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Thermodynamic modeling of CatLiq® biomass conversion process

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Introduction

Process:
A second generation catalytic liquefaction process for the production of bio-oil.

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 (K_2CO_3) and a heterogeneous (Zirconia) catalyst.

Products:
Main components are bio-oil, H_2O, CO_2, and water-soluble organic compounds.

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

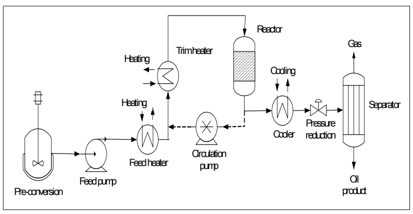


Figure 1. CatLiq® process scheme

DDGS *Oil + water soluble organic compounds* *CatLiq® bio-oil*

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% CO_2 + 84.8% H_2O + 0.1% Ethanol + 0.1% Acetic acid + 8.0% Octanoic acid) as a model system for CatLiq® process.

Figure 2. JEFRI-DBR mercury free PVT system

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.

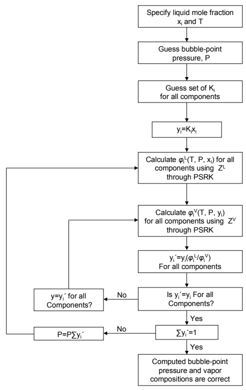


Figure 3. The proposed algorithm for bubble pressure calculation

T/°C	Pexp/bar	Pcal/bar	Rel. Dev. (%)[a]
40	156.73	138.53	11.6123
50	190.88	169.22	11.3474
60	224.48	202.08	9.9786
75	258.97	253.85	1.9770
		AAD %[b]	8.728863

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

[a]Relative Deviation (%) = (Pexp – Pcal)/Pexp×100

[b]Average Absolute Deviation (%) = (∑ |error %|) /number of data points

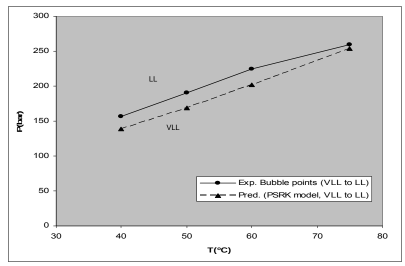
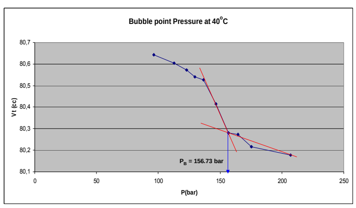
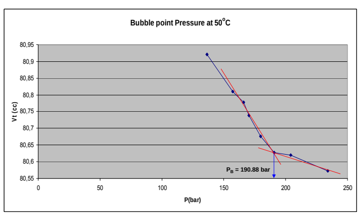
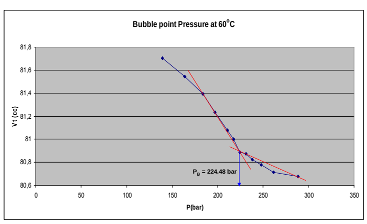


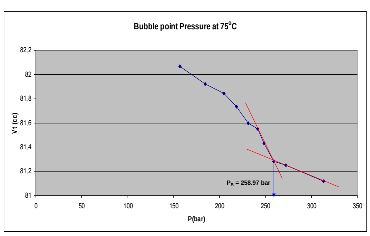
Figure 4. Measured and predicted phase boundaries for the model system

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.

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