most commonly used types of industrial fungus for cellulase manufacture, *Trichoderma reesei*. The model assumes that 47% of the soluble sugars go to cell mass production and 53% go to enzyme production. An iterative cost optimization was done to determine the minimum cost when vessel aspect ratio and air flow rate were allowed to vary. This optimization included mass-transfer calculations constrained to provide a minimum oxygen-transfer rate in the vessels of 80 mmol/L·h.

Area 500: Product Recovery and Water Recycle. Distillation and molecular sieve column designs in this study represent a significant improvement over previous design studies, particularly given the ability to use ASPEN PLUS for the rigorous design of the distillation columns. In addition, many practical tips from Delta-T Corporation contributed to making the design of this whole area more practical and representative of best industry practices. For example, Delta-T recommended the use of a water scrubber to recover ethanol from all vents. Merrick Engineering's recommendations for waste treatment led to the addition of a multiple effect evaporator to treat stillage water. The evaporator produces a syrup that is burned, in lieu of sending this water to the waste treatment system. Though this addition to the process design was not an obvious way to reduce cost, Merrick's analysis demonstrated that the savings in wastewater treatment system costs outweighed the added cost of the evaporator (11).

Table 6. Total Project Investment (\$1997)

total equipment costs	\$135,000,000
warehouse	\$2,000,000
site development	\$6,600,000
total installed cost	\$143,600,000
indirect costs	
field expenses	\$28,700,000
home office & construction fee	\$35,900,000
project contingency	\$4,300,000
total capital investment	\$212,500,000
other costs	\$21,300,000
total project investment	\$233,800,000

Area 600: Wastewater Treatment. Waste treatment includes an equalization basin that feeds into an anaerobic digestion system, which produces 4.2 million Btus of a medium-Btu methane/CO₂ fuel that is burned for process energy. Ninety percent of the organic loading in the wastewater is removed in the anaerobic digester. An aerobic digester is used to remove most of the remaining 10%. Sludge produced in this last step is burned.

Area 700: Product and Chemical Storage. Requirements for this part of the plant were based on recommendations from Delta-T Corporation. This area includes storage capacity for 7 days of denatured ethanol product. Chemical storage ranges from four to 7 days.

Area 800: Burner, Boiler, and Turbogenerator. A fluidized bed combustor burns three available waste fuels streams: residual lignin solids, medium-Btu methane gas from the anaerobic digesters, and a concentrated syrup from the multiple-effect evaporator. The boiler produces 103.1 atm (510 °C) steam that is fed to a cogenerating turbine. Steam is pulled off the turbine at 12.3 and 4.4 atm for use in the process. The turbine generates 38 MW of electricity, of which 32 MW is used in the process and 6 MW is sold to the grid.

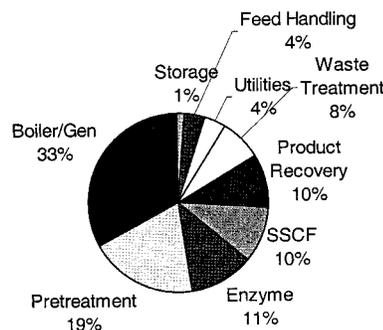
Area 900: Utilities. This area includes chilled water, cooling water, plant and instrument air, process water, and clean-in-place solution.

Results

The Cost of Ethanol for the Near-Term Enzyme-Based Plant Design. All of the costs reported here are indexed to 1997 dollars. Capital investment estimates are accurate to around $\pm 25\%$. For this level of accuracy, we felt it was reasonable to use a factored analysis for determining the installed cost of equipment. We used installation factors from Walas (35). Delta-T Corporation reviewed these factors for consistency with their experience in constructing ethanol facilities. Other factors were applied for warehouse, site preparation, and other project-related costs.

Capital Cost. Table 6 summarizes the capital requirements for a 2000 MT per day facility. Total project investment for the near-term enzyme-based plant design is \$234 million. The overall yield of ethanol from biomass is 68 gallons per dry U.S. ton. For the 2000 MT per day capacity, this amounts to an annual production capacity of 198 million liters (52.2 million gallons) of ethanol. At \$4.48 per gallon of capacity, this design is more capital-intensive than today's corn ethanol facilities, which have capital costs of around \$2 per gallon of annual ethanol capacity (36). This is not surprising, considering the cogeneration and enzyme production capability built into our design.

Figure 4 shows the percentage breakdown of installed equipment costs. The power plant and pretreatment sections are the two largest ticket items and together represent 52% of the capital investment for equipment. Biological processing (enzyme production and SSCF) is

**Figure 4.** Breakdown of installed equipment cost for near-term enzyme-based process.**Table 7. Operating Costs for a Near-Term Enzyme-Based Process (\$1997)**

item	MM \$/yr	cents/gal ethanol
biomass feedstock	19.31	37.0
chemicals	4.0	8.0
nutrients	3.22	6.2
diesel	0.48	0.9
makeup water	0.45	0.9
utility chemicals	0.59	1.2
solid waste disposal	0.61	1.2
electricity credit	-3.68	-7.2
fixed costs	7.50	13.3
total	32.48	61.5

^a \$25 per MT. ^b Megawatts (10.942) of excess electricity sold to grid at 4 cents per KWh.

the next largest contributor to capital cost, representing 22% of the total installed equipment cost.

Operating Costs. Fixed and variable costs are summarized in Table 7. Fixed costs include labor, overhead, maintenance, insurance, and taxes. They are based on estimates provided by Delta-T Corporation and from standard rules of thumb. The table presents total annual cost and costs per gallon of ethanol. Variable costs include feedstock and other raw materials, as well as solid waste disposal costs and a credit for excess electricity sold to the grid.

The Bottom Line. Once the capital and operating costs have been established, a discounted cash flow analysis can be used to determine the minimum selling price per gallon of ethanol produced. The discounted cash flow analysis iterates on the selling cost of ethanol until the net present value of the project is zero. We assume a discount rate of 10%, on the basis of arguments presented by Short in his description of how to perform economic evaluations of renewable energy technologies for the U.S. Department of Energy (37). His view is that "In the absence of statistical data on discount rates used by industrial, transportation and commercial investors for investments with risks similar to those of conservation and renewable energy investments, it is recommended that an after tax discount rate of 10%..." be used. We assume a 20-year plant life and 100% equity financing.

Table 8 summarizes the economics of a near-term enzyme-based process for bioethanol. At a feedstock cost of \$25 per ton, ethanol has a minimum selling price of \$1.44 per gallon, making it a higher-cost alternative to corn-derived ethanol, which typically sells for around \$1.20 in today's fuel market.

"Best of Industry" Near-Term Case. The price of \$1.44 per gallon for bioethanol is, as we have discussed, based on the current status of research that is complete or nearly so. Thus, a grassroots facility based on the enzyme process *as tested in our lab* is approaching (but

Table 8. Summary of Economics for Near-Term Enzyme-Based Bioethanol Process (\$1997)

production cost of ethanol	\$1.44/gal
ethanol yield	68 gal/ton
ethanol production	52.2 MM gal/yr
total project investment (capital)	\$234 MM

Table 9. Summary of Economics for a Near-Term "Best of Industry" Enzyme-Based Bioethanol Process (\$1997)

production cost of ethanol reduced	from \$1.44/gal to \$1.16/gal
yield increased	12% to 76 gal/ton
production increased	12% to 58.7 MM gal/yr
capital reduced	12% to \$205 MM

is not quite ready for) commercialization, at least for the assumptions about feedstock costs. There are other technologies available to the project developer. Specifically, it is been suggested that pretreatment can produce higher conversions of hemicellulosic sugars (38) and that the current cellulase industry could provide a microorganism to produce the enzyme more efficiently. Also, there are other ethanologens (39, 40) that will ferment the other hemicellulose sugars (arabinose, galactose and mannose) to ethanol.

Table 9 summarizes these "best of industry" improvements over the near-term case we have already described. Taking advantage of the best technology reported to be available today brings the cost of bioethanol down to \$1.16 per gallon. This suggests that an enzyme-based facility could be built in the near term that competes successfully in today's fuel ethanol market. However, the technology is commercially "unproven". Our process model assumes an "nth" plant that does not carry with it any allowance for the added risk of a "first-of-its-kind" facility. The question of risk is further exacerbated by the high capital investment required.

The Impact of Proposed Research Activities.

Facilities that are being engineered today all have some niche that allows them a special advantage in the short term for a small market segment. This could be feedstock costs (very low or negative for environmental wastes), used equipment (utilization of related equipment that has been shutdown), colocation with existing facilities (biomass burners and waste treatment facilities) or a combination of all of these. Certainly, the development of higher value products from sugars would contribute to plant profitability. Research and development is needed to lower the cost of producing sugars. In this section, we describe briefly our strategies for improving the economics of bioethanol production over the next 10–15 years. We also show what kinds of cost reductions can be expected from the successful completion of these strategies.

Research Strategies and Targets for Cellulase Enzymes. Because of the importance of cellulase enzymes in the process, DOE and NREL sponsored a series of colloquies with experts and stakeholders in industry and academia to determine what types of improvements in enzyme production and performance offer the greatest potential for success in the short term (41). There was a clear consensus in these discussions that the prospects for enzyme improvement through protein engineering are very good. We identified the following targets for protein engineering:

- **Increased Thermal Stability.** Simply by increasing the temperature at which these enzymes can operate, we can dramatically improve the rate of cellulose hydrolysis. The genetic pool available in our labs and in others around the world includes thermo-tolerant, cellulase-producing

organisms that represent a good starting point for engineering new enzymes.

- **Improved Cellulose-Binding Domain.** Cellulase enzymes contain a catalytic domain and a binding domain. Improvements in the latter will lead to more efficient interaction between the soluble cellulase enzymes and the insoluble surface of the biomass.

- **Improved Active Site.** In addition to modifying the binding domain, we plan to modify amino acid sequences at the active site. Even minor modifications of the enzyme can lead to dramatic improvements in catalytic activity of the enzyme.

- **Reduced Nonspecific Binding.** Enzyme that adsorbs on lignin is no longer available for hydrolysis. Genetic modifications of the enzyme will be geared toward adjusting its surface charge to minimize such unwanted binding.

We have identified two approaches for achieving these goals, both representing the state-of-the-art in biotechnology research. The first is a rational design approach known as site-directed mutagenesis. It uses sophisticated 3-D modeling tools to identify specific amino acids in the protein sequence that can affect the enzyme properties listed above (42–44). The second is a more recent strategy known among biotechnologists as "directed-evolution" (45). It combines advanced genetic engineering techniques with highly automated laboratory robotics to randomly evolve new enzymes with the features required. The enzyme performance goals that are indicated in the future cases are based on the projected progress for these research strategies. By 2005, improvements in thermostability of the enzymes should yield a 3-fold improvement in specific activity. By 2010, enhancements in the cellulose binding domain, the active site, and protein surface charge will lead to an increase in enzyme performance of 10 fold or more.

In parallel with the protein engineering work, our program plan calls for research aimed at improving the productivity of the enzyme expression systems. Two targets for research are being pursued:

- Improved microbial organisms genetically engineered for high productivity of enzymes

- Genetically engineered crops harvested as feedstock, which contain high levels of cellulase enzymes

Higher efficiency microorganisms for use in submerged culture fermentors should be available by 2005.

Research Strategies and Goals for Improved Ethanologens. Research over the past 10 years on ethanol-producing microorganisms has yielded microorganisms capable of converting hexose and pentose sugars to ethanol (33, 39, 40). These ethanol-producing microorganisms ferment xylose and glucose mixtures to ethanol with high efficiency. This represents a major advance in technology, as previous conversion of pentose sugars by natural yeasts was not industrially attractive. Furthermore, these new ethanologens have eliminated the need for separate pentose and hexose fermentation trains.

Substantial improvement in biomass conversion can be achieved by making the following additional improvements in ethanol-producing microorganisms:

- Ethanol-producing microorganisms capable of producing 5% ethanol at temperatures greater than or equal to 50 °C and

- Ethanol-producing microorganisms capable of converting cellulose to ethanol.

We have recently shown that a doubling of the rate of biomass hydrolysis for every 20 °C increase in temperature of saccharification can be expected if *T. reesei*-like cellulases are used. The development of ethanologens

capable of fermentation at temperatures greater than 50 °C can potentially reduce the cost of cellulase enzyme by one-half. This is because the current industrial ethanologens can only meet desired performance at temperatures of 30–33 °C.

The most advanced processing option is one in which all biologically mediated steps (e.g., enzyme production, enzymatic cellulose hydrolysis, and biomass sugar fermentation) occur in a single microorganism (46). This process, also known as direct microbial conversion (DMC) or Consolidated Bioprocessing (CBP), can be carried out to various extents by a number of microorganisms, including fungi, such as *Fusarium oxysporum* and bacteria, such as *Clostridia* sp. However, known DMC strains often exhibit relatively low ethanol yields and have not yet been shown to be effective in handling high concentrations of biomass.

Our program plan calls for introducing a high-temperature ethanologen by 2005. This new organism should be able to operate at 50 °C, while maintaining the best characteristics of the current ethanologens. One company has already disclosed early development work on a thermotolerant ethanologen capable of operating at temperatures as high as 70 °C (47), which suggests that our goal is readily attainable.

Strategies for Process Development and Integration. The cellulase enzymes and the fermenting organisms are the major thrusts of our applied research efforts. Integrating these into a complete process is critical to commercial success. Pilot and bench scale optimization of an integrated process is expected to lead to the following kinds of improvements:

- Optimal yields and operating conditions for the concurrent pretreatment step
- Optimal yields and operating conditions for the simultaneous saccharification and co-fermentation step
- Testing of improved organisms and enzymes as they become available

An optimized and integrated process using cellulase enzymes and concurrent pretreatment technology should be available by 2005.

Strategies and Goals for Feedstock Improvements. Although still in its early stages, research on genetic engineering of agricultural crops holds great promise. We see tremendous opportunities to integrate biomass characteristic enhancement with the conversion process to lower the cost of ethanol production. Plant characteristics that could lower ethanol cost include (1) carbohydrate composition increase, (2) plant structure modification to facilitate pretreatment in milder conditions or with hemicellulases, (3) enzyme expression in the biomass, and (4) combinations of these suggestions or other ideas. We have analyzed the impact of one change, carbohydrate composition increase, which provides a direct improvement in the yield of ethanol. Because the feasibility and details of a research program targeted at higher carbohydrate content have not been worked out, we look at this as a long-term improvement. In our analysis, the fruits of such a research program are reflected in our year 2015 case study.

Price Trajectories for Bioethanol Based on Research Targets. The improvements in enzyme and ethanologen performance will impact the process in 2005 and 2010. Genetically engineered feedstocks with higher carbohydrate content might happen in 2015, though the timing for this last item needs to be determined more precisely. Figure 5 shows the decline in bioethanol pricing based on these research targets. The upper and lower

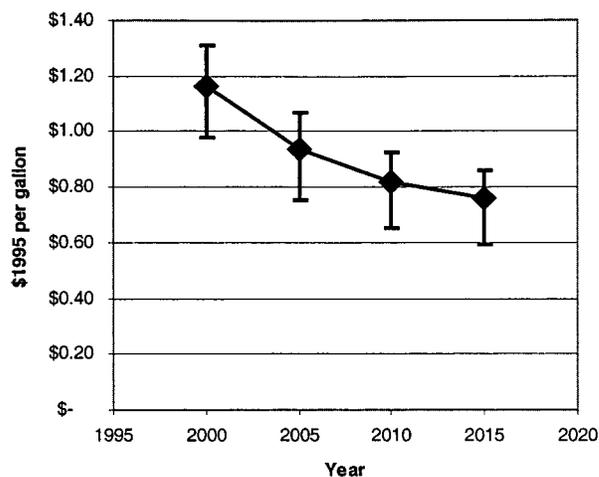


Figure 5. Price trajectory for enzyme-based process technology.

bounds on the error bars reflect the results of sensitivity studies to assess the effect of feedstock price. The lower bound is a price projection for \$15 per U.S. ton (dry) (\$17.50 per MT) feedstock, and the upper bound is a price projection for \$40 per U.S. ton (dry) (\$44 per MT) feedstock. The year 2000 price shown is for the “best of industry” scenario.

Conversion technology improvements could provide a 34 cents per gallon cost reduction over the next 10 years. Feedstock costs represent the largest contributor to operating costs (see Table 7). Thus improvements in yield that occur in pretreatment, in enzyme production, and in the SSCF step improvements are major factors in reducing cost. In addition, the dramatic improvements in enzyme activity help to reduce the high cost of enzyme production. Combining these improvements with genetically engineered feedstocks brings the savings to 40 cents per gallon.

We show these projections not so much to claim any accurate forecast of the technology’s future over the next 10 years but to demonstrate how our process model can be used to understand the value of proposed research targets. These targets are, by their nature, somewhat conservative. They are based on the application of research advances that build on the same process configuration.

Conclusions

We have presented the results of two years of effort to upgrade our biomass-to-ethanol process model and to utilize the model and the latest biotechnology tools to establish future technology performance targets. Our model is an improvement over previous work and shows that, with near-term cost projections bracketed between \$1.44 and \$1.16 per gallon, this technology (with on-site production of enzymes) is competitive in today’s ethanol market. We have also shown that future improved enzymatic conversion processes offer low-cost sugar and ethanol production capability. As we continue to improve performance and industry demonstrates commercial production of bioethanol, we expect biomass conversion with cellulase enzymes to emerge over the next five years. The introduction of low-cost cellulase enzyme technology will expand the growth of bioethanol production beyond the base established by “pioneer plants” working in niche markets.

In the meantime, we plan to continue to improve the core of the model and to expand our process modeling

activities beyond the process configuration presented here. Future potential technologies to be evaluated include

- Counter-current pretreatment technology (both with and without the use of enzymes)
- Consolidated bioprocessing in which cellulose hydrolysis and fermentation are carried out by one organism
- Advanced power generation technologies

References and Notes

- (1) Sheehan, J.; Himmel, M. Enzymes, Energy and the Environment: Cellulase Development in the Emerging Bioethanol Industry. *Biotechnol. Prog.* **1999**, *15*, xxxx–xxxx.
- (2) Lynch, M. Future Oil Supplies: Is Wolf Really at Door? *Forum for Applied Research and Public Policy*, Spring 1992; pp 23–27.
- (3) Annual Energy Outlook 1999 with Projections to 2020. Energy Information Administration. Report No. DOE/EIA-0383(99). U.S. Department of Energy, Washington, D.C. 1999.
- (4) Kerr, R. The Next Oil Crisis Looms Large—and Perhaps Close. *Science* **1998**, *281*, 1128–1131.
- (5) Wright, J.; D'Agincourt, C. Evaluation of Sulfuric Acid Hydrolysis Processes for Alcohol Fuel Production. *Biotechnol. Bioeng. Symp. No. 14*, **1984**, 105–123.
- (6) Wright, J. D. Ethanol from Lignocellulose: An Overview. *Energy Prog.* **1988**, *8* (2), 71–78.
- (7) *Technical and Economic Evaluation of Wood to ethanol Process*. A report prepared for Solar Energy Research Institute, Chem Systems, Terrytown, NY, 1990.
- (8) Hinman, N.; Schell, D.; Riley, C.; Bergeron, P.; Walter, P. Preliminary Estimate of the Cost of Ethanol Production for SSF Technology. *Appl. Biochem. Biotechnol.* **1992**, *34/35*, 639–649.
- (9) ASPEN Plus, Release 9.2–1, Aspen Technology, Inc., Cambridge, MA, October 1995.
- (10) Wooley, R. J.; Putsche, V. Development of an ASPEN PLUS Physical Property Database for Biofuels Components. NREL/MP-425–20685, April 1996.
- (11) *Wastewater Treatment Options for the Biomass-To-Ethanol Process*; NREL Subcontract AXE-8-18020-01, Final Report, Merrick & Company, Aurora, CO, 10/20/98.
- (12) Wooley, R.; Ruth, M.; Sheehan, J.; Majdeski, H.; Galvez, A. *Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis Current and Futuristic Scenarios*; Report No. NREL/TP-580-2615. National Renewable Energy Laboratory, Golden, CO, July 1999, (http://www.ott.doe.gov/biofuels/process_engineering.html).
- (13) ICARUS Process Evaluator, Version 4.0, ICARUS Corporation, Rockville, MD, June 30, 1997.
- (14) See <http://www.arkenol.com>.
- (15) Anonymous. Bagasse-to-Ethanol Plant Proposed. *Ethanol Report*. January 8, 1998.
- (16) Wald, M. L. A New Bacterium Helps Turn Agricultural Waste Into Energy to Fuel Cars. *The New York Times*, October 25, 1998.
- (17) Thomas, S.; Laymon, R.; Chou, Y.; Tucker, M.; Vinzant, T.; Adney, W.; Baker, J.; Nieves, R.; Mielenz; Himmel, M. Initial Approaches to Artificial Cellulase Systems for Conversion of Biomass to Ethanol. *Enzymatic Degradation of Insoluble Carbohydrates*, ACS Symposium Series No. 618; American Chemical Society, Washington, D.C., 1995; pp 208–236.
- (18) Himmel, M.; Adney, W.; Baker, J.; Elander, R. Advanced Bioethanol Production Technologies: A Perspective. *Fuels and Chemicals from Biomass*; ACS Symposium Series #666; American Chemical Society: Washington, D.C., 1997; pp 2–45.
- (19) *Bioethanol Strategic Road map: A planning framework for development of biomass-to-ethanol technology (Preliminary Draft)*. National Renewable Energy Laboratory, Golden, CO, December 1998.
- (20) Farmer, J.; Hayward, T.; Newman, M.; Ruth, M.; Tucker, M.; McMillan, J. *Milestone Completion Report: Demonstrate process technology meeting or exceeding process qualifier performance in the mini-pilot biochemical conversion system and assess continuous SSCF performance to recommend future work*. Internal Report, National Renewable Energy Laboratory, Golden, Colorado, September, 1997.
- (21) McMillan, J. Bioethanol Production: Status and Prospects. *Renewable Energy* **1997**, *10* (2/3), 295–302.
- (22) Walsh, M.; et al. *The Evolution of the Fuel Ethanol Industry: Feedstock Availability and Price*. Internal report to the Office of Transportation Technologies. Oak Ridge National Laboratory. Oak Ridge, Tennessee. June 5, 1997.
- (23) Glassner, D.; Hettenhaus, J.; Schechinger, T. Corn Stover Collection Project. In *BioEnergy '98—Expanding Bioenergy Partnerships: Proceedings*; Madison, WI, 1998; Vol. 2, pp 1100–1110.
- (24) Graham, R. L.; Allison, L. J.; Becker, D. A. The Oak Ridge Energy Crop County Level Database. December 20, 1996. Available at www.esd.ornl/bfdp/orecl/database.html.
- (25) Wilke, C. R.; Yang, R. D.; von Stockar, U. Preliminary Cost Analyses for Enzymatic Hydrolysis of Newsprint. *Biotechnol. Bioeng.* **1976**, *6*, 155–175.
- (26) Gauss et al. U.S. Patent No. 3990944, November 9, 1976.
- (27) Huff et al. U.S. Patent 3990945, November 9, 1976.
- (28) Platz, B. Sunda Defibrator, Inc., personal communication, April, 1998. Results of experimental work conducted at TVA, Muscle Shoals Laboratories. Date of tests unknown.
- (29) Platz, B. Sunda Defibrator, Inc., personal communication, August, 1998.
- (30) Ranatunga, T. D.; Jervis, J.; Helm, R. F.; McMillan, J. D.; Hatzis, C. Identification of Inhibitory Components Toxic Toward *Zymomonas mobilis* CP4(pZB5) Xylose Fermentation. *Appl. Biochem. Biotechnol.* **1997**, *67*, 185–198.
- (31) Ranatunga, T. D.; Jervis, J.; Helm, R. F.; McMillan, J. D.; Wooley, R. J. The overliming of dilute acid pretreated lignocellulosics, Part 1. The fate of inorganics, uronic acids and other soluble organics. *Enzyme Microb. Technol.* In preparation.
- (32) McMillan, J. D.; Tucker, M. P.; Hayward, T. K.; Hatzis, C.; Glassner, D. *Process Qualifier Milestone*. Internal Report, National Renewable Energy Laboratory, Golden, CO, 31 August 1996.
- (33) Zhang, M.; Eddy, C.; Deanda, K.; Finkelstein, M.; Picataggio, S. Metabolic Engineering of a Pentose Metabolism Pathway in *Zymomonas Mobilis*. *Science* **1995**, *267*, 240–243.
- (34) Hamilton, J. Cellulase Production Experiment No. 36: Air/Oxygen 22 Factorial Design. Enzymatic Process Development Team Internal Report. National Renewable Energy Laboratory, Golden, CO, December 1998.
- (35) Wales, S. M. *Chemical Process Equipment Selection and Design*; Butterworth Publishing, NY, 1988.
- (36) Grethlein, H.; Nelson, T. *Projected Process Economics for Ethanol Production from Corn*; Final Report to U.S. Department of Agriculture North Atlantic Area Eastern Regional Research Center, Philadelphia, PA, July 17, 1992.
- (37) Short, W.; Packey, D. J.; Holt, T. *A Manual for the Economic Evaluation and Energy Efficiency and Renewable Energy Technologies*; Report No. NREL/TP-462-5173. National Renewable Energy Laboratory, Golden, CO, March 1995.
- (38) Katzen, R. Personal Communication, January 1998.
- (39) Ingram, L. O.; Conway, T.; Alterthum, F. *Ethanol Production by Escherichia coli strains coexpressing Zymomonas PDC and ADH Genes*; US Patent 5,000,000. Issued March 19, 1991.
- (40) Ingram, L. O.; Conway, T.; Clark, D. P.; Sewell, G. W.; Preston, J. F. Genetic Engineering of Ethanol Production in *Escherichia coli*. *Appl. Environ. Microbiol.* **1987**, *53*, No. 10, 2420–2425.
- (41) Hettenhaus, J.; Glassner, D. *Milestone Completion Report: Enzyme Hydrolysis of Cellulose: Short-Term Commercialization Prospects for Conversion of Lignocellulosics to Ethanol*; National Renewable Energy Laboratory Internal Report, Golden CO, 1997
- (42) Himmel, M. E.; Karplus, P. A.; Sakon, J.; Adney, W. S.; Baker, J. O.; Thomas, S. R. Polysaccharide Hydrolase Folds Diversity of structure and Convergence of Function. *Appl. Biochem. Biotechnol.* **1997**, *63/65*, 315–325.

- (43) Warren, R. A. J. Structure and Function in β -1,4-Glycanases. In *Carbohydrases from T. reesei and Other Microorganisms*; Claeysens, M., Nerinckx, W., Piens, K., Eds.; The Royal Society of Chemistry: Cambridge, U.K., 1998; pp 115–123.
- (44) Thomas, S. R.; Adney, W. S.; Baker, J. O.; Chou, Y.-C.; Himmel, M. E. *Method for Increasing Thermostability in Cellulase Enzymes*; U.S. Patent No. 5712142. July 1, 1997.
- (45) Arnold, F. H.; Moore, J. C. Optimizing Industrial Enzymes by Directed Evolution. *Adv. Biochem. Eng./Biotechnol.* **1997**, *58*, 1–14.
- (46) Lynd, L.; Elander, R.; Wyman, E. Likely Features and Costs of Mature Biomass Ethanol Technology. *Appl. Biochem. Biotechnol.* **1996**, *57/58*, 741–761.
- (47) *AGRE-0063: High Temperature Ethanol Fermentation of Lignocellulosic Waste*; NF-2000 Online Database Information, 1 July 1992 to 30 June 1993. See www.nf2000.org.

Accepted August 9, 1999.

BP990107U