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Process simulation of ethanol production from biomass gasification and syngas fermentation

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ABSTRACT

The hybrid gasification-syngas fermentation platform can produce more bioethanol utilizing all biomass components compared to the biochemical conversion technology. Syngas fermentation operates at mild temperatures and pressures and avoids using expensive pretreatment processes and enzymes. This study presents a new process simulation model developed with Aspen Plus® of a biorefinery based on a hybrid conversion technology for the production of anhydrous ethanol using 1200 tons per day (wb) of switchgrass. The simulation model consists of three modules: gasification, fermentation, and product recovery. The results revealed a potential production of about 36.5 million gallons of anhydrous ethanol per year. Sensitivity analyses were also performed to investigate the effects of gasification and fermentation parameters that are keys for the development of an efficient process in terms of energy conservation and ethanol production.

1. Introduction

The Energy Independence and Security Act targeted a production of ethanol of 36 billion gallons by 2022 (Schnepf, 2011), and expects cellulosic materials to be used as a sustainable feedstock for renewable ethanol. The biochemical platform of ethanol production ferments sugars obtained from hydrolyzates of pretreated biomass. However, this platform is unable to degrade lignin, which is a major portion of biomass. Therefore, the potential ethanol yield is reduced significantly. In addition, the biochemical platform requires expensive pretreatment processes to make the polymeric sugars in the biomass amenable to enzymes. These problems can be avoided by first gasifying the lignocellulosic biomass to synthesis gas (syngas), containing primarily CO and H_2 along with some CO_2. The syngas is converted to alcohols and organic acids by acetogenic microorganisms via the Wood-Ljungdahl metabolic pathway (Henstra et al., 2007; Liew et al., 2016; Phillips et al., 2017). Different acetogenic microorganisms have the ability to produce different alcohols, including ethanol, butanol, propanol, and hexanol, and their corresponding organic acids. However, most acetogenic microorganisms produce ethanol and acetic acid, which are the focus of the present study. The stoichiometric equations for the production of ethanol and acetic acid are displayed below:

$$4CO + 2H_2O \rightarrow CH_3\,COOH + 2CO_2 \tag{1}$$

$$2CO_2 + 4H_2 \rightarrow CH_3\,COOH + 2H_2O \tag{2}$$

$$6CO + 3H_2O \rightarrow C_2\,H_5OH + 4CO_2 \tag{3}$$

$$2CO_2 + 6H_2 \rightarrow C_2\,H_5OH + 3H_2O \tag{4}$$

Clostridium ljungdahlii (Tanner et al., 1993), *Clostridium carboxidivorans* (Phillips et al., 2015; Ukpong et al., 2012), *Clostridium ragsdalei* (Devarapalli et al., 2017; Saxena and Tanner, 2011), and *Alkalibaculum bacchi* (Liu et al., 2012) are examples of microbes that produce alcohols and organic acids via syngas fermentation. The main advantages of syngas fermentation include potential of high product yield due to utilization of all biomass fractions, including lignin, as well as operation at mild pressures and temperatures. However, there are challenges in syngas fermentation, such as low gas-liquid mass transfer rates and the cost of medium. These issues have been partially addressed in the literature (Devarapalli et al., 2017; Gao et al., 2013; Orgill et al., 2013; Phillips et al., 2017).

To date, little efforts have been directed to process simulation of the hybrid gasification-syngas fermentation. To our knowledge, there are few published studies on process simulation of syngas fermentation. One of these studies was focused on the production of polyhydroxylalkanoate and hydrogen rather than ethanol (Choi et al., 2010). Another study used process simulation for modeling the production of ethanol via syngas fermentation, although it was based on a small-scale process (Rao, 2005). Piccolo and Bezzo (2009) presented techno-economic analyses for two ethanol production processes. One

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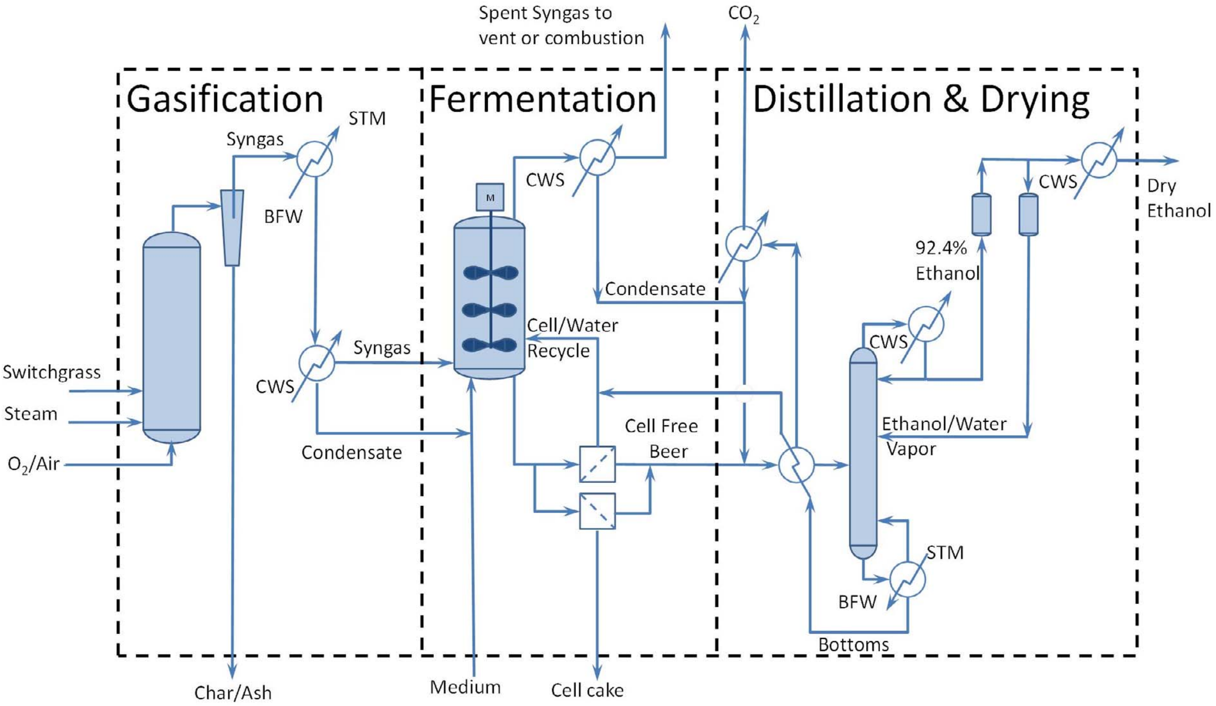

Fig. 1. Process flow diagram (PFD) depicts flow of material through the simplified equipment for gasification of switchgrass and syngas fermentation to produce ethanol. BFW: boiler feedwater system; STM: steam; Syngas: synthesis gas; CWS: circulating water system.).
Adapted from Phillips et al. (2017

process was the conventional hydrolysis of biomass followed by fermentation, and the other process was gasification followed by syngas fermentation. Martín and Grossmann (2011) optimized energy use for gasification of biomass and compared conversion of syngas to alcohols using catalytic and fermentation processes. Ardila et al. (2014) presented a simulation model for gasification of sugarcane bagasse followed by syngas fermentation without including the amount of feedstock used, ethanol yield or separation process. In addition, none of the previous studies examined effects of critical syngas fermentation parameters such as specific gas uptake rate, ethanol concentration and substrate gas conversion efficiencies on required reactor volume and energy requirement. As evident from the above, there is a need for developing detailed simulation models for investigating the hybrid gasification-syngas fermentation process. This study aims to fulfill that need in the existing literature.

Modeling and simulation of the biomass gasification-syngas fermentation process can provide a powerful tool for evaluation of this technology at a commercial scale. Process simulation software packages, such as Aspen Plus®, or Aspen Hysys®, SimSci™ Pro/II, have been used in the chemical industry for performing techno-economic analysis of multiple types of processes. The objective of the present study was to design a new model in Aspen Plus® of an integrated gasification-syngas fermentation plant for ethanol production from switchgrass as a model lignocellulosic biomass. This study should thus provide a framework for defining the gasification, fermentation, and product recovery units to support equipment specification, and will be the basis for a future comprehensive techno-economic analysis.

2. Model description

2.1. Simulation software

The model describing the various unit operations used for gasification fermentation and product separation was developed in Aspen Plus® version 8.2 (AspenTech, Inc.). For the purpose of designing the gasification and fermentation stages of the process, both Aspen Plus blocks and user-defined calculator blocks were integrated. These two types of calculation tools exchanged data until the mass and energy balances converged.

Aspen Plus® provides different thermodynamic packages to calculate the phase equilibria throughout the simulation. The non-random-two-liquid (NRTL) model was the main thermodynamic model used for this study (Renon and Prausnitz, 1969). The thermodynamic package chosen should be capable of accurately describing the phase equilibrium between different components in the mixture, including a water-ethanol azeotrope that exists in these systems. Further the gasification process requires an equation of state approach. In this study, the Redlich-Kwong-Soave equation of state (Soave, 1972) with Boston Mathias alpha function (RKS-BM) was used to calculate the phase equilibria during gasification, and the ASME steam table correlations were used for calculating steam properties.

2.2. The hybrid gasification-syngas fermentation process

A process flow diagram depicts the gasification of biomass, fermentation of CO and H_2 into ethanol and recovery of ethanol by distillation and drying (Fig. 1). This simplified depiction of the equipment and material flows is represented mathematically within the Aspen Plus® model. Switchgrass is fed into a gasifier and converted by partial combustion to syngas containing mainly CO and H_2 along with some CO_2. The syngas is converted into ethanol and acetic acid in the fermenter by acetogenic microorganism like *Clostridium ragsdalei*. Ethanol produced is removed from the fermentation broth or beer by distillation and dried in packed beds of molecular sieves with a recovery of water and ethanol.

2.3. Biomass feedstock

Switchgrass (*Panicum virgatum*) is a herbaceous species that has been identified as a good candidate for being used as a sustainable energy crop for biofuel production because of its high yield and efficient use of water and nutrients (Sanderson et al., 1996). The available