Renewable Energy 89 (2016) 135–143

Contents lists available at ScienceDirect

Renewable Energy

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

Evaluation of biorefinery configurations through a dynamic model-based platform: Integrated operation for bioethanol and xylitol co-production from lignocellulose

Ricardo Morales-Rodriguez [a,*], Eduardo S. Perez-Cisneros [b], Jose A. de Los Reyes-Heredia [b], Divanery Rodriguez-Gomez [c]

[a] *Departamento de Ingeniería Química, Universidad de Guanajuato, Noria Alta s/n, 36050, Guanajuato, Gto., Mexico*
[b] *Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, C.P. 09340, México, D.F., Mexico*
[c] *Departamento de Biotecnología, Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, C.P. 09340, México, D.F., Mexico*

ARTICLE INFO

Article history:
Received 28 May 2015
Received in revised form
25 October 2015
Accepted 7 December 2015
Available online 17 December 2015

Keywords:
Biorefinery
Xylitol
Bioethanol
Model-based evaluation
Process configurations

ABSTRACT

This study presents a feasibility analysis of simultaneous bioethanol and xylitol production from lignocellulosic materials. In addition with the *in situ* power generation analysis employing the residual solids not converted in the process. This work is an extension of the Dynamic Lignocellulosic Bioethanol 1.0 modelling platform (Morales-Rodriguez et al., Bioresour Technol 2011; 102: 1174–84) in four process configurations that included operation in both continuous and continuous with recycling of unconverted materials. The benchmarking criteria employed was the potential profit of combined bioethanol and xylitol products. The best process configuration was simultaneous saccharification and co-fermentation in continuous with recycling and continuous production of xylitol with 11.4% higher for combined production of bioethanol and xylitol compared with the selected base case (simultaneous saccharification and continuous co-fermentation). Besides, integrating the energy generation using the remaining solid materials and energy balance, allowed to determine that the energy necessary for the production process configurations could be generated with the residues from each configuration. The energy produced from solid material combustion was in the range of 1.9 and 2.2 times higher than the energy needed for each configuration. The potential depleted carbon dioxide from crude oil for energy production was up to 32,194 kg/h.

1. Introduction

The accelerated growth of the world's population and the use of global resources have led to the increase of greenhouse gases and subsequent global environmental effects. Besides, the consensus about the gradual shift from a petroleum-based economy to a more carbohydrate-based economy, have predicted that by 2030, 20% of transportation fuel and 25% of chemicals must be produced from biomass [1]. Therefore, continued research has been conducted into developing production processes for conversion of biomass from agroindustrial residues into biofuels (*e.g.* bioethanol, biohydrogen, biobutanol, biomethanol, Fischer-Tropsch diesel, etc.), added-value bioproducts (such as xylitol, furfurals, aldehydes, sorbitol, etc.) and the subsequent conversion of some of them to high carbon number alkanes by an experimental approach [2,3].

For instance, xylitol is a five-carbon sugar alcohol widely used in the food, odontological, and pharmaceutical industries due to the significant benefits for human health. It has been mainly used as a sweetener in chewing gums, mints and toothpaste due to its anti-cariogenic properties. Moreover, it has also been utilized to prevents acute otitis media in small children [4] and as a suitable substitute for sugar for diabetics, as well [5,6].

In 2007, the annual production of xylitol was between 20,000 and 40,000 tons per year with an estimated market value of 40–80 M€ [7]. Chen et al. [8] estimated that the global market was about USD$340 million year^{-1}, according to the current D-xylitol price of 4–5 USD$/kg.

The conventional chemical production of xylitol includes the

* Corresponding author.
E-mail address: ricardo.morales@ugto.mx (R. Morales-Rodriguez).

http://dx.doi.org/10.1016/j.renene.2015.12.019
0960-1481/

hydrogenation of pure xylose in the presence of a Raney nickel catalyst at elevated temperature (373–418 K) and pressure conditions (up to 5066 kPa) [9]. More recently, xylitol has been produced with some Ruthenium-based catalyst that also needs extreme operating conditions [10]; which increase the production cost and subsequently the market prices of xylitol.

On the other hand, recently the biotechnological production of xylitol has reached importance because microbial production could be an alternative without operating at high pressure and elevated temperatures [11]. Among the diverse microorganisms, yeasts have been the preferred producers of xylitol. *Candida* strains have become important over *Saccharomyces cerevisiae* because they are a natural D-xylose consumer and maintain the reduction–oxidation balance during xylitol accumulation [4].

In *Candida* sp., once xylose is converted to xylitol, some of it is excreted, and the rest is converted to xylulose to generate biomass and maintenance energy. When an easily metabolized carbon source, such as glucose, is present in the medium it can be used by the cell in order to keep higher xylitol yields; however, high concentrations of glucose have been known to inhibit xylose transport into the cell and repress induction of relevant enzymes by xylose [12].

Up till, the process design and development have been mostly done using an experimental approach, which can be expensive from the economic and time-consuming perspective, for instance, some studies have been focused on the production of xylitol from the residues of bioethanol production [13], the conversion of lignocellulosic materials into xylitol by a previous pretreatment and enzymatic saccharification [14–16], the direct conversion of xylan into xylitol by engineered modified strains [11], in addition to the inhibition effect analysis of critical factors such as, enzyme load, pH, furfural compounds, phenolic compounds, aeration, the presence of other hemicellulosic sugars, etc. [6].

As far as a mathematical model approach for xylose fermentation process is concerned, the mathematical models available in the literature have been proposed from different points of view, for example, stoichiometric analysis [17], the use of response surface methodology and statistical analysis from several factors [18], sequential production of lactic acid and xylitol from vine trimming residues [19], direct xylitol production from xylose [20], xylitol production from xylose in the presence of glucose [12] and the extension of the former mathematical model by Hernandez-Escoto et al. [21] for a continuous reactor operation including some control scenarios and the search for an optimal feeding policy during xylitol fed-batch production [22]. The previous works have only been applied to model lab and bench scales processes. Thus, a systematic model-based simulation could be an alternative to analyze the production process at industrial scale from the economic and feasibility point of view.

Previously, Morales-Rodriguez et al. [23] presented a dynamic model-based approach for second generation (2G) bioethanol production, developing a Dynamic Lignocellulosic Bioethanol (DLB 1.0) modelling platform, which allowed to perform quantitative simulations and the comparison of 12 different process configurations based on the yield (kg-ethanol/kg dry-biomass), final product concentration and number of unit operations. The benchmarking criteria were based on the mass balance results obtained from the modelling of three sections of the process (pretreatment, enzymatic hydrolysis and co-fermentation) in 9 process configurations; and 3 extra process configurations including the pretreatment and simultaneous saccharification and co-fermentation (SSCF), using the former mathematical model proposed and validated by Morales-Rodriguez et al. [24] and implemented by Hernandez-Escoto et al. [25].

However, the DLB 1.0 platform did not include the downstream processes and conversion of other added-value bioproducts (such as xylose into xylitol) in the process route, which can be strategically added to the modelling platform since glucose and xylose are still present in the waste stream of the bioethanol production process.

Therefore, the objective of this study was to present an extension of the DLB 1.0 model platform through the addition of the dynamic modelling downstream processes and the conversion of xylose into xylitol. The comparison of selected process configurations and operations was carried out based on the combined production cost for bioethanol ($USD/L-ethanol) and xylitol ($USD/kg-xylitol) and their potential profit ($USD). This study allowed to decide, from an economical point of view on the introduction of a xylitol production section in the original bioethanol production process. Moreover, showing and analyzing the reliability of having a biorefinery platform by including xylitol co-production into the process and the *in situ* energy generation by the combustion of the residual unreacted solids in the process. The study assumed that the process plant has been already constructed and the necessary additional equipments for the xylitol production are already available at the plant location.

2. Methods

The development of this work for the extension of the DLB 1.0 computational platform followed 3 main steps, which included other sub-steps. Fig. 1 illustrates the systematic methodology proposed and implemented in this study.

2.1. Extension of the DLB 1.0: downstream processes and heat exchangers equipment addition

The extension of the DLB 1.0 modelling platform with respect to downstream processes and heat exchangers was performed

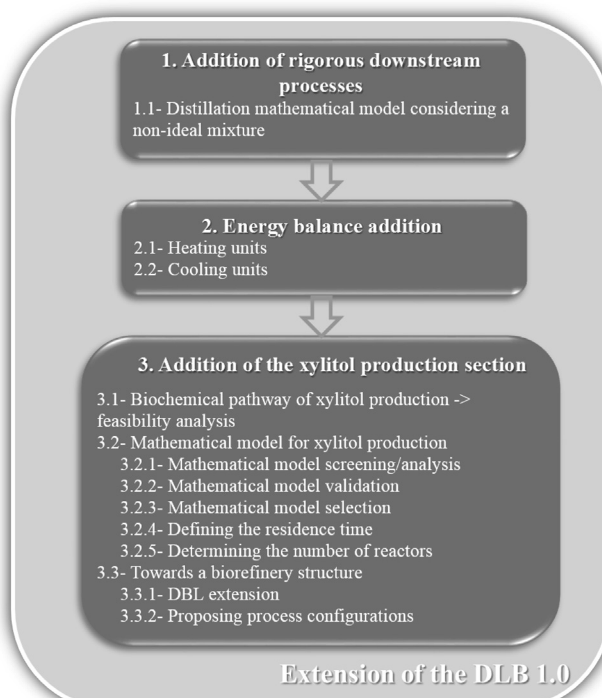

Fig. 1. Systematic methodology for the DLB 1.0 modelling platform extension. Towards a biorefinery approach.