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Upgrading of lignocellulosic biorefinery to value-added chemicals: Sustainability and economics of bioethanol-derivatives

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ABSTRACT

In this study, several strategies to upgrade lignocellulosic biorefineries for production of value-added chemicals are systematically generated and evaluated with respect to economic and sustainability objectives. A superstructure-based process synthesis approach under uncertainty integrated with a sustainability assessment method is used as evaluation tool. First, an existing superstructure representing the lignocellulosic biorefinery design network is extended to include the options for catalytic conversion of bioethanol to value-added derivatives. Second, the optimization problem for process upgrade is formulated and solved for two different objective functions: *i*) maximization of operating profit (the techno-economic criterion); and *ii*) minimization of the sustainability single index ratio (the sustainability criterion). These results indicate first that there is a significant potential of improvement of operating profit for biorefineries producing bioethanol-derived chemicals (247 MM$/a and 241 MM$/a for diethyl ether and 1,3-butadiene, respectively). Second, the optimal designs for upgrading bioethanol (i.e. production of 1,3-butadiene and diethyl ether) performed also better with respect to sustainability compared with the petroleum-based processes. In both cases, the effects of the market price uncertainties were also analyzed by performing quantitative economic risk analysis and presented a significant risk of investment for a lignocellulosic biorefinery (12 MM$/a and 92 MM$/a for diethyl ether and 1,3-butadiene, respectively). The multi-product biorefinery presented a more robust and risk-aware upgrading strategy considering the uncertainties that are typical for a long-term investment horizon.

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1. Introduction

Concerns regarding limitation of fossil resources, environmental problems, and sustainability in general, have become important drivers to develop efficient processes in the chemical and biochemical sectors. These concerns are also motivating the development of tools that support the design of more sustainable alternatives for processing renewable feedstock into fuels, chemicals, polymers and all types of bio-based materials.

An important concept related to the efficient processing of renewable feedstock into bio-based products is the "integrated biorefinery", which aims to convert all biomass fractions into a range of marketable products. This concept can be identified as "*the integrated production of bio-based chemicals, biofuels, bio-based polymers, pharmaceuticals, food and/or feed*" (adapted from Cherubini and Strømman [1]). However, for this integrated production there are usually multiple bio-based feedstocks and conversion technologies that match a range of pre-defined products, resulting in a large number of potential processing combinations and production paths for the conceptual design of biorefineries [2]. Therefore, during the early-stage of planning and design, it is important to quickly reduce the number of potentially feasible alternatives by identifying the most promising biorefinery processing paths with respect to specific design criteria (e.g. techno-economics, resource consumption, environmental impacts, and sustainability). A methodology capable of rapidly reducing the number of alternatives, and thus reducing the complexity of the design problem, would strongly support decision-making in the early-stage of the conceptual design [3].

There are, however, a number of challenges related to the synthesis and design of biorefinery systems [4], for example: (*a*.) challenges to achieve the maximum efficiency with improved designs as well as expansion by integration of conversion platforms (*e.g.* biochemical and thermochemical) or upstream and downstream processes; (*b*.) challenges to account for a wide range of feedstock and formulate local/regional solutions instead of solutions on a global basis as is the case for fossil-fuel based processes; (c.) challenges to take several dimensions of the design problem into account (*i.e.* feedstock characteristics, feedstock quality and availability; trade-offs between energy consumption for feedstock and product distribution, production and product market prices).

To overcome these challenges, a number of studies on lignocellulosic biorefineries have been performed in the past covering different areas, e.g. supply-chain, process synthesis and design, and product design. These studies looked at different aspects of biorefinery concept such as type of feedstock, processing technologies, and products as reviewed by Yuan et al. [5]. These studies provided interesting methodological approaches and insights into promising biorefinery configurations. However each of these studies has focused only on a limited number of alternatives or design options, which directly impact the optimal biorefinery design and concept. In our earlier work [6], a decision support toolbox for designing a biorefinery was developed to collect the large number of alternatives available in thermochemical and biochemical biorefinery platforms and to identify the optimal design using an optimization approach.

Moreover, most of these aforementioned studies deal with bioenergy and biofuels production, in particular, bioethanol as end product. However bioethanol can be used as intermediate feedstock to further synthesize and produce a large number of higher value-added chemicals, which can improve the overall economy of the biorefinery [7,8]. This study therefore expands the scope of biorefinery concept in two ways: *(a)* by simultaneously considering both thermochemical and biochemical conversion technologies in the design space and *(b)* by considering upgrading bioethanol to produce value-added chemicals.

Therefore, the main aim of this study is to address the problem of finding an optimal upgrading strategy for lignocellulosic biorefineries towards production of bioethanol derived value-added chemicals. We use a systematic evaluation methodology developed on the basis of earlier work [6,9]. In particular, we present the following: *i)* an extension of the lignocellulosic biorefinery superstructure by including the processes needed for bioethanol upgrading into value-added chemicals to improve the overall economics; and *ii)* a comparison of two objective functions (*i.e.* techno-economic and sustainability) under market uncertainties. The techno-economic objective function considers the operating profit, while the sustainability objective function is a multi-criteria index that compares the bio-based reference system to its equivalent petrochemical counterpart, and that considers: techno-economic aspects of feedstock and products, greenhouse gas emission (GHG) and cumulative energy demand (CED) of raw materials and processes, hazards indicators of all chemicals present in the system and economic aspects related to external agents.

The next section presents the superstructure-based optimization approach where the two objective function criteria, *i.e.* techno-economic and multi-criteria sustainability, are described. Then, the optimal processing paths under product price uncertainties are analyzed regarding the two mentioned objective functions. And finally the results of the techno-economic and sustainability objective functions are compared and discussed.

2. Methodology

The method for systematic synthesis and design of processing networks integrated with uncertainty analysis is briefly described below; more details can be found in Quaglia et al. [10] and Cheali et al. [6,9].

The framework consists of 7 steps which can be grouped in two main stages: *(i)* problem formulation and database generation; *(ii)* mathematical formulation and solution.

(i) Problem formulation (Step 1) includes the definition of the problem scope, the selection of suitable design specifications with respect to economic, engineering, and sustainability metrics. The processing networks (i.e. the group of different processing paths connecting feedstock with processing technologies and products), or the so called superstructure, is also generated in this step. The data regarding feedstock composition and technology efficiency (i.e. yield, reaction, separation, utilities/chemicals usage) is furthermore collected and verified. In case there is a significant deviation in the data