A STRATEGY FOR PRODUCTION OF 1,4-PENTANEDIOL FROM CELLULOSE AND HEMICELLULOSE OF LIGNOCELLULOSE BIOMASS

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Abstract

Many studies have developed simulation models of bio-based process for production of liquid transportation fuels (bio-gasoline and biodiesel) from lignocellulosic biomass (containing cellulose, hemicellulose and lignin) and conducted economic analysis of the process. However, because of a sharp decrease in the price of crude oil based liquid transportation fuels in entire world today, lignocellulosic biofuels process cannot yet compete with the crude oil based process. Alternatively, production of value-added chemicals instead of biofuels has been considered as a viable option using lignocellulosic biomass. In this study we develop a catalytic process and perform an economic analysis for production of 1,4-pentanediol from lignocellulosic biomass. 1,4-pentanediol was used in the preparation of poly(ortho ester). In the process, the cellulose and hemicellulose are simultaneously converted to levulinic acid (LA) using γ-valerolactone (GVL) as a solvent. The LA is then converted to GVL in the presence of GVL and subsequently to 1,4-pentandiol. The simulation models of bio-based process are developed using ASPEN Plus simulator. Moreover, in order to reduce the total process energy requirements, heat integration of the process has conducted using Aspen Energy Analyzer. Our energy analysis shows that the total energy requirements could be satisfied from combustion of the biomass residues (lignin). Our economic analysis shows that minimum selling price of 1,4-pentanediol is $1.57 per kg which is compete with the market price of crude oil based one.

Key words
Lignocellulosic biomass, Economics, GVL, 1,4-pentanediol

Introduction

Because of increased usage of fossil fuel in entire world, alternative energy sources are in the spotlight in order to escape the difficulties of fossil fuel supply. Lignocellulosic biomass is available as an option of a carbon source that can be substituted for the production of transportation fuels to meet the energy needs of the future. So, there are many researches for economic analysis about production of biofuel using lignocellulosic biomass [1-3]. Past long years, extensive conversion technologies were developed for efficient usage of lignocellulosic biomass [4-6]. Lignocellulosic biomass consists of three polymeric components: hemi-cellulose, cellulose and lignin. Hemi-cellulose and cellulose can be converted into various types of biofuels, such as bioethanol, bio-butanol and bio-gasoline. And lignin is used to produce steam and electricity as fuel. Until now, many researches were studied about the reaction after separating the hemi-cellulose, cellulose and lignin [5, 7-9]. But even high efficiency of LA converted, these processes require high total cost (capital + operating cost) because pretreatment process of lignocellulosic biomass is needed. So, as a method for increasing the economics, the research for simultaneous conversion of hemicellulose and cellulose in same reactors had been studied [10]. Unlike previous studies, if hemicellulose and cellulose at the same time was converted, yield of LA converted was decreased relatively. But the economics of the entire process, will be increased because there aren't pretreatment processes of biomass. And it requires a large amount of heat utility in biomass conversion processes. So, there is a study applying heat integration for further improving the economics of the overall process [1]. As a trend of sharply falling price of fossil fuels in the world, economics about production of transportation fuels using lignocellulosic biomass have decreasing. Therefore it can be possible to improve the economics by producing chemical products using lignocellulosic rather than transportation fuels.

Our studies have calculated the economics of process about production of chemical products rather than transportation fuels using lignocellulosic biomass. In section 2, we describe an overview of the technologies we, and in section 3 we describe a different alternative design. In section 4, we present the results of techno-economic analysis.

Technology overview

In this study, 1,4-pentanediol was produced from lignocellulosic biomass in simultaneous conversion of hemicellulose and cellulose.

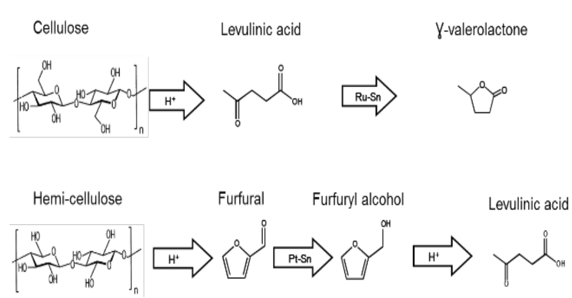

Fig. 1 Simultaneous conversion of cellulose and hemicellulose to gamma-valerolactone (GVL)

In here, our strategy combines three catalytic conversion systems for (1) the simultaneous conversion of cellulose and hemi-cellulose to LA, (2) LA converted to GVL and (3) GVL conversion to 1,4-pentanediol.

In the initial reaction, cellulose and hemi-cellulose is converted to Levulinic acid (LA) [Fig.1]. LA is used as materials for the production of liquid hydrocarbon fuels and fuel additives as well as various chemical substances. LA can be produced by the hydrolysis of cellulose followed by the dehydration of glucose using diluted acid [11]. Hemi-cellulose was converted to furfural by process of hydrolysis and after it conversion, furfural was converted to furfuryl alcohol over Pt-Sn catalyst [12]. And furfuryl alcohol was converted to LA by dehydration of furfuryl alcohol [12]. And LA can be upgraded to GVL over a RuSn2/C catalyst [13]. After production of GVL, GVL can be converted to 1,4-pentanediol chemical product over Rh-MnOx/SiO2 [Fig. 2][14].

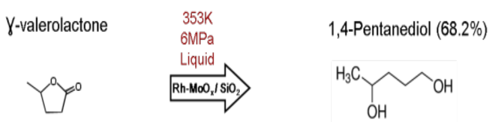

Fig. 2 1,4-pentanediol production

Process development

Basic design

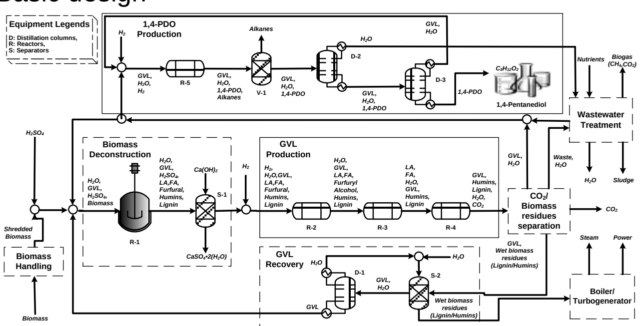

Fig. 3 Process flowsheet for the integrated conversion systems.

First, we develop an integrate process for the conversion of biomass-derived cellulose and hemi-cellulose to chemical product. The integrated conversion systems consists of eight main sections, as shown in fig. 3: biomass handling, biomass deconstruction, GVL production, GVL recovery, CO2 and biomass residues separation, 1,4-pentanediol production, wastewater treatment, and boiler/turbo-generator.

In the first step of biomass conversion process, the pre-treatment process performs to remove residues prior to entering the biomass conversion process. And in the second process, hemi-cellulose and cellulose were converted to LA in biomass separation process. LA was converted to GVL in GVL solvent in third process of biomass conversion process. Using GVL from LA conversion process, GVL go to the process of production of 1,4-pentanediol and produce the 1,4-pentanediol chemical product. GVL is used as a solvent in the separation process of biomass. And GVL is high cost solvent so these have to recycle to the process of separation process of biomass in order to reduce total cost of entire process.

Alternative configuration

In the base model, there are alkanes (1-pentaneol and 2-pentaneol) are created when the process create 1,4-pentanediol from GVL to generate to steam and electricity and these energy generated from alkanes have met the demand of total heat. However, we thought that there are insufficient amount of the alkanes to produce steam and electricity. Thus, the alkanes in order to improve the economics of the process were conducted to evaluate the strategy for selling on the market as a fuel.

Techno-economic evaluation

Design basis and assumptions

A simulation model was developed using Aspen plus process simulator. Based on the simulation results with experimental results, using the Aspen process economic analyzer, unit cost was calculated. And installed equipment cost for power generation and waste treatment and handling of biomass was estimated based on the NREL reports. Equipment and utility cost in order to reduce the heating requirement were calculated using Aspen energy analyzer program.

Minimum selling price

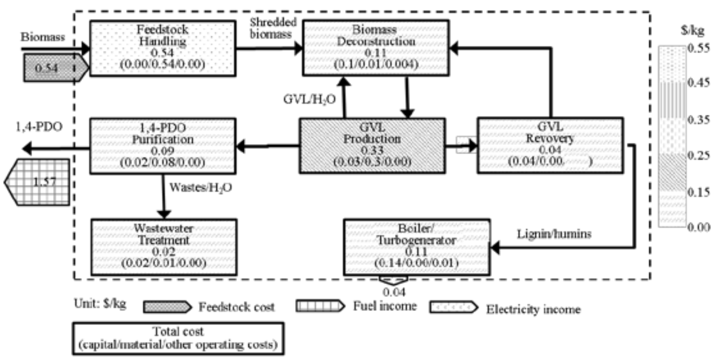

Fig. 4 capital/material/operating costs for entire process.

The capital cost/material/operating costs of the base case design are given in Fig. 4. Considering the capital, material and operating costs, we determine a minimum selling price (MSP) of 1,4-pentanediol chemical product that makes the net present value of the present equal to zero. The minimum selling price of 1,4-pentanediol chemical product is USD $ 1.57 per kg 1,4-pentanediol: raw material of biomass ($0.54/kg), Feedstock handling ($0.54/kg), biomass deconstruction ($0.11/kg), GVL production ($0.33/kg), GVL recovery ($0.04/kg), Boiler/Turbo-generator ($0.11/kg), Wastewater treatment ($0.02/kg), and 1,4-pentanediol production and purification ($0.09/kg). The processes having a high price of MSP are raw material of biomass and feedstock handling process. And the process having a low price of MSP is the process of wastewater treatment. Therefore, it is important to reduce the price of raw material biomass and the cost of the biomass handling process.

Heat integration

This process requires great amounts of heat requirement. Among the components of lignocellulosic biomass, lignin, one of the components in lignocellulosic biomass, is used as fuel and is used to produce the heat required to the entire process of biomass conversion process. So, heat integration technique was used in order to reduce the amount of heat utilities used because the amounts of heat utilities are significantly high. By developing the heat and cold network among the streams of entire process, the amounts of hot and cold utilities can be reduced after identifying the hot & cold stream of biomass conversion process.

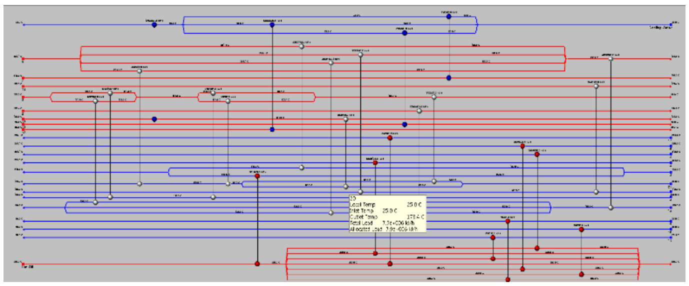

Fig. 5 heat exchanger network of biomass conversion process

Through Aspen Energy Analyzer program, we can configure the heat exchanger network [Fig. 5]. And if it configured to reflect a process, new heat exchanger network may be ways to reduce the heating requirements.

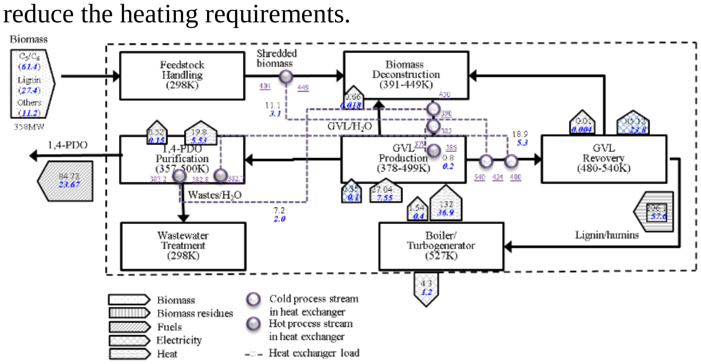

Fig. 6 networks of heat exchange between hot and cold streams.

Through the heat exchanger network among biomass conversion process, the amount of energy required can be reduced. And heat exchange network among processes was presented in figure 6.

Alternative designs

Unlike the basic design model, by using the alkanes from the process of 1,4-pentanediol production, the alkanes was not used for the production of steam and electricity. And production process for steam and electricity was not included. Also, the production of steam and electricity for the cost does not paid because alkanes does not produce steam and electricity. Therefore, we thought that would be a better economics. Under economic evaluation results, the MSP about selling alkanes to market as fuel is better than the MSP about producing the steam and electricity. The MSP is $1.54 per kg about selling alkanes to market as fuel.

Conclusions

Through this study, we developed a strategy for the simultaneous conversion of hemicellulose and cellulose in lignocellulosic biomass to chemical products based on catalytic conversions. Heat integration technology was identified as a fairly good way to improve the economics of the process. And we found that when 1,4-pentanediol is produced and electricity is generated on site, the MSP is $ 1.57 per kg for 1,4-pentanediol. And the MSP is $ 1.54 per kg when no electricity is generated on site and alkanes from 1,4-pentanediol production process is selling to other industry site.

Acknowledgements

This work is financially supported by Korea Ministry of Environment (MOE) a「Knowledge-based environmental service (Waste to energy recycling) Human resource development Project」

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