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Technoeconomic analysis for biofuels and bioproducts

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Technoeconomic analysis (TEA) is an approach for conducting process design and simulation, informed by empirical data, to estimate capital costs, operating costs, mass balances, and energy balances for a commercial scale biorefinery. TEA serves as a useful method to screen potential research priorities, identify cost bottlenecks at the earliest stages of research, and provide the mass and energy data needed to conduct life-cycle environmental assessments. Recent studies have produced new tools and methods to enable faster iteration on potential designs, more robust uncertainty analysis, and greater accessibility through the use of open-source platforms. There is also a trend toward more expansive system boundaries to incorporate the impact of policy incentives, use-phase performance differences, and potential impacts on global market supply.

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Introduction

Low-carbon liquid biofuels are critical to the rapid decarbonization of transportation, particularly long-haul freight and aviation. For any new renewable fuel, competitive production cost is a prerequisite to making a measurable impact on fossil energy demand and greenhouse gas emissions. While some consumer products can be advertised as low-carbon or otherwise sustainable to sell for a premium, liquid fuels are highly regulated and require massive scale to justify the approval processes and infrastructure needed to produce and distribute them. This may be why many of the earliest technoeconomic analysis (TEA) studies focused on biofuel production [1,2]. It is useful to guide and prioritize early stage research and development targets by using lab-scale or pilot-scale data to design and analyze a theoretical scaled-up process. This is what TEA aims to provide: a combination of process and/or product design, simulation, and cash flow analysis to produce mass and energy balances as well as a variety of economic metrics that can be used to gauge the viability of a technology before it has been commercialized. It is an exercise in full system design, virtual scale-up, and evaluation, grounded in empirical data wherever possible. The mass and energy balances are also crucial inputs for life-cycle assessment (LCA) [3], and the two types of analysis are often conducted together. Recent studies have pushed the boundaries of biofuel and bioproduct TEA in the complexity and novelty of systems being modeled, the approaches for quantifying and reporting uncertainty, and the development of simplified open-source models [4•]. This article builds on the fundamentals of TEA [5] and technology-specific reviews of TEA studies [6–9] by providing a technology-agnostic summary of best practices and recent trends in TEA research. We discuss conventional process simulation, lightweight open-source alternatives, and highlight some of the challenges specific to biofuels and bioproducts.

Conventional process design and simulation

Conventional process design and simulation is the starting point for most biofuel and bioproduct TEAs. Groups employing this approach typically use commercial chemical engineering software packages such as SuperPro Designer® [10–13] and Aspen Plus® [14–18]. The Aspen-based Humbird *et al.* [19•] model and report on corn stover conversion to ethanol using dilute acid pretreatment have been widely cited and used as a basis for comparison for many other biofuel production processes, in part because the model is carefully and extensively documented. Commercial process modeling tools provide a platform to build a rigorous process model and handle a complex biorefinery with multiple recycle loops. This level of detail is essential to capture the complexities and potential for integration in heating and cooling utilities, wastewater treatment, and on-site cogeneration, as demonstrated by Meramo-Hurtado *et al.* [20]. Although most commercial software defaults to sequential modular mode, which is more expedient for simple calculations, equation oriented modeling approaches provide more

flexibility, transparency, and speed for highly integrated processes. In some cases, these software packages are used to do deeper analyses on single unit processes, as Humbird *et al.* conducted to understand cost drivers for stirred tank and bubble column reactors [21].

Although useful for building detailed designs, complex full-system models can be time-consuming to construct, slow to run, and do not necessarily lend themselves to brute force uncertainty analysis or frequent updates to facility design. Most prior studies using conventional tools are limited to scenario and single-point sensitivity analyses [10,14,15,17,22,23]. Some studies included more extensive uncertainty analysis [16,24,25], although only cost parameters varied, including capital expenses and prices of feedstock and process chemicals, which are typically modeled in a separate cash flow analysis without passing input variables through the process model itself. Full scale process model-based uncertainty analyses that include variations in capital and operating data inputs, intermediate and final product yields, and economic parameters are limited [26,27]. These chemical process simulation tools are also challenging to integrate with models for other components of the supply chain that can impact cost and mass/energy balances, including feedstock supply and logistics and use-phase impacts (see Figure 1).

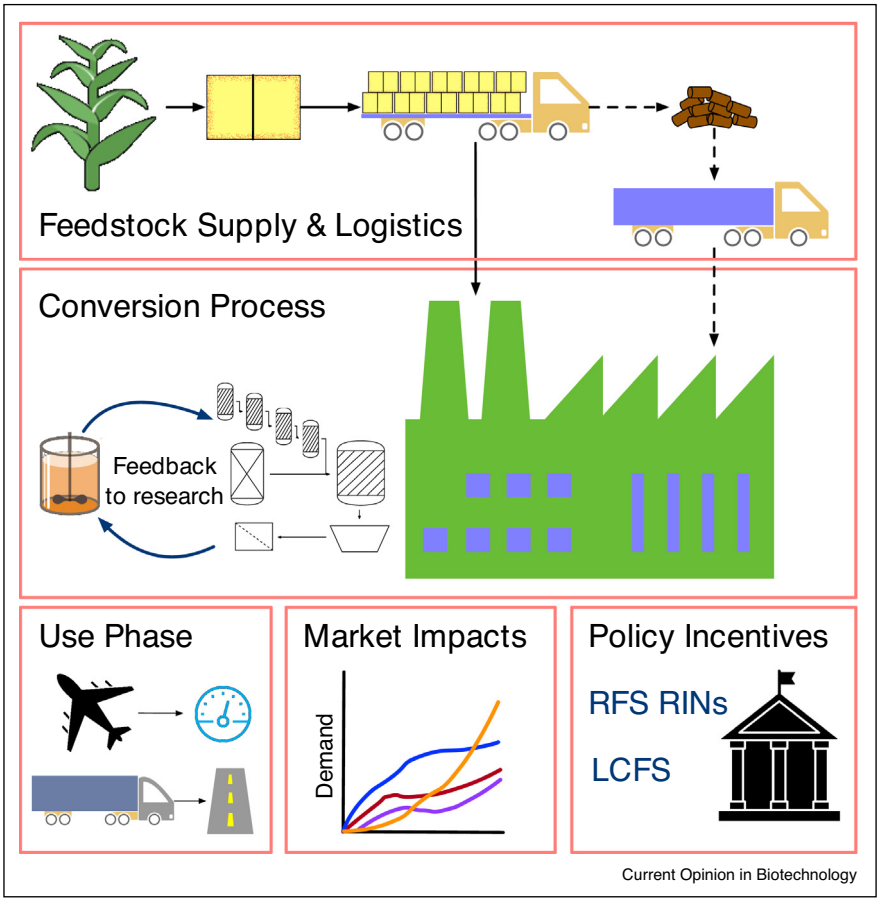
Lightweight and open-source process models

Without building a complex process model, there are simple methods that can be used to evaluate operating expenditures (OPEX). For example, Blanch [28] demonstrated the simple stoichiometric theoretical yield calculations one can apply to estimate glucose requirements for biological fuel or chemical production. This calculation alone, provided yield is adjusted appropriately, is likely to capture a large fraction of the OPEX. For perspective, the feedstock for a corn ethanol facility using dry milling makes up around 58% of the total production cost (CAPEX and OPEX), with other operating costs comprising 17% and capital costs (direct and indirect) contributing 25% [29,30]. The relative importance of feedstock cost is diminished for processes that utilize lower-cost feedstocks such as lignocellulosic biomass or organic wastes; the same is true for processes that involve resource intensive or multi-step pretreatment and conversion. For example, Baral *et al.* [31] found that the biomass feedstock cost for a lignocellulosic biorefinery using aerobic bioconversion to produce isopentenol makes up less than one third of total production costs in most scenarios.

There have also been recent efforts to develop simplified publicly-available models that go beyond these basic calculations but do not require the same level of expertise as traditional process design and simulation software. For example, Viswanathan *et al.* recently released a spreadsheet tool aimed specifically at hybrid biological/catalytic process called ESTEA2 (Early State Technoeconomic Analysis, version 2) [30] and validated results for corn ethanol production and sorbic acid production against more detailed SuperPro Designer® simulations, showing 3–22% variation of minimum selling price (MSP) relative to published values. Another recently released model, Biorefinery Simulation and Techno-Economic Analysis Modules (BioSTEAM) [4•], is a flexible Python-based platform that was validated against the co-production of biodiesel and ethanol from lipid-cane (modeled in SuperPro Designer) and second-generation ethanol from corn stover (modeled in Aspen Plus). Additional examples of simplified models include a comprehensive Microsoft Excel-based model using thermodynamic empirical equations [32] and a simplified MATLAB-based modeling approach [33,34].

Accuracy, reliability, utility, and scalability of these modeling approaches are dependent on the sources of data inputs, appropriateness/accuracy of the selected thermodynamic models, and level of detail applied to unit operations. In particular, large databases of thermophysical properties, empirically derived constants and coefficients, and predicted values for gaps in empirical data can vary in their availability and accessibility for open-source applications. Thus, lightweight TEA models are likely to be useful for estimating costs and mass balances for processes with a limited number of unit operations and recycle streams. Based on results reported in the literature, a limitation of currently available simplified process models seems to be their ability to accurately predict the net steam and electricity needs of the facility. While this has a minimal impact on minimum selling price due to historically low fuel and electricity prices [4•], energy balances are one of the most important inputs for life-cycle greenhouse gas (GHG) inventories, given that electricity exports to the grid alone can reduce life-cycle GHG emissions by 10–20 gCO_{2e}/MJ of fuel depending on the local grid mix [31,35]. The carbon intensity of biofuels is directly linked to economics, since these estimates determine Renewable Identification Number (RIN) values and Low Carbon Fuel Standard (LCFS) credits [36•]. To minimize the potential for misuse of simplified models, these tools should be accompanied by explicit guidance as to which types use cases are appropriate, both in terms of specific types of conversion processes as well as metrics (cost, mass balances, energy balances). For example, a model populated with default values and equations that are useful for biochemical processes is unlikely to work well for a thermochemical conversion process. These issues are by no means exclusive to simplified TEA models; default thermodynamic models in many of the unit processes included in SuperPro Designer are best suited for liquid-phase, relatively low-pressure conditions most common in biochemical processes.

Figure 1



Key Considerations for Biofuel and Bioproduct Technoeconomic Analysis.

Economic metrics

There exists a considerable gap between how TEA is used in the research community and how it is leveraged in private industry. TEA conducted with the purpose of informing and prioritizing process development and optimization will typically focus on total capital investment (TCI or CAPEX, measured in total dollars), annual operating cost (AOC or OPEX, measured in dollars per year) and minimum product selling price (MSP, measured in dollars per kg product or volume of fuel) after cash flow analysis [27,37•]. MSP is a commonly reported metric in published TEAs, and is determined based on the unit price needed to reach a net present value (NPV) of zero for an established facility lifetime, given a set internal rate of return (IRR), which is often set at 10% for biorefineries to remain consistent with the Humbird *et al.* report [19•]. In contrast, private companies seeking to evaluate potential investments are generally more interested in simpler profit-related indicators that do not account for the time value of money, such as revenues (Eq. (1)), gross margin (%) (Eq. (2)), return on investment (ROI, %) (Eq. (3)) and payback period (in years) (Eq. (4)) [38,39]. Policymakers have an entirely different objective in using the results of TEAs. For policy-making, the question is whether a novel renewable fuel or product can be viable in the long term and what level of economic incentives are needed to make near-term production profitable. Hannon *et al.* [36•] provided an excellent example of results that directly inform researchers, industry, and policymakers by estimating payback time with and without RINs and LCFS credits across multiple potential fuel selling prices and Yang *et al.* employed a similar approach to explore the economics of carbon capture in biorefineries with and without policy supports [40].

$$Revenue, \$/yr = Product\ Sales, kg/yr \times Product\ selling\ price, \$/kg \quad (1)$$

$$Gross\ margin, \% = \frac{Annual\ revenue, \$ - Annual\ operating\ cost, \$}{Annual\ revenue, \$} \times 100 \quad (2)$$

$$Return\ on\ investment\ (ROI), \% = \frac{Annual\ net\ profit, \$}{Total\ capital\ investment, \$} \times 100 \quad (3)$$

$$Payback\ period, yr = \frac{Total\ capital\ investment, \$}{Annual\ average\ net\ cash\ flow, \$} \quad (4)$$

High-value co-products and market impacts

Like petroleum refineries, biorefineries can produce multiple biofuel and non-fuel bioproducts to diversify their revenue streams [41•]. Identifying ideal bio-based co-products depends on a range of criteria including product price, market volume, market maturity, feedstock flexibility, expected demand growth, external funding support, and the competitive edge over conventional production routes [41•]. Generally, TEA studies calculate revenue from co-products over the entire plant life based on market price of the product, balance it against additional costs of extracting, purifying, and producing the products, and apply the net credit towards the minimum selling price of biofuel(s). However, the implicitly assumed price stability of the co-product may not hold true. Studies have addressed price fluctuations by incorporating historical product market price (generally 5, 10, 15-year averages) in their sensitivity or uncertainty analysis [42–44]. Huang *et al.* used cost parity for ethanol as a target to back-calculate the MSP of their co-product, 1,5-pentanediol. Their findings demonstrated that 1,5-pentanediol's MSP was significantly below current market price (19% of the actual market price) and variation in the 1,5-pentanediol MSP had a large effect on minimum ethanol selling price [45].

Market size of the co-product relative to the proposed level of production and the price elasticity of demand for the product are both important for evaluating the merits of high-value co-products. In the case of 1,5-pentanediol, the existing market size is relatively small (around 2700 tonnes/year), and one biorefinery would produce an order of magnitude more than this [45]. The majority of studies have relied on qualitative discussions and simple back-of-the-envelope calculations to address potential market impacts. For example, Biddy *et al.* demonstrated the potential of bringing down the selling price of a renewable fuel blendstock by co-producing bio-based succinic acid [43]. However, their biorefinery production estimates would have increased total production of succinic acid by fourfold, so they supplemented the analysis with a discussion on expanding the market by considering derivative chemicals of succinic acid. Huang *et al.* provided a similar qualitative discussion of expanding the market size by considering potential chemicals that could be replaced with 1,5-pentanediol [45]. Yang *et al.* showed that the global market for some specialty chemicals accumulated *in planta* would be satisfied by just 5–10 biorefineries, while large polymer markets could support well over 1000 commercial scale facilities and very high-value pharmaceutical markets would be flooded by just a fraction of one facility [46•]. This tradeoff between high value and market volume was also highlighted by Markel *et al.* [47]. A few studies have adopted market size as an initial screening criterion such that only products with total demand exceeding 1 million metric tons are considered [42,48,49]. McManus and Taylor recommended that a framework similar to that of life-cycle assessment be used to incorporate market dynamics as well as a broader range of policy scenarios in more sophisticated economic models [50]. Market size and impact considerations become even more challenging to capture if a bioproduct or fuel does not obviously result in a one-to-one replacement of an incumbent product.

Use-phase impacts of biofuels and bioproducts

The system boundary for most TEAs ends at the biorefinery gate, and researchers select a functional unit that allows for direct comparison between the conventional product and its bio-based alternative. The goal is to define a unit of analysis based on the function a fuel or product provides during its use phase, which refers to the span of time when a finished fuel or product is used for its intended purpose before reaching its end-of-life. For example, costs per volume of fuel may be reported in liters of diesel- or gasoline-equivalent to adjust for differences in volumetric heating value. Even in the case of fuels, this adjustment is not straightforward; fuel properties may impact costs associated with blending, fueling infrastructure, and engine performance/longevity, but most of these performance characteristics are unknown at early stages of research when experiments yield biofuel and bioproduct volumes far too small for most standard testing procedures [51•]. Baral *et al.* used a simplified method for quantifying the monetary value of potential per-passenger energy savings associated with aircraft lightweighting through the use of more energy-dense biojet fuel [27]. However, the resulting increase in aircraft range is more challenging to monetize. Recently, there have been sophisticated modeling efforts to understand the impact of advanced jet fuels on externalities that could be assigned dollar values, such as aircraft noise around airports [52]. The task of quantifying economic impacts during the use phase becomes even more complex when considering bioproducts that might be used for multiple applications, such as packaging, textiles, or durable goods. A simple mass-based cost comparison becomes inappropriate if a manufacturer will choose to use more or less of a new bio-based material to achieve comparable strength, durability, or aesthetics. Linking TEA with efforts to measure or computationally predict the impacts of biofuel or bioproduct properties may help to address this disconnect.

Future research directions

There is an emerging trend in TEA towards more agile modeling that can quickly iterate over a larger solution space and enables the construction of basic models by non-experts [4•,30,32–34], even if this capability comes at the expense of some accuracy. In many early-stage research applications, this is likely a worthwhile tradeoff, particularly if cost is of more interest than life-cycle emissions. Another approach for improving the accuracy of reduced-form models, at the expense of flexibility, is the use of regressions/machine learning (ML) to approximate the relationship between input parameters and key outputs using outputs of more rigorous models as training data. This approach, sometimes referred to as surrogate modeling has been employed for other fields, such as atmospheric fate and transport and fluid flow [53,54]. Surrogate models may treat either a section of a biorefinery or the entire facility as a black box and these choices will impact the model's flexibility in handling altered configurations.

These simplified or black box models can be both a tool for, and barrier to, addressing another important need: more robust, transparent uncertainty analysis. TEA models are subject to epistemic uncertainty (reduceable with better data) and aleatory uncertainty (irreducible, also referred to as variability). Any modeling approach can be leveraged to conduct scenario analysis, whereas lightweight modeling techniques and equation-oriented simulations are particularly well suited for brute-force Monte Carlo simulations, which require thousands of model runs [18,55,56]. Regardless of modeling approach, using scenario analysis to convey the impacts of epistemic uncertainty and using Monte Carlo simulations to capture aleatory uncertainty can be a useful approach for communicating researchers' level of confidence in their results and key conclusions.

Another interesting potential future direction is the integration of TEA modeling with high-throughput experimental pipelines capable of processing hundreds or thousands of samples from raw feedstock inputs through the generation of final products. Recent articles in *Nature* have highlighted the promise of robotic pipelines where both organic synthesis and hypothesis generation are automated to some degree [57,58]. These advances, combined with the general trend of more lightweight agile models, offer the opportunity to insert TEA models into this rapid research and development feedback loop. The use of technical and biological replicates from these high-throughput studies can also enable TEA models to more fully account for different sources of uncertainty in key input parameters. Through further advancements in integration of process simulation with high-throughput experimental pipelines, improved uncertainty analysis, and additional efforts to leverage ML and optimization methods, TEA has the potential to play a central role in shaping the future bioeconomy.

Conflict of interest statement

Nothing declared.

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