

# Flash calculation for butanol production through ABE fermentation

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## 【Module Learning Objectives】

- Flash calculation based on K-value correlations and Raoult's law.

## 【Associated Sections in Selected Textbooks】

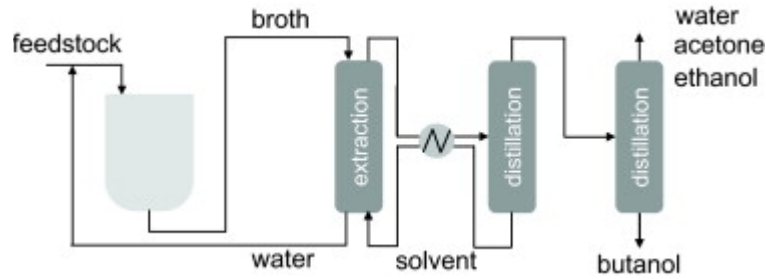
- Introduction to Chemical Engineering Thermodynamics [1] Sec. 10.6

## 【Associated Web Modules】

## 【Process Background and Problem】

Butanol was traditionally produced by ABE fermentation - the anaerobic conversion of carbohydrates by strains of *Clostridium* bacteria into acetone, butanol and ethanol. However, cost issues, relatively low-yield and sluggish fermentations, as well as problems caused by end product inhibition and phage infections, meant that ABE butanol could not compete on a commercial scale with butanol produced synthetically and almost all ABE production ceased as the petrochemical industry evolved [2].

However, there is now increasing interest in use of biobutanol as a transport fuel. 85% butanol/gasoline blends can be used in unmodified petrol engines. It can be transported in existing gasoline pipelines and produces more power than ethanol. A variety of alternative hybrid separation processes for extracting butanol from the fermentation broth have therefore been proposed: these are based on gas stripping, liquid-liquid extraction, pervaporation, perstraction, and adsorption. Besides reduced energy demands for butanol separation, these methods also offer the advantage that they can be applied inside the fermenter to decrease product inhibition. Adsorption and extraction combined with distillation are the most energy efficient alternatives. Hybrid processes with pervaporation or extraction are most attractive for integrated product removal. Extraction in combination with distillation may also be preferred since these techniques are conventional in unit operations [3].



**Figure 1. Simplified Hybrid Downstream Process of Extraction and Distillation [3].**

After separating butanol in a distillation column, the vapor phase consists of water (1), acetone(2) and ethanol(3) as shown in Figure 1. If the vapor phase, with overall composition of  $z_1 = 0.80$ ,  $z_2 = 0.15$  and  $z_3 = 0.05$ , is brought to vapor-liquid equilibrium with the condition of  $80^\circ\text{C}$  and  $60\text{ kPa}$ , determine  $L$ ,  $V$ ,  $\{x_i\}$ , and  $\{y_i\}$ . Assume that Raoult's law is appropriate to approximately describe the system.

## Bibliography

- [1] J. Smith, H. Van Ness and M. Abbott, Introduction to Chemical Engineering Thermodynamics, 7th Ed. ed., New York: McGraw Hill, 2005.
- [2] European Biofuels Technology Platform, "Biobutanol," [Online]. Available: <http://www.biofuelstp.eu/butanol.html>. [Accessed 04 April 2014].
- [3] K. Kraemer, A. Harwardt, R. Bronneberg and W. Marquardt, "Separation of butanol from acetone--butanol--ethanol fermentation by a hybrid extraction--distillation process," *Computers & Chemical Engineering*, vol. 35, pp. 949--963, 2011.