Bioresource Technology 236 (2017) 212–224

Contents lists available at ScienceDirect

Bioresource Technology

journal homepage: www.elsevier.com/locate/biortech

A generalized disjunctive programming framework for the optimal synthesis and analysis of processes for ethanol production from corn stover

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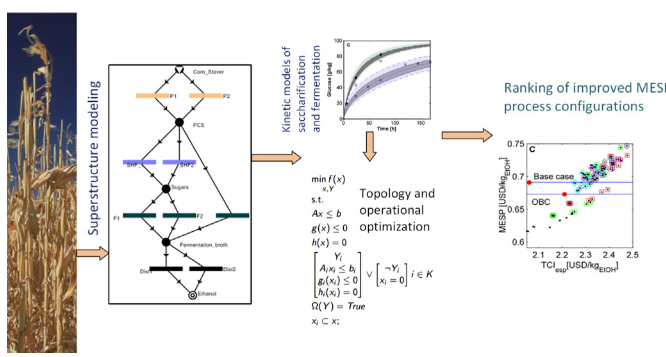
HIGHLIGHTS

- An optimization framework for process design of ethanol plants is presented.
- 150 different process configurations are compared and analyzed.
- New process configurations outperform the NRELs base case.
- Lower MESPs were found when solid-liquid separators are included.
- Energy in products ranges from 44% to 62.4% of the energy in corn stover.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 31 January 2017
Received in revised form 28 March 2017
Accepted 29 March 2017
Available online 4 April 2017

Keywords:
Solid-liquid separation
Biofuels
Techno-economic analysis
Process optimization

ABSTRACT

The aim of this study is to analyze the techno-economic performance of process configurations for ethanol production involving solid-liquid separators and reactors in the saccharification and fermentation stage, a family of process configurations where few alternatives have been proposed. Since including these process alternatives creates a large number of possible process configurations, a framework for process synthesis and optimization is proposed. This approach is supported on kinetic models fed with experimental data and a plant-wide techno-economic model. Among 150 process configurations, 40 show an improved MESP compared to a well-documented base case (BC), almost all include solid separators and some show energy retrieved in products 32% higher compared to the BC. Moreover, 16 of them also show a lower capital investment per unit of ethanol produced per year. Several of the process configurations found in this work have not been reported in the literature.

1. Introduction

With an increasing concern about global warming and long-term sustainability of fossil fuels and chemicals, products obtained from lignocellulosic biomass have been intensively studied during the last decades as sustainable substitutes to petroleum based products (Dale et al., 2014). Lignocellulosic ethanol is the first

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http://dx.doi.org/10.1016/j.biortech.2017.03.180
0960-8524/

biofuel produced from lignocellulosic materials instead of edible feedstock (Dale, 2015), an advance made possible by extensive research and development, an existing infrastructure for ethanol distribution and use in some countries, and national renewable fuel policies and subsidies such as the Renewable Fuel Standard in the United States (Whistance et al., 2017). However, there is room for improvement, as much as the one observed in the evolution of the first petroleum refineries into the modern ones. A large effort has been made by the Process System Engineering community to develop decision-making tools based on optimization to select among the myriad of feedstock, technologies, processes and product alternatives. These efforts include optimization of the entire manufacturing system, including supply chain design and analysis (Giarola et al., 2012; Osmani and Zhang, 2014; You et al., 2012), selection of optimal processing plants including feedstock and products (Tsakalova et al., 2015) and individual plant sections and technologies (Gabriel and El-Halwagi, 2013; Matthews et al., 2015).

However, the current industry of ethanol production from corn stover requires an analysis focused at the equipment level to retrofit its existing ethanol plants and to design more sustainable (both economically and environmentally) new ones. In this regard, previous studies on improving the economics of lignocellulosic ethanol production generally fix the topology (this is the combination of processes, equipment and their interconnection) to analyze one process configuration at a time. For every topology, heat and mass balances are calculated using a process simulation software and an economic analysis is carried out to calculate a minimum product selling price, net present value or any other financial metric. In this way, some of the leading pretreatments for agricultural biomass have been analyzed in a techno economic study (Tao et al., 2011) showing that, despite significant variation in investments, the minimum product selling price varies little between the pretreatments. Moreover, several process configurations for the saccharification and fermentation of pretreated corn stover (PCS) have been analyzed, and in some cases compared, including separated saccharification and fermentation, SHF, and simultaneous saccharification and fermentation, SSF (Bura et al., 2007; Saha et al., 2011). More advanced processing alternatives include separate processing of pulp and pretreatment liquor (Dutta et al., 2009) and several highly integrated bioprocesses, such as consolidated bioprocessing (CBP) where enzyme production, saccharification and fermentation are integrated into one system (Brethauer and Studer, 2014). However, a thorough comparison between process configurations is not possible due to an inexistent common framework of economic parameters and pretreatment conditions. Using the Attainable Region concept, Scott et al. (2013) showed that for the saccharification and fermentation of PCS the reactor networks that minimize the residence time can be constructed using plug flow reactors and continuously stirred tank reactors, despite the complexity of the reaction networks and underlying kinetics. However, no solid separators were included in this analysis. Including multiple reactors and solids separators in the saccharification and fermentation areas creates a combinatorial process synthesis problem, which calls for an optimization approach to determine the best process configurations from an economic perspective. Solid separators can be used to remove the unhydrolyzed cellulose and hemicellulose, allowing the separated fermentation of the released sugars. Thus, after combining the cell-free fermentation liquor with the separated solids, saccharification can resume with a reduced concentration of glucose and xylose. Although this alleviates product inhibition over the enzymatic reactions rates (Hodge et al., 2008; Teugjas and Väljamäe, 2013), the use of solid separators increases the investment costs, thus creating a new trade-off in the superstructure. This trade-off, have been recognized in the open literature (Sievers et al., 2014; Tao et al., 2012), however, no attempts have been made to analyze the optimal sequence of separation-reactor units in the saccharification and fermentation stages. This paper aims at filling this gap in the techno-economic analysis of process configurations in the saccharification and fermentation stages of a second generation ethanol plant using corn stover, through proposing and comparing process configurations beyond the conventional SHF, SSF and CBP processes by incorporating solid separators. We propose a systematic, optimization-driven, framework for the search of economically improved process configurations (modeled at the equipment level) of a stand-alone and energy self-sufficient plant producing ethanol, electricity and solid fuel from corn stover. Recognizing that a unique (optimal) solution is uninformative for decision makers, optimal and suboptimal process configurations will be ranked.

The novelty of this work is twofold. Firstly, a framework for the synthesis of processes producing ethanol from corn stover, able to handle a mathematical representation of the superstructure and to compare it against a rigorous process simulation is presented. This framework allows the assessment of a large number of process configurations in a common technical and economic basis, or the optimization of the superstructure to find a process configuration with optimal economic performance. The methodology used to create the superstructure results in a more compact formulation compared to previously reported ones based on Mixed Integer non-linear Problem formulations (MINLP) (Baliban et al., 2013; Martín, 2016), a reduced computational burden and a more natural modeling approach. Secondly, its application produced several new process configurations for ethanol production from corn stover, which have not been reported in the literature and show improved Minimum Ethanol Selling Price (*MESP*) values respect to a benchmark.

2. Materials and methods

This section introduces the Generalized Disjunctive Programming (GDP) formulation and the construction of the superstructure, this is, the mathematical representation of the process alternatives embedded in a plant-wide model. It is organized as follows. The problem is formally stated in Section 2.1, the conceptual design of the superstructure is presented in Section 2.2 and its mathematical representation is given in Section 2.3 along with the optimization problems that will be solved to find process configurations with improved *MESP*. Finally, in Section 2.4 the implementation of the problem is given, including the calibration of the superstructure against a rigorous simulation in Aspen HYSYS™.

2.1. Problem statement

The problem addressed by this framework can be formally stated as follows (equations are deferred to the Electronic Supplementary Information, ESI). Given is a superstructure for ethanol production from corn stover; this is, a mathematical representation of the pretreatment, saccharification, fermentation, distillation, combined heat and power production (CHP) and wastewater treatment (WWT) stages. Every plant design uses dilute sulfuric acid pretreatment and must be energy self-sufficient; generating heat and power from the lignin rich subproduct obtained after enzymatic hydrolysis, without consumption of gas, coal or oil. At the fermentation and saccharification stages, a number of process alternatives (equipment) are available to be included. They are represented by saccharification reactors, fermentation reactors and solid separators. Properly arranged, a combination of process alternatives can represent well-known process configurations, such as SHF or SSF, or new ones, including processes using pulp separation and cell recycle. The saccharification