XYLITOL AND BIOETHANOL PRODUCTION FROM LIGNOCELLULOSES: A SYSTEMATIC MODEL-BASED SIMULATION FOR A BIOREFINERY PROCESS EVALUATION

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...\Introduction

...\Objective

...\Xylitol mathematical model and production pathway

...\Towards a biorefinery structure: addition of the xylitol production section to the extended version of the dynamic lignocellulosic bioethanol 1.0 model platform

...\Benchmarking criteria for the comparison of the extended process models

...\Results and conclusions

...\What Next..?
According to The European commission predictions, 20% of the transportation fuel and 25% of chemicals should be produced from biomass by 2030 [1].

Recent advances on producing bioproducts from biomass (Biorefinery concept) has triggered out continued research on developing new production processes, such as xylitol.

**Xylitol**: Value added product, five-carbon sugar alcohol, used for health (dental caries and acute otitis media) and lately for the production of alcanes (C7-C12) for obtaining a biodiesel through a chemical route.

Industrially, xylitol is produced by chemical route [2].

Recently, the biotechnological production of xylitol has reached importance due to this is produced by yeast metabolism, where Candida strains has become important over Saccharomyces cerevisiae by being a natural D-xylose consumer and maintaining the reduction–oxidation balance during xylitol accumulation.
Conventional process configuration for bioethanol production via biological route for DLB 1.0

1. Pretreatment

2. Simultaneous Saccharification Co-Fermentation (SSCF)

3. Lignin

4. Cellulases

5. Yeast

6. Downstream

Ethanol
Dynamic lignocellulosic bioethanol (DLB) 1.0 model platform and extension

### Operational Scenario

<table>
<thead>
<tr>
<th>SHCF</th>
<th>Acronyms</th>
<th>Ethanol/DM ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1)</td>
<td>H: Fed-batch – CF: Fed-batch</td>
<td>FB-FB</td>
</tr>
<tr>
<td>2)</td>
<td>H: Fed-batch – CF: Continuous</td>
<td>FB-C</td>
</tr>
<tr>
<td>3)</td>
<td>H: Fed-batch – CF: Continuous-Recycle</td>
<td>FB-C_RECY</td>
</tr>
<tr>
<td>4)</td>
<td>H: Continuous – CF: Fed-batch</td>
<td>C-FB</td>
</tr>
<tr>
<td>5)</td>
<td>H: Continuous – CF: Continuous</td>
<td>C-C</td>
</tr>
<tr>
<td>6)</td>
<td>H: Continuous – CF: Continuous-Recycle</td>
<td>C-C_RECY</td>
</tr>
<tr>
<td>7)</td>
<td>H: Continuous-Recycle – CF: Fed-batch</td>
<td>C_RECY-FB</td>
</tr>
<tr>
<td>8)</td>
<td>H: Continuous-Recycle – CF: Continuous</td>
<td>C_RECY-C</td>
</tr>
<tr>
<td>9)</td>
<td>H: Continuous-Recycle – CF: Continuous-Recycle</td>
<td>C_RECY-C_RECY</td>
</tr>
<tr>
<td>10)</td>
<td>Fed-batch</td>
<td>SSCF-FB</td>
</tr>
<tr>
<td>11)</td>
<td>Continuous</td>
<td>SSCF-C</td>
</tr>
<tr>
<td>12)</td>
<td>Continuous-recycle</td>
<td>SSCF-C_RECY</td>
</tr>
</tbody>
</table>

H: Enzymatic Hydrolysis, CF: Co-Fermentation

### Benchmarking performance criteria: Ethanol/Dry-Biomass Ratio

\[
R_{Et/dry-biomass} = \frac{\text{Total Mass Et}}{\text{Total Mass Dry Biomass}}
\]

### Extension of DLB 1.0:
- Heat exchangers
- Distillation columns

[7-9]
To present an *extension* of the *DLB 1.0 model platform* by the *addition* of the dynamic modeling for the *conversion* of *xylose* into *xylitol*. In order to *evaluate* the *technological* and *economical feasibility* through a model-based *simulation*. 
• Once xylose is inside the cell, it is reduced to xylitol by the enzyme xylose reductase.
• Part of xylose is excreted as a xylitol and the other is converted to xylulose that is consumed for producing cell mass and maintenance energy.
• Glucose (easily metabolized sugar) is used for producing energy and biomass, reducing xylitol consumption.
• High glucose concentration can inhibit xylose transport into the cell [11].
Mathematical model [10]:

- Biomass growth rate,
- The rate of glucose and xylose uptake related with biomass concentration
- The production rate of intracellular and extracellular xylitol.

Original model for xylitol production considers a reactor operating in batch.

The model was extended for a continuous operation mode, considering the residence time with higher xylitol production...!!
Towards a biorefinery structure: addition of the xylitol production section to the extended version of the dynamic lignocellulosic bioethanol 1.0 model platform

The xylitol production by yeast can be affected by several factors such as, culture conditions, initial xylose concentration, and the presence of inhibitor (such as glucose, acetic acid, furfural, 5-hydroxymethylfurfural (HFM) and phenolic compounds) released by acid hydrolysis.

The inhibition effect of ethanol on Candida genus has not been completely studied and none available information was found.

Where do we add the xylitol production section?

For the sake of the process design, the xylitol production section was added after ethanol was eliminated from process streams.
Towards a biorefinery structure: addition of the xylitol production section to the extended version of the dynamic lignocellulosic bioethanol 1.0 model platform
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Implementation using MatLab
Benchmarking criteria for the comparison of the extended process models

• Production costs and potential profit for bioethanol and xylitol as the benchmarking criteria.

• The production costs considered were:
  – feedstock
  – utilities (low-pressure steam, high-pressure steam and cooling water)
  – additives (enzyme loading in the enzymatic hydrolysis and sulfuric acid loading in the pretreatment)

\[
\text{Production Cost Ethanol} = c_{\text{Feedstock}} + c_{\text{Utilities}} + c_{\text{Additives}} = \frac{\text{USD}}{\text{gal} - \text{ethanol}}
\]

\[
\text{Production Cost Xylitol} = c_{\text{Utilities}} = \frac{\text{USD}}{\text{gal} - \text{xylitol}}
\]

Note that only utilities cost (cooling water) is considered for xylitol production, since after the distillation columns the temperature at the waste streams must be decreased to carry out the fermentation of xylose to xylitol.
### Results

<table>
<thead>
<tr>
<th>Process configuration</th>
<th>Production cost for bioethanol, USD/gal-ethanol</th>
<th>Production cost for xylitol, USD/gal-xylitol</th>
<th>% of difference on bioethanol profit with respect to SSCF configuration</th>
<th>% of difference on potential profit with respect to SSCF configuration</th>
<th>% of difference on total profit with respect to SSCF configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_RECY-C</td>
<td>2.42</td>
<td>0.0078</td>
<td>-90.4%</td>
<td>20.9%</td>
<td>-44.4%</td>
</tr>
<tr>
<td>C_RECY-C_RECY</td>
<td>2.15</td>
<td>0.0078</td>
<td>-49.8%</td>
<td>20.3%</td>
<td>-20.8%</td>
</tr>
<tr>
<td>SSCF-C</td>
<td>1.53</td>
<td>0.0054</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>SSCF-C_RECY</td>
<td>1.71</td>
<td>0.0077</td>
<td>29.9%</td>
<td>18.4%</td>
<td>25.1%</td>
</tr>
</tbody>
</table>

- **C_RECY-C – SSCF-C**: xylitol potential profit 20.9% higher for the C_RECY-C, the ethanol production cost was 58.2% higher for SSCF-C process configuration, for total profit analysis was 44.4% less in the C_RECY-C than in the SSCF-C.

- **C_RECY-C_RECY – SSCF-C**: for xylitol profit the results were quite similar, but for the bioethanol production cost this was 1.4 times higher than SSCF-C and the bioethanol profit was lower by 20.8%.

- **SSCF-C – SSCF-C_RECY**: xylitol potential income for SSCF-C_RECY was 1.84 higher than the reference process configuration and the variation for bioethanol production cost was found to be 11.8% more expensive for SSCF-C_RECY, but the total potential income for ethanol and xylitol production was 25.1% higher for the SSCF-C_RECY.
• At first relying on the production cost, the SSCF-C seemed to be the best process configuration, but whether the incomes from bioethanol and xylitol productions were taken into account, the best process configuration was the SSCF-C_RECY.

• A previous study [7] showed that ethanol/dry-biomass ratio was 0.18 and 0.12 for SSCF-C_RECY and SSCF-C, respectively. The obtained profit for SSCF-C_RECY was reasonability understandable since the production was 1.5 times higher with respect to SSCF-C.

• Xylitol production: difference was due to the flowrate in the streams leaving from the distillation columns. In the SSCF-C_RECY, the amount of xylose and glucose available in the streams was higher when compared with SSCF-C.
This study has presented the addition of a xylitol production section to the previous extended version of the DLB 1.0 modeling platform biorefinery modeling platform.

Detailed analysis in terms of the likely profit; where the best process configuration when combining both products was the SSCF-C_RECY having 25.1% more incomes compared to the SSCF-C.

A multidisciplinary team in the process design step, due to the intrinsic complexity of the biological processes.
Concluding remarks

✓ Future work:

• Extension in the DLB 1.0 modeling platform for the remaining process configurations presented by Morales-Rodriguez et al. [7],
• Addition of the unit operations for the production of xylitol and other high value-added products through a chemical and biological route under the biorefinery concept, thereby, providing a global vision of the scope of biomass processing.
• Control strategies for the different unit operations. (Poster: 936, simulación y control)
• Risk analysis in the process configurations. (Poster: 737, energía)
Thank you for your attention
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