

Technical University of Denmark



Equilibria of ternary system acetic acid-water-CO₂ under subcritical conditions

Gutierrez, Jose M. Jimenez; Mussatto, Solange I.; Tsou, Joana; Verlinden, Rob; Straathof, Adrie J J; van der Wielen, Luuk A. M.

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Gutierrez, J. M. J., Mussatto, S. I., Tsou, J., Verlinden, R., Straathof, A. J. J., & van der Wielen, L. A. M. (2017). Equilibria of ternary system acetic acid-water-CO₂ under subcritical conditions. Poster session presented at Biotechnology, creating opportunities, Wageningen, Netherlands.

DTU Library
Technical Information Center of Denmark

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

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

EQUILIBRIA OF TERNARY SYSTEM ACETIC ACID–WATER–CO₂ UNDER SUBCRITICAL CONDITIONS

back

Jose M. Jimenez Gutierrez¹ (J.M.JimenezGutierrez@tudelft.nl), Solange Mussatto², Joana Tsou³, Anton Hoppel⁴, Rob Verlinden⁴, Adrie Straathof¹, Luuk van der Wielen¹ ¹Delft University of Technology; ²Technical University of Denmark, ³AkzoNobel Industrial Chemicals, Amsterdam; ⁴Bioprocess Pilot Facility B.V., Delft

Carbon dioxide has been subject of research in the past decades, with special attention targeting different uses of this “greenhouse” gas as raw material, technological fluid, building block or as a carbon supply for fuels, turning it from a pollutant to a green resource. Albeit likely it will be returned to the atmosphere (as part of the carbon cycle), CO₂ is an inexpensive and clean source with numerous industrial applications in diverse fields: from chemical processes to biotechnological purposes [1].

Many of these studies have been focused on supercritical CO₂, due to its broad potential uses in a very wide range of applications. However, those conditions, especially the levels of high pressure required at larger scale, involve certain equipment limitations. An alternative to overcome those restrictions is to use subcritical carbon dioxide.

In order to understand the different systems to be tackled within the bio-process design comprising subcritical CO₂, and therefore to improve its applicability, it becomes necessary to investigate the behaviour of such gas at different conditions. Some bioprocesses which require CO₂ might also involve the presence of other substances in the medium, such as acetic acid in fermentations [2, 3]. Thus, from a biotechnological perspective, it is highly interesting to research on the system CO₂—H₂O with different concentrations of acetic acid (HAc). Based on previous studies [4, 5], this project aims to investigate the vapour/liquid equilibria (VLE) of the ternary system HAc—H₂O—CO₂ at different subcritical conditions. A proposed computer model could be validated with experimental data, leading to a certain degree of adjustment due to specific factors, such as the binary interaction parameter k_{ij} , used in the model based on the Peng-Robinson EoS coupled with the mixing rules, or in the calculation of the cross second virial coefficients proposed by Prausnitz [6].

References:

1. Aresta, M., *Carbon dioxide as chemical feedstock*. 2010: John Wiley & Sons.
2. Straathof, A.J.J., *Transformation of biomass into commodity chemicals using enzymes or cells*. *Chemical reviews*, 2014. 114(3): p. 1871-1908.
3. Cabrera-Rodríguez, C.I., et al., *Recovery and esterification of aqueous carboxylates by using CO₂-expanded alcohols with anion exchange*. *Green Chemistry*, 2017.
4. Rumpf, B., J. Xia, and G. Maurer, *Solubility of carbon dioxide in aqueous solutions containing acetic acid or sodium hydroxide in the temperature range from 313 to 433 K and at total pressures up to 10 MPa*. *Industrial & engineering chemistry research*, 1998. 37(5): p. 2012-2019.
5. Bamberger, A., G. Sieder, and G. Maurer, *High-pressure (vapor+ liquid) equilibrium in binary mixtures of (carbon dioxide+ water or acetic acid) at temperatures from 313 to 353 K*. *The Journal of Supercritical Fluids*, 2000. 17(2): p. 97-110.
6. Prausnitz, J.M., R.N. Lichtenthaler, and E.G.d. Azevedo, *Molecular thermodynamics of fluid-phase equilibria*. 2nd ed. ed. 1986, Englewood Cliffs, N.J.: Prentice-Hall.

back

A

B

C

D

pst



NBC 17

Biotechnology, creating opportunities



Did you like the programme?
Please give us some feedback! It only takes 1 minute...
[Evaluation form >>](#)

A

B

C

D

pst

created by Agri Information Partners