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Evaluating and guiding the development of sustainable biorenewable chemicals with feasible space analysis

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ABSTRACT

The economic and environmental performance of a biorenewable chemical process is analyzed by defining its cost, energy, and greenhouse gas feasible design spaces in terms of process parameters. Delimiting the feasible space of a process allows developers to set development targets and quantify performance trade-offs among unit processes. Feasible space analysis is demonstrated for the biocatalytic synthesis of C10 saturated fatty acid from glucose. Capric acid yield from glucose of $\geq$0.25 g g^{-1}, titer of $\geq$40 g l^{-1}, and volumetric productivity of 2 g l^{-1} h^{-1} are found to result in cost, greenhouse gas emissions, and energy consumption as good as or better than the conventional process for production of fatty acids from coconut oil.

1. Introduction

There is growing interest in biorenewable chemicals because of their perceived economic and environmental benefits [1]. It is expected that production from renewable, plant-derived sugars should, in the long-run, allow a low cost of production relative to conventional petrochemicals. Environmental benefits are also expected through the use of biorenewable feedstocks, particularly in terms of carbon footprint. Unfortunately, none of these benefits are certain and recent biorenewable chemical investments have included some high-profile disappointments [2]. To avoid such disappointments, the economic potential and environmental sustainability of a new biorenewable chemical production process should be determined before large irreversible investments are made in process development and scale-up to production scale.

The techno-economic analysis (TEA) and life cycle assessment (LCA) methods are often used to assess the economic and environmental performances of new chemical processes [3,4]. One process configuration or a single combination of process parameters (yield, selectivity, etc.) is usually evaluated when assessing the potential of a new chemical process [4]. If such analyses indicate that a process is not economically viable and environmentally sustainable, then further development may be stopped. The economic and environmental feasibility of a new chemical process, however, still may be achieved by further improvement of the process. It is, therefore, necessary to assess the performance of a new chemical process over a range of combinations of process parameters in order to determine the combinations that would be economically and environmentally feasible. In this manner, one can avoid eliminating processes that are currently unviable but could potentially be made viable. Knowledge of which combinations of process parameters would make the process viable can guide the efforts of process development teams, allowing them to focus on improving those process parameters that, on the basis of the current stage of technology, are not in the feasible range.

A new biomass conversion technology (biological, chemical, and thermo-chemical) has to pass through multiple stages of process development (laboratory-, pilot-, and demonstration-scale) before it is implemented at commercial scale. Often the transition from early research to commercialization takes 10 years or more and requires large capital investment [5]. Reducing technology development time will enable faster access to markets. Technology development can be accelerated by coordinating efforts between multiple development teams working on different process technologies, such as catalytic conversion and separations. In this case, the economic performance of a new chemical process might be improved by developing a separation process that can be used to easily recover and recycle unconverted raw material, if it is diffi-

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cult to improve the catalyst conversion. Technology development efforts tend to have an asymptotic return on investment, such that the economic benefit per dollar invested in improving process performance grows smaller. Determining the economic benefits of improving process parameter values will allow research and development teams to focus on improving those process parameters that have the potential to provide better economic performance.

A semi-quantitative method has been proposed by Patel et al. [6] that integrates economic and environmental indicators to provide a generic 'feasibility score' that is useful as a way to sift through many novel biorenewable chemical routes early in the development process [6]. This method, however, is not used to quantitatively assess the economic viability of a process for the production of the biorenewable chemical over a range of process parameters and to determine process trade-offs among process parameters. Understanding the consequences of process trade-offs allows the setting of meaningful performance targets for the technology development team. This paper provides a new approach by combining feasible space analysis (FSA), TEA, and LCA methods to evaluate and guide the development of biorenewable chemical technologies. The shortcomings of existing approaches for the assessment of biorenewable chemical production processes can be overcome by combining these methods.

The FSA method maps the trade-offs in process parameters into production performance metrics, such as the production cost of a process. Such a mapping defines a "space" of process parameters that will result in a commercially viable process for chemical production. The FSA method has been used to optimize the cost performance of chemical processes [7,8]. In addition to cost considerations, new and existing chemical production processes must meet environmental objectives, as there is a growing concern over the increasing greenhouse gas (GHG) concentrations in the atmosphere [9]. Therefore, it would be useful to extend the FSA method to take environmental objectives into account, which has not been done before.

We used the minimum selling price (MSP) as an economic performance metric, and energy consumption and GHG emissions as environmental performance metrics [10]. The MSP of a biorenewable chemical that is synthesized using a biocatalyst, for example, is driven by the costs of feedstock, fermentor, and separations [11]. Feedstock cost is dominated by the yield of chemical per unit of feedstock and the price of feedstock [12]. The separations cost is driven by the product titer [13]. The production rates influence the capital and operating costs of the fermentor [14]. Similar to the MSP, the GHG emissions and the energy consumption of a biocatalytic process are largely influenced by productivities, titers, and yields. The feedstock production might cause the largest life cycle environmental impact in the biorenewable chemical production system. The yield determines the amount of feedstock required for making the chemical and thus the feedstock contribution to the overall energy consumption and GHG emissions. The energy requirement of the fermentation process depends on the agitator power (kW), which, in turn, depends on production rates. The fermentation titer impacts the energy demand and GHG emissions of downstream processes.

In the current work, the production of fatty acid from glucose using *Escherichia coli* (*E. coli*) was used as a model system to demonstrate the assessment of a new biorenewable chemical process by combining the methods of FSA, TEA, and LCA. Fatty acids are platform molecules that can be transformed into a range of industrial chemicals, such as fatty alcohols [15], α-olefins [16], ethyl esters [17], and alkanes [18]. Global consumption of fatty acids is increasing at a rate of 3% annually [19]. Currently, fatty acids are primarily made from natural oils, such as coconut oil [20]. The hydrolysis of these natural oils results in a mixture of fatty acids that is further fractionated into pure fatty acids. The environmental impact of conventional fatty acid production is high, as the fractionation process consumes large amounts of fossil energy [20]. The new market opportunities for fatty acids and negative environmental impacts of the conventional process have driven interest towards developing efficient biocatalysts to synthesize fatty acids from sugars [21]. Producing fatty acids in a microorganism would allow tailoring properties, such as chain length and functionality, which can add special value by addressing the needs of specific industries, such as the detergent industry [22].

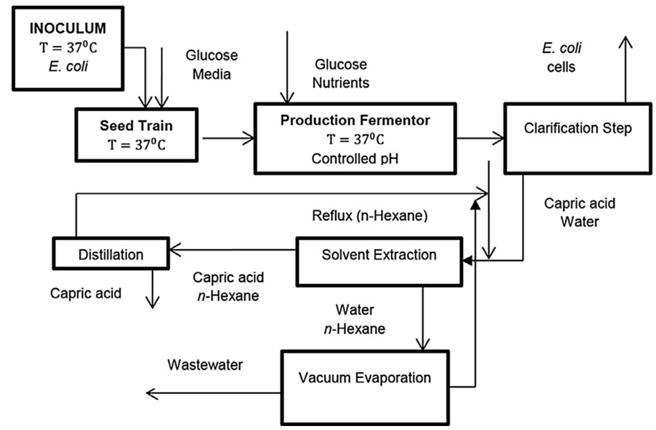

Fig. 1. Proposed process for the production of capric acid from glucose.

In this work, capric acid was used as a model fatty acid molecule. A process flow diagram (PFD) for the synthesis of capric acid was developed. The PFD was modeled to determine material and energy balances of the capric acid production process for various combinations of yield, titer, and volumetric productivity. These balances were used to estimate MSP, energy use, and GHG emissions of the capric acid production process. Such estimates were utilized to generate cost, energy, and GHG performance surfaces. Finally, a feasible space for the glucose-based capric acid production process in terms of yield, titer, and productivity was defined using performance surfaces and constraint planes of cost, energy, and GHG. The constraint planes were determined by estimating performance metrics of the coconut-oil-derived capric acid production process. The assessment of glucose-based capric acid production by combining FSA, TEA, and LCA indicated that this process has the potential to compete with the conventional technology in terms of economic and environmental performances. However, the biocatalyst development team must achieve capric acid yield from glucose of greater than 0.25 $g\,g^{-1}$ and a titer greater than 40 $g\,l^{-1}$ if the process is to meet the performance of the conventional technology in terms of cost, energy use, and GHG emissions.

2. Process description and modeling

In the patent published in 2014 by San and Han, a strain of *E. coli* was used to synthesize capric acid from glucose [21]. The biocatalyst development team has attained a capric acid yield of 0.25 $g\,g^{-1}$, a volumetric productivity of 0.8 $g\,l^{-1}\,h^{-1}$, and a titer of 15 $g\,l^{-1}$ (personal communication from the development team). We created a PFD of this process (Fig. 1). An annual plant capacity of 40,000 metric tons of glucose conversion and a plant life of 20 years were assumed. The PFD has three major sections: seed fermentation, product fermentation, and separation/purification, which are described in detail in the following subsections.