

## Process Simulation of Ethanol from Straw – Validation of Scenarios for Austria

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In this work the production of ethanol from straw is assessed from an energetic point of view. For that purpose process simulation with the simulation software IPSEpro is used. For a process based on steam pretreatment and enzymatic hydrolysis, several scenarios for utilization of stillage are simulated. Ethanol yield is 78,3 %, based on C6 sugars in the raw material and overall energy efficiencies range from 38 % to 78 %.

### 1. Introduction

In the EU the target for renewable energy in transport has been defined to be 10 % at 2020 (EU, 2009). Biofuels are one strategy to reach this target and thus biofuels must reach an energy based market share of 5,75 % by 31 December 2010 (EU, 2003). In Austria this share is successfully implemented via blending of diesel with bio-diesel and gasoline with bio-ethanol respectively. Currently ethanol produced from wheat is employed to reach the 5,75 % target as far as gasoline is concerned. In the long run however, the demand for fuels in general and for bio-ethanol in particular will increase consequently new resources for bio-ethanol production have to be tapped.

For two main reasons lignocellulosic materials are good choices for bio-ethanol production. First, the greenhouse gas mitigation potential compared to both, fossil fuels and bio-ethanol from starchy crops is high (Eisentraut, 2010; Wang et al., 2007) and second usage of additional acreage can be avoided if residual materials from food production or forest industry are employed.

In this work we investigate the production of ethanol from straw from an energetic point of view. Several process scenarios based on steam pretreatment and enzymatic hydrolysis are compared using the steady state process simulation software IPSEpro.

### 2. Process Simulation

For calculation of mass and energy balances the equation oriented, steady state flowsheeting software IPSEpro is employed. A model library for handling the complex materials present in lignocelluloses to ethanol process was constructed (Schausberger et al., 2010) and is improved and augmented continuously. To guarantee optimal use of energy heat exchanger network synthesis was performed with in-house optimization software.

### 3. Process Description

Figure 1 summarizes the scenarios considered in this work. As can be seen, the scenarios are identical as far as the upstream process, ethanol recovery and stillage separation are concerned.

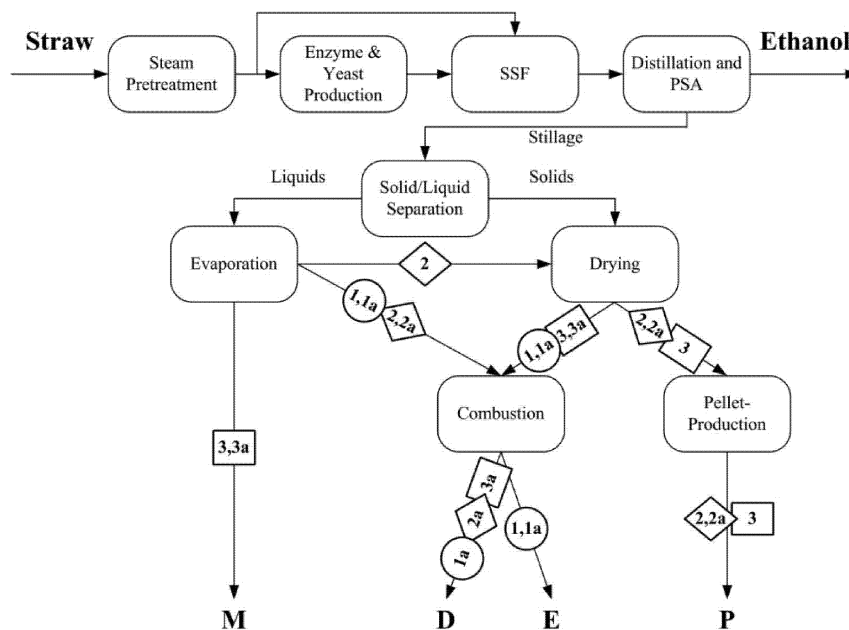


Figure 1: Schematic summary of process scenarios for the production of ethanol from straw. Byproducts are abbreviated as follows: M: C5-Molasses, D: district heating, E: Electricity, P: Pellets. Lines without numbering are identical in all the scenarios.

For all the scenarios process steam is generated by burning part of the stillage reducing the processes' demand for fossil energy largely. The remaining streams are used to create the byproducts electricity (E, Scenarios 1 and 1a), Pellets (P, 2 and 2a) and C5-molasses (M, 3 and 3a). In Scenarios 1a, 2a and 3a additional district heating (D) is produced. Ethanol production capacity is 100,000 t/y, operating time is 8,000 h/y.

#### 3.1 Steam Pretreatment

Baled straw with a moisture content of 10 % (w/w) is shredded to smaller pieces, wetted to reach a moisture content of 65 % (w/w) and preheated close to the boiling temperature of water. The moistened and preheated straw is impregnated with 1 % (w/w)  $\text{SO}_2$  based on dry matter. Subsequent steam pretreatment is performed at 190 °C. Heat losses are assumed to be 10 % of total heat transferred. As suggested by Wingren (Wingren et al., 2003) the pressure release after steam pretreatment is performed in two steps, first at 4 bar and then at 1 bar. In steam explosion, 80 % of hemicelluloses sugars are released as sugar monomers, 15 % are degraded. For cellulose 10 % and 2 % of sugars are released

as monomers and degraded, respectively. Formation of sugar oligomers is not considered.

### 3.2 Simultaneous saccharification and fermentation, enzyme production and yeast propagation

The slurry after steam pretreatment is neutralized using  $\text{NH}_4(\text{OH})$ , cooled and split into three streams. The major part is directly fed to simultaneous saccharification and fermentation (SSF) and minor parts are used for enzyme production (EP) and yeast propagation (YP). The massflows of the streams to EP and YP are a result of the conversions in the reactors on the one hand and enzyme and yeast requirements in SSF on the other hand.

In YP the pretreated straw is enriched with molasses to reach approximately equal amounts of C6 sugars from straw and molasses respectively. Moreover corn steep liquor (CSL) and Diammumphosphate (DAP) are added as nutrients. 60 % of C6 sugars fed to yeast propagation are converted to yeast and 35 % are converted to  $\text{CO}_2$  and  $\text{H}_2\text{O}$ , corresponding to a biomass/sugar yield of approximately 0.5 kg/kg.

In contrast to yeast *T.reesei* can also utilize C5 sugars, hemicelluloses and cellulose. Consequently no molasses but only CSL and DAP are added to the pretreated slurry. In EP 50 % of carbohydrates are converted to  $\text{CO}_2$  and  $\text{H}_2\text{O}$ , 35 % are converted to enzyme and 10 % are converted to biomass, corresponding to an enzyme/sugar yield of 0.28 kg/kg. Specific enzyme activity is assumed to be 600 FPU/g Enzyme.

SSF is performed for 72 h at 37 °C and 12 % (w/w) water insoluble solids (WIS) with an enzyme loading of 15 FPU/g cellulose and an initial yeast concentration of 2 g/l. Cellulose to C6 conversion and C6 to Ethanol conversion are both set with 92 %, yielding a final ethanol concentration of approximately 4 % (w/w). Again, CSL and DAP are added to meet the yeast's requirements.

### 3.3 Ethanol recovery and purification

For ethanol recovery two parallel stripper columns and one rectifier column as suggested by Wingren (Wingren et al., 2008) are used. Evaporation in the bottom of the high-pressure stripper takes place at 133 °C and condensation in the head of the rectifier at 54 °C. The 92.5 % (w/w) ethanol head product is compressed, superheated to 130 °C and sent to pressure swing adsorption (PSA). In PSA ethanol is purified to 99.5 % (w/w). 25 % of the purified ethanol are used for recovery of the loaded bed and thereafter returned to the rectifier. Purified ethanol is condensed and cooled to 30 °C.

Ethanol containing vapors from SSF and ethanol condensation are sent to the scrubbing system. In accordance with emission standards for volatile organic carbon (VOC) final ethanol concentration in the vapors leaving the scrubber are set to reach 100 mg C/Nm<sup>3</sup>.

### 3.4 Stillage utilization

The stillage from distillation containing all the solids, water and byproducts of prior conversion steps is sent to a filter press, separating liquids and soluble solids from insoluble solids. The drymatter content of the insoluble solid stream is assumed to be 50 % (w/w), corresponding to a WIS content of approximately 41 % (w/w). Retention for insolubles is assumed to be 99 %. The liquid fraction containing most of the soluble solids is concentrated in a 5 effect evaporation train working in co-current mode. A part

of the vapors from evaporation is recycled, the rest is disposed of. Insoluble Solids are dried to 90 % drymatter in a superheated steam dryer, working at 4 bar.

Now several ways to utilize the residual streams exist, as indicated by the numbers 1 through 3a in Figure 1. For all of the scenarios a part of the residual streams is burnt in a boiler to provide process steam at two levels. The boiler is operated at 820 °C with air recirculation and a lambda of 1.7. Flue gas temperature is 120 °C or 130 °C (depending on scenario), resulting in a boiler efficiency of approximately 88 %.

#### **3.4.1. Combined heat and Power**

In Scenarios 1 and 1a the dried insoluble solids as well as the concentrated soluble are burnt in a boiler. Steam is produced at 63 bar and 650 °C and expanded in a turbine to produce electricity for the process. Excess electricity can be sold to the grid. Process steam is extracted at the two pressure levels required. Isentropic and mechanical turbine efficiency are 87 % and 97 %, respectively. Electric and mechanical generator efficiency is 97 %. In Scenario 1 wet steam coming from the turbine is condensed at 50 °C using cooling water. In Scenario 1a steam is condensed at higher temperature and together with high temperature cooling water of the ethanol process used for district heating. Supply and return temperature of the district heating system are 110 °C and 50 °C.

#### **3.4.2. Pellets**

In Scenarios 2 and 2a process electricity is supplied from the grid. The dried insoluble solids are pelletized and can be sold as solid fuel. Since the energy content of the concentrated soluble solids is more than sufficient to meet the processes heat demand, two options for excess solubles are possible. In Scenario 2 excess solubles are dried and pelletized together with the insoluble solids. In Scenario 2a all the solubles are burnt, excess heat and high temperature cooling water of the ethanol process are used for district heating.

In Scenario 2C5 (not explicitly included in Figure1) it is assumed, that yeast can co-ferment C5 sugars to produce ethanol. Conversions of C5 to ethanol and biomass are 75 % and 5 %, respectively. All the solids are dried and the amount required to meet the processes' heat demand is burnt, excess solids are pelletized.

#### **3.4.3. C5-Molasses**

In Scenarios 3 and 3a process electricity is supplied from the grid. The dried solids are used as fuel for the boiler, whereas the concentrated solubles (C5 sugars and other soluble components) can be sold as a product. One possible use is feed for animals (Larsen et al., 2008). Since the energy content of the dried solids exceeds the processes heat demand, excess solids can be either pelletized (scenario 3) or used to produce district heating (Scenario 3a, see also sections 2.4.1 and 2.4.2).

## **4. Results and Discussion**

Table 1 summarizes most important mass and energy flows for the scenarios. In all the cases, except 2C5 ethanol yield is 0,171 kg/kg, corresponding to 78.3 % of theory, based on C6 sugars in the raw material. In case 2C5 ethanol yield is 0,249 kg/kg dry, corresponding to 70.4 % of theory based on C5 and C6 sugars in the raw material.

Table 1: Summary of mass and energy flows for the scenarios, all massflows are 100 % drymatter. Abbreviations: E: Electricity, EtOH: Ethanol, M: C5-Molasses, P: Pellets, D: district heating

	1	1a	2	2C5	2a	3	3a
Straw In [t/y]	58,257	583,257	583,257	401,809	583,257	583,257	583,257
E In [MW]	-	-	8.9	9.0	8.9	8.8	8.9
EtOH Out [t/y]	100,000	100,000	100,000	100,000	100,000	100,000	100,000
M Out [t/y]	-	-	-	-	-	191,850	191,850
P Out [t/y]	-	-	245,118	108,615	188,495	55,290	-
D Out [MW]	-	125.3	-	-	72.5	-	68.9
E Out [MW]	47.4	38.1	-	-	-	-	-

Figure 2 shows the energy balance for the scenarios (for material flows the lower heating is used to derive energy content). Energy outputs are expressed as percentage of energy in inputs. In cases 1 and 1a, straw is the only energy input, whereas in cases 2 through 3a electricity is also considered as input. For scenarios where only C6 sugars are utilized for ethanol production, 25 % (2, 2a, 3, 3a) to 26 % (1,1a) of energy input is recovered in ethanol, whereas for case 2C5 36 % of energy input is contained in ethanol.

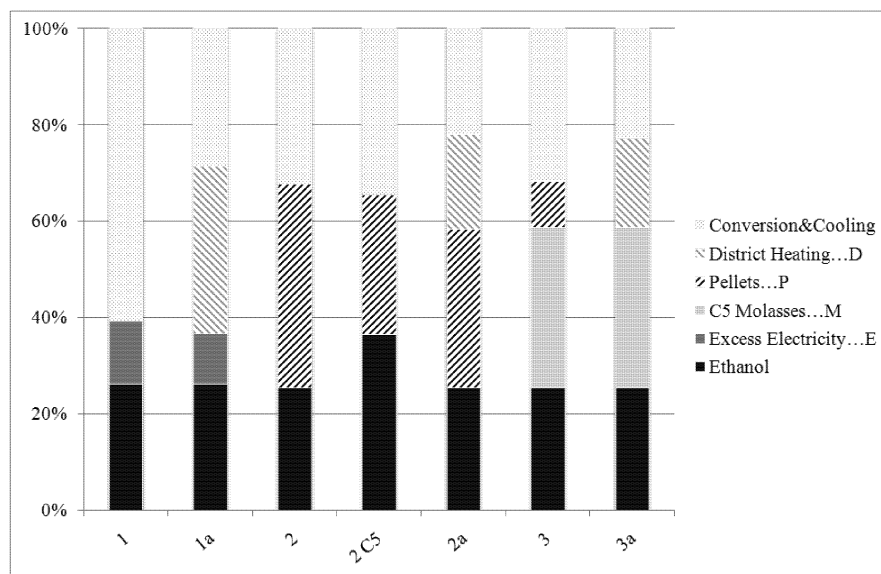


Figure 2: Energy balance for the production of Ethanol from Straw, expressed as percentage of energy inputs straw (cases 1 and 1a) and straw + electricity (other cases).

As can be seen, total process efficiency ranges from 38 % for case 1 to 78 % cases 2a and 3a. As generally known utilization of off-heat for district heating (1a, 2a, 3a) leads

to high efficiency processes, demand for district heating however is limited and strongly dependent on plant-location. From an energetic point of view the relatively low efficiency for cases where electricity is produced on-site (1, 1a) favors Scenarios 2, 2a, 3 and 3a.

## 5. Conclusions and Outlook

Several scenarios for the production of ethanol from straw were investigated from an energetic point of view, using process simulation. For all the scenarios, process heat demand is supplied by burning residual materials. Process electricity is produced on-site or purchased. With overall energy efficiency between 38 % and 78 % the production of ethanol from straw is a highly efficient process.

Future work will be dedicated to economic evaluation and life cycle analysis, determining socio-economic perspectives of the technology.

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