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Authors
Yang, Minliang
Dahlberg, Jeff
Baral, Nawa Raj
et al.

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Identifying Forage Sorghum Ideotypes for Advanced Biorefineries

Minliang Yang, Jeff Dahlberg, Nawa Raj Baral, Daniel Putnam, and Corinne D. Scown*

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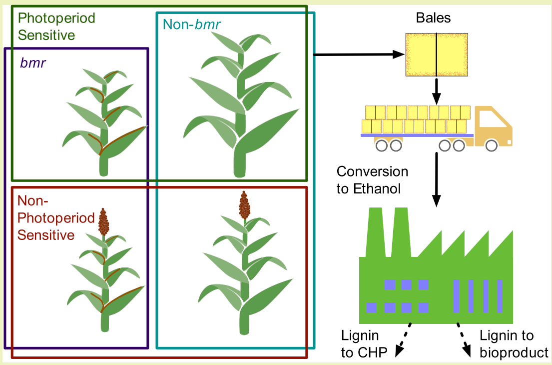
ABSTRACT: Forage sorghum is a promising feedstock for the production of biofuels and bioproducts because it is drought tolerant, high-yielding, and familiar to farmers across the world. However, sorghum spans a diverse range of phenotypes, and it is unclear which are most desirable as bioenergy feedstocks. This paper explores four forage sorghum types, including brown-midrib (*bmr*), non-*bmr*, photoperiod sensitive (PS), and photoperiod insensitive (non-PS), from the perspective of their impact on minimum bioethanol selling price (MESP) at an ionic liquid pretreatment-based biorefinery. Among these types, there are tradeoffs between biomass yield, lignin content, and starch and sugar contents. High biomass-yielding PS varieties have previously been considered preferable for bioenergy production, but, if most starch and sugars from the panicle are retained during storage, use of non-PS sorghum may result in lower-cost biofuels (MESP of \$1.26/L-gasoline equivalent). If advances in lignin utilization increase its value such that it can be dried and sold for \$0.50/kg, the MESP for each scenario is lowered and non-*bmr* varieties become the most attractive option (MESP of \$1.08/L-gasoline equivalent). While *bmr* varieties have lower lignin content, their comparatively lower biomass yield results in higher transportation costs that negate its fuel-yield advantage.



KEYWORDS: *biofuels, forage sorghum, Sorghum bicolor, Brown-midrib (bmr), photoperiod sensitive (PS), ionic liquid pretreatment, technoeconomic analysis*

■ INTRODUCTION

The U.S. produced 16.9 billion gallons per year of fuel ethanol as of 2019, largely from corn [*Zea mays* L.] ethanol plants in the Midwest.[1] Because corn is resource-intensive to produce, research efforts across the world have focused on identifying, engineering, breeding, and evaluating alternative bioenergy crops that can be deconstructed to constituent sugars and lignin intermediates for conversion to biofuels.[2−5] Although low-input high-yielding perennial grasses are attractive feedstocks from an environmental perspective,[6] they require substantial upfront investment by farmers in the establishment phase, which may not be recouped if a stable market for biomass does not exist over the 15−20 year lifetime of the crop. Grasses such as switchgrass [*Panicum virgatum*] and Miscanthus [*Miscanthus* × *giganteus* J.M. Greef & Deuter ex Hodkinson & Renvoize [*sacchariflorus x sinensis*]] also do not have well-established alternative markets, although prior studies have noted switchgrass may be viable as a forage crop.[7] Sorghum [*Sorghum bicolor* (L.) Moench spp. *bicolor*], a highly productive C4 annual crop, is a promising alternative that may be less risky for farmers to adopt because of its established commercial production and supply chain.[8,9] The United States is already the largest sorghum producer in the world.[10] Sorghum is a naturally drought-tolerant crop, making it attractive in semiarid regions without sufficient rainfall to support corn production.[11] Additionally, targeted breeding over the past 50 years has increased sorghum biomass yield, carbohydrate content, insect resistance, and drought tolerance.[2,11] Breeding efforts have also resulted in a highly diverse set of phenotypes, ranging from grain types to high-yielding forage types.

Sorghum is grown for animal feed grain, forage, alcohol, food, and fiber.[12] Sorghum acreage in the United States is dominated by sorghum grown for grain, with a much smaller fraction of land area devoted to silage or forage.[13] Grain types maximize grain production, while forage types are optimized for biomass yield and digestibility and can grow up to 3 m tall.[14] The two types are not mutually exclusive, as some dual-purpose varieties achieve both high grain and biomass yield. Forage sorghum is typically chopped, including any grain head present, and ensiled for use as animal feed. Some varieties can be "ratooned," grazed, or harvested multiple times.

Although the bioenergy research community often refers to "biomass sorghum" or "bioenergy sorghum" generically to mean a very high biomass-yielding forage type with little or no

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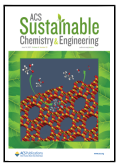

Table 1. Average Biomass Dry Matter Yield (Mg ha^{-1}) and Chemical Structural Compositions (Dry Basis) of Different Forage Sorghum Hybrids[25,a]

parameter	unit	*bmr* (5 varieties)	non-*bmr* (13 varieties)	PS (3 varieties)	non-PS (15 varieties)
biomass yield (DM)	Mg ha^{-1}	15.1 (11.1−17.5)	18.1 (15.6−21.1)	18.7 (16.3−20.1)	17.0 (13.5−21.1)
lignin	%	10.4 (9.9−11.3)	13.1 (10.7−16.3)	12.9 (11.3−13.9)	12.3 (9.9−16.3)
glucan	%	24.5 (18.7−35.3)	24.9 (18.8−34.3)	32.0 (29.8−35.3)	23.4 (18.7−34.3)
xylan	%	15.3 (12.6−19.9)	15.3 (13.1−18.3)	18.4 (17.4−19.9)	14.7 (12.6−18.3)
arabinan	%	2.6 (1.4−2.9)	2.5 (2.1−3.0)	2.9 (2.7−3.0)	2.4 (2.1−3.0)
galactan	%	1.0 (0.9−1.1)	1.0 (0.8−1.2)	1.0 (0.8−1.1)	1.0 (0.9−1.2)
soluble sucrose	%	1.2 (0.6−1.7)	1.2 (0.2−2.4)	2.1 (1.6−2.4)	1.0 (0.2−1.7)
structural starch	%	15.5 (0.0−23.7)	12.2 (0.0−21.7)	0.0 (0.0−0.0)	15.8 (0.0−21.7)
soluble starch	%	2.2 (0.0−7.9)	1.9 (0.0−3.3)	0.0 (0.0−0.0)	2.4 (0.0−3.3)
protein	%	5.1 (4.4−6.4)	4.9 (1.7−5.9)	4.8 (4.6−4.9)	5.0 (1.7−6.4)
ash	%	8.6 (7.6−9.4)	8.9 (7.3−10.9)	9.7 (9.3−10.5)	8.6 (7.3−10.9)

[a] The ranges of biomass yield and chemical composition are listed in the parentheses.

grain head, there exists a wide variety of commercially available forage sorghum genotypes with differences in composition and yield. The question of which phenotypes are ideal for bioenergy applications remains unresolved.[2] In this study, we explore photoperiod sensitive (PS), photoperiod insensitive (non-PS), brown midrib (*bmr*), and non-*bmr* sorghum. PS sorghum does not begin flowering until the photoperiod (day length) falls below 12 h and 20 min per day, which occurs in September for the continental United States. This means that PS sorghum will remain in the vegetative stage longer (relative to non-PS varieties that flower about 2 months after planting), thus accumulating more biomass by the end of the growing season.[15] Brown midrib mutants can be either PS or non-PS, and these *bmr* types are recognizable because of the reddish-brown pigmentation of the central vein on their leaves.[16] These sorghum varieties have lower lignin content, which makes them more attractive for animal feed markets despite their typically lower yields,[17] but could also be suitable for biofuel production since the lignin fraction of biomass is one of the major obstacles for the existing biomass deconstruction and subsequent bioconversion technologies.[18]

In this study, we use a combination of field trial data and technoeconomic analysis to quantify the cost tradeoffs associated with varying yield and composition across major genotypes of forage sorghum. The goal of the analysis is to identify which type is likely to be most cost effective for bioenergy production. The biorefinery model is based on an ionic liquid (IL) pretreatment process, followed by enzymatic hydrolysis to liberate monosaccharides for downstream conversion, although the results are intended to be generalizable across a range of deconstruction processes. Most published technoeconomic studies have been conducted on sweet sorghum-based bioethanol production. Studies focused on the impact of forage sorghum phenotypes remain sparse.[9,19−23] Dahlberg et al.[24] found that forage sorghum-based bioethanol has a similar minimum selling price compared to corn stover-based bioethanol. In this article, we aim to inform both the selection of available commercial sorghum varieties for biofuel production and research efforts aimed at engineering sorghum for improved performance as a bioenergy crop. To accomplish this goal, we quantify the minimum selling price of ethanol (MESP) for IL-based biorefineries utilizing *bmr*, non-*bmr*, PS, and non-PS sorghum and conduct sensitivity analyses based on biomass yield and utilization of lignin in high-value products.

MATERIALS AND METHODS

In this study, four forage sorghum types *bmr*, non-*bmr*, PS, and non-PS were simulated as the sole feedstock for commercial-scale cellulosic biorefineries. These groups are not all mutually exclusive; *bmr* varieties represented in this study include both PS and non-PS, as do non-*bmr*, while both PS and non-PS average yield and composition are based on samples that include *bmr* and non-*bmr*. Agronomic data of these four plant types were collected from field trials conducted by Dahlberg et al.[25] A total of 18 hybrids (also referred to as varieties) were chosen for compositional analyses. There were 3 PS and 15 non-PS hybrids. In terms of brown midrib mutants, there were 5 *bmr* and 13 non-*bmr* hybrids. The non-PS lines varied in maturity class, with two medium early hybrids, five medium, five medium late, and three late. Each hybrid was harvested for dry matter yield when the grain reached the soft dough stage. Additional details are provided in the Supporting Information (SI), Tables S1 and S2.

Biomass Composition. The average composition of these four forage sorghum types is summarized in Table 1. Although actual composition and yield will vary by geography, soil type, specific variety, fertilizer and irrigation application, and a host of other factors, these average compositions are meant to capture typical differences across the four major forage sorghum types. Unless explicitly intended to explore the impacts of deficit irrigation or low nutrient inputs, most field trials are designed such that plant growth is not limited by water or nutrient availability. Still, local climate conditions can impact the results, as can the specific varieties selected for cultivation within each major type (PS/non-PS and *bmr*/non-*bmr*). In California, field trial results showed that PS varieties, when averaged, had the highest yield (18.7 dry Mg ha^{-1}) and *bmr* types had the lowest yield (15.1 dry Mg ha^{-1}) over the 6-year period;[26−30] in Texas, similar results were observed between PS (19 Mg ha^{-1}) and *bmr* (12 Mg ha^{-1}) varieties at an irrigation level of 300 mm.[31] Compositional analysis from the California trial showed that *bmr* varieties had the lowest lignin content (10.4%) and PS varieties had the highest lignin content (12.3%). The *bmr* varieties had the highest cellulose fraction compared to other sorghum varieties and the PS varieties had less starch relative to other varieties (Table 1). Other published studies[16−18] have found similar chemical structural compositions of the different sorghum varieties.

Forage Sorghum Feedstock Supply Cost. The forage sorghum supply cost at the biorefinery gate is calculated using our bioenergy sorghum supply logistics model, which is documented in Baral et al.[9] Among the different potential supply systems analyzed previously,[9] including chopped ensiled biomass, dry bales, and densely packed modules, this study considers the direct-supply bale system because it is the least GHG-intensive option if the farm-to-biorefinery distance is between 80 and 248 km.[9] Briefly, the direct-supply bale system involves windrowing and in-field drying to 20% moisture content, after which the dried material is baled and directly loaded onto trucks at the field for transport to the biorefinery. To remain consistent with the nutrient regime followed in the field trial, we assume that uniform fertilizer amounts are applied to all hybrids: 131.38 kg/ha of nitrogen,

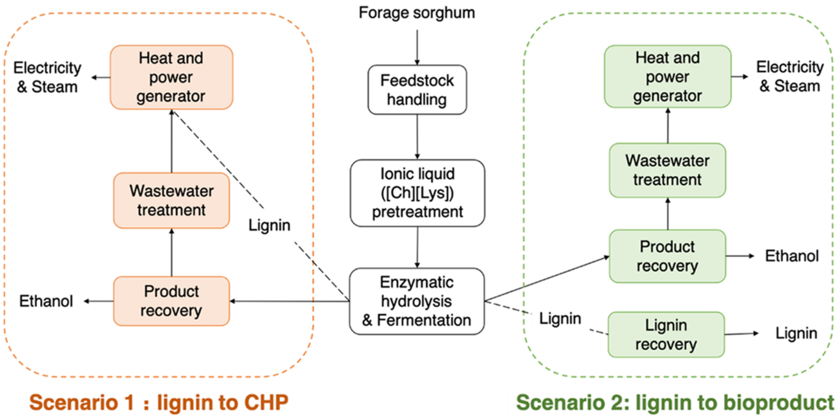

Figure 1. Simplified flowchart of the bioethanol process from forage sorghum. Scenario 1 refers to the lignin combustion for onsite energy generation and Scenario 2 refers to the lignin utilization as a byproduct.

33.96 kg/ha of phosphorous, and 212.48 kg/ha of potassium. As documented in Baral et al.,[9] we assume dry matter losses totaling 11.6% over the entire supply chain a land utilization factor (referring to the fraction of land surrounding the biorefinery that is cultivated with sorghum) of 5%. The transportation distance from farm to biorefineries changes from variety to variety due to yield differences and land utilization. Sorghum varieties with lower yields are more costly to cultivate on a per-biomass yield basis and transport to the biorefinery; a lower-yielding biomass must be transported a longer distance on average to satisfy the same biorefinery feedstock requirement. Additionally, 5% structural starch loss is assumed during the logistic supply for all varieties. However, it is important to note that grain heads (containing higher starch) in non-PS sorghum degrade more quickly than the remaining biomass, and this may impact the results.

Biochemical Conversion Process. The downstream conversion process includes feedstock handling, IL-based biomass pretreatment, simultaneous enzymatic saccharification and fermentation (SSF), ethanol recovery, wastewater treatment, and onsite combustion of biogas from wastewater treatment and lignin (Scenario 1) or separate recovery of lignin as a coproduct (Scenario 2). A simplified process flow diagram is shown in Figure 1. The feedstock handling stage includes biomass handling using belt and screw conveyors and a short-term storage before the pretreatment process. This study considers an integrated one-pot high-gravity ionic liquid-based biomass deconstruction process.[32] Briefly, biomass is mixed with water and IL ([Ch][Lys]) at IL-to-biomass ratio of 0.29 wt % at a total solids loading ratio of 30 wt % in the pretreatment reactor. The mixture is heated to 140 °C for 3 h. Following the IL pretreatment, the slurry is cooled down to room temperature and H_2SO_4 is added to adjust the pH to around 5. Then, enzymes (CTec2 and HTec2 from Novozymes) are added at 10 mg per g of glucan for saccharification at 50 °C for 72 h. The ILs used in this process are compatible with the enzymes and microbes, meaning the IL can remain in solution through simultaneous saccharification and cofermentation (SSCF). Glucan to glucose and xylan to xylose conversion rates are assumed to be 90%.[33] The operating conditions for the fermentation and the downstream processes, including ethanol recovery and separation, wastewater treatment, and lignin combustion, are consistent with the 2011 National Renewable Energy Laboratory (NREL) report.[34] Glucose to ethanol and xylose to ethanol conversion rates are assumed to be 95 and 85%, respectively. Following the fermentation, 97% of the IL is recovered using a pervaporation system and recycled back to the pretreatment section.[33] Ethanol is recovered through distillation and molecular sieve adsorption. Apart from lignin combustion to generate process heat and electricity (Scenario 1), a lignin-utilization scenario (Scenario 2) is considered for analysis in this study in which lignin is recovered through the centrifugation and subsequent drying processes (Figure 1). The dried lignin (moisture content of 5%) is assumed to be sold for $0.50/kg to a separate facility capable of utilizing lignin for value-added products. According to Bajwa et al., the value of lignin can range between 280 and 500 $/t.[35] In this study, we selected the upper bound of $0.5/kg as an optimistic selling price of lignin because, with the rapid development of chemical and biological/chemical approaches to upgrading lignin, it has the potential to be converted to a range of fuel blendstocks and specialty chemicals, which could increase its value in the near future.

Technoeconomic Analysis. In this study, *SuperPro Designer* v11 is used to develop technoeconomic models. The biorefinery capacity is 2000 dry metric tons (Mg) per day. We used an annual operating time of 7920 h per year (330 days per year and 24 h per day). Bioethanol is the main product from this biorefinery, and two byproducts are produced (electricity in Scenario 1 and lignin and electricity in Scenario 2, Figure 1). Feedstock arriving at the biorefinery was modeled based on an assumed 20% moisture content, although lower moisture contents may be required in practice for some facilities. Following the mass and energy balance analysis, total capital investment (TCI), annual operating cost (AOC), and MESPs were determined. The direct and indirect capital cost factors in this model are consistent with the 2011 NREL report.[34] Piping was assumed to be 4.5% of main installed equipment cost, project contingency is 10% of the direct cost, and working capital is assumed to be 5% of fixed capital investment. Other assumptions impacting the TCI are documented in the SI, Table S3.

AOC consisted of raw materials cost, utility cost, labor cost, and facility-dependent costs, including maintenance, property taxes, and insurance. Apart from biomass feedstock, electricity cost and other raw materials costs were obtained from the previously documented database at JBEI. Historical industrial electricity price was collected from the U.S. Energy Information Agency.[36] Several distributions were considered to determine their best-fit distributions, including normal, lognormal, chi-square, exponential, and logistic distribution. The best-fit distribution was determined by Kolmogorov−Smirnov goodness-of-fit test. Based on the best-fit distributions of historical industrial prices, electricity price is $0.057/kWh (average value) with normal distribution. The results are presented in the SI, Figure S1. The required labors are consistent with the 2011 NREL study.[34] Their corresponding salaries are obtained according to the 2018 labor market price. Additionally, maintenance and insurance are assumed 3 and 0.7% of the installed equipment cost.

Discounted cash flow analysis was used to determine the MESP. The discount rate and plant life were set to 10% and 30 years, respectively. The depreciation method used for analysis in this study was the Internal Revenue Service (IRS) Modified Accelerated Cost Recovery System for both general plant and steam plant. The depreciation rate was based on the IRS Publication 946 on how to depreciate property.[37] Income tax rate was set to 35%. Construction time for this biorefinery was considered to be 36 months, and start-up time was set to 6 months.

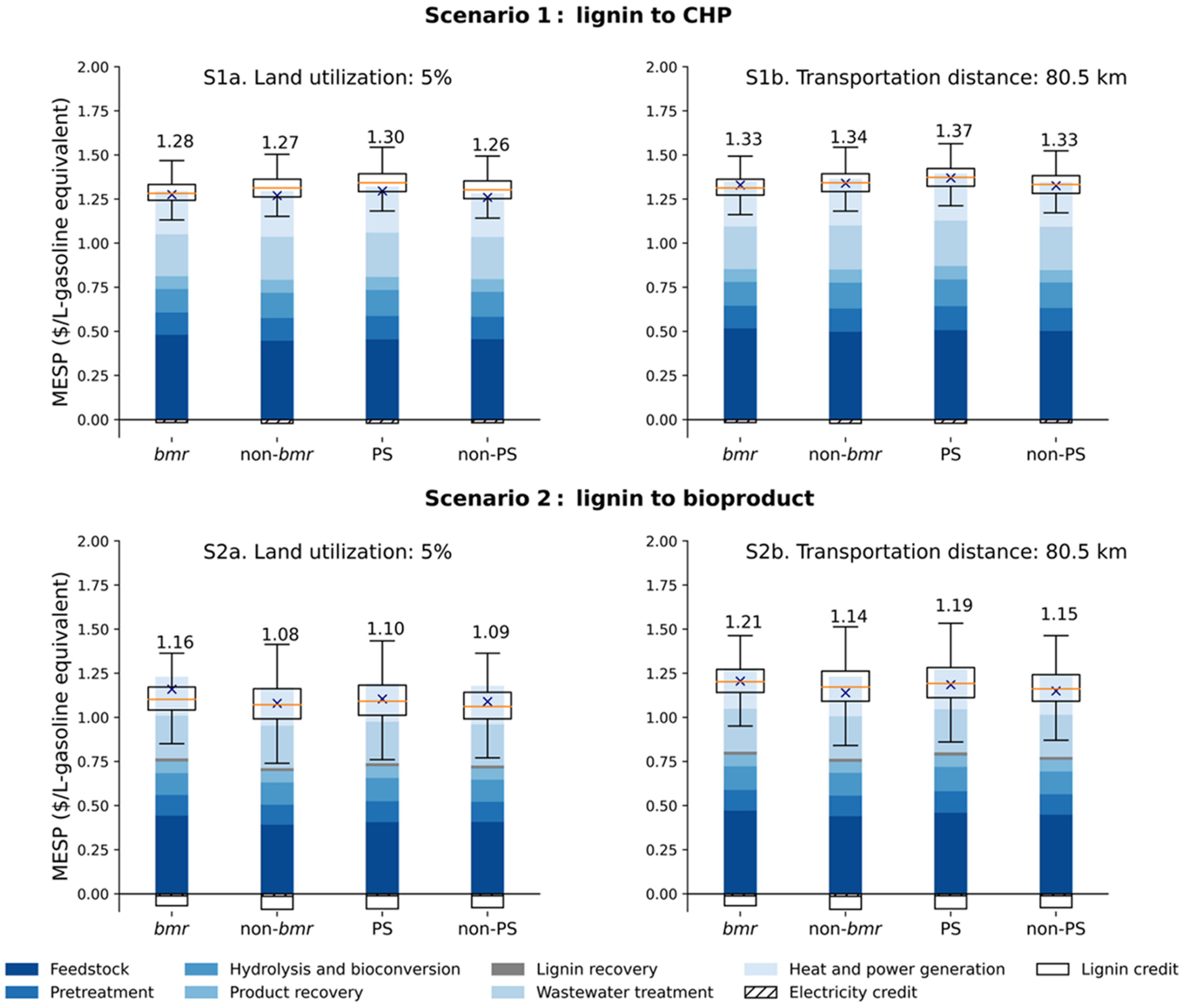

Figure 2. Cost contribution from capital investment and operating costs in both scenarios. Scenario 1 (S1) refers to the lignin combustion for onsite energy generation and Scenario 2 (S2) refers to the lignin utilization as a byproduct. Minimum selling prices of ethanol (MESPs) are shown as the black x in each grouped bar. The box and whisker plots indicate the Monte Carlo simulation results, with the whiskers denoting the maximum and minimum values. Please refer to Table S5 for numerical results.

Sensitivity and Uncertainty Analyses. A key limitation of this study is its reliance on theoretically calculated sugar and fuel yields based on the measured composition of each sorghum variety. For instance, some previous studies have shown that *bmr* sorghum can achieve increased fuel yields relative to non-*bmr* sorghum types.[16,17] Additionally, a single field trial cannot capture the range of yields and composition that would be observed in the national-scale production of forage sorghum for bioenergy. Process parameters can also impact sugar and fuel yields, and these may be adjusted to achieve optimal outcomes for a particular variety; in our study, we have held the process parameters fixed and explored possible variations as part of the sensitivity and uncertainty analysis. A study published recently explored the use of ensiled biomass sorghum and indicated that similar sugar yields could be achieved at half the IL loading required for dry biomass, suggesting that how biomass is handled postharvest also has an impact on sugar and fuel yields.[38] Although not every possible variable can be explored, we conducted Monte Carlo simulations and single-point sensitivity analysis to better understand the influence of process parameters and economic modeling assumptions on the resulting MESP. Single-point sensitivity analyses for each of the lignin-utilization scenarios were conducted to explore the relative influence of each input parameter on the MESP. We also explored the relationship between biomass yield, and its impact on delivered feedstock costs, and MESP. Then, we investigated the impact of major chemical composition (lignin, glucan, xylan, starch, and protein) on final MESPs. In this analysis, we sought to understand the composition of the forage sorghum ideotype. Hence, we used the average data of 18 forage sorghum hybrids as the baseline and altering each composition by ±25 and ±50% while maintaining the fraction of other components constant. In other words, when varying the amount of each composition, other components are reduced or increased proportionally. Monte Carlo simulations were also used to capture uncertainty. In the Monte Carlo simulation, multiple parameters were varied over 5,000 trials. All parameters used for the sensitivity and uncertainty analyses are summarized in the SI, Table S4.

RESULTS AND DISCUSSION

Technoeconomic Analysis Results. Biomass yield per hectare proves to be the primary driver of delivered biomass costs, assuming all other logistics and dry matter losses are similar. Thus, it is not surprising that the logistics model produced higher delivered costs for lower-yielding *bmr* sorghum and lower costs for PS varieties. Based on a 5%

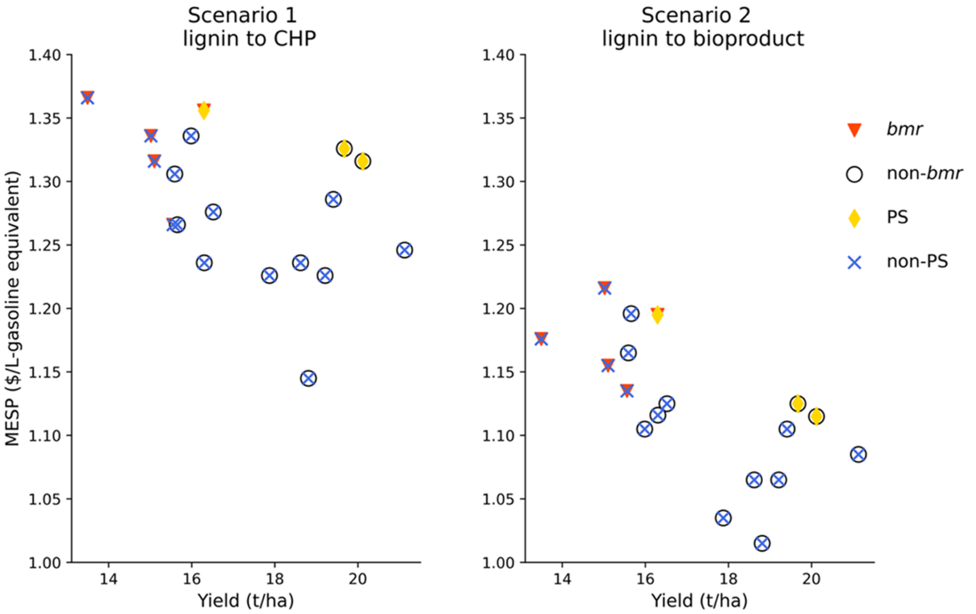

Figure 3. Relationship between minimum ethanol selling price (MESP: $/L-gasoline equivalent) and biomass yield t/ha (Mg ha^{-1}) using four forage sorghum types (18 hybrids) in cellulosic biorefineries. Scenario 1 refers to the lignin combustion for onsite energy generation and scenario 2 refers to the lignin utilization as a byproduct. Results are based on 5% land utilization. Please refer to the SI, Table S6, for numerical results.

land utilization factor surrounding the biorefinery, the average feedstock supply costs at the biorefinery gate are $131, $117, $115, and $122 per dry metric ton for *bmr*, non-*bmr*, PS, and non-PS, respectively. Lower yields mean sorghum must be sourced from a larger area to achieve the same level of supply; the one-way average transportation distances are 61, 56, 55, and 57 km for *bmr*, non-*bmr*, PS, and non-PS, respectively. However, transportation distances are not the only driver of cost differences. The cost of on-farm logistics and some inputs are also higher for lower-yielding varieties on a per-metric ton basis. If the farm-to-biorefinery transportation distance is fixed at 80.5 km (50 miles), the average feedstock supply costs are $141, $130, $128, and $133 per dry metric ton for *bmr*, non-*bmr*, PS, and non-PS, respectively. Corresponding land utilization for *bmr*, non-*bmr*, PS, and non-PS are 2.9, 2.4, 2.3, and 2.5%, respectively within an 80.5 km radius. The remaining question is whether the more favorable composition and fuel yields per-metric ton of *bmr* and non-PS types compensate for their higher delivered feedstock costs.

Figure 2 shows the total MESP for each sorghum type, broken down by key contributors under the lignin onsite combustion scenario (S1) and the lignin-utilization scenario (S2). For each scenario, we generate results based on a fixed land utilization factor of 5%, allowing transportation distances to adjust based on the average yield and required catchment area, and a separate set of results for a fixed farm-to-biorefinery transportation distance of 80.5 km (50 miles). The fixed-distance results eliminate the impact that sorghum yield per unit land area otherwise has on average transportation distances. Scenario 2, where lignin is sold for $0.50/kg as a byproduct for conversion to a high-value product, results in lower MESPs across all sorghum types relative to Scenario 1 (where lignin is combusted onsite for energy).

Most notable in the results (Figure 2) is the fact that MESP variations across sorghum types are small. In S1 (onsite lignin combustion), biorefineries using non-PS sorghum as a feedstock achieve the lowest MESP of $1.26/L-gasoline equivalent in the 5% land utilization case and $1.33/L-gasoline equivalent in the 80.5 km transportation case. In both cases in the SI, however, the gap between the highest- and lowest-cost options is only $0.04/L-gasoline equivalent. PS sorghum has the lowest delivered feedstock cost ($115/t with a fixed land utilization factor and $128/t with fixed transportation distance), but the total ethanol production is lower because PS sorghum has lower carbohydrate content and higher lignin (204 million liters of ethanol in PS-based biorefineries as compared to 223 million liters in *bmr*-based biorefineries). The TCIs in S2 are about $15−20 million higher relative to S1 because of lignin separation and recovery processes. In S2, lignin is modeled as a lucrative coproduct as opposed to a low-value fuel for onsite combustion, so feedstocks with higher lignin content become preferable. As expected, *bmr* sorghum (low-lignin mutants) results in the highest MESPs for S2, exceeding the lowest-cost option by as much as $0.08/L-gasoline equivalent. Biorefineries using non-*bmr* sorghum (the combined average of all non-*bmr* PS and non-PS) lead to the lowest MESP of $1.08/L-gasoline equivalent with 5% land utilization and $1.14/L-gasoline equivalent with 80.5 km transportation distance.

In both scenarios, the utility and wastewater treatment sections are the largest contributor (~20% for each section) to the capital investment (see the SI, Figure S2 for results). In biorefineries processing PS sorghum, less biogas is produced in the wastewater treatment process due to higher ash and extractives contents, which are sent to combustor directly, are reported in PS chemical composition than other forage sorghum varieties (see Table 1 for composition data); despite the highest lignin content in PS type, it requires less capital investment in the utility section (~65 million $ of PS-based biorefineries vs. ~70 million $ of non-PS-based biorefineries). The utility costs in S2 are generally higher than those in S1 because, although less lignin is sent to the turbine-generator for heat and power in S2, the drying unit makes the lignin recovery process more energy intensive. Regardless of the forage sorghum type, materials cost accounts for ~50% of the AOC. Feedstock supply is the largest contributor to the total

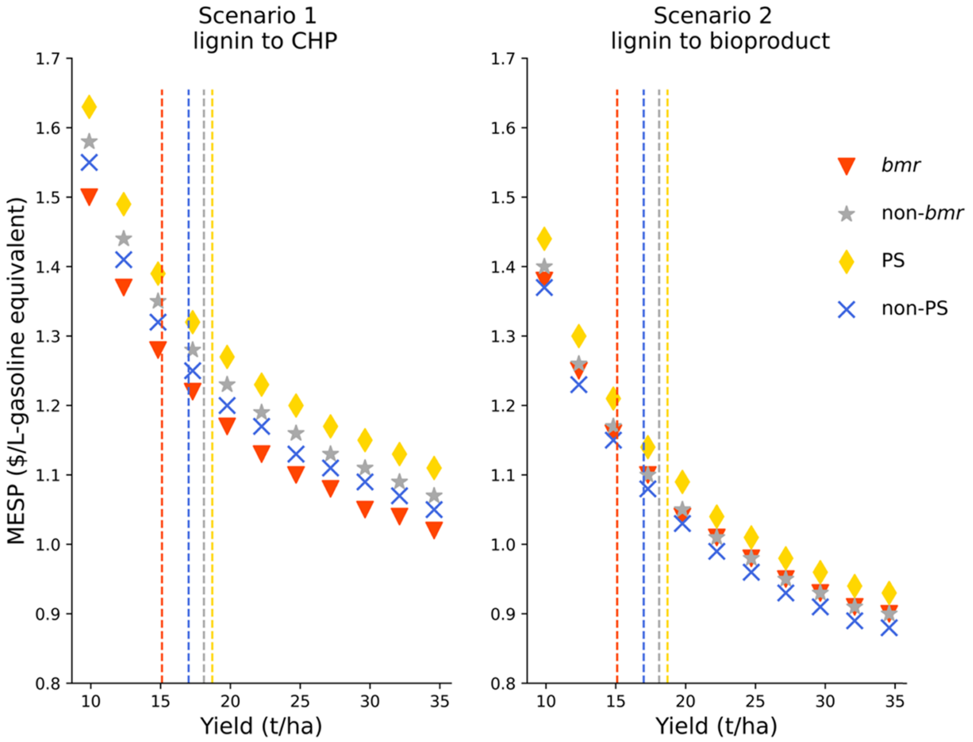

Figure 4. Correlation between forage sorghum yield (t/ha (Mg ha^{-1})) and the minimum selling price of bioethanol (MESP: $/L-gasoline equivalent). Scenario 1 refers to the lignin combustion for onsite energy generation and Scenario 2 refers to the lignin utilization as a byproduct. Vertical dash lines are the reported yield used in this study. Both scenarios are based on 5% land utilization. Please refer to the SI, Table S7, for numerical results.

raw material costs, and *bmr* sorghum results in the largest feedstock supply cost on average due to its lower biomass yield (15.1 t/ha). PS varieties have the lowest carbohydrate content (including cellulose, hemicellulose, starch, and soluble sugars) per unit of incoming biomass, which results in the lowest operating cost in both scenarios for a fixed quantity of incoming biomass, but also translates into lower fuel production per commercial-scale biorefinery. Additionally, the PS type has the highest lignin content resulting in the highest byproduct revenue of 15 million $ in S2 when lignin is sold at $0.5/kg as a byproduct. The *bmr* type has the lowest lignin content; thus, it generates the lowest byproduct revenue of $12 million.

The MESP results for averaged sorghum types shown in Figure 2 suggest that, at least within the varieties compared in the underlying field study, there is not a significant advantage associated with growing PS sorghum for bioenergy, even in an *nth* plant scenario where cellulosic ethanol production is a mature technology. In fact, the lowest MESPs corresponded to the average of non-PS varieties in S1 and non-*bmr* varieties in S2. If all of these four types are supplied at the same price (for instance, $100/t), *bmr* sorghum would result in the lowest MESP in S1 because of its low-lignin trait and the average of non-PS varieties would be lowest cost in S2 (SI, Figure S2). Dahlberg et al.[25] noted that the maturity class of non-PS varieties, while not explored explicitly in this paper, appeared to also have an impact on composition, including sucrose, whole and structural starch, glucan, xylan, and galactan. It is clear that maturity class, along with the PS/non-PS and *bmr*/non-*bmr* distinction, would be worth exploring, particularly in larger field trials with a greater number of hybrids.

By developing specific technoeconomic models of the 18 forage sorghum hybrid samples described in the Materials and Methods section (see the SI, Table S2, for detailed biomass compositions), we were able to better understand how much variation there is across individual varieties that were tested (Figure 3). There is considerable variation in modeled MESP across the different non-PS non-*bmr* varieties and those varieties achieved the lowest MESP in both scenarios, although this result also likely to be tied to sample size (fewer *bmr* and PS varieties were grown in the field trial). The average yield for PS sorghum varieties proved to be higher than non-PS, but the individual results show that one non-PS variety (a late-maturing hybrid) did achieve higher biomass yields than all PS sorghums (refer to the far-right blue data point in Figure 3). However, it is notable that the highest-yielding variety did not result in the lowest cost in either scenario because of its comparatively low carbohydrate content. In an effort to isolate the effects of composition from the effects of yield on MESP, the SI, Figure S4, shows the MESP for S1 and S2 across each sorghum type if the sorghum supply cost is fixed at $100/t (so all cost differences would be attributable to differences in ethanol yield). The sale of lignin for upgrading in S2 resulted in uneven reductions in MESP depending on feedstock composition. When treating lignin as a byproduct rather than burning onsite, selling prices of PS-non-*bmr* sorghum-based ethanol achieve a larger reduction (~$0.25/L-gasoline equivalent) relative to the MESP from the PS-*bmr* type ($0.15/L-gasoline equivalent).

Sensitivity Analysis. We found a relationship between sorghum yield at the field and MESPs ($/L-gasoline equivalent) for both the lignin onsite combustion scenario (S1) and lignin-utilization scenario (S2) (Figure 4). Regardless

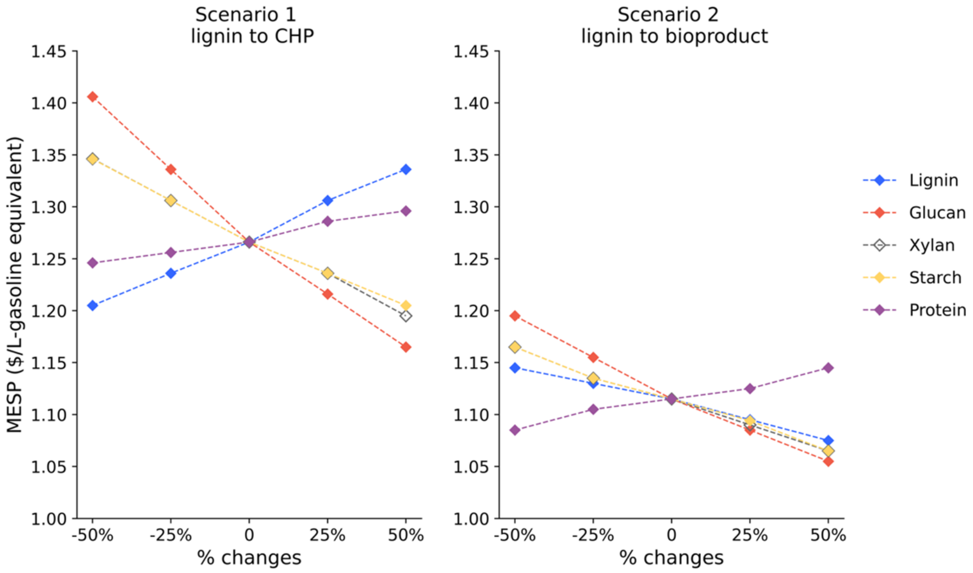

Figure 5. Sensitivity analysis of major chemical composition of forage sorghum to minimum ethanol selling price (MESP). Scenario 1 refers to the lignin combustion for onsite energy generation and Scenario 2 refers to the lignin utilization as a byproduct. Results are based on 5% land utilization. Please refer to the SI, Table S8, for numerical results.

of sorghum types and lignin-utilization scenarios, increasing the forage sorghum yield reduces the MESP. The sorghum biomass yield alters feedstock supply cost by changing the feedstock collection area or supply radius, nutrients input, and cost of field operations. Among four sorghum types, the PS type has the highest yield (yellow dash line in Figure 4), followed by non-*bmr* (gray dash line), non-PS (blue dash line), and *bmr* type (red dash line). In both scenarios, PS-based biorefinery has the highest MESPs because of less sugar accumulated in the plant. The lowest MESPs reported under the same dry matter yield are *bmr*-based biorefineries in S1 and non-PS-based biorefineries in S2. In S2, due to a lower lignin content in *bmr* type, less revenue is earned in the lignin stream in *bmr*-based biorefineries. In addition, increasing the biomass yield from 10 to 35 t/ha results in a similar level of reduction on the MESPs. These results indicate that while compositional differences across different types do impact the MESP, diverting lignin for a higher-value application may have a greater effect on the economics.

To further identify the chemical composition of forage sorghum ideotype applying in cellulosic biorefineries, we conducted a sensitivity analysis of major chemical compositions (glucan, xylan, lignin, starch, and protein content) on MESPs in both scenarios (see Figure 5). We used the average data of the 18 forage sorghum samples described above as the baseline and conducted the sensitivity analysis with both ±25 and ± 50% of the glucan, xylan, lignin, protein, and structural starch to explore their individual impacts on the final MESPs. We find that for both scenarios, glucan is the most sensitive parameter to the final MESPs because glucan makes up a larger fraction of the total biomass than other components (Figure 5 shows a range from $1.17/L-gasoline equivalent to $1.41/L-gasoline equivalent). Starch and xylan content have similar economic impacts in both scenarios, assuming a cofermenting microbial host capable of utilizing pentose sugars. Increasing lignin content, while holding the breakdown of other components constant, results in cost increases in S1 and cost decreases in S2. This indicates that the selling price of lignin in S2 ($0.5/kg assumed in this study) is sufficient to convert it from a net cost driver to a driver of profits. However, even in S2, it is more economically attractive to increase glucan content on a relative basis than it is to increase lignin content. Protein, although favorable in animal feed markets, is not attractive for bioenergy production. However, to our knowledge, there has not been extensive work exploring the benefits of feedstock protein content on the performance of various microbial hosts in biorefineries. The presence of some amino acids may be beneficial to microbial hosts and this is a topic worth further exploration, particularly in the context of sorghum.[39]

In addition to the direct impact of biomass yield to MESPs, the biomass feedstock cost and lignin selling price are the most influential input parameters to MESPs in S1 and S2, respectively. The SI, Figure S5, depicts the single-point sensitivity analysis results for all four sorghum types with two different lignin-utilization scenarios. Following the overall feedstock supply cost, ethanol yield, interest rate, and project contingency (reflected by TCI) are other most influential parameters to MESPs for both scenarios. The glucan to glucose conversion rate is another sensitive parameter to MESPs as the microbe metabolizes glucose more effectively than xylose (glucose is also present as a larger fraction of total dry weight compared to xylose), and this drives the total production of ethanol. That said, there has been a large variation in xylan to xylose conversion rates reported in the literature, and it can have a measurable impact on the price if it is decreased from 90 to 60%.[34] Residence times required for enzymatic hydrolysis, pretreatment, and fermentation are also important as these have impacts on the equipment cost and utility costs. If the hydrolysis time is reduced from 72 to 48 h, the MESP decreases by ~$0.02/L-gasoline equivalent in both lignin-utilization scenarios.

As noted earlier, this study relies on theoretical calculations for glucan to glucose and xylan to xylose yields as well as the same sugar to ethanol conversion rate because there is not yet experimental data available to compare these sorghum types. This may underestimate the advantages of low-lignin *bmr* hybrids. For example, higher ethanol conversion efficiency with *bmr* sorghum varieties relative to other varieties has been demonstrated in some bench-scale experiments.[16,17] Additionally, the presence of inhibitors can result in unexpected effects on fuel yields and this warrants future studies that leverage empirical data collection to explore the sensitivity of sugar and fuel yields across many different varieties under varying process conditions. Finally, additional field trials, paired with empirical testing in a deconstruction and conversion process, can elucidate the impact of maturity class (medium, medium early, medium late, or late) on composition and conversion efficiency, which is an intriguing area of future research.

■ CONCLUSIONS

In this study, we used field trial data combined with technoeconomic analysis for 18 commercially available PS, non-PS, *bmr*, and non-*bmr* sorghum varieties. Although additional field data with a larger sample size might provide greater confidence, these preliminary results suggest that the exclusive focus on high-yielding PS varieties (bioenergy sorghum or biomass sorghum) may not be entirely justified by the available data. Perhaps the most surprising finding is that variations in MESP across averaged sorghum types are relatively small. In Scenario 1 (lignin combustion onsite), the highest and lowest MESPs only differed by $0.04/liter-gasoline-equivalent. The results also suggest that non-PS sorghum varieties may be more economically attractive on average (by a small margin) and particular non-PS non-*bmr* varieties perform substantially better than the PS and *bmr* varieties included in this study. In Scenario 2, where lignin is sold as a coproduct for conversion to high-value products, the difference between the highest and lowest MESPs widens slightly to $0.08/L-gasoline equivalent. In this case, low-lignin *bmr* sorghum varieties are at a disadvantage because of their combination of low lignin content and lower yield. An important caveat in this study is that all sugar and ethanol yields are based on simulations using compositional data collected as part of the field study. We have also not attempted to analyze scenarios in which the grain is harvested separately and sold as food or feed, although the flexibility to earn revenue from multiple markets may be attractive to farmers. Future research is required to explore the impacts of a wider set of sorghum samples and gather empirical data on the impacts of composition on saccharification and fuel yields, ideally for a range of process conditions and microbial hosts.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.1c01706.

> The Supporting Information includes tables of chemical compositions of the forage sorghum explored in this study, tables of input parameters used for technoeconomic modeling and uncertainty analyses, tables of numerical results for each figure in the Results and Discussion section, MESPs under a fixed biomass supply cost, and sensitivity analyses results (PDF)

■ AUTHOR INFORMATION

Corresponding Author

Corinne D. Scown − *Joint BioEnergy Institute, Emeryville, California 94708, United States; Biological Systems and Engineering Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States; Energy Analysis and Environmental Impacts Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States; Energy & Biosciences Institute, University of California, Berkeley, Berkeley, California 94720, United States;* orcid.org/0000-0003-2078-1126; Email: cdscown@lbl.gov

Authors

Minliang Yang − *Joint BioEnergy Institute, Emeryville, California 94708, United States; Biological Systems and Engineering Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States; Energy Analysis and Environmental Impacts Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States;* orcid.org/0000-0002-4670-7947

Jeff Dahlberg − *Joint BioEnergy Institute, Emeryville, California 94708, United States; University of California Agricultural and Natural Resources—Kearney Agricultural Research & Extension Center, Parlier, California 93648, United States*

Nawa Raj Baral − *Joint BioEnergy Institute, Emeryville, California 94708, United States; Biological Systems and Engineering Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States;* orcid.org/0000-0002-0942-9183

Daniel Putnam − *Joint BioEnergy Institute, Emeryville, California 94708, United States; Department of Plant Sciences, University of California, Davis, Davis, California 95616, United States*

Complete contact information is available at: https://pubs.acs.org/10.1021/acssuschemeng.1c01706

Notes

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