**Theory:**

In a separation unit, we have two phases . Assume that the system is closed, and pressure and temperature are constant. Therefore, . With respect to have to phases, we can rewrite the equation as: (General Point of View)

In microscopic point of view, we have that:

Regards to fugacity definition, we have:

The fugacity can be driven from session 3 notes. The parameter is calculated from EOS, and is calculated from EOS + mixing rules. This calculation process is difficult and boring!

For the case of real gas and ideal mixture, we can write the equilibrium as:

In case of *ideal gas*, the fugacity coefficient () equal to 1.

In other hand, we can use method to calculate the fugacity. The activity coefficient can be calculated from several defined equations!

The term “” is a correction term, which allows us to compute fugacity in any another pressure.

In real world, the term approximately equals to 1, so:

If the mixture behaves as an ideal mixture, the term will be equals to 1. Hence,

If the gas phase behaves in Ideal Gas Model context, we have:

*Note that the gas phase is Real Mixture, and the liquid phase is Real Mixture too.*

In VLE problem, the first duty is to calculate the Dew and Bubble points. With knowledge of these points, we can determine the separation conditions and criteria.

In Dew point, we have:

In Bubble point, we have:

The simplest model for separation system is Flash Unit. The inlet stream consists of both gas and liquid phase, and the outlet stream is divided to pure vapor stream and pure liquid stream. We can define Recovery Ratio in Liquid phase as

V, y

F, z

Fixed T, P

L, x

Figure 1- Schematic of a Flash Separation Unit

At the exit of a Methanol Reactor, we must separate the products to achieve Methanol with desired purity. The Flash unit works in same pressure as reactor pressure (because of the reflux stream). A throttle valve is installed in the outlet path of pure Liquid stream to reduce the pressure and inject it in another flash separator. In the second flash separator, the pure vapor stream will be purged, and the pure liquid stream (L2, x2) will be chosen as the final product!

A diagram of a machine

Description automatically generated

Both flash separators are working in , and the inlet flow rate and composition are known!

The solution process is:

1. Dew Temperature at feed in Ideal Gas case (Ideal Mixture), or Real Mixture (Real Gas) case should be calculated.
2. The volatility factor should be calculated:
3. The volatility factor should be calculated:
4. The input energy to the second flash separator should be calculated (in order to conduct energy balance)

For the first stream, first, we have to determine the phase of stream. The process is:

1. P and z are known. Hence, we can calculate dew temperature and determine the phase by parameter, and approach!

In the case of ideal gas, we have:

We can solve these equations with iteration method (there’s the only possible method!). First, we have to guess xi,D (the best guess in this case is to consider it as ideal gas)! Hence, xi,D = 0. by compute TD from , we can re-estimate xi,Dnew. Finally, the phase of the stream will be determined.

**First Flash Separation Unit:**

**Quests: Condition: Real gas!**

We can impose a global material balance:

Then, we have to write a component material balance:

The vapor-liquid equilibrium for each component is written as:

Finally, we should write stochiometric equation:

**2nd Separation Flash Unit:**

The pressure in comparison to the 1st unit is fairly low. Assume the gas phase behaves like *ideal gas*. The solution algorithm is same as previous unit, but there’s a little difference:

**Energy Balance:**

We can neglect from the enthalpy contribution of dissolved supercritical component in stream!

A control Volume (CV) should be defined, which consists of the inlet stream to valve. Then, we have to define a convention that Q>0. The thermodynamic scheme in this case is *ideal gas*. Finally, we have to set a reference condition in one of the streams, then calculate the parameters in the others. The enthalpy balance is written as follows:

A chalkboard with math symbols

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