Thermodynamic modelling of CatLiq® biomass conversion process

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Publication date:
2010

Document Version
Accepted author manuscript, peer reviewed version

Link to publication from Aalborg University

Citation for published version (APA):
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Introduction


Raw Material: DDGS (Dried Distilled Grain with Solubles), a byproduct in first generation ethanol production.

Process conditions: 280-350 °C and 225-250 bar, in the presence of homogeneous (K₂CO₃) and a heterogeneous (Zirconia) catalyst.

Products: Main components are bio-oil, H₂O, CO₂, and water-soluble organic compounds.

Capacity: 10-20 L/h of wet biomass pilot plant with fixed-bed reactor.

Thermodynamic model

The results were correlated with PSRK model proposed by Holderbaum and Gmehling, which is predictive Soave-Redlich-Kwong EOS with the modified Huron-Vidal first-order (MHV1) mixing rule of Michelsen coupled with the UNIFAC model.

Table 1. Experimental and PSRK-estimated bubble point pressures for model system

<table>
<thead>
<tr>
<th>Temp/°C</th>
<th>Pexp/bar</th>
<th>Pcal/bar</th>
<th>Rel. Dev. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>156.73</td>
<td>138.53</td>
<td>11.612</td>
</tr>
<tr>
<td>50</td>
<td>190.88</td>
<td>169.22</td>
<td>11.347</td>
</tr>
<tr>
<td>60</td>
<td>224.48</td>
<td>202.08</td>
<td>9.978</td>
</tr>
<tr>
<td>75</td>
<td>258.97</td>
<td>253.85</td>
<td>1.977</td>
</tr>
</tbody>
</table>

AAD % = (Pexp – Pcal)/Pexp × 100

Results

Conclusion

Experimental and predicted data shows that the capability of the PSRK model is reasonably good in predicting the phase behaviour of such a model system for CatLiq® process.

This modelling work is useful for the CatLiq® process design, development and optimization, which provides a general thermodynamic approach on how to model biomass conversion processes.

References


Acknowledgement

The authors would like to thank the SCF Technologies A/S for giving the opportunity to perform this research. Thanks are also due to Tor Austad and Sivert for his help in the experimental work at the Department of Petroleum Engineering, Stavanger University, Norway.