Process simulations for wheat and wheat straw based ethanol biorefinery concepts

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Abstract: Bioconversion of wheat straw to ethanol is becoming an attractive alternative to ethanol production from conventional grain crops, especially with wheat straw being a low commercial value, high volume agricultural by-product and grain prices continuously increasing. Similarly, using wheat straw as energy source in the ethanol biorefinery has become a subject of interest in recent years. In this light, the aim of present work is to compare ethanol production from wheat grain and wheat straw for commercial scale plants. Using same configuration for the two feedstocks, change in ethanol and by-products' outputs is simulated. The simulated biorefinery is based upon the established technologies within the bioethanol industry. In the two models same by-products are produced, namely: dried distillers grain solubles (DDGS), acetic acid, glycerol and furfural. Results show that 20% less ethanol is produced per ton for wheat stalk than when wheat grain is used.

Keywords: Biorefinery, Ethanol, Fermentation, Dry Grind Process

1. INTRODUCTION

In recent years cereal grains such as wheat and corn have become important feedstock for ethanol biorefineries with corn being mainly used in American biorefineries and wheat in the European biorefineries. The cereals to fuel ethanol industry is relatively small and not as developed as the cane to ethanol or ethanol from starch industry. Nonetheless, in a short span cereals have become a significant part of bio-fuel feedstock. While wheat is actively used and researched as the feedstock for ethanol (e.g. [5], [11]), low value high volume wheat straw is largely treated as a by-product. However, in recent years research and interest in using wheat straw as ethanol source has increased (e.g. [9]), especially for the fact that for every kg of wheat grain 1.3–1.4 kg of wheat straw is produced [12] and costs are one fourth the price of wheat grain. A typical 100 kg of wheat grain (10% moisture, wb) produces 29 kg of pure ethanol, 44 kg of DDGS (8% moisture, wb) and 28 kg of CO₂ [11], while 100 kg of wheat stalk produces around 23 kg of ethanol.

In recent years, ethanol production from wheat straw has progressed on to demonstration scale and a few pilot biorefineries have been setup. Iogen is operating one such biorefinery in Ottawa, Canada, using their proprietary enzyme hydrolysis and

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fermentation techniques to daily produce 930 tonne ethanol from 2900 tonne of wheat and corn stalk [3]. Chempolis, Finland is producing cellulosic ethanol, biochemicals and fibres from 68 tonne/day of variety of non-food biomass, particularly straw and bagasse [4]. TMO Renewables of UK genetically modified a bacteria from a strain found in compost heaps to produce ethanol from cellulosic feedstock, naming the bacteria TM242 [6], [14]. The main feedstocks include grasses, wheat straw, newspaper, municipal waste and distillers' grains. Abengoa, Spain is operating two wheat straw to ethanol biorefineries. The first one in Salamanca, Spain, has a processing capacity of 70 tons of agricultural residues, such as wheat straw, each day and produces over 11 tons of fuel grade ethanol [1] while the second plant operating in York, Nebraska (USA) uses both corn stover and wheat straw [2]. Other than these there are numerous biorefineries under construction throughout the globe, optimally designed to utilize wheat straw for ethanol production or in some cases a variety of biomass sources to produce cellulosic ethanol.

There are two main processes for production of ethanol from grains and straw; dry milling and wet milling. Of the two, mostly dry grind milling process is used for producing ethanol, though wet milling is increasingly being employed in newer biorefineries. Main advantage of wet milling is that it produces a number of valuable co-products, however, it is capital intensive and produces less ethanol when compared with dry milling. In wet milling the feedstock such as corn kernels are steeped and fractionated in order to produce co-products. In dry milling whole grain is milled, liquefied, saccharified and fermented, producing ethanol and DDGS as a co-product. The top-level block diagram of a typical dry-milling process is shown in the following figure (1).



Figure. 1. Dry Milling Process.

In a typical dry milling process, wheat grain is milled and mixed with water. The mash or slurry is then cooked to help prepare it for fermentation. The mash is removed from cookers and allowed to cool. It is then liquefied by adding enzymes which break down complex carbohydrates (starch) to dextrins (complex sugars). It is important that liquefaction and proceeding reactions take place in optimum temperature and pH ranges. Step following liquefaction is called saccharification where hydrolysis of soluble polysaccharides (i.e. complex carbohydrates such as starch, cellulose) into monosaccharide components (i.e. simple sugars) takes place. The monosaccharides are easily fermented by the bacteria/fungi into ethanol during the next step which is fermentation. There is a variety of organisms; bacteria or fungi (such as yeast) which ferment carbohydrates into ethanol under oxygen-free conditions to obtain energy (in the form of adenosine triphosphate) and are thus dependent upon ethanol production for growth and long-term survival [10].

Theoretically, the optimum reaction yield is 0.51 kg of ethanol and 0.49 kg of CO₂ per kg of sugar for wheat grain [7] and nearly 0.41 kg of ethanol per kg of sugar for wheat straw [9]. The overall fermentation reaction can be described by the following equation [10].

Carbohydrates + Fungi/bacteria \rightarrow Ethanol + CO₂ + more Fungi/bacteria

At the completion of fermentation process the mash is heated again. During this heating process, ethanol evaporates into a vapour that is collected, while some biomass and enzyme solids remain behind. This is the distillation process from which ethanol vapour is cooled and condensed into liquid form. This liquid is dehydrated to remove excess water leaving behind "anhydrous" ethanol suitable for blending with gasoline. The distillation process also produces a highly valuable co-product from the leftovers of the fermentation. They are composed of unfermented and unhydrolyzed biomass and enzyme solids. This stream of stillage which exists from the distillation column is centrifuged into thin stillage which is further concentrated by evaporation to produce distillers' dried grains with soluble (DDGS).

The efforts to optimize ethanol production from biomass has yielded numerous modifications of the typical dry grind milling process. These modified processes range from adaptations in pre-treatment processes to recycling in the fermentation process, however all of these are at the experimental stages.

In the current study a dry milling process using wheat has been developed and simulated in ECLIPSE simulation software. Wheat grain is used as feedstock in the basecae, which is then compared with wheat stalk as the feedstock. Structure of the paper is as follows. Simulations for the two feedstock are produced and outputs compared. In second section of the paper, composition of wheat grain and wheat stalk are discussed while in section three the technical model is presented. Fourth section discusses the simulation result, while the paper concludes in section five.

2. COMPOSITION OF WHEAT GRAIN

Composition of biomass not only greatly affects the ethanol output but it also helps select best suited technologies for ethanol production. Wheat grain is a complex structure composed of different tissues that have distinct functions and biochemical compositions (figure 2). On the whole the grain can be divided into three sections, namely: endosperm, bran and wheat germ. Endosperm is 80–85% of the wheat grain and is mostly composed of starch and proteins, while most of the fibre, vitamins, minerals and antioxidants are concentrated in the outer layers, i.e. bran (12–17% of the grain) and the wheat germ (3% of the grain) [8]. Bran itself is composed of three layers, namely: i) Pericarp layer: rich in fiber; ii) Aleurone Layer: rich in vitamins, minerals and antioxidant compounds; and iii) Testa Layer: composed of hydrophobic material containing non polar compounds [8].



Figure. 2. Structure of wheat grain (1) and of the constitutive layers of wheat bran (2).P: pericarp (fibrous and porous: empty cells); T: testa (hydrophobic layer); A: aleurone (full cells with cellular content rich in proteins, lipids and minerals) [8].

2.1 Ultimate and Proximate Analysis

Proximate and ultimate analyses of wheat grain were obtained through the PHYLLIS database [13]. According to the proximate analysis wheat grain contains 7.3% (wt.) of ash in dry form. The ultimate analysis of wheat grain and wheat stalk are provided in the following table (I).

Element	Wheat Straw	Wheat Grain
Carbon	42.15	49.4
Hydrogen	5.83	5.4
Oxygen	50.84	44.3
Nitrogen	0.70	0.37
Sulphur	0.00	0.06
Chlorine	0.48	0.464
Total	100	100

Table I. Composition of Wheat Straw and Wheat Grain (Daf%)

3. TECHNICAL MODEL

As already discussed, the current biorefinery model is built upon the dry milling concept using the established technologies within the bioethanol industry. Same model has been used to simulate both wheat grain and wheat stalk based biorefineries (Figure 3). Wheat grain and wheat stalk are delivered at the factory gate. Feedstock is stored at the site in short term storage silos. Biomass then goes to pre-treatment where it is washed, cleaned and shredded. Water is then added to help prepare the mash. This mash is then heated at 120 °C to sterilize it. Warm mash is then cooled and passed through Separate Hydrolysis and Fermentation (SHF) process. In this process mash passes through liquefaction, saccharification and fermentation stages in separate tanks. Temperature, pH and residence time for all three are different, dependent upon the biomass and enzyme used.

3.1 Biorefinery System

Refinery size for the current study is 2,000 dry ton/day. Wheat grain/stalk is delivered at the refinery gates where it is stored in short-term storage silos. Refinery consists of pretreatment, conversion and product storage technologies. Utilities are taken off the grid and all products are transferred to and from the refinery via trucks. Operating scale of the biorefinery is as follows (table II).

	Table II.	Biorefinery	Operating	Scale
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	Scale
Wheat Grain	2000 tons/day
Operating Temperature	15 °C
Operating Pressure	1 bar

The amount of different feedstock used during the biorefinery operations are listed below (table III).

Feedstock	Ton/day
Wheat grain/stalk	2000
Glucoamylase	2.306
Alpha-amylase	1.598
Yeast	0.554
Water	1333.34

Table III. Daily Biorefinery Consumption



Figure. 3.Biorefinery Model

3.2 Assumptions

During the simulation it was assumed that per ton of wheat straw and wheat grain used, same quantity of enzymes and water would be used to complete the process.

4. SIMULATION RESULTS AND DISCUSSION

With a feedstock input of 2000 ton/day the system produces 672 tons of ethanol for wheat grain and 534 tons of ethanol for wheat stalk. Daily production of different products is provided in the following table (IV).

Product	Wheat Grain	Wheat Stalk
Ethanol	672.365	534.125
CO ₂	655.603	520.819
DDGS/residue	839.981	919.872
Furfural	16.848	13.435
Acetic Acid	39.571	31.449
Glycerol	44.755	35.597

Table IV. Wheat Grain and Wheat Stalk Products (tons/day)

4.1 Ethanol and Residue

Wheat stalk produces less ethanol compared to wheat grain, but it also produces more residue. This is mainly because less percentage of wheat stalk is fermented as compared to wheat grain. In wheat grain's case the residue is dried into DDGS but the residue from stalk being higher in lignin and lower in protein content cannot be compared to DDGS obtained from wheat grain. Wheat grain produces nearly 20% more ethanol than wheat stalk per ton, while the change in residue output is 9%. For other products, furfural, acetic acid and glycerol is also produced less per ton for wheat stalk.

5. CONCLUSION AND FUTURE RESEARCH

The aim of this research activity was to prepare a technical comparison between wheat grain and wheat stalk for production of ethanol. As the simulation results show, wheat stalk produces 20% less ethanol than wheat grain per ton of the biomass. The wheat stalk ethanol output, however, is an optimum theoretical system. The current lignocelluloses biorefineries are operating at considerably lower efficiencies. However, as with other technologies, with time and technological advancement the theoretical limits might be achieve.

Technically this paper has shown the feasibility for wheat straw to be used as a feedstock for ethanol production. The next step is to build economic models for the two feedstocks. The techno-economic models would then help determine the viability of wheat straw to

be as ethanol feedstock.

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