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Abstract
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Development and validation of a technoeconomic analysis tool for early-stage evaluation of biorenewable processes

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1. Introduction

Bio-based chemicals represent an opportunity to produce value-added products from sugars. These chemicals are an attractive alternative to biofuels because of their higher market prices compared to biofuels. In a 2004 study, Werpy and Petersen identified ten chemicals that presented the greatest short-term opportunity for bio-based chemical production in the U.S., spurring tremendous efforts to increase the economic viability of these bio-based chemicals (Sánchez et al., 2005; Song and Lee, 2006; Werpy and Petersen, 2004). Aggressive research and development efforts have led to increasing productivities and yields for these chemicals, but little is known about the economics of producing these value-added bio-based chemicals at commercial scale.

One chemical that does possess a good deal of process information is ethanol due to its large-scale deployment as a 1st-generation biofuel. The broad ethanol literature encompasses process improvements, technoeconomic analyses (TEAs), and life-cycle assessments, and can provide fundamental knowledge to inform studies about other bio-based chemicals (Kwiatkowski et al., 2006; Michael et al., 2007). Robust TEA's, in particular, have the ability to illuminate process bottlenecks and to clarify how process alternatives will impact production costs. Typically, these TEA's require extensive knowledge of process parameters and design details only available during the latter stages of a project. However, early-stage cost estimation is critical to helping companies and applied academic research centers chart a course through translational research and towards economic viability.

As novel metabolic pathways are explored or novel hybrid fermentative-catalytic processes are proposed (Nikolau et al., 2008); comprehensive and accurate process data necessary for detailed TEAs of these operations at full-scale will be years away. And yet, strong evidence regarding the economic viability of a particular chemical is needed early in the process to warrant continued investment of resources. By making simplifying assumptions and estimates for key variables, it is possible to develop an early-stage TEA of novel processes. Strong TEA capabilities exist commercially in tools such as Aspen Process Economic Analyzer and Intelligen SuperPro Designer®, both of which provide estimations of capital and operating costs. But these tools also require a level of detail that is typically unavailable at early stages in process evaluation. While preliminary cost evaluation methods have been outlined by several authors (Peters et al., 2003; Turton et al., 2010), we are unaware of any widely-available early-stage TEA model or tool for bio-based chemicals. To address this gap, we developed a spreadsheet-based tool to provide early-stage TEAs of bio-based chemicals named BioPET (Biorenewables Process Evaluation Tool). Key criteria used in the development of BioPET were as follow: (1) ease of use, (2) minimal data inputs, (3) results comparable to simplified models implemented in existing cost-modeling software, and (4) simple graphical reporting of estimated minimum selling prices and cost breakdowns. To operate the tool, users need a basic knowledge (or educated guesses) for each unit operation comprising their overall process design of interest. Once developed, BioPET was compared against SuperPro Designer® and results from Patel (2006) (Patel, 2006) for a suite of three chemicals: ethanol, succinic acid, and adipic acid. The objective of this research was to (1) develop a tool capable of informing economic decisions regarding new pathways developed for bio-based chemicals and (2) provide a platform for future early-stage TEA's.

2. Methods

2.1 Methods for BioPET development

BioPET was designed with the objectives of evaluating multiple processes with (re)construction of new process flow diagrams (PFD) with each new evaluation. With organisms capable of consuming many types of feedstocks, the model remained agnostic to where the feedstock was derived. In doing so, the tool does not consider upstream processes such as starch hydrolysis or pretreatment and hydrolysis of lignocellulosic biomass – these were considered outside the scope of the model and the feedstock price was considered as a lumped parameter to include the costs of the initial source and conversion technology if required. The feedstock can then be directly fed to fermentation or catalysis, and any other subsequent unit operations.

BioPET assumes the following carbon flow: fermentation, followed by a separation stage, followed by up to three catalytic processes, finishing with up to two purification stages with different unit operations allowed within each stage. All stages in the tool can be toggled on and off to allow for process flexibility. The following approach was taken to accommodate inherent complexity of the separation, catalysis, and purification processes while allowing for a relatively simple user interface: The types separation and catalytic methods along with assumptions are listed in the following sections. This shields the user from having to provide full process details that are often not available at early stages of a project. Finally, within the hypothetical plant, BioPET only examines a stream of material consisting of a primary product and solvent. This binary system uses mass balance equations and relationships to characterize all steps post-fermentation. Using a series of

inputs and assumptions, process cost estimations can be made.

BioPET assumes that fermentation operates as a batch process and using user-defined inputs of productivity, titer, and yield, BioPET computes baseline fermentation time and sugar demand. The baseline fermentation time is then augmented by 20% to account for downtime between runs for vessel emptying, cleaning, and refilling. The required fermentation volume is computed based on the required mass flow of product and on the downtime-corrected productivity. The number of equal-volume fermenters necessary is then calculated; each primary fermenter is also associated with a seed fermenter having a volume that is 10% of the primary fermenter.

BioPET includes a centrifugation stage immediately downstream of fermentation to account for removal of cell mass from the broth. This stage is automatically present in any process scheme that uses fermentation, and cannot be deselected. All feedstock that does not end up in the final fermentation product is assumed to be converted into cell mass and metabolic by-products that are then combined into a single waste stream. No co-product credits are assumed, which is a conservative assumption given the likely use of genetically modified microbes in the biorenewable chemicals industry.

Adsorption is typically used to remove dilute contaminants or products from a stream – and large-scale adsorption is primarily focused on pollutant removal rather than product recovery. When increasingly large adsorption column volumes are needed, we assumed they are achieved by adding multiple additional units, not by simply making a single unit larger. The number of columns computed in BioPET is done so with non-integer results allowed (e.g., a plant could have 8.6 columns). The cost of the adsorbent in the model therefore follows that of activated carbon with a cost of $1.00/kg.

Crystallization is a viable separation technique for several potential bio-based chemicals. Several techniques exist for producing crystals from their respective solution. Two of these techniques rely on steam for cooling or for evaporation of the solvent to generate a saturated solution from whence the crystals can then be separated. Another method relies on the addition of a mass-separating agent to the solution to initiate precipitation. This method utilizes less energy but often produces a secondary product at the expense of the mass-separating agent. Crystallizers come in such drastically different configurations to provide different levels of separation based on product requirements that often a highly specific crystallizer design must be implemented (Jones, 2002). As this highly specialized process does not easily lend itself to process generalizations, an external forced circulation crystallizer was selected because of its ability to run continuously and at a high production rate, typically between 5000 kg hr^{-1} and 50,000 kg hr^{-1} (Walas, 1990).

Distillation costs can be estimated using the Fenske-Underwood sizing calculations. Fenske-Underwood assumes a constant relative volatility to construct the necessary number of equilibrium stages.

Liquid-liquid extraction was costed using the Kremser assumptions.

The chemical reaction pathways for bio-based chemicals are likely to be more temperature sensitive those of petrochemical pathways (Chia et al., 2012). This implies the widespread use of isothermal packed-bed reactors for catalysis. These reactors were modeled as large-tube heat exchangers with an outside diameter of 0.0508m. A solvent density of 810 kg/m^3, typical of many organic solvents, such as n-butanol, was applied if the separation step prior was adsorption; otherwise the solvent density assumed was that of water.

Chemical plants incur two significant types of costs; capital and operating costs. Operating expenses such as utilities and feedstocks, can dominate the total cost of production, upwards of 75% of total manufacturing costs (Cysewski and Wilke, 1978). To account for these costs and other major pieces of specific unit operations, such as the metal for a catalyst, cost factors were assumed (data not shown). In addition to these operating costs, labor was estimated as a function of capital cost. Annual labor costs typically ranging between 10-20% of the total capital, 10% was chosen for a majority of processes with unit operations such as crystallization increasing it by 5% per added unit operation. These, while potentially overgeneralizing, provide a basis for evaluating tradeoffs of processes under identical assumptions.

3. Results

For overall cost, BioPET produced an ethanol production cost estimate, 0.52 USD kg^{-1}, within 1% of SuperPro Designer®, 0.52 USD kg^{-1}, under the same assumptions. The majority of the cost was a result of the feedstock for both models. The most significant differences were in the capital and utilities costs. Nutrients and labor were both within 5% of each other and appeared to produce adequate results.

4. Discussion

The largest source of error tended to be in operating expenses as opposed to fixed costs, which can be expected as operating expenditures tend to have a larger impact on final cost due to the annual occurrence versus the one-time expenditure that is amortized. While SuperPro estimates these costs as a function of each unit operation, the uncertainty of the designed process prior to commercialization presents a greater source of error and BioPET appeared to perform within an acceptable range of estimates. To better model these costs would require more data regarding the commercial-scale processes, which have not yet been achieved for the bio-based chemical industry.

5. Conclusion

A new tool for preliminary cost estimation has been developed and tested against modeling software and published literature. The results displayed a tool capable of predicting feedstock and capital cost near identical to SuperPro Designer®. While incapable of replacing a program such as SuperPro Designer® due to the level of detail that a modeling program as such can produce, the value of an early-stage cost estimation tool has been demonstrated. BioPET has also been shown to produce results within the range of previous literature helping further validate this technique.

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