SUNLIBB

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Deliverable 7.3
"*In silico* optimisation studies from lab scale data completed"

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SUNLIBB deliverables

Del No: 7.3	**Deliverable Name:** In-silico optimisation studies from lab scale data completed			
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*PU = Public ; PP = Restricted to other programme participants (including the Commission Services); RE = Restricted to a group specified by the consortium (including the Commission Services); CO= Confidential, only for members of the consortium (including the Commission Services).

1. Objective

The objective of this deliverable is to carry out simulations of lab scale fermentation experiments and identify the optimisation potential of these experiments.

2. Description of work

Fermentation experiments were carried out (Mahendra Raut) using bagasse and miscanthus hydrolysate sent to the University of Sheffield by partner 1 (University of York). Data from these experiments was used to simulate these experiments in Aspen Plus, which is a process simulation software package. Figure 1 shows the fermentation model that was built in Aspen plus using lab data.

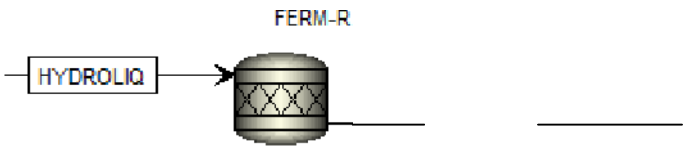

Figure 1: Fermentation model in Aspen Plus

Bagasse

The modelling work focused only on the fermentation experiments that resulted in the highest ethanol yields. In the case of bagasse, results showed that ethanol yields are higher for bagasse that was pretreated using 1N NaOH at 180^{o}C. There were three bagasse hydrolysate samples for these pretreatment conditions (1N NaOH 180^{o}C) which were sent from York (samples 115-117). The three samples had to be mixed due to sample constraints (not enough quantity) in order to conduct the fermentation experiments. For the modelling study we had to take this into consideration, thus we assumed that the sugar content of the final hydrolysate sample used for the fermentation experiments was the average of all three samples (see Table 1).

Table 1: Average sugar content (mg/g biomass used) in the bagasse hydrolysate sample

	Average (mg/g biomass)
Fucose	0
Arabinose	41.74522
Galactose	16.5988
Glucose	**79.99946**
Xylose	78.10217
Mannose	2.076317
Galactose A	0.958228
Glucose A	1.04482
Total (including other sugars)	**236.17**

The ethanol yields from the fermentation experiments were included in the report for deliverable 7.2. The highest ethanol yield achieved was 2.5 g/litre or 0.23 % ethanol on a mass basis (g ethanol per g fermented liquor).

Miscanthus

Miscanthus hydrolysate samples were sent from partner 1 to Sheffield to use for fermentation experiments with *Clostridium acetobutylicum*. Results showed that ethanol yields are higher for miscanthus that was pretreated using 0.2 NaOH. The ethanol yield reported was 0.04 g/litre or 0.0039 % ethanol on a mass basis (g ethanol per g fermented liquor). Additionally, the sugar content was examined before and after fermentation and results are shown in Table 2. This is very useful for the modelling study, as we can use these conversion rates to model the fermentation process.

Base case models

We built three base case models of a biorefinery plant using either bagasse, miscanthus or maize stover as the feedstock. These models were based on literature and real plant data. Subsequent models that are based on SUNLIBB technologies will be compared with the base case models in terms of process performance and costs. Results from the three base case models were presented in the last project meeting which took place in Wageningen. The bagasse base case model is shown in Figure 2. The other two models (miscanthus, maize stover) were not included here as their structure is similar to the bagasse model.

Table 2: Sugar content (mg/ml) before and after fermentation of miscanthus hydrolysate samples

Sugars	**Before fermentation**	**After fermentation**	**Conversion** (%)
Arabinose			
H2O	22.7	5.8	74.5
0.2N H2SO4	325.4	12.7	96.1
0.2N NaOH	196.0	3.4	**98.3**
Glucose			
H2O	31.0	1.7	94.5
0.2N H2SO4	121.5	1.1	**99.1**
0.2N NaOH	72.9	0.6	**99.2**
Mannose			
H2O	62.2	0.7	**98.8**
0.2N H2SO4	279.9	248.3	11.3
0.2N NaOH	110.3	35.2	68.0
Xylose			
H2O	33.9	0.0	100.0
0.2N H2SO4	1245.9	27.7	**97.8**
0.2N NaOH	439.8	2.0	**99.5**

3. Results

Regarding the fermentation process which is the focus of this deliverable, we used a conversion rate of 90% for hexoses (mainly glucose) and 80% for pentoses (mainly xylose) for the base case models [1, 2]. These are lower than the conversion rates reported in Table 2 so it seems that *Clostridium acetobutylicum is* a promising alternative to other yeast and bacteria species used for fermentation [1-3].

Regarding ethanol yields, the base case models showed that ethanol at approximately 5 wt% (g/g) is produced during fermentation. This is significantly higher than the ethanol yields achieved from the fermentation model which was based on lab data (see previous section). This might be due to the relatively low sugar content in the hydrolysate and the low retention time (54 hours for bagasse and 120 hours for miscanthus) of the fermentation experiments.

4. Conclusions

Aspen Plus simulations of fermentation experiments showed that *Clostridium acetobutylicum* has a lot of potential for fermenting sugars to ethanol. Ethanol yields could be increased with higher retention times and by improving the upstream pretreatment process to result in higher sugar content in the biomass hydrolysate.

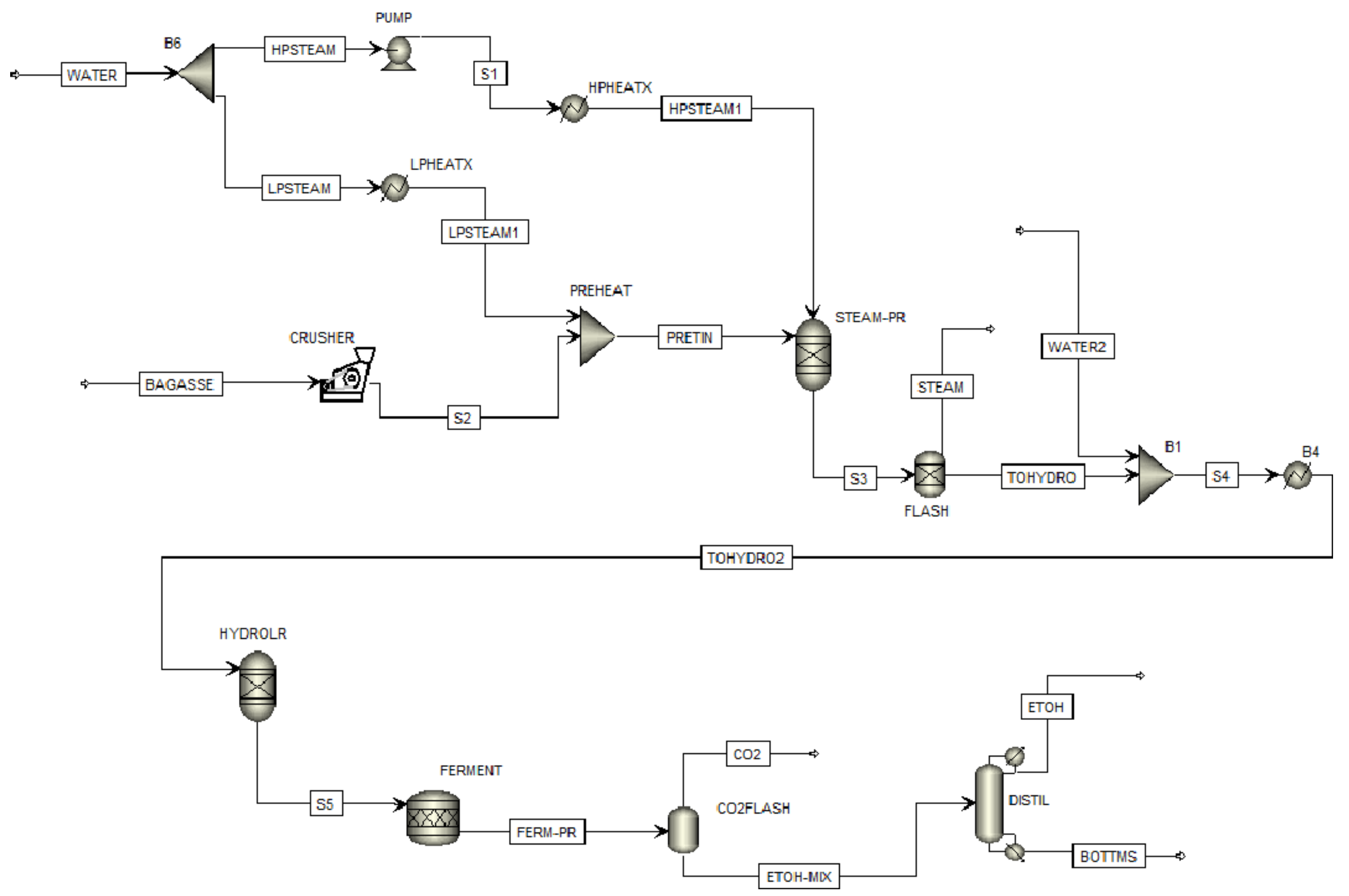

Figure 2: Bagasse base case model in Aspen Plus

5. Future Work

- ☐ Continue building Aspen Plus models based on technologies examined within the SUNLIBB project. Investigate the performance and costs of various scenarios (D7.7).
- ☐ Develop kinetic models of the fermentation process to compare with lab results. This could be included in a future publication of the fermentation experimental results.

6. References

1. Humbird, D., et al., *Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol,* Report NREL/TP-5100-47764, National Renewable Energy Laboratory, May 2011.
2. Piccolo, C. and F. Bezzo, *A techno-economic comparison between two technologies for bioethanol production from lignocellulose.* Biomass and Bioenergy, 2009. **33**: p. 478-491.
3. Bloomberg, D., *Personal Communication,* Processum, September 2013.