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Thermodynamic modeling of CatLiq® biomass conversion process

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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.

Aim
Measurement and Prediction of bubble point pressures of selected model system to investigate phase boundaries of the CatLiq® process.

Experiment
The experimental study was carried out in a mercury free JEFRI-DBR high pressure PVT phase behavior system using composition of (7.0% CO₂ + 84.8% H₂O + 0.1% Ethanol + 0.1% Acetic acid + 8.0% Octanoic acid) as a model system for CatLiq® process.

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

Results

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

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Pexp/bar</th>
<th>Psrk/bar</th>
<th>Rel. Dev. (%)</th>
<th>AAD (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>156.73</td>
<td>138.53</td>
<td>11.612</td>
<td>8.7286</td>
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<tr>
<td>50</td>
<td>190.88</td>
<td>169.22</td>
<td>13.853</td>
<td>9.9786</td>
</tr>
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<td>60</td>
<td>224.48</td>
<td>202.08</td>
<td>11.612</td>
<td>9.9786</td>
</tr>
<tr>
<td>75</td>
<td>258.97</td>
<td>253.85</td>
<td>2.0759</td>
<td>8.7286</td>
</tr>
</tbody>
</table>

Figure 2. JEFRI-DBR mercury free PVT system

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


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