Estimate VLE models by Margules, Van Laar and Wilson equations for a batch fermentation VLE data

【Module Learning Objectives】

- VLE models by Margules, Van Laar and Wilson equations

【Associated Sections in Selected Textbooks】

- Introduction to Chemical Engineering Thermodynamics [1] Sec. 12.1-12.2

【Associated Web Modules】

- http://biofuelsacademy.org/web-modules/process/fermentation/batch-fermentation/

【Process Background and Problem】

Batch fermentation is the most simplistic approach of producing ethanol. The overall process of producing ethanol involves the following steps: milling, cooking, fermentation, and distillation. Milling and cooking are pretreating steps that facilitate proper conditions for fermentation; the milling step essentially breaks down the sugar containing feed to very small particles, and the cooking step allows for the yeasts to reach the proper reaction temperature to start the fermentation [2].

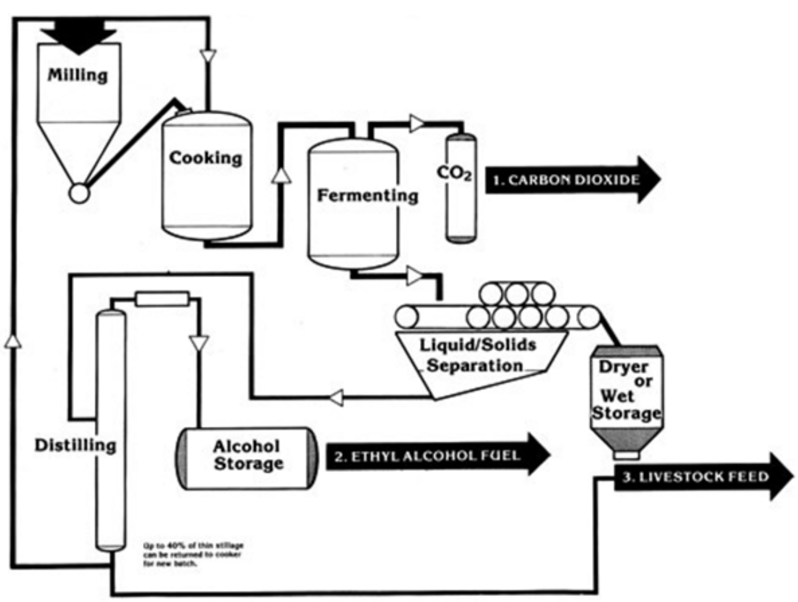

Figure 1. Flow Diagram of Batch Fermentation for Ethanol Production [3]

Removal of the ethanol is the key function of distillation; other byproducts will be removed in this step because of the difference in boiling points. After liquids/solids separation, the main components going into the distillation column are ethanol and water. It is important to understand the vapor-liquid equilibrium data of mixture systems in order to design a good recovery and purification system. Do the following calculations based on the following set of VLE data for the system ethanol(1)/water(2) at 333.15 K (extracted from K. Kurihara et. al, *J. Chem. Eng. Data*, vol. 40, pp. 679-684, 1995) [4].

P/kPa	x_1	y_1	P/kPa	x_1	y_1
31.647	0.0742	0.4130	43.756	0.4808	0.6682
34.540	0.1071	0.4742	44.935	0.5800	0.7070
36.840	0.1511	0.5196	45.881	0.6764	0.7468
38.387	0.1899	0.5473	46.547	0.7656	0.7968
41.230	0.3168	0.6006	46.998	0.8538	0.8616
43.368	0.4548	0.6502	47.060	0.9091	0.9095

The saturation pressures of ethanol and water can be determined through Antoine equation with parameters from the textbook [1] or through a steam table.

(a) Basing calculations on Eq. (12.1), find parameter values for the Margules equation that provide the best fit of G^E/RT to the data, and prepare a P-x-y diagram that compares the experimental points with curves determined from the correlation.
(b) Repeat (a) for the van Laar equation.
(c) Repeat (a) for the Wilson equation.
(d) Using Barker's method, find parameter values for the Margules equation that provide the best fit of the P-x_1 data. Prepare a diagram showing the residuals δP and δy_1 plotted vs. x_1.
(e) Repeat (d) for the van Laar equation.
(f) Repeat (d) for the Wilson equation.

Bibliography

[1] J. M. Smith, H. C. Van Ness and M. M. Abbott, Introduction to chemical engineering thermodynamics, Boston: McGraw-Hill; 7th ed., 2005.

[2] Q. P. He and J. Wang, "Biofuels Academy," 2012. [Online]. Available: http://www.biofuelsacademy.org/index.php?p=3_45. [Accessed 03 March 2014].

[3] M. E. News, "Mother's Alcohol Fuel Seminar," 1980. [Online]. Available: http://journeytoforever.org/biofuel_library/ethanol_motherearth/meCh1.html. [Accessed 25 March 2014].

[4] K. Kurihara, T. Minoura, K. Takeda and K. Kojima, "Isothermal vapor-liquid equilibria for methanol+ ethanol+ water, methanol+ water, and ethanol+ water," *Journal of Chemical and Engineering Data*, vol. 40, pp. 679--684, 1995.