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Technoeconomic analysis of biofuels: A wiki-based platform for lignocellulosic biorefineries

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ABSTRACT

We present a process model for a lignocellulosic ethanol biorefinery that is open to the biofuels academic community. Beyond providing a series of static results, the wiki-based platform provides a dynamic and transparent tool for analyzing, exploring, and communicating the impact of process advances and alternatives for biofuels production. The model is available for download (at <http://econ.jbei.org>) and will be updated based on feedback from the community of experts in biofuel-related fields. By making the assumptions and performance metrics of this model transparent, we anticipate this tool can provide a consensus on the energy-related, environmental, and economic performance of lignocellulosic ethanol.

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1. Introduction

Biofuels, particularly lignocellulosic ethanol, have attracted significant attention as one of the routes to address the world's concerns on energy and climate, though their potential as a sustainable solution remains somewhat controversial. Principally, substantial doubts remain regarding the economic and greenhouse gas (GHG)-abatement performance of biofuels [1–4]. In the background of these discussions, researchers have continued to focus on solving the challenges that have hitherto limited the

commercialization and adoption of lignocellulosic biofuels. It is the outcome of these efforts that will assist in moving toward a consensus, and thus the technological and economic progress brought about by biofuels research must be carefully and repeatedly evaluated.

Several technoeconomic studies based on process models have provided assessments of the potential of biofuels and have provided invaluable guidance to research, investment, and policy endeavors [5–8]. These studies usually rely on experimentally-derived or assumed parameters to estimate process performance values, including capital and operating

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costs, GHG emissions, and biofuel yield as a function of feedstock, among others. They have been also used to analyze how changes in the input parameters translate into changes in overall system performance. Naturally, but unfortunately, these studies can only study a limited set of scenarios, and it is impossible for them to address all possible parameter choices or designs that could be of interest to the biofuels community. Moreover, research in the field is highly dynamic and advances brought about by one research group are rarely considered in models developed by others primarily because there is, at present, no avenue for such an exchange to take place.

In response to these challenges, we have constructed a technoeconomic model of a lignocellulosic ethanol biorefinery that is accessible to the biofuels community at large. The model has been deposited online and is available for download. Each unit operation in the process flowsheet has a dedicated discussion thread, making it possible for experts in different fields to collectively and publicly address issues associated with different sections of the biorefinery, contributing in their respective areas of expertise. To make the model interactive and dynamic, and to ensure its accuracy, the parameters and assumptions will be updated in response to feedback obtained from the community of users. This is an essential feature of the present contribution, as the results of any model are strongly dependent on the assumptions made, and the community as a whole will have the opportunity to monitor all parameter values. The goal is to provide a tool that: (1) incorporates assumptions in a transparent manner, (2) allows comparative analyses to be made from the same starting point, (3) permits its users to analyze the scenarios that are of most interest to them, (4) gathers meaningful parameters and other information from experts across disciplines in a centralized model, (5) directs research efforts by communicating what parameters are in most need of experimental verification, and (6) disseminates findings across different, and many times unrelated, fields.

2. Methods

The technoeconomic model we present is based on a process flowsheet of a lignocellulosic ethanol biorefinery, built with the aid of the SuperPro Designer software (Intelligen, NJ, USA). The process flowsheet built with the program includes all of the unit operations and process flows that are needed to transform the inputs (corn stover, process water, etc.) into outputs (ethanol, CO₂, electricity, etc.). The model consists of: (1) all equations that describe the flow of materials in and out of each unit operation and the overall biorefinery (material balances); (2) all equations that describe the flow of energy in and out of each unit operation and the overall biorefinery (energy balances); and (3) all equations needed to price the purchase and installation of equipment required for each unit operation. The solutions of the equations within sets (1) and (2) allow for the determination of the use of utilities and raw materials, equipment sizing, plant throughput, and related dependent variables. This information, along with the equations within set (3) and the cost of raw materials and labor, allow for the determination of the capital and operating costs. It is not practical to list all of the equations utilized and solved

by SuperPro Designer, but a detailed description of the approach can be obtained from specialized sources [9] and from the software's manual.

2.1. Description of the base case

A diagram illustrating the base case process is found in Fig. 1. The conditions of this case were chosen based on available literature; thus, the base case was such that it would represent the performance that could be achieved in a plant today (see also Section 3). Briefly, corn stover, priced at 60\$ t⁻¹ (at the farmgate), is transported ~50 km to the biorefinery, where it is unpacked from the bales, washed, and shredded. It enters the pretreatment reactor along with sulfuric acid, where high-pressure steam is used to heat the vessel to ~180 °C (~450 K) at a pressure of ~1–1.5 MPa. The mixture is flash-cooled and the slurry is passed through a belt filter. The liquid filtrate is overlimed and neutralized to remove toxins before being slurried back with the solids, which contain most of the cellulose. This mixture enters the saccharification tank, cellulase enzymes are added to 20 g kg⁻¹ cellulose, and the reaction is allowed to proceed at 50 °C (323 K) for ~5 days. At this point, the cooled saccharified slurry enters the fermentation section, where it supplies the substrates for yeast growth (in a train of seed fermentors) and ethanol fermentation. An engineered yeast strain that co-utilizes C5 and C6 sugars is used. The fermentation proceeds until the C6 sugars are exhausted (see Section 4.2), though some of the C5 sugars are also utilized. The exiting beer is passed through two distillation columns before entering the molecular sieve columns, from which ethanol exits almost pure (~99.5%). The bottoms (i.e. the stillage) from the first distillation column, containing most of the lignin and other non-fermentable solids, are sent to a series of multi-effect evaporators for partial dewatering. Water is recycled back or treated in the wastewater treatment (WWT) section. The lignin and other solids, along with the biogas produced in the WWT digestors, are burned in a boiler, producing high-pressure steam. This is used to run the turbogenerator for electricity production and for generation of low-pressure steam used in the pretreatment, product recovery, and water recovery sections.

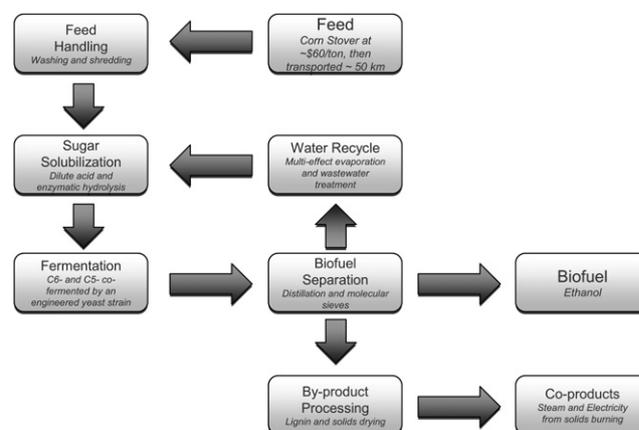


Fig. 1 – General schematic of the lignocellulosic ethanol biorefinery.

The reader is invited to obtain the parameters and assumptions, as well as the literature sources used for those values, from the wiki online (<http://econ.jbei.org>); thus, detailed lists of specifications and references are omitted here. The model is freely available to all non-commercial users, and is meant to be a community-updatable tool: we encourage and welcome suggestions, corrections, and modifications to the assumptions and parameters used.

3. Scenario mapping

In order to show how different groups can benefit from the model, we highlight different targeted biorefinery scenarios. It must be noted that none of our cases has been optimized for a particular performance value, which is best left to the commercial sector [1]; these cases are offered mainly as an illustration of how groups with different aims can explore parameter variations. We therefore stress that the main goal of this report is to contribute a tool for wide use, rather than to provide a series of static results. Nonetheless, the model is intended to have immediate applicability within the biofuel community. All the parameters of the model were either taken from published studies or were chosen according to established industrial practice, and, regardless of whether the results provide optimistic or pessimistic outlooks, they are certainly representative of current technology (i.e. of what could be achieved today if successful scale-up was accomplished).

3.1. Scenario 1: reducing acetate content of the biomass feedstock

Acetyl functional groups are found in the hemicellulose and lignin constituents of biomass, and are liberated and solubilized during dilute acid pretreatment. Acetic acid is inhibitory to fermenting microorganisms, and especially to *Saccharomyces cerevisiae*, in addition to interfering with enzymatic hydrolysis during saccharification [10,11]. Plant biotechnologists are targeting reducing the content of acetate in bioenergy crops. In this scenario, a reduction of 20% in the acetate content in biomass was modeled, relieving toxicity during fermentation. A reduction in saccharification time or enzyme loading was not modeled in this scenario, since we were not aware of published reports that quantified such an effect.

3.2. Scenario 2: increasing cellulolytic enzyme activity

Cellulolytic enzymes are the second largest material costs after the feedstock material itself, even at the highly optimistic price of 2.70\$ kg⁻¹ of enzyme (corresponding to about 92.47\$ m⁻³ (0.35\$ gal⁻¹) ethanol in our base case). Efforts in protein engineering have strived to reduce this contribution to the operating costs, for example, by increasing the kinetic activity of the enzymes during saccharification [12]. Some have proposed enzymes that do not absorb as easily to lignin as native enzymes do [13], or that are engineered for stability [14]. Consequently, a lower loading could be used in the process or the residence time of saccharification could be reduced. Here, we explored a 2-fold improvement in enzyme activity, which would halve the required enzyme loading.

3.3. Scenario 3: reducing lignin content of the biomass feedstock

The effects of lignin have been described as some of the major hurdles that lie in the way of an effective process for lignocellulosic ethanol. Notably, lignin interferes with sugar solubilization by limiting the accessibility of enzymes to the cellulose fibers during saccharification and by adsorbing active enzyme [13,15]. The toxicity of lignin monomers to fermenting organisms has been reported [16]. In this scenario, we modeled the use of biomass modified to have 20% lower lignin content with respect to the base case. This reduction was assumed to be compensated by an increase in cellulose, based on previously reported studies in transgenic aspen [17]. While the saccharification residence time was left unchanged, the sugar released during hydrolysis was increased by ~50% [18]. Fermentation time was either left unchanged (scenario 3a), or increased so that the glucose was exhausted (scenario 3b), similar to the base case (see Section 4.2). To partly compensate for the lost lignin and higher conversion, purchased natural gas was added in scenario 3b to the combustor for adequate steam and electricity production.

3.4. Scenario 4: increasing the rate of xylose-fermentation by yeast

S. cerevisiae is the preferred industrial organism for the production of ethanol from cane or grain-derived sugars, because of its natural ability to quickly ferment six-carbon sugars even in the presence of oxygen and its tolerance to the alcohol product [19,20]. Wild-type *S. cerevisiae*, however, cannot metabolize five-carbon sugars such as xylose, effectively reducing the overall yield of ethanol on biomass and increasing the cost of production. To overcome this limitation, several groups have focused on engineering strains for uptake of five-carbon sugars [21]. To model the effect of an increase in xylose metabolism, we doubled the growth rate on xylose in the anaerobic fermentors, while leaving fermentation time unchanged.

3.5. Scenarios 5 and 6: increasing the tolerance of yeast to acetic acid and ethanol

Acetic acid has a pronounced toxic effect in yeast; the minimum inhibitory concentration (MIC) of the undissociated form of acetic acid can be as low as 10 g L⁻¹ or less [22,23]. Typical fermentation conditions for yeast have a starting pH of ~4.5 (pK_a = 4.75), so that even relatively low concentrations of the acid can have a detrimental effect on fermentation performance. Ethanol is also toxic, and overcoming its negative effects on fermentation has been the area of intense study. In order to account for toxic effects, the inhibition of both ethanol and acetic acid were included in the fermentation kinetic models. The decrease in growth rate with increasing concentrations of both compounds was assumed to be linear, based on previous studies [23–25]. For scenario 5, the MIC of acetic acid (assuming a pH of 4.5) was increased by 50%. A similar case was studied with ethanol (scenario 6).

4. Results

4.1. Base case results

A summary of the base case economic performance metrics is given in Table 1. The capital investment, at approximately 340 M\$ (in 2009\$, financed with 60% debt), corresponds to a facility processing 2000 t d⁻¹ of wet biomass (moisture content ~15% w w⁻¹). A section that describes the assumptions for cost estimation, and its associated discussion thread, has been placed on the wiki. As part of our analysis, we plotted the contributions of materials, utilities, labor, and facility-dependent payments to the annual operating cost (AOC) for the base case (Fig. 2). In addition, we plotted the distribution of different raw materials in the contribution of the material-associated costs (Fig. 3). As shown in the figures, the majority of the AOC is made up by facility-dependent and raw material costs. The stover is by far the largest contribution to the material costs, with the cost of enzymes being second. This trend may not hold had we not made such optimistic assumptions regarding the cost of enzymes: a base case value of approximately 92.47\$ m⁻³ (0.35\$ gal⁻¹) of ethanol based on literature estimates [5].

4.2. Sugar conversion

As explained in the preceding section and is apparent in Figs. 2 and 3, the feedstock cost contributes significantly to the production cost; therefore, the yield of ethanol on biomass affects the minimum ethanol selling price (MESP), corresponding to a zero net present value of the project over its lifetime, that is, 25 years with a 10% discount rate). In turn, the fermentation residence time influences the yield, as higher conversion of sugars can be achieved if the yeast is allowed to metabolize for longer periods of time. In general, longer times translate into larger or more fermentor units to maintain the same throughput, and thus there is a tradeoff that arises from increasing the residence time of

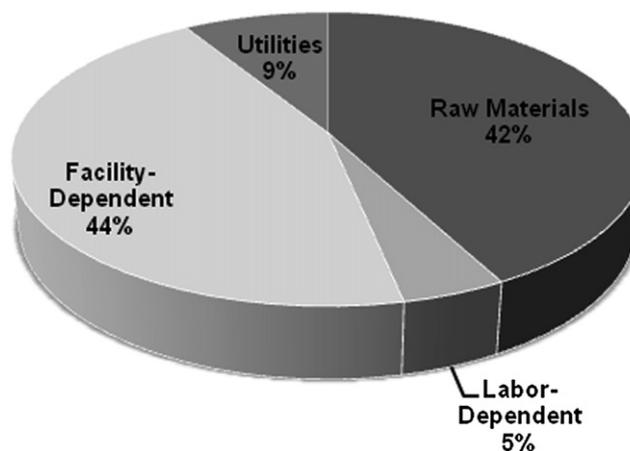


Fig. 2 – Annual operating cost (AOC) breakdown for the base case.

fermentation. To explore this effect, the dependence of MESP on fermentation residence time was graphed using the base case model, as shown in Fig. 4. The relative MESP is defined such that the MESP at the time where all C6 sugar is consumed has the value of 1. For the base case, there is a clear and sharp decrease in MESP until ~140 h, the time at which the C6 sugars are depleted. After that, the decrease in MESP decelerates. Even though the cost of production continues to decrease, other performance values become less favorable, for example, electricity consumption increases quickly. To make the results of the scenarios comparable across all cases, the fermentation time was set to 140 h and not changed, regardless of when C6 sugars were consumed, except for scenario 3b (lower lignin). For this case, for which the C6 sugar content of the fermentor feed increases dramatically, the same rationale was used to select an appropriate residence time.

Because the extent of solubilization of C5 and C6 sugars varies during pretreatment and saccharification and the dynamics of sugar fermentation to ethanol depends on the

Table 1 – Summary of the explored scenarios^a

Case	Annual Throughput ^b	Yield ^c	TPI ^d (M\$)	AOC ^e (M\$ y ⁻¹)	MESP ^f	Δ MESP ^g
Base case	117.1 (30.9)	167 (44.2)	337.1	138.5	\$ 1207.40 (\$ 4.58)	\$–
CS low acetate	131.4 (34.7)	188 (49.7)	336.7	139.0	\$ 1086.44 (\$ 4.11)	\$ 120.96 (\$ 0.47)
Lower Enzyme	116.8 (30.9)	167 (44.1)	335.3	133.2	\$ 1165.13 (\$ 4.41)	\$ 42.27 (\$ 0.17)
CS low lignin (a)	132.9 (35.1)	190 (50.2)	315.5	135.4	\$ 1051.22 (\$ 3.98)	\$ 156.18 (\$ 0.60)
CS low lignin (b)	166.0 (43.9)	238 (62.8)	367.7	148.5	\$ 932.41 (\$ 3.53)	\$ 247.99 (\$ 1.05)
Fast xylose metabolism	133.3 (35.2)	191 (50.4)	334.7	138.5	\$ 1063.91 (\$ 4.03)	\$ 143.49 (\$ 0.55)
Acetate tolerance	140.0 (37.0)	200 (52.9)	338.1	139.7	\$ 1025.25 (\$ 3.88)	\$ 182.15 (\$ 0.70)
Ethanol tolerance	119.9 (31.7)	172 (45.3)	334.5	138.0	\$ 1175.25 (\$ 4.45)	\$ 32.15 (\$ 0.13)

a Use of indigenous units has been permitted as the working units inside the model are those in common usage in the USA today. All dollar amounts are in 2009\$.

b Units: dam³ per year; in parenthesis, million gallons per year.

c Yield in L t⁻¹ of biomass (wet basis, 15% moisture); in parenthesis, gal t⁻¹.

d Total project investment in million \$.

e Annual operating cost, including facility-dependent in million \$.

f Minimum ethanol selling price in \$ per m³; in parenthesis, \$ per gallon.

g Difference to base case in \$ per m³; in parenthesis, \$ per gallon.

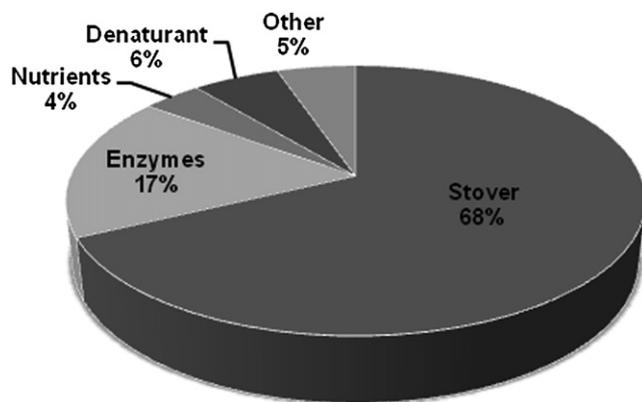


Fig. 3 – Contributions of different raw materials to total material cost.

ability of yeast to use the substrates, sugar conversion varies in the different scenarios (Fig. 5). Highest C6 conversion is observed in the case for low lignin, mainly because delignification enhances the sugar solubilized during enzymatic saccharification. Highest C5 conversion is observed for the faster xylose-metabolizing yeast, evidencing the importance in metabolic engineering efforts for introducing the xylose-utilizing pathway into these hosts.

4.3. Carbon emissions and electricity production

Without performing a full life-cycle analysis, one can analyze the greenhouse gas (GHG) emission reduction that stems from operating a biorefinery. Though the results of such analysis are by definition incomplete, they are useful for comparing different scenarios, i.e., when they are evaluated in relative terms. In essence, we performed the calculations expecting that the results could be used as part of the data needed in a full life-cycle analysis. Factors occurring outside of the biorefinery, such as biomass origin and cultivation practices, are therefore not part of the present treatment.

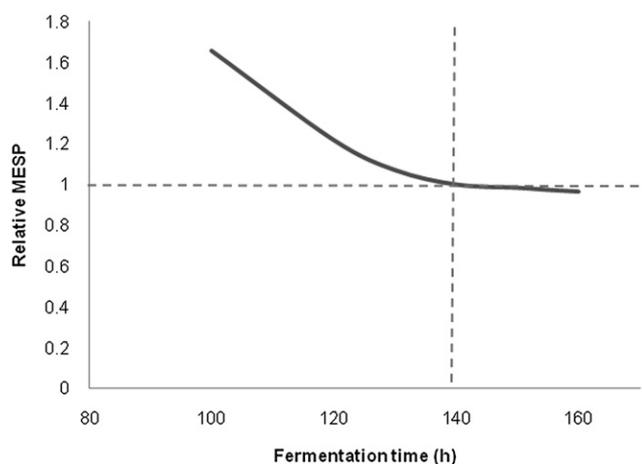


Fig. 4 – Dependence of the minimum ethanol selling price (MESP) on fermentation residence time. The relative MESP in this plot is defined such that the MESP at the time where all C6 sugar is consumed has the value of 1.

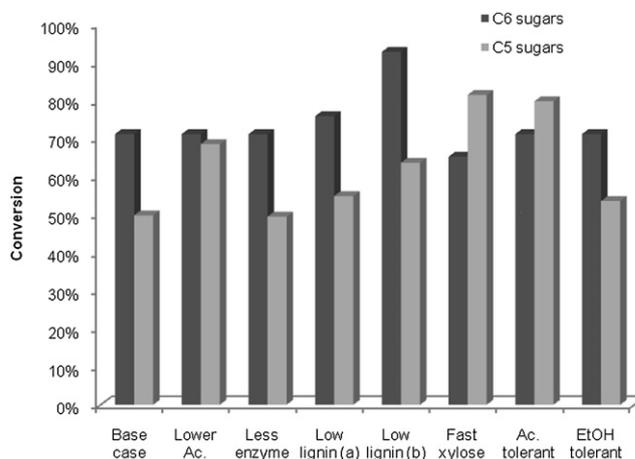


Fig. 5 – Percentage of C5 and C6 sugars in the biomass feedstock that are converted to ethanol.

In a simple case, a biorefinery can potentially diminish fossil fuel-generated CO₂ by two mechanisms: (1) the electricity displaced by that produced from burning biomass residues, and (2) the gasoline displaced by ethanol (assuming the biomass used was grown for biofuel production [26]). To quantify the “credits” from such displacements, we calculated the CO₂ that would be “saved” because green alternatives were used instead of fossil fuels. For fossil fuel-based electricity, we assumed that emissions are those of the US, on average 606 kg MWh⁻¹ of CO₂ equivalent [27]. For ethanol, the value was calculated by assuming that gasoline produces 2.32 t m⁻³ of CO₂ (8.8 kg gal⁻¹) [28], and adjusting for ethanol’s lower energy content. In the cases where natural gas was used to supplement the energy contained in biomass residues, the emissions from completely burning the gas were subtracted from the CO₂ credit to give a lower number.

Credits, as defined above, are graphed for each scenario in Fig. 6. In all cases where conversion of biomass to ethanol increases with respect to the base case, a concomitant reduction in electricity production is observed, as less biomass is available for burning (Fig. 7). A tradeoff between credits due to fossil fuel displacement and fossil electricity displacement arises. This is particularly seen in scenario 3b, where natural gas is assumed to be purchased to supply the steam and electricity needed for plant operation. The CO₂ credit is highest for this scenario, however, because producing more ethanol offsets methane-associated emissions.

5. Ethanol selling price

The investment and cost results from the different scenarios are summarized in Table 1. The capital investment for all scenarios was comparable, at roughly 315–370 M\$ (2009\$), but the MESP varies significantly in the different scenarios. As mentioned in Section 4.2, the strong dependence of the production cost on feedstock cost implies that gains in yield have a large effect in the minimum ethanol selling price

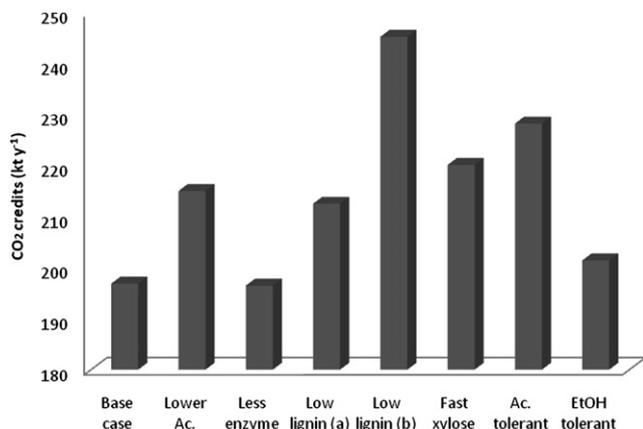


Fig. 6 – Carbon emission credits associated with the production of ethanol and electricity in the biorefinery. This information can be used to compare the GHG-abatement potential of the different technologies explored in this paper when used as part of a full life-cycle analysis.

(MESP). To explore this, we graphed the dependence of MESP on yield and observed a clear nearly linear correlation (Fig. 8). The apparent approximate linearity is due to the fact that the capital costs for the different scenarios are similar, and therefore the return on operating costs, closely related to yield in our analysis, has a pronounced effect on MESP. Even though different scenarios explored technologies that bring about benefits through different mechanisms, gains in yield are the main reason for decreases in MESP across the study.

Even for our base case scenario, the performance values of our process – the MESP, operating cost, yield on biomass, etc. – contrast significantly to others in the literature. While the capital expenditure is approximately the same as previous estimates for this configuration [5], the conversion of sugars is much lower, which has a marked effect on yields and, thus, on operating cost per unit of output. The main reason for this is our choice of fermentation and sugar solubilization technologies [21,29–32]. The parameters and performance assumptions for these operations were derived from studies in the literature that were complete enough to be accurately represented in our simulations (more references are found in the

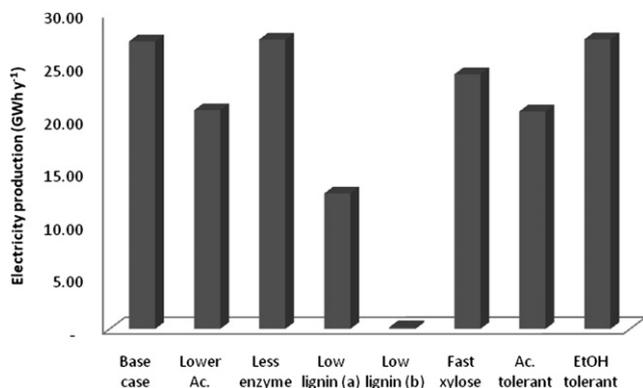


Fig. 7 – Surplus electricity production from burning the residual solids and methane from wastewater treatment.

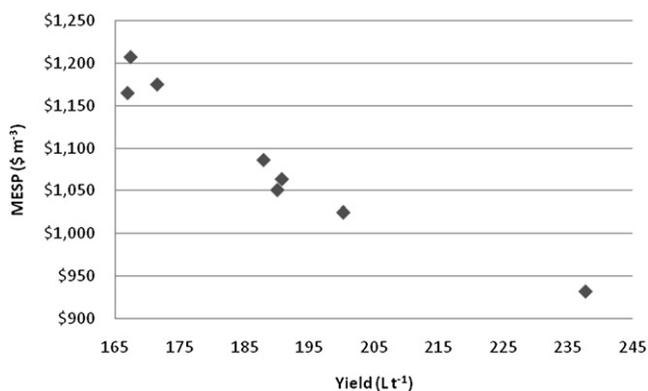


Fig. 8 – Correlation between the MESP and the yield of ethanol on the biomass feedstock (wet basis, moisture content 15%).

wiki). This approach ensured that our choices were representative of current technology. Future experimental work will be needed to obtain the necessary details for alternative technologies to be modeled, and we invite the biofuels research community to contribute their results in these areas.

6. Conclusions

We present the first open and collaborative model of a lignocellulosic ethanol biorefinery. Although the present model is specifically formulated for corn stover to ethanol using a specified configuration, the flowsheet can serve as a starting point for considering alternative configurations. For example, a new pretreatment technology can be modeled by changing the unit operations of this section, while leaving most other sections unchanged (obviously, one must consider heat and water integration). New fuels can be considered as well, by modifying the fermentation and product recovery sections accordingly.

The model can be used not only to calculate performance values for a particular configuration or fuel, but also for sensitivity analyses to suggest possible future directions for biofuels research. For example, plant genetic engineering strategies offer great potential for aiding commercialization of lignocellulosic ethanol (see scenarios 1 and 3), though their economic impact has not been properly studied. Strain and enzyme engineering also offer interesting prospects, although some of these are in areas different from those explored most extensively (e.g. acetate impairs yeast fermentation more than ethanol does; see scenarios 5 and 6). One main reason behind why these and other observations may escape experts is the lack of time and resources needed to develop a full technoeconomic model. Even if each research group were to create a model of their own, the likelihood of different studies agreeing in the assumptions and parameters is quite low, making the observations and conclusions non-comparable and diminishing their usefulness. Partial analyses are common and have continued to be a weakness in the field, fostering unrealistic expectations that cannot be fulfilled by

any single technology. It may still be possible, however, to bring about economical and environmentally sustainable renewable liquid fuels derived from biomass, and the process will be facilitated if new technologies are developed and evaluated in the context of other advances from a common scientific and economic perspective. The aim of this study was not to determine what technology is best, but rather to make available a dynamic learning tool and a communication avenue for such exchanges to occur. Without a concerted effort, diverging arguments about the advantages and limitations of biofuels and different biofuel technologies might significantly limit progress in the area.

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