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ANALYSIS

An optimization-based assessment framework for biomass-to-fuel conversion strategies†

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We develop a framework for the identification and evaluation of biomass-to-fuel production strategies. We generate a *technology superstructure* that consists of a wide range of conversion technologies along with the corresponding feedstocks, intermediates, and final products. The superstructure includes both known technologies as well as technologies that can be developed based on results available in the literature. Technical (yields and energy requirements) and economic (production cost) parameters, for both existing and potential new technologies, are calculated from the literature or estimated using a systematic approach. The superstructure along with the associated data is used to develop optimization models which allow us to identify and evaluate new and existing biofuel strategies as well as to perform sensitivity analyses and identify the major cost drivers of these strategies. The proposed framework can be used to study a range of interesting questions: *What is the best strategy for the production of a specific fuel? What is the best utilization strategy for a specific feedstock?* We illustrate our methodology using the production of ethanol from hard woody biomass as a case study.

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Broader context

While advances in fundamental research have resulted in the development of large number of biomass-to-fuel processing and conversion technologies, it is still unclear what mix of products would make biofuel production economically viable; and even for a given set of final products, it is unknown which chemistries and what types of conversion technologies should be integrated and how. Accordingly, to speed the development of a competitive, integrated biorefinery, we develop a system-level methodology for the synthesis and evaluation of a wide range of biomass-to-fuel strategies. In particular, we generate a *biomass utilization superstructure* (BUS) which consists of a wide range of conversion technologies along with the corresponding feedstocks, intermediates, and final products; and we develop optimization models for the evaluation of the embedded strategies using alternative criteria. Our framework establishes a methodology and suite of tools for the systematic comparison of biofuel strategies, the identification of the major technology gaps and cost drivers, and the assessment of the impact of technology uncertainty.

1 Introduction

Currently, most chemicals and energy carriers are derived from fossil fuels.[1] The demand for transportation fuels, which accounts for nearly 25% of the total net primary energy and 70% of the energy provided by petroleum,[2] is expected to increase, while oil prices are also expected to remain high due to strong demand in the developing world. To meet this challenge, it is necessary to increase energy supplies through the development of renewable and alternative energy sources. Biomass, the only renewable source of carbon-based fuels, offers promising alternatives to satisfy energy demand while reducing the environmental impact.[3,4] Furthermore, biomass resources are widely abundant.[5] In the last few decades, many technologies have been developed to produce biomass-derived chemicals[6–8] and fuels[9–15] through the formation of platform chemicals[16,17] (see Huber *et al.*[18] for a review).

A large number of studies focuses on the economic assessment of biomass-to-fuel strategies that rely on biochemical,[19–24] catalytic[25,26] or thermochemical (pyrolysis[27,28] and gasification[29–32]) technologies utilizing a range of biomass alternatives[33] including energy crops[34] and biomass wastes.[35–38] Also, researchers have explored improvements *via* the optimization of energy[39] and water consumption,[40] and waste treatment systems,[41] as well as the integration of new strategies with existing infrastructure.[42,43] It is envisioned that the conversion of biomass to fuels, chemicals and power will take place in an integrated facility, the *biorefinery*.[44–46] Several review papers on the design and analysis of biorefineries are available in the literature.[1,47,48] Finally, a number of studies, primarily in the field of *industrial ecology*, focus on the analysis of the environmental impact of biofuel strategies.[49–53]

Despite the large number of system-level analyses in the literature, there are limited methods available for (i) the

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identification (and assessment) of new biofuel production strategies, and (ii) the simultaneous assessment and comparison of alternative strategies. Most technology assessment studies in the literature focus on specific systems, *i.e.*, systems with a specified feedstock, series of conversions, and final products. Accordingly, the goal of this paper is the development of a systematic framework for the identification and assessment of biofuel strategies, which can be used to study a wide range of questions. In developing this framework, we first generate a biomass utilization superstructure (BUS), which includes more than 170 technologies and 120 compounds (Section 2). Second, we evaluate technical and economic parameters for the technologies; parameters for existing technologies are obtained from the literature, whereas those for new technologies are estimated based on similar existing technologies (Section 3). Third, we develop network optimization (linear programming and mixed-integer programming) models for the underlying superstructure (Section 4). Based on these models, we discuss methods to generate alternative strategies, identify bottlenecks and technology gaps, and perform sensitivity analyses (Section 5). Finally, in Section 6, we use our framework to study the production of ethanol from hard woody biomass.

2 Biomass utilization superstructure

2.1 Technologies

Biomass can be converted to fuels, fuel additives, and chemicals *via* multiple production strategies, where each strategy starts from a biomass feedstock and through a series of conversion technologies leads to the production of one or more targeted fuel(s). We develop a technology superstructure that consists of all major conversion technologies and the corresponding compounds, thus embedding all potential strategies. To simplify the representation, we group similar *technologies* into *technology groups*, as shown in Fig. 1.

To generate the superstructure, we performed an extensive review of the literature. In some cases, research papers describing a single conversion technology were used while in other cases we studied papers that describe integrated production systems. In the latter case, we divided the known systems into a series of technologies. For instance, the production of *ethanol* from *corn stover* is decomposed into three technologies, *dilute acid pretreatment*, *enzymatic simultaneous saccharification and fermentation (SSF)*, and *distillation* with two

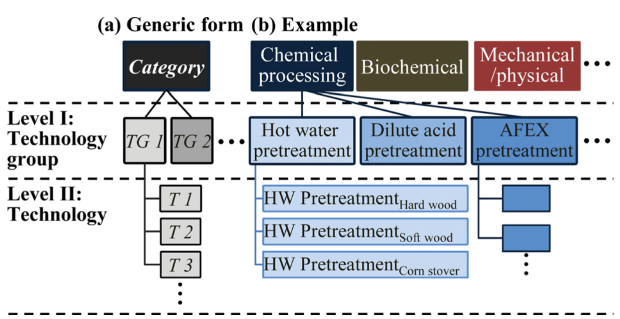

Fig. 1 Technology groups (for superstructure representation) and technologies.

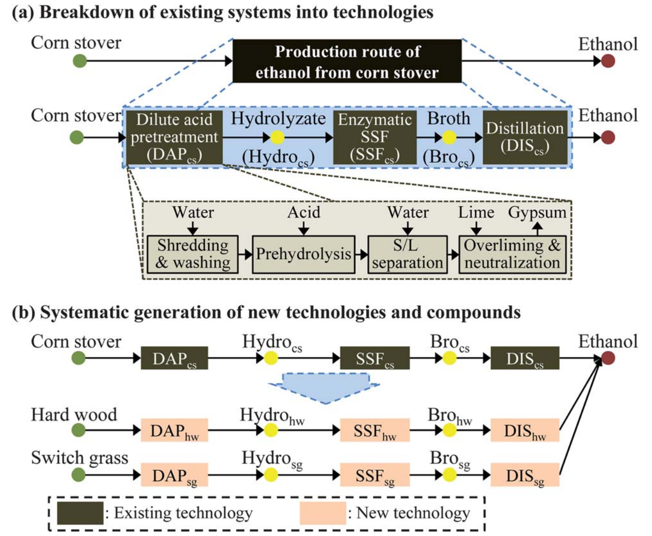

Fig. 2 (a) Breakdown of a production system into a series of technologies and (b) systematic generation of new technologies and compounds utilizing different feedstocks.

corresponding intermediates, *hydrolyzate* and *broth* as shown in Fig. 2a.

It is important to stress here that each technology does not correspond to a single operation. For example, *dilute acid pretreatment* (DAP_{cs}) includes four operations: (i) shredding and washing, (ii) prehydrolysis, (iii) S/L separation, and (iv) overliming and neutralization (see Fig. 2a). Thus, although each technology is treated as a block, the calculation of its technical and economic parameters is based, as we discuss in Section 3, on detailed modeling of the individual operations comprising a technology, the intra-technology streams, and the corresponding operational costs (including

Table 1 Major technology groups in each category; number of technologies in each group in parentheses

Category	Technology group[a]
Mechanical/ physical	Handling and drying (9), milling and shredding (6), liquefaction (2), syngas, conditioning (4), distillation (22), pervaporation (18), residue separation (12), residue treating (2), residue upgrading (1), hydrolyzate conditioning (12), extraction (1)
Biochemical	Acidic fermentation (10), SSF (12)
Chemical	Dilute acid pretreatment (5), hot water pretreatment (5), AFEX pretreatment (5), hydrolysis (10), acidic treatment (6), syngas production (4), MeOH synthesis (2), acetic acid production (1), MTG process (1), hydrogenation (1), glycerol upgrading (1), FT synthesis (1), hydrogen production (3), hydrocracking (1), esterification (1)
Thermochemical	Gasification (10), pyrolysis (5), power generation (14)

[a] AFEX: ammonia fiber expansion, FT: Fischer–Tropsch, MeOH: methanol, MTG: methanol to gasoline, SSF: simultaneous saccharification and fermentation.

Table 2 Major compound groups in each compound category; number of compounds in each group in parentheses

Category	Compound group[a]
Feedstock (biomass)	Soybean (1), corn (1), sugarcane (1), bagasse (1), corn stover (1), hard wood (1), soft wood (1), switch grass (1)
Intermediate	Chopped particle (5), slurry (24), hydrolyzate (12), triglycerides (1), broth (24), glycerol (1), chopped dry corn (1), steeped wet corn (1), glycerol (1), cane juice (1), levulinic acid (1), syngas (2), methanol (1), GVL (1), raw acetic acid (1), bio-oil (7), butene (1), solid (16)
Final product (biofuels)	Gasoline (1), diesel (1), bio-diesel (1), FT-fuels (1), ethanol (1), butanol (1), DBK (1), SNG (1), hydrogen (1), ethyl levulinate (1), fuel additives (1), mixed alcohol (1)
By-product	Electricity (1), DDGS (1), gluten (1), xylose (1), formic acid (1), acetic acid (1)

[a] DBK: 5-nonanone; DDGS: dried grains with soluble; FT: Fischer–Tropsch; GVL: γ-valerolactone; SNG: synthesized natural gas.

utility, wastewater, and material costs). An example illustrating the development of technology models is presented in the ESI.†

If alternative feedstocks are used, then the composition of the compounds and the yields will be different, so new technologies and compounds should be introduced. For example, we generate two alternative technologies, DAP_{hw} and DAP_{sg}, which utilize *hard wood* and *switch grass* feedstocks, respectively, based on the existing technology utilizing *corn stover*. In this case, intermediate compounds $Hydro_{hw}$ and $Hydro_{sg}$ are also generated for the new technologies (see Fig. 2b).

We classify technologies into four categories according to their processing characteristics:[54]

• *Mechanical/physical*: a compound is separated or its size is reduced without changes in its chemical structure.

• *Biochemical*: microorganisms or enzymes are used for the conversion.

• *Chemical*: a compound is transformed at mild pressure and temperature.

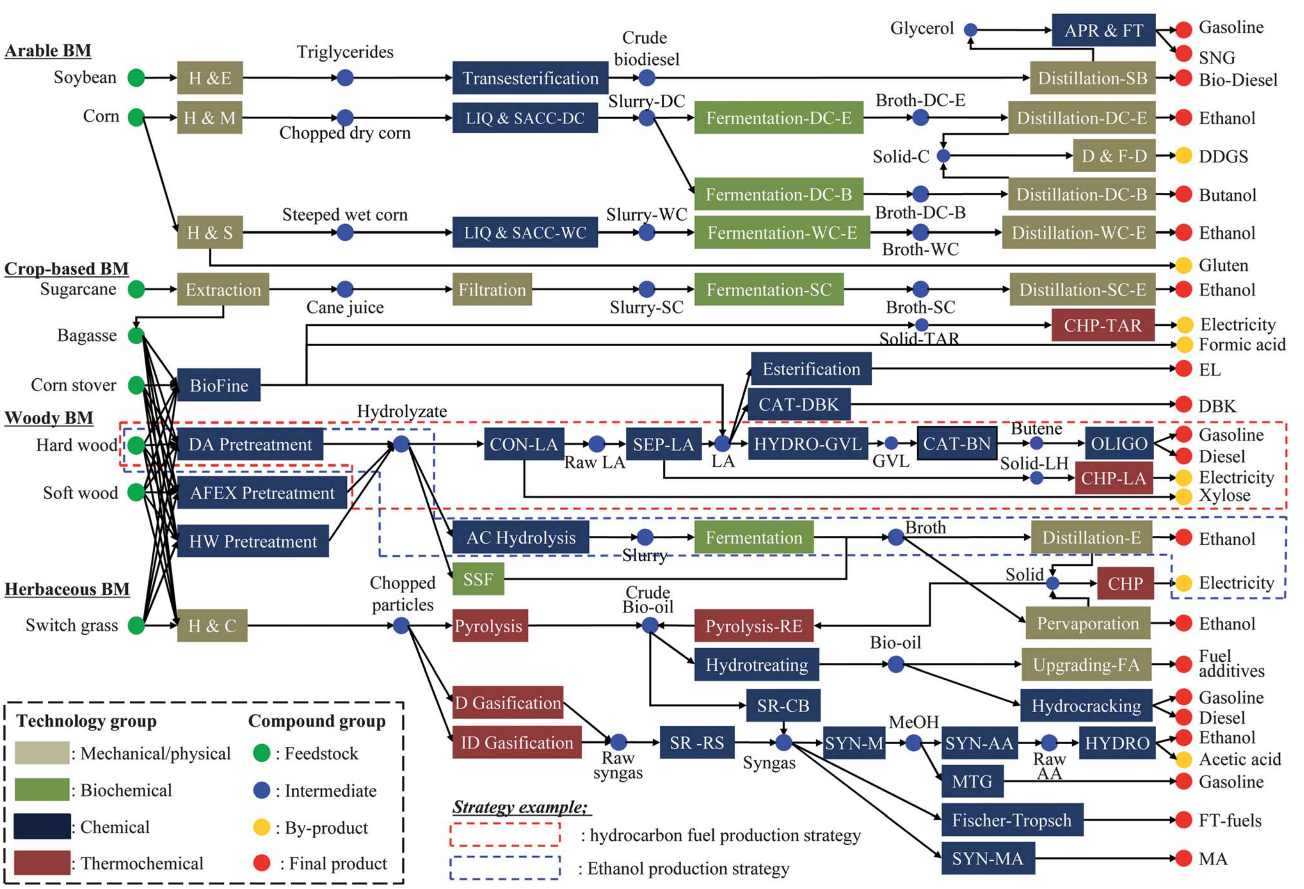

Fig. 3 Biomass utilization superstructure; representation based on technology and compound groups. *Technologies*. AC: acidic, AFEX: ammonia fiber expansion based pretreatment, APR: aqueous phase reforming, CAT: catalytic conversion technology, CHP: combined heat and power generation, CON: conditioning, D: direct, DA: dilute acid, D&F: drying and filtering, FT: Fischer–Tropsch, HW: hot water, HYDRO: hydrogenation, H&C: handling and chopping, H&E: handling and extraction, H&M: handling and milling, H&S: handling and steeping, ID indirect, LIQ and SACC: liquefaction and saccharification, MTG: methanol to gasoline technology, OLIGO: oligomerization, SEP: separation, SR: steam reforming, SSF: simultaneous saccharification and fermentation, SYN: chemical synthesis technology. *Compounds*. AA: acetic acid, AL: alkanes, B: butanol, BM: biomass, BN: butene, BO: bio-oil, C: corn, CB: crude bio-oil, DBK: dibutyl ketone, DC: dry corn, DDGS: dried grains with soluble, E: ethanol, EL: ethyl levulinate, FA: fuel additives, GVL: γ-valerolactone, LA: levulinic acid, LH: lignin and humans, M: methanol, MA: mixed alcohols (ethanol, propanol, butanol and pentanol), RS: raw syngas, SB: soybean, SC: sugarcane, SNG: synthesized natural gas, TAR: tar residue, WC: wet corn.

- *Thermochemical*: extreme temperature and pressure conditions are used for the conversion.

Table 1 shows the major technology groups of each category and the number of technologies included in each technology group.

2.2 Compounds

Compounds are classified into four categories; biomass feedstocks, intermediates, final products (fuels or fuel additives) and by-products. Feedstock composition varies regionally, while the composition of intermediates and final products depends on the technology they are produced from and the composition of the input compound. Compounds are also grouped into *compound groups*, as shown in Table 2. The BUS includes 8 feedstocks, 18 compound groups for intermediates, 6 by-products, and 12 final products. Note that we also consider compounds which can be upgraded (blended) to value-added fuels such as ethyl levulinate.

2.3 Biomass utilization superstructure generation

Based on an extensive search of the literature and the systematic generation of alternative technologies described in subsection 2.1, we formulated a superstructure that consists of 172 technologies and 125 compounds. A complete technology list is given in the ESI,† along with the references that were used to evaluate the associated parameters. Fig. 3 shows the same superstructure represented using technology and compound groups. Note that feedstocks can be converted to fuels in multiple ways and, in general, a fuel can be produced by multiple feedstocks. For example, the compound group *hydrolyzate* (which can be produced from different feedstocks through different pretreatment technologies) can be used to produce ethanol through a combination of hydrolysis and fermentation or it can be used to produce liquid hydrocarbon fuels through catalytic conversion technologies.

3 Parameter evaluation

The methodology for evaluating technical and economic parameters for existing and new technologies is outlined in Fig. 4.

3.1 Existing technologies

3.1.1 Technical parameters. As discussed in subsection 2.1, a detailed process model was developed for each technology in order to calculate two key parameters, the product yield(s) (the mass ratio of product over primary reactant) and energy requirement (kW per unit processing rate), which are then used to develop a simple block technology model in the superstructure. The detailed models used for the calculation of these parameters consider the consumption of auxiliary inputs, such as makeup water, enzymes, solvents and catalysts, as well as the consumption of utilities. However, since auxiliary inputs do not appear as compounds in the final superstructure, they are not included in the calculation of yields. The generation of detailed technology models based on the literature is illustrated in the ESI† through an example.

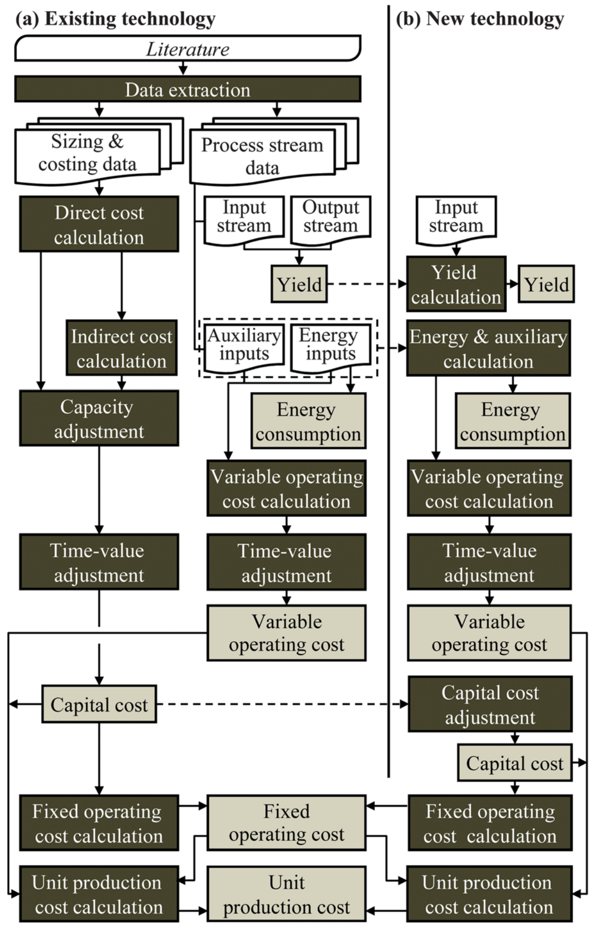

Fig. 4 Procedure for evaluation of technical and economic parameters for (a) existing and (b) new technologies; dark boxes denote evaluation tasks, light boxes represent parameters.

3.1.2 Economic parameters. The main economic parameter is the unit production cost, which has capital and operating cost components. The capital cost consists of direct costs, which include equipment, installation, piping and instrumentation costs, and indirect costs, which include engineering and construction costs, fees and tax, and project contingency costs. Based on sizing and costing data, direct costs are estimated using the installation factors given in Table S7 of the ESI† and the total capital cost is estimated using the project investment factors given in Table S8.† To compare the economics of different strategies accurately, we adjust the capacity of all technologies. Specifically, we consider capacities that would be suitable for a plant that processes 2000 dry tons of biomass per day based on *benchmark* reports in the literature.[55] In other words, the first technology in a strategy utilizes 2000 dry tons of biomass per day as input and the capacities of the following technologies are modified accordingly. The capacity-adjusted capital cost, C_p, is estimated using a power-law expression,

$$C_p = C_{po}(Q/Q_o)^a \quad (1)$$

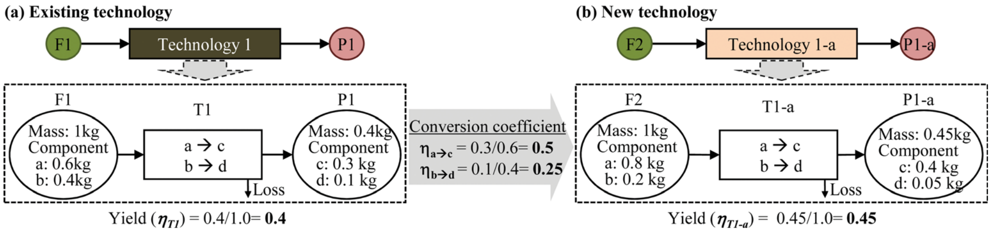

Fig. 5 Yield estimation of a new technology from component-based conversion coefficients of an existing technology.

where C_{po} is the capital cost of the baseline design, Q is the adjusted capacity, Q_o is the capacity of the baseline design and a is the scaling exponent, which is assumed to be 0.67.[22]

The amortized capital cost, ACC, is then calculated with time-value adjustment,

$$ACC = \varepsilon \times CCF \times C_p \tag{2}$$

Table 3 Technical and economic parameter ranges for the major technology groups[a]

	Reactant	Product	Yield	Production cost ($ per kg)	Energy requirement (kW h kg^{-1})
Mechanical/physical					
Handling and drying	Lignocellulosic	Dried BM	0.54–0.80	0.01–0.03	<0.01
Milling and shredder	Lignocellulosic	Shredded BM	0.67–1.16	<0.01	0.02–11.98
Liquefaction	Corn powder, slurry	Liquefied mash	1.59–2.67	0.01	<0.01
Syngas conditioning	Raw syngas	Syngas	0.55–0.63	0.05–0.07	0.01–0.07
Distillation	Broth, fermented mash	Ethanol	0.01–0.11	0.09–0.36	<0.01
Pervaporation	Broth, fermented mash	Ethanol	0.02–0.05	0.20–0.46	656.7–983.3
Residue separation	Residue	Lignin	0.63–0.71	<0.01	<0.01
Residue treating	Residue	DDGS	0.04–0.14	0.14–0.44	8.87–21.40
Residue upgrading	Residue	Raw bio-oil	0.25–0.27	0.15	944.20
Hydrolyzate conditioning	Hydrolyzate	Treated solid	0.98–1.02	<0.01	1.01–1.24
Extraction	Soybean	Triglyceride	1.05	0.01	<0.01
Biochemical					
Fermentation	Liquefied mash	Broth	0.56–1.11	<0.01	0.01–0.02
Enzymatic SSF	Hydrolyzate	Broth	0.95–1.03	<0.01	12.05–37.48
Thermochemical					
Gasification	Dried biomass	Raw syngas	0.84–1.19	0.02–0.03	0.06–0.08
Pyrolysis	Dried biomass	Raw bio-oil	0.75–0.77	0.02–0.03	1.74–1.83
Power generation[b]	Residue	Electricity	0.25–1.93	0.05–0.09	144.6–245.4
Chemical					
Dilute acid pretreatment	Lignocellulosic	Hydrolyzate	3.12–3.24	0.01–0.02	61.52–94.84
Hot water pretreatment	Lignocellulosic	Hydrolyzate	4.08–4.24	0.01	89.11–109.33
AFEX pretreatment	Lignocellulosic	Hydrolyzate	3.39–3.41	0.01	52.39–68.02
LA-hydrolysis	Lignocellulosic	Levulinic acid	0.12–0.15	0.01	0.08–0.10
Acidic treatment	Hydrolyzate	Acidic slurry	0.98–1.02	<0.01	1.01–1.25
Syngas production	Raw syngas	Syngas	0.54–0.63	0.05–11.22	0.02–0.07
MeOH synthesis	Syngas	Methanol	0.86–0.93	0.04–0.07	0.02–0.06
AA production	Methanol	Acetic acid	1.81	0.19	0.015
MTG process[c]	Methanol	Gasoline	0.32	0.25	0.21
		Diesel	0.12		
Hydrogenation	Acetic acid	Ethanol	0.76	0.26	<0.01
Glycerol upgrading[c]	Glycerol	Gasoline	0.20	0.01	0.27
		Diesel	0.06		
FT synthesis[c]	Syngas	Gasoline	0.13	0.46	0.67
		Diesel	0.05		
H_2 production	Syngas, bio-oil	Hydrogen	0.02–0.07	0.53–8.97	0.59–21.40
Hydrocracking[c]	Bio-oil	Gasoline	0.41	0.16	132.80
		Diesel	0.18		
Esterification	Triglyceride	Crude biodiesel	1.1	0.02	<0.01

[a] Abbreviations given in Fig. 3. [b] The units of yield and production cost are given in terms of kW h kg^{-1} of reactant and $ per kW h, respectively. [c] The costs are calculated based on the main product (*e.g.*, gasoline).

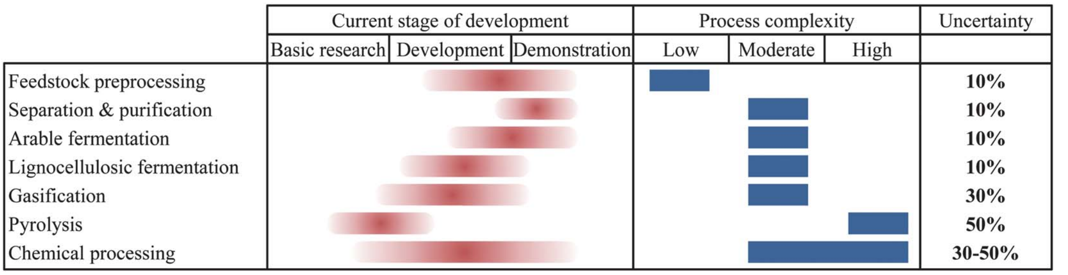

Fig. 6 Production cost uncertainty based on technology maturity and complexity.[56,57]

where ε is the time-value adjustment factor, and CCF is the capital charge factor,

$$\mathrm{CCF} = \frac{r(1+r)^n}{(1+r)^n - 1} \tag{3}$$

where r is the interest rate and n is the lifetime of the plant, which are 10% and 20 years, respectively; thus the CCF is 0.1175.

The operating cost (OC) consists of fixed and variable costs. The fixed operating cost includes labor charges, overhead, maintenance, and general and administration costs; these sub-items are assumed to be a percentage of the capital cost as shown in Table S9 of the ESI.† The variable operating cost accounts for auxiliary inputs and utilities including steam and electricity as well as waste treatment costs. The reference year is 2007 (see Table S10 of the ESI† for the time-value index factor).

Finally, the unit production cost (UPC) of a technology is calculated based on the capital and operating costs as well as the annual production rate (APR) of that technology,

$$\mathrm{UPC} = \frac{\mathrm{ACC} + \mathrm{OC}}{\mathrm{APR}} \tag{4}$$

The detailed methods for the calculation of UPC are described in the ESI.†

3.2 New technologies

3.2.1 Technical parameters. The yields of new technologies are estimated using component-based conversion coefficients of existing technologies, as shown in Fig. 5. For instance, technology T1 converts 1 kg of F1, consisting of components a and b, to 0.4 kg of P1. Based on the conversion coefficients of components a and b (for conversions $a \rightarrow c$ and $b \rightarrow d$), we calculate the yield of new technology T1-a with feed F2. In other words, the yield of a new technology is estimated based on the composition of the input compound. The feedstock compositions considered in this study are given in Tables S11 and S12 in the ESI.†

3.2.2 Economic parameters. The capital cost, C_n, of a new technology is,

$$C_\mathrm{n} = C_\mathrm{p}(R_\mathrm{n}/R_\mathrm{p})^a \tag{5}$$

where C_p is the capital cost of the existing technology, R_p is the amount of reactant in the existing technology, and R_n is the amount of reactant in the new technology. Similarly, operating costs are estimated based on the mass ratio of the reactants in the new and existing technologies ($R_\mathrm{n}/R_\mathrm{p}$), assuming that the consumptions of energy and auxiliary materials are generally proportional to the amount of feed. Ranges for the technical and economic parameters for the major technology groups are shown in Table 3.

3.3 Technology uncertainty

While we have tried to estimate production costs for industrial scale production accurately, there is still a significant amount of uncertainty in the projected production cost of most technologies in the BUS, since most of them are still in their infancy. In general, the level of uncertainty depends on the maturity and complexity of a technology, as well as the quality of information we found in the literature.[27] To address this shortcoming, we quantified the uncertainty in production cost based on the following indicators:

- *Process maturity*: we consider three levels: basic research, development, and demonstration; technologies at a later stage have lower uncertainty.
- *Process complexity*: we consider three levels: low, moderate, and high; a higher level results in higher uncertainty.

Based on these indicators, each technology is assigned an uncertainty level (see Fig. 6). We use three levels: low (10%), intermediate (30%) and high (50%). In Section 5, we show how these levels can be used for the analysis and comparison of different strategies. Note that the uncertainty we consider here is in addition to the uncertainty that is typically considered through the addition of contingencies to the indirect cost.

4 Optimization models

To identify promising strategies, we develop a linear programming (LP) model based on the network representation of the BUS and the parameters we evaluate. Technologies and compounds are represented as nodes; consumption and production of compounds by technologies, as well as feedstock purchases and final product sales, are represented as arc flows[58] (see Fig. 7). We use uppercase bold letters to represent sets, lowercase italics for set indices, uppercase italics for variables, and lowercase Greek characters for parameters.

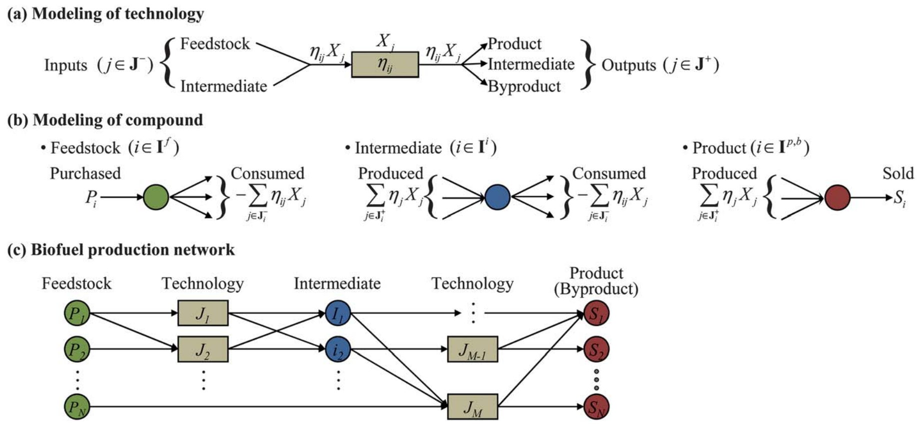

Fig. 7 Representation of the network-based model.

The model consists of:

(i) A set of compounds, $i \in \boldsymbol{I}$; $\boldsymbol{I}^{\mathrm{F}}$, $\boldsymbol{I}^{\mathrm{I}}$, $\boldsymbol{I}^{\mathrm{P}}$ and $\boldsymbol{I}^{\mathrm{B}}$ are the subsets of feedstocks, intermediates, products, and by-products, respectively; λ_i, φ_i, γ_i, δ_i, and ω_i are the compound price, heating value, minimum purchase and availability (for feedstocks), and demand (for products), respectively.

(ii) A set of technologies, $j \in \boldsymbol{J}$, with capacity β_j; $\boldsymbol{J}_i^+$ and $\boldsymbol{J}_i^-$ are the subsets of the technologies that produce and consume, respectively, compound i; ρ_j, and υ_j are the unit production cost and unit energy requirement, respectively; and η_{ij} is the yield of compound i in technology j ($\eta_{ij} < 0$ for inputs and $\eta_{ij} > 0$ for outputs).

We introduce three nonnegative continuous variables:

(i) X_j: production level of technology j.

(ii) P_i: amount of feedstock, $i \in \boldsymbol{I}^{\mathrm{F}}$, purchased.

(iii) S_i: amount of product/by-product, $i \in \boldsymbol{I}^{\mathrm{P}} \cup \boldsymbol{I}^{\mathrm{B}}$, sold.

Compound material balance: the purchases and production (incoming flows) of a compound should be equal to its sales and consumption (outgoing flows):

$$P_i + \sum_{j \in \boldsymbol{J}_i^+} \eta_{ij} X_j = S_i - \sum_{j \in \boldsymbol{J}_i^-} \eta_{ij} X_j, \quad \forall i \tag{6}$$

Technology capacity: the production level of each technology is bounded by its capacity:

$$X_j \le \beta_j, \ \forall j \tag{7}$$

Demand satisfaction: demands for final products should be satisfied:

$$S_i \ge \omega_i, \ \forall i \in \boldsymbol{I}^{\mathrm{P}} \tag{8}$$

Feedstock availability and minimum purchase: feedstock purchase is upper bounded by its availability and lower bounded by a minimum purchase amount:

$$\gamma_i \le P_i \le \delta_i, \ \forall i \in \boldsymbol{I}^{\mathrm{F}} \tag{9}$$

Eqns (6) and (7) are common constraints in all LP models, while the inequalities in eqns (8) and (9) are selectively used according to the type of question we seek to address. For example, the minimum purchase inequality in eqn (9) is used in problems where our goal is to identify strategies utilizing a specific feedstock.

Strategy evaluation can be performed using various criteria. For example, the objective function in eqn (10) seeks the strategy that leads to the minimum production cost (for the production of a fixed amount of a targeted fuel),

$$\min Z_1 = \sum_{i \in \boldsymbol{I}^{\mathrm{F}}} \lambda_i P_i + \sum_j \rho_j X_j - \sum_{i \in \boldsymbol{I}^{\mathrm{B}}} \lambda_i S_i \tag{10}$$

If our goal is to find the strategy with the minimum energy consumption (for the production of a fixed amount of a targeted fuel), then we use the following objective function:

$$\min Z_2 = \sum_j \upsilon_j X_j \tag{11}$$

Finally, the strategy that leads to the maximum profit can be expressed as follows,

$$\max Z_3 = \sum_{i \in \boldsymbol{I}^{\mathrm{P}} \cup \boldsymbol{I}^{\mathrm{B}}} \lambda_i S_i - \sum_{i \in \boldsymbol{I}^{\mathrm{F}}} \lambda_i P_i - \sum_j \rho_j X_j \tag{12}$$

Other objective functions that can be used include the maximization of fuel production (from a given amount of a specified feedstock) and the minimization of environmental impact as well as other life cycle assessment metrics.

5 Strategy identification and analysis

Using the equations of the previous section, we can formulate different optimization models to address different types of questions. For example, we can formulate models to find different strategies for the production of a specific fuel, or strategies that are based on a specific feedstock. This is accomplished by carefully selecting the equations included in the LP model and the corresponding parameters. Also, for each type of question, we can use different assessment criteria (*i.e.*, objective functions). In the next subsections, we present a few examples, but we stress that our framework can be used as the basis for the formulation of multiple models to address a large number of questions. A model is denoted by $\boldsymbol{M_{qc}}$, where q is the type of question and c the assessment criterion.

5.1 Identification of the optimal strategy

5.1.1 Question 1: optimal production strategy for a given product. The first question we consider is the identification of the optimal strategy for the production of a specific product, $i' \in \boldsymbol{I}^{\mathrm{P}}$. This includes the selection of the feedstock to be used as well as the technologies to be employed. To address this question, we formulate a model where the demand of fuel i' is equal to 1, all other fuels have zero demand, and the availability of all feedstocks is unlimited, so that all strategies can be chosen. If the assessment is based on the minimization of cost (objective Z_1), then we formulate model $\boldsymbol{M_{11}}$: min $\{Z_1$: eqns (6)–(9), with $\omega_{i'} = 1$; $\omega_i = 0$ if $\boldsymbol{I}^{\mathrm{P}} \ni i \neq i'$; $\gamma_i = 0$, $\delta_i = M$, $\forall i \in \boldsymbol{I}^{\mathrm{F}}\}$, where M is a sufficiently large number.

The solution of $\boldsymbol{M_{11}}$ yields feedstock purchase, P_i, and technology production levels, X_j, from which we can construct the optimal strategy.

5.1.2 Question 2: optimal utilization strategy for a given feedstock. In this case, we want to identify the best way to utilize a specific feedstock, $i'' \in \boldsymbol{I}^{\mathrm{F}}$. We formulate a model that requires that one unit of feedstock i'' should be purchased ($\gamma_{i''} = \delta_{i''} = 1$), which, since sales of intermediates are not allowed, leads to the production of one or more final products. If we are interested in determining the strategy that is more competitive against existing technologies today, then we use the maximization of profit (eqn (13)) as the objective function to formulate the model, $\boldsymbol{M_{23}}$: max $\{Z_3$: eqn (6), (7) and (9); $\gamma_{i''} = \delta_{i''} = 1$; $\gamma_i = 0$, $\delta_i = M$ if $\boldsymbol{I}^{\mathrm{F}} \ni i \neq i''$; $\omega_i = 0$, $\forall i \in \boldsymbol{I}^{\mathrm{P}}\}$.

Note that since the production cost of biofuels is typically higher than the market prices of fossil-based fuels, the profit will be negative, which means that the identified strategy is the one that is closer to becoming competitive.

5.1.3 Question 3: optimal strategy for a given feedstock and product. This question arises when there are multiple strategies to convert a specific feedstock, $i'' \in \boldsymbol{I}^{\mathrm{F}}$, to a specific product, $i' \in \boldsymbol{I}^{\mathrm{P}}$. To address this question, we set the availabilities of all other feedstocks to 0, and require the production of one unit of product i'. If our goal is to find that strategy that requires the least amount of energy inputs (besides biomass), we use model $\boldsymbol{M_{32}}$: min $\{Z_2$: eqn (6)–(9); $\omega_{i'} = 1$; $\omega_i = 0$ if $\boldsymbol{I}^{\mathrm{P}} \ni i \neq i'$; $\gamma_i = 0$, $\forall i \in \boldsymbol{I}^{\mathrm{F}}$; $\delta_{i''} = M$; $\delta_i = 0$ if $\boldsymbol{I}^{\mathrm{F}} \ni i \neq i''\}$.

Note that since the objective is the minimization of energy use, exactly 1 unit of fuel i' will be produced at the optimal solution, which means that the optimal objective function value, Z_2^*, is equal to the energy required to produce one unit of fuel i', or, equivalently, the efficiency of the optimal strategy is $\varphi_{i'}/Z_2^*$.

5.2 Identification of alternative strategies

Given the high uncertainty in the field, it is important to be able to (i) identify alternative strategies, and (ii) evaluate how changes in production costs affect the selection of the optimal strategy. Towards the first aim, we develop a mixed-integer programming (MIP) model that can be used iteratively to identify the best K strategies. Towards the second aim, we generate production cost intervals for the alternative strategies using the uncertainty levels discussed in Section 3.

To formulate the MIP model, we first introduce binary variable Y_j and replace eqn (7) with,

$$X_j \leq \beta_j Y_j, \ \forall j \tag{7*}$$

Eqn (7*) essentially *activates* binary Y_j when technology j is utilized at the optimal solution; *i.e.*, $Y_j = 1$ if $X_j > 0$. Also, we introduce eqn (13)

$$\sum_{j \in \boldsymbol{J}^l} Y_j \leq \left|\boldsymbol{J}^l\right| - 1, \quad l = 0, 1, \ldots, k-1 \tag{13}$$

where $\boldsymbol{J}^l$ is the set of technologies selected in iteration l; $\boldsymbol{J}^0$ is the set of technologies selected using LP model $\boldsymbol{M_{qc}}$ (iteration 0). Eqn (13) for $l = 0$ cuts off any strategy that employs the technologies employed in the optimal strategy identified by $\boldsymbol{M_{qc}}$. At iteration $\boldsymbol{k} > 1$, we solve model $\boldsymbol{M_{qc}^k}$, which consists of eqn (6), (7*), (8), (9) and (13) to identify the *next best strategy*. In general, the inequalities in eqn (13), which are termed as *integer cuts*, prevent model $\boldsymbol{M_{qc}^k}$ from finding strategies that were previously found or strategies that include the technologies in a previously found strategy as a subset of $\boldsymbol{J}^k$. Different types of cuts can be used if it is allowed to have $\boldsymbol{J}^l \subset \boldsymbol{J}^k$ for some $l < k$.

The procedure for the identification of K alternative strategies, after we solve $\boldsymbol{M_{qc}}$ once to obtain $\boldsymbol{J}^0$, is as follows:

0. Choose K; set $k = 1$;
1. Solve $\boldsymbol{M_{qc}^k}$; obtain $\boldsymbol{J}^k$; *i.e.*, the k^{th} alternative strategy;
2. If $k < K$, set $k = k + 1$ and go to 1.

5.3 Strategy analysis

After we identify a set of alternatives, we can perform cost contribution and sensitivity analyses on the results. For the minimum cost problem with $\omega_{i'} = 1$, the objective function essentially gives the total production cost (TPC). By breaking down TPC into individual contributors (*e.g.*, feedstock and technologies), we can identify the major cost drivers. Also, we can carry out a sensitivity analysis on the major parameters to understand the effects of their variations on the objective function value.

Furthermore, based on the technology uncertainty levels discussed in Section 3.3, we can determine an interval for the total production cost, TPC_k, of strategy k,

$$TPC_k \in \left[\frac{\sum_{i \in \boldsymbol{I}^{\mathrm{F}}} \lambda_i P_i^k + \sum_{j \in \boldsymbol{J}^k} \left(1 - \xi_j\right) \rho_j X_j^k}{S_{i(k)}^k}, \frac{\sum_{i \in \boldsymbol{I}^{\mathrm{F}}} \lambda_i P_i^k + \sum_{j \in \boldsymbol{J}^k} \left(1 + \xi_j\right) \rho_j X_j^k}{S_{i(k)}^k} \right] \tag{14}$$

where $\boldsymbol{J}^k$ is the subset of technologies included in strategy k (*i.e.*, the strategy identified at iteration k by model $\boldsymbol{M_{qc}^k}$); $\xi_j \in \{10\%, 30\%, 50\%\}$ is the cost uncertainty of technology j; P_i^k and X_j^k are the values of variables P_i and X_j in the optimal solution of model $\boldsymbol{M_{qc}^k}$ (or model $\boldsymbol{M_{qc}}$ for $k = 0$); and $S_{i(k)}^k$ is the value of variable $S_{i(k)}$ in the optimal solution of $\boldsymbol{M_{qc}^k}$, where $i(k)$ is the primary product of strategy k.

5.4 Sensitivity analysis

The focus of this paper is on the development of a framework for the study of conversion strategies. While our framework allows us to study how technological uncertainty impacts the economics of the most promising strategies, there are a number of other factors that play a key role in the development and adoption of biofuel strategies, most notably, constraints originating from the cultivation of biomass, the existing transportation fuel infrastructure, and the market of fuels (and chemicals). One way to study the effect of these factors is through sensitivity analysis. For example, we can calculate how the total production cost of a set of strategies changes as the price of feedstock changes and determine the threshold values at which the optimal strategy changes. Similar analyses can be performed for other parameters, such as the price of by-products, which impacts the economics of a strategy through the by-product credit.

6 Case study: ethanol production from hard woody biomass

6.1 Model and assumptions

We use the production of ethanol from hard woody biomass to illustrate the types of analyses that can be performed using the proposed framework. Our goal in this case study is to identify the most cost-effective strategy. Fig. 8 shows the corresponding superstructure which includes biochemical and thermochemical conversion strategies. For the baseline, we assume that the prices of hard wood, acetic acid, and electricity are \$110.7 per dry ton,[21] \$0.882 per kg[21] and \$0.065 per kW h,[22] respectively; all technical and economic parameters are provided in Table S13 of the ESI.†

6.2 Results

6.2.1 Strategy identification. The optimal strategy (S1) is the production of ethanol from methanol synthesis *via* indirect gasification followed by acetic acid production and hydrogenation at \$3.50 per gallon of ethanol. Strategy S1 and the top four alternative strategies are given in Table 4. We observe that the TPC of the directly heated gasification strategy (S2) is slightly higher than the indirectly heated gasification strategy (S1) despite its higher ethanol throughput. In gasification-based strategies, CO and H_2 are used to synthesize acetic acid and ethanol, respectively, and their costs account for a major fraction of the operating cost.[21] Our results show that the high consumptions of CO and H_2 lead to a higher operating cost for S2, as well as that the need for a pressurized gasifier and an air separation plant for oxygen supply results in a high capital cost for S2. The detailed characteristics of the two configurations were compared in a previous study.[21]

Although gasification-based strategies (S1 and S2) have higher capital and operating costs, their TPCs are lower than the fermentation-based strategies (S3, S4 and S5) because their ethanol yields are higher by two to four times as shown in Table 4. Furthermore, the by-product of gasification-based strategies, acetic acid, leads to a lower TPC, because it can be sold at a high price.[21] The credit from acetic acid sales reduces the TPC by 24.6%, which is significantly higher than the credit from excess electricity sales in the fermentation-based strategies (5.8–7.3%). Finally, dilute acid pretreatment appears to be more effective than other pretreatment technologies due to its higher yield. Our findings in terms of yields and costs are similar to a previous study[22] although a different biomass feedstock was considered.

6.2.2 Cost contribution analysis. Fig. 9 shows the cost contributions of each technology as well as the feedstock cost and the by-product credit to the TPC of each strategy. For the gasification-based strategies, the major cost driver is the acetic acid production system, followed by the hydrogenation system and feedstock cost, whereas for the fermentation-based strategies, the largest contributor is the feedstock cost, followed by the simultaneous saccharification and fermentation systems. This means that the economics of the gasification-based strategies can be improved primarily through processing modifications (*e.g.*, cheaper catalyst), while lower feedstock prices can lead to lower TCP for the fermentation-based strategies.

6.2.3 Production cost uncertainty. We estimate intervals for the TPC of the selected strategies using eqn (14), as shown in Fig. 10. Combining the uncertainties of the technologies of a strategy, we calculate that gasification-based strategies have an overall uncertainty between 32 and 33%, while fermentation-based strategies have a 22–24% uncertainty. The main reason for this difference is that the former are more complex than the latter.

6.2.4 Sensitivity analysis. In addition to conversion efficiency, market considerations, at both ends of our superstructure, play a key role in the adoption of biofuels. Specifically, if a feedstock were to be used for mass biofuel production, then its price would be expected to increase. On the other end, if a chemical is a by-product in a widely employed strategy, then its price would be expected to decrease, which would in turn make

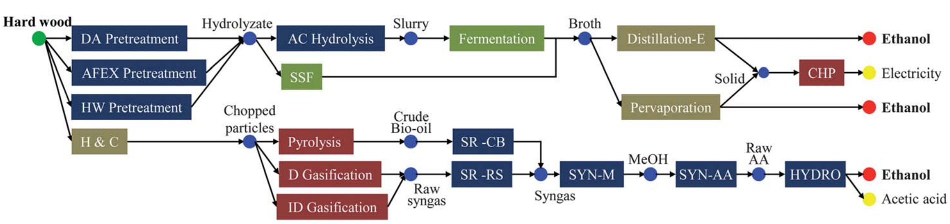

Fig. 8 Superstructure for ethanol production from hard woody biomass (abbreviations given in Fig. 3).

Table 4 Alternative strategies for ethanol production; TCC: total capital cost, TOC: total operating cost, TPC: total production cost; calculations based on processing 2000 dry tons of aspen wood per day[a]

		Product (gal/h)	By-product (/gal ethanol)	TCC (M$)	TOC (M$/year)	TPC ($/gal)
S1	Hard wood → H&C → ID gasification → SR-RS → SYN-M → SYN-AA → HYDRO	11 225	Acetic acid (1.29 kg)	567	261	3.50
S2	Hard wood → H&C → D gasification → SR-RS → SYN-M → SYN-AA → HYDRO	15 860	Acetic acid (1.29 kg)	644	449	3.70
S3	Hard wood → DA pretreatment → SSF → distillation-E	5425	Electricity (3.40 kW h)	372	94	4.38
S4	Hard wood → AFEX pretreatment → SSF → distillation-E	4554	Electricity (5.11 kW h)	271	84	4.66
S5	Hard wood → HW pretreatment → SSF → distillation-E	3840	Electricity (5.40 kW h)	329	81	5.64

[a] Abbreviations given in Fig. 3.

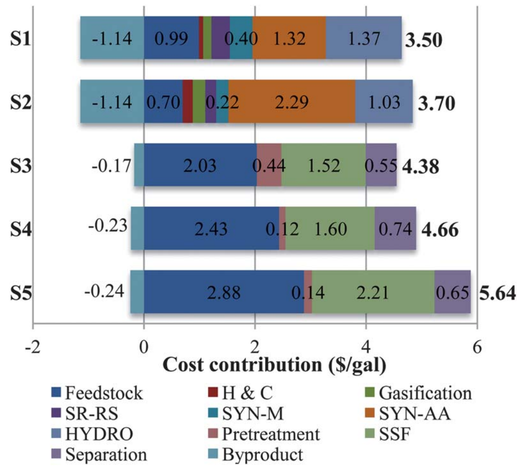

Fig. 9 Cost contributions in alternative strategies; abbreviations given in Fig. 3.

the specific strategy less attractive. To study these effects, we carry out sensitivity analyses for the hard woody biomass price and the price of the acetic acid, which is a by-product of the gasification process.

The TPC of fermentation-based strategies is sensitive to variations in the feedstock price as shown in Fig. 11a.

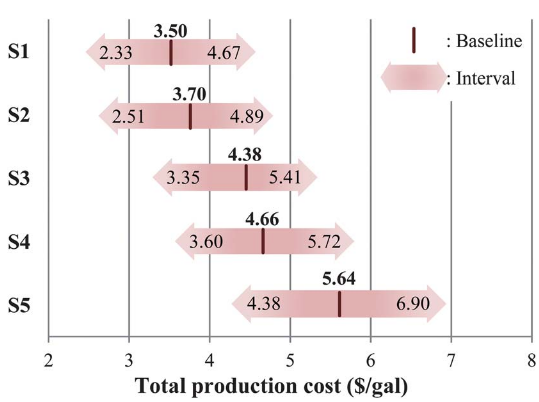

Fig. 10 TPC intervals for the selected strategies.

When the feedstock price decreases, the TPC of the fermentation-based strategies decreases rapidly compared to the gasification-based strategies. At prices below $18 per dry ton, S4 becomes the most cost-effective strategy, while ethanol production through S2 is expected to have the least cost at prices higher than $160 per dry ton. Sensitivity analysis results with respect to the acetic acid price for the gasification-based strategies are shown in Fig. 11b. A 36% increase in the price ($1.2 per kg) decreases the TPC by 11.1–11.4% (3.11 $ per gal and 3.28 $ per gal for S1 and S2, respectively). On the other hand, when the acetic acid price is less than $0.15/kg, S3 leads to a lower TPC than that of gasification-based strategies.

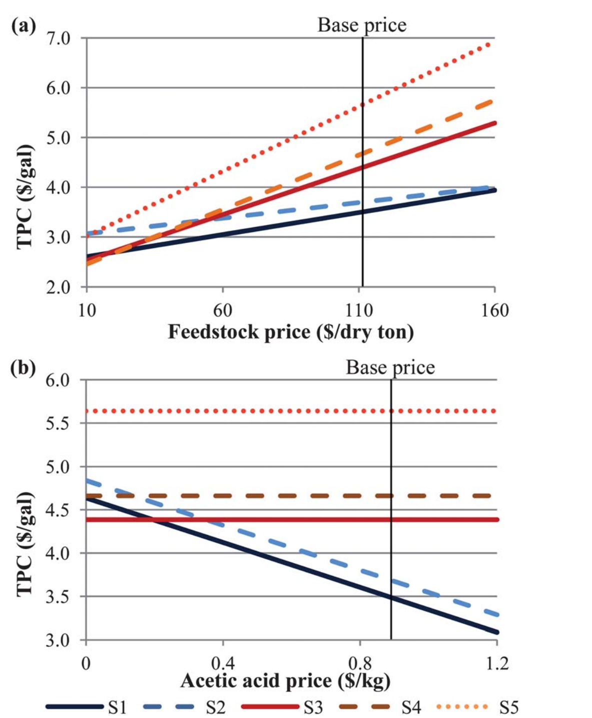

Fig. 11 Sensitivity analyses with respect to (a) feedstock and (b) acetic acid prices.

It is important to note that while sensitivity analysis is useful, it does not fully capture the relationship between the optimization decisions (adoption of strategy and corresponding feedstock consumption) and the variability of the parameter (feedstock price). Specifically, it does not account for the endogenously generated price change. A rigorous treatment of this subject would require the modeling of this interaction, but this is beyond the scope of this conversion-centric framework.

7 Conclusions

We developed a framework for the systematic assessment of biomass-to-fuel conversion strategies. Our framework is based on a superstructure of technologies that have been reported in the literature as well as technologies that can be developed in the future. Based on this superstructure, we developed two types of optimization models that allow us to: (i) generate novel strategies combining technologies that were previously thought to belong in *parallel* production systems; (ii) assess strategies based on a range of criteria; (iii) identify a set of promising alternative strategies; and (iv) perform sensitivity analysis studies with respect to *external* (*e.g.*, feedstock process) and *internal* (*e.g.*, technology maturity) parameters. These models can be used to examine a wide range of questions.

Our framework establishes a methodology and suite of tools for the systematic comparison of competing strategies, the identification of technology gaps and cost drivers in existing strategies as well as synergies between distinct strategies. It also enables us to study trade-offs and assess the impact of technology uncertainty. We hope that researchers in the field of biofuels will not only use our framework to explore new strategies, but also help us enrich it with emerging conversion technologies and improve it with more accurate data where appropriate. We are currently developing a software tool that will allow users with no optimization background to use it effectively. Also, building upon this work, we will extend our framework to study combinations of feedstocks and/or combinations of final products, include life cycle assessment (LCA) methods,[59] study the effect of biomass supply chain as well as market constraints, and employ more rigorous approaches to study the impact of uncertainty.

Nomenclature

Parameter evaluation

α	scaling exponent for technology capacity adjustment
ε	time-value adjustment factor
C_n	capital cost of new technology
C_p	adjusted capital cost of existing technology
C_{po}	capital cost of baseline design
n	lifetime of plant
Q	adjusted capacity of existing technology
Q_o	capacity of baseline design
r	interest rate
R_n	amount of reactant in new technology
R_p	amount of reactant in existing technology
ACC	amortized capital cost [$ per year]
APR	annual production rate [kg per year]
CCF	capital charge factor
TCC	total capital cost of technology [$]
TOC	total operating cost of technology [$ per year]
UPC	unit production cost of technology [$ per kg]
TPC	total production cost for a strategy [$ per kg].

Mathematical programming model

Sets.

$i \in \boldsymbol{I}$	compounds
$j \in \boldsymbol{J}$	technologies.

Subsets.

$\boldsymbol{I}^F/\boldsymbol{I}^I/\boldsymbol{I}^P/\boldsymbol{I}^B$	feedstocks/intermediates/final products/by-products
$\boldsymbol{J}_i^+/\boldsymbol{J}_i^-$	technologies producing/consuming compound i
$\boldsymbol{J}^l/\boldsymbol{J}^k$	technologies included in the strategy identified in iteration l/k.

Parameters.

β_j	maximum capacity for technology j
γ_i	minimum purchase of feedstock $i \in \boldsymbol{I}^F$
δ_i	availability of feedstock $i \in \boldsymbol{I}^F$
η_{ij}	yield of compound i in technology j
λ_i	price of compound i
ξ_j	cost uncertainty of technology j
ρ_j	unit production cost of technology j
υ_j	unit energy requirement level of technology j
φ_i	heating value of compound i
ω_i	demand for product $i \in \boldsymbol{I}^P$.

Binary variables.

Y_j	$= 1$, if technology j is selected.

Continuous (non-negative) variables.

P_i	amount of compound $i \in \boldsymbol{I}^F$ purchased
S_i	amount of compound $i \in \boldsymbol{I}^P \cup \boldsymbol{I}^B$ sold
X_j	production level of technology j.

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