Energy Analysis of Butanol Extraction Using Supercritical Carbon Dioxide
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Abstract
The goal of this project was to model a butanol extraction process using supercritical carbon dioxide (CO₂) in Aspen Plus and then complete an energy analysis for various probable process models. A large part of modeling the process was determining an Equation of State (EOS) that accurately modeled the CO₂/Water/Butanol ternary system at critical conditions. Following the design of a process model and the completion of the energy analysis, recommendations were proposed on the best method of butanol production from an energy standpoint.

Background
Butanol has the potential to be a better renewable liquid fuel option than ethanol because of its superior energy density. Supercritical extraction of higher alcohols implements supercritical fluids as solvents, most commonly CO₂, to extract an alcohol product. This method of extraction has been found to be a simpler and a more economic process than other extraction methods, and is more energy efficient. The Massachusetts Institute of Technology (MIT) recently discovered that a butanol producing bacteria (B. megaterium) can survive at CO₂ supercritical conditions. With butanol extraction using supercritical CO₂, now a possibility, butanol production has the potential to be energy efficient.

Objectives
1. Determine an EOS that accurately models the ternary system CO₂/Water/Butanol at supercritical conditions
2. Perform a sensitivity analysis on the basic process model to determine optimal parameters
3. Design different models for the butanol extraction process in Aspen Plus
4. Determine the most energy efficient and viable process design with heat integration and energy analysis
5. Provide recommendations for further research and development

Equation of State Results
We explored three equations of state (EOS) that we predicted would best model the ternary system CO₂/Water/butanol at our desired temperature and pressure: SRK, LK-PLCBS, and PENGROB. SRK equation of state accurately predicts the phase composition of the CO₂/Water/butanol at our desired temperature and pressure.

Table 1: Altered EOS analyzed for accuracy of representing CO₂/Water/butanol system at critical conditions

<table>
<thead>
<tr>
<th>Compound</th>
<th>Gas</th>
<th>Liquid 1</th>
<th>Liquid 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>0.92%</td>
<td>0.009</td>
<td></td>
</tr>
<tr>
<td>Butanol</td>
<td>18%</td>
<td></td>
<td>0.007</td>
</tr>
<tr>
<td>Water</td>
<td>82%</td>
<td>0.010</td>
<td>0.031</td>
</tr>
</tbody>
</table>

Table 2: Results for the four analyzed process models

<table>
<thead>
<tr>
<th>Mass % Butanol in Product</th>
<th>Regular</th>
<th>Total Depressurization</th>
<th>Total Recycle</th>
<th>Post Pressurization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product Energy Requirement</td>
<td>2.0</td>
<td>3.1</td>
<td>1.2</td>
<td>8.0</td>
</tr>
<tr>
<td>Butanol Energy Requirement</td>
<td>2.0</td>
<td>3.2</td>
<td>1.3</td>
<td>8.3</td>
</tr>
</tbody>
</table>

Final Models and Results
Unless specified: 3:1 CO₂ to butanol mass ratio and 100 bar pressure was used in the reactor. Pressure of the first separator set to 65 bar.

- Regular model: CO₂ recycle ratio of 0.6
- Total depressurization: pressure of the first separator is 1 bar. Therefore no CO₂ recycle stream or third separator.
- Total recycle: no inlet CO₂ and a CO₂ recycle ratio of 0.71.
- Post pressurization: the reactor is at atmospheric conditions and pressurization and extraction post reaction.

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