



Thermodynamic modelling of CatLiq® biomass conversion process

Toor, Saqib Sohail; Rosendahl, Lasse; Rudolf, Andreas

Publication date:
2010

Document Version
Accepted author manuscript, peer reviewed version

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Toor, S. S., Rosendahl, L., & Rudolf, A. (2010). *Thermodynamic modelling of CatLiq® biomass conversion process*. Poster presented at International Conference on Renewable Resources and Biorefineries, Düsseldorf, Germany.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal -

Take down policy

If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

Thermodynamic modeling of CatLiq[®] biomass conversion process

Toor, S. S.¹, Rosendahl, L.¹, Rudolf, A.²

¹Department of Energy Technology, Aalborg University, DK-9220 Aalborg, Denmark

²SCF Technologies A/S, Smedeholm 13B, DK-2730 Herlev, Denmark

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 (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.

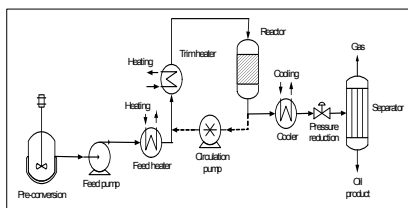


Figure 1. CatLiq[®] process scheme



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.

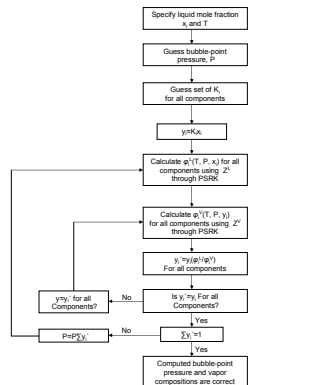


Figure 3. The proposed algorithm for bubble pressure calculation

T/°C	P _{exp} /bar	P _{cal} /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

^aRelative Deviation (%) = (P_{exp} - P_{cal})/P_{exp} × 100

^bAverage Absolute Deviation (%) = (Σ |error %|) / number of data points

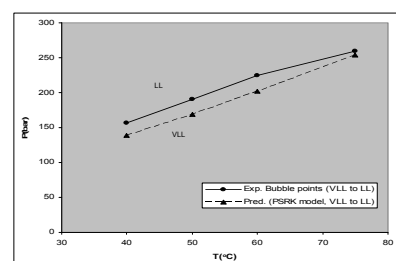
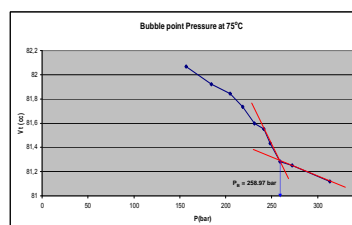
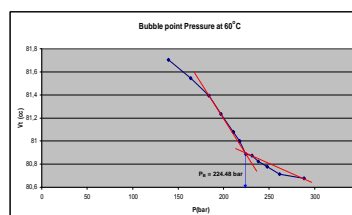
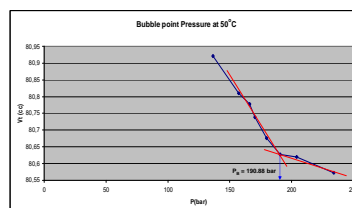
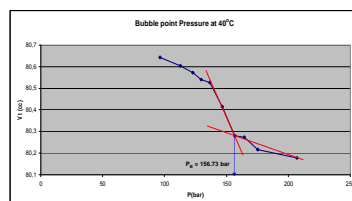


Figure 4. Measured and predicted phase boundaries for the model system

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.

References

- Holderbaum, T., Gmehling, J., 1991. PSRK: A group contribution equation of state based on UNIFAC. Fluid Phase Equilibria 70, 251-265.
- Michelsen, M.L., 1990. A modified Huron-Vidal mixing rule for cubic equations of state. Fluid Phase Equilibria 60, 213-219.
- Sandler, S. I., Orbey, H., 1998. Modeling Vapor-Liquid Equilibria- Cubic Equations of State and Their Mixing rules. Cambridge University Press ISBN: 0-521-62027-9 (hb).
- Bruusgaard, H., Beltrán, G.J., Servio, P., 2008. Vapor-liquid water-hydrate equilibrium data for the system N₂ + CO₂ + H₂O. Journal of Chemical and Engineering Data 53, 2594-2597.
- Beltrán, G.J., Servio, P., 2008. Equilibrium studies for the system Methane + Carbon Dioxide + Neohexane + Water. Journal of Chemical and Engineering Data 53, 1745-1749.

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.



Figure 2. JEFRI-DBR mercury free PVT system

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.