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Aim:-

Develop a MATLAB code implementing the boundary value design method for simple ternary distillation using bottom-up and top-down tray-by- tray calculation.

Assumption:-

CMO condition is valid for this problem and relative volatility is constant throughout the distillation column.

Given Data:-

For moderate (2) and difficult (1.2) adjacent relative volatility of the feed, which is an equimolar ABC ternary of 100 kmole/h which is to be processed and the desired key impurity in the product stream are 1 mole % each.

Theory:-

A tertiary feed could be split into two different ways:-

1. **Direct Split:** In Direct Split light component will be in the distillate stream and will be separated first with impurities of heavy component and heaviest component (very little) and heavy components will leave the distillation column through bottom stream with impurities of A in it.
2. **Indirect Split:** In Indirect Split light components will be in the distillate stream and will be removed first with impurities of heaviest component and heaviest components will be separated first from the feed with impurity of moderate component and a little impurity of lightest component.

DOF Analysis:-

We are using boundary value design method to solve this problem so we need to know reflux ratio, distillate and bottom composition. We are assuming CMO is valid so we know the value of L, V at each tray in rectifying section where L is equal to liquid coming from the condenser and V is equal to sum of L, D. We can calculate D, B from overall mass balance so D is known, B is also known because B = R*D so we know V, L. Now we have Reflux ratio and composition in bottom and top. For top

compositions, we know key component composition will be .01. So the and if we specify the heaviest/lightest component composition then D, B as well as, we can get bottom composition using overall mass balance. Now we know that for our feed is at bubble point so L′ = L + F where L′ is liquid coming from feed tray so we can calculate Boil up ratio using L′, V. So we have only two DOF and that is reflux ratio and composition of lightest (Indirect Distillation) or heaviest component (Direct Distillation).

Procedure:-

1. **Give necessary input variable:-**

   To proceed we need to specify value of the two DOF variables that is reflux ration and composition of lightest (Indirect Distillation) or heaviest component (Direct Distillation).

   Key component impurity in bottom = 0.01
   Key component impurity in distillate= 0.01

2. **Overall mass balance:-**

   We can calculate composition of top (Direct case) because we know key component mole fraction and we specified value of highest component so we can calculate lightest component composition and we know lightest component composition in bottom so we can apply material balance on lightest component and by using overall material balance we can find the Distillate and Bottom product rate. And now using this we can find the compositions of all components in both the streams.

3. **Tray by tray Calculation:-**

   For rectify section:

   We know the distillate stream composition so composition of vapour stream coming out from tray 1 will be the same as the distillate, by using the relative volatility correlation we can find composition of liquid stream coming out from tray 1. And after doing that we can do material balance over tray 1 and condenser to find the vapour composition coming to the tray 1. And by repeating

these steps we will find the liquid and vapour stream compositions on each tray.

For stripping section:

For stripping section vapour will be same as rectifying section and liquid will be liquid in rectifying section plus feed. Now we know the bottom stream composition so composition of liquid stream coming out from tray 1 will be the same. So by using the relative volatility correlation we can find composition of vapour stream coming out from tray 1. Now, we can do material balance over tray 1 and reboiler to find the liquid stream composition coming to the tray 1. And by repeating these steps we will find the liquid and vapour stream compositions on each tray.

We calculate the composition tray-by- tray until we got the difference in the composition of any component between the consecutive trays to be too small. This is the pinch point for the given section.

Results and Calculations:-

F=100 kmol/hr

Z = [0.33 0.33 0.33]

- **Minimum Reflux Calculation for direct Split:**

For minimum reflux in this case we just need to set a value of reflux ratio so that stripping profile just touches the rectifying profile. We will take a large number of trays and the value of component other than key component will be too small.

1. **For moderate adjacent component relative volatilities:**

   Alpha = [4 2 1]

   Here we specified the 3^{rd} component impurity in distillate = 1e (-14)

   2^{nd} component impurity in distillate = 0.01

   1^{st} component impurity in bottom = 0.01

   So at R_{min} = 2.14, the stripping profile just touches the rectifying profile.

   Value of L = R*D

D in this case is 32.98
So L = 2.14*32.98 = 70.5772

Optimum Reflux ratio = 1.2* R_{min} = 2.568

2. **For Difficult adjacent component relative volatilities:**

Alpha = [1.44 1.2 1]
3^{rd} component impurity in distillate = 1e (-14)
2^{nd} component impurity in distillate = 0.01
1^{st} component impurity in bottom = 0.01

So at R_{min} = 11.3 stripping profile just touches the rectifying profile.
Optimum Reflux ratio = 1.2*R_{min} = 13.56

- **Minimum Reflux Calculation for Indirect Split:**

In Indirect split minimum reflux rate will be finding by when the rectifying profile will just tough the stripping profile.

1. **For moderate adjacent component relative volatilities:**

Alpha = [4 2 1]
Here we specified the 1^{st} component impurity in bottom = 1e (-14)
2^{nd} component impurity in distillate = 0.01
1^{st} component impurity in bottom = 0.01

So at R_{min} = .99 rectifying profile just touches the stripping profile.

Optimum Reflux ratio = 1.2* R_{min} = 1.188

2. **For Difficult adjacent component relative volatilities:**

Alpha = [1.44 1.2 1]
1^{st} component impurity in bottom = 1e (-14)
2^{nd} component impurity in distillate = 0.01
1^{st} component impurity in bottom = 0.01

So at R_{min} = 5.5 rectifying profile just touches the stripping profile.
Optimum Reflux rate = 1.2* R_{min} = 6.6

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Effect of third product stream mole fraction on column design:-

- **For direct split:-**
  Reflux rate increases as we increase the 3rd component impurity in distillate and number of trays decrease.
  So when we decrease impurity of 3rd component, no. of rectifies trays increase and minimum reflex decreases. But after some value of impurity if we further decrease it, reflux rate doesn't decrease much but no. of trays increases rapidly. So it will be more costly to decrease impurity of 3rd component further.

- **For indirect split:** -
  Reflux rate increases as we increase the 1st component impurity in bottom and number of trays decrease.
  When we decrease impurity of 1st component, no. of stripping trays increase and minimum reflex decreases. But after some value of impurity if we further decrease it, reflux rate doesn't decrease much but no. of trays increases rapidly. So it will be more costly to decrease impurity of 3rd component further.