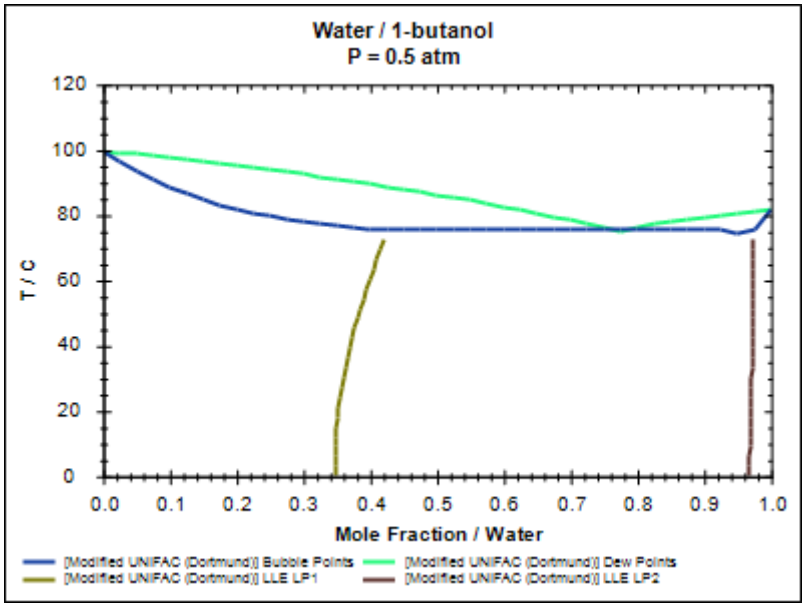
# HETEROGENEOUS AZEOTROPIC DISTILLATION OF BUTANOL AND WATER

## Background:

The recent surge in crude-oil prices and issues of energy independence and carbon dioxide emissions have generated new interest in bio fuels. Ethanol is now being produced on a fairly large scale for blending into gasoline. Qurishi et al discuss the advantages of n-butanol over ethanol: lower heat of vaporization, lower vapour pressure, higher octane number, and higher energy density.

Some opportunities that can change the dynamics of the n-butanol industry in the years to come include the demand supply-gap in China(being a major importer), rising investments in Saudi Arabia's oil & gas downstream sector, and increasing demand of biobased butanol. However, the concentration of n-butanol produced in the batch fermenter is quite low (20 g/L) because of toxicity problems. In addition, acetone and ethanol are also produced, which must be removed from the mixture coming from the fermenter. Traditional Bio based processes produce n-butanol amongst the other isomers. Butanol forms an azeotrope




with water at 0.5 atm,78$^0$C with compositions around 77.85% water, 22.15% n-butanol . Breaking the azeotrope ; with the vapour from two absorbers coupled with a decanter forms the basis for the separation. The flow sheeting source is

## DESCRIPTION :

Feed at 78$^0$C is admitted to a re-boiled absorber at an intermediate stage of a 10 stage column. The aqueous liquid from the decanter(Recycle to the 1st column) at 70$^0$C is fed to the top stage. A small fraction of vapour in the feed, at a higher temperature and the liquid undergo a flash at each stage. The feed composition of 0.98 water,0.02 butanol on the right extreme of azeotropic composition; ensures the fraction of water in vapour is reduced(as evident from the T-X-Y diagram above) leaving the over-head product richer in butanol as compared to that in feed.

The organic phase from the decanter(also a recycle) is fed to a 10 stage re-boiled absorber. The composition of over-head vapour almost near to the azeotrope. The vapours from the 2 columns are fed to a

mixer which in turn is cooled to $70^0$C , to bring it to a liquid-liquid phase.(as seen in T-X-Y Diagram). Now, the liquid is fed to a decanter(with appropriate models defined for Liquid-Liquid Separation) where the aqueous and organic phases are separated , which in turn are used as reflux for the respective columns.

## Results:

All the relevant data can be obtained by clicking the respective streams after simulation.
The data for some main streams is below.

| | WATER | ORGANIC | FEED | BUTANOL | AQUEOUS |
|---|---|---|---|---|---|
| Temperature | 81.204 | 70 | 77.975 | 94.3286 | 70 C |
| Molar Flow | 979.999 | 64.2774 | 1000 | 20.0016 | 134.35 kmol/h |

## Conclusions & Recommendations :

1. The process is highly sensitive to change of property methods during simulation. Methods such as UNIQUAC, MODIFIED UNIFAC(DORTMUND),NRTL support VLLE for flash calculations.
2. Generate a phase diagram while using a given property method. For the T-X-Y drawn above, the NRTL method won't give desired results for the given system. 98% feed water in NRTL model is usually a region, not outside the LLE; while one expects to be outside.
3. The Re-boiled absorber unit operation in DWSIM usually takes longer time to converge. One has to know how to set the tolerance limits if the basis is on mole fraction of the bottom. For simulation of sensitive azeotropic mixtures, a CAPE OPEN plugin model is used. The Prausnitz interaction parameters for this system is loaded from ChemSep. Make sure to install ChemSep to simulate and view detailed results.
4. The reboiler load for 10 or 20 stages is not so much significant. 10 stages are usually taken to reduce capital costs. A new DWSIM plugin to evaluate process costs is also available

5. Process takes place at 0.5 atmosphere, which decreases boiling points of the respective components(Refer T-X-Y diagram) so that cooling water can be used in a cooler for a desired temperature reduction.

6. Extensive Temperature Control on the top plate of the column, rigorous decanter modelling to include settling time has to be done for dynamic control of the system. Disturbances in feed is a major factor.

7. The feed is introduced at an intermediate stage if the butanol composition is below 2%. The configuration is different for higher mole %. It is directly fed to decanter in such cases.

## References:

1. William L.Luyben, I-Lung Chien Design and Control of Azeotropic Distillation Columns.

2. Markets and Markets..Trend of Butanol until 2020.
3. Flow sheeting source http://www.chemsep.com/downloads/index.html

4.Image Source: Phase Envelope Utility DWSIM