RESEARCH ARTICLE

SIMULATION OF A THERMALLY-COUPLED COLUMN FOR SEPARATION OF ALCOHOLS.

Olugbenga. A. G.
Department of Chemical Engineering, Federal University of Technology Minna.

Abstract

The design of an energy saving distillation plant has been carried out. The procedure included all the design of the conventional distillation plant with a deviation from a single column to three-thermally coupled distillation columns. The coupled column was designed by configuring a linkage of three columns together with the overhead and bottoms stream without heat exchangers. The first column was made the pre-fractionator which evaporates the lightest component; the second column separates both the lightest and middle components, while a last column was connected in the bottom where both the middle and the bottom components were separated. The feed included a 100kgmol/hr and the liquid fraction was one. The relative volatilities of each distillation are 7.5, 5.0, 2.1 and 1.9 for a feed composition of Methanol, Ethanol, n-propanol and i-propanol respectively. Each component has a feed composition of 25%. The recoveries were 66%, 34%, 50% and 50% respectively. Conceivable mixes of parallel blends were made and the base energy was calculated for each. The underwood technique was utilized to get least reflux proportion.

Introduction:-

The majority of the procedures in chemical industry are associated with purifying components. As a result, a substantial piece of the energy use in modern industry can be ascribed to separation processes. Distillation is the predominant separation techniques in the chemical industries regardless of its high energy consumption. Distillation takes around 3% of the all energy expended universally (Caballero and Grossman, 2004) Since numerous separation under takings need to proceed with this innovation, techniques needed to decide the insignificant energy utilized as a part of a given refining assignment have turned out to be essential. For detachments of a multicomponent blend, one approach to decrease the energy necessities is utilizing thermally coupled distillation sections rather than the traditional direct arrangement. These new techniques allow energy savings of over 30% when compared to conventional distillation columns. In addition, the current ascent in energy costs and demands additionally underlines the importance of this distillation process. Distillation is a physical procedure for the separation of liquid mixtures that depends on contrasts in the boiling points of the constituent parts. Distillation is the most generally accepted separation processes utilized in most industry.

Distillation takes around 95% of all current physical separation process. It has been utilized as part of chemical industries, pharmaceutical and food production processes, ecological innovations and in oil refineries. It has been widely utilize by attachment to a reactor where a few component is required to be distilled over. Refining is utilized

Corresponding Author:- Olugbenga. A. G.
Address:- Department of Chemical Engineering, Federal University of Technology Minna.
as a part of request to isolate the coveted item from the rest getting a high purified component. Cases of the most vital applications in food industries are concentrating essential oils and flavours; the de-odorization of fats and oils or in liquor distillations. Some pharmaceutical procedures in view of grouping of antibiotics are additionally related with distillation segments. Then again, Distillation is the primary part in oil refineries. The crude petroleum which contains an unpredictable blend of hydrocarbons is separated into a number of refining section keeping in mind the end goal to be separate fractions obtained at various temperatures.

By exploiting the recycle flow streams from the main column, the second column is connected to the top stream while the third column is connected into the simple column with vapour phase defined as Equation (1).

\[ y_l = \frac{x_i P_i}{P} \]  

Where \( y_l, x_i, P_i, P \) are the mole fraction of the vapour phase, mole fraction of the liquid phase, partial pressure and pressure in the distillation column respectively. For a non-ideal mixture such as that used for this work overall material balance is given in Equation (2). The componential balance is given in Equation (3).

\[ F = B + D \]  
\[ Fx_f = Bx_R + Dx_D \]  

For the multi-component systems, the material balance around the rectifying segment is given by Equation (4), the minimum number of plate is given by Equation (4) and (5) the fraction in the vapour phase is defined by Equation (6) expressed as \( V_T \) in equation (7).

\[ V_{min} y_{Ln+1} = L_{min} x_{Ln} + D x_{LD} \]  
\[ \frac{N_{min}}{ln \frac{y_{R}}{x_{R}}} \]  
\[ w_l = V_{n+1} y_{Ln} - L_{n+1} x_{Ln+1} \]  
\[ V_T = \sum_{i=1}^{N} \frac{w_l x_i \alpha_i}{\alpha_i \beta} \]

Distillation is utilized to isolate a mixture into at least one individual material by utilizing a temperature difference (Errico, et. al., 2009a). In this way, the creating item will contain the desired purity by controlling the condenser and re-boiler (Errico, et. al., 2009b). Both simple and thermally coupled distillation takes advantage of volatilities.

Though simple distillation column has been used for experimental purposes in laboratories for the separation of binary mixtures, little or no work has been reported for the separation of a multicomponent mixture which are actively implemented for various industrial applications in Nigeria. Although the use has been reported in Japan (Midori and Nakahashi, 1999). Currently no practical application of thermally coupled distillation column for practical work scheme. Like the internally heat-integrated distillation column (HIDiC), a significant percentage of energy is saved from the thermally coupled distillation column. The extended pilot design of the column requires proper answers for the design and operation, which is yet to be understood. The thermally coupled replacing the simple column system has one reboiler instead of three reboilers for the conventional system. Some other arrangements of coupled columns (Sargent and Gaminibandara, 1976; Kaibel, 1987; Agrawal, 1996), and the combination of a main column and two satellite columns of the figure proposed by Agrawal (1996). Another example of a similar research work was carried out by Lee at al., (2001) which uses a known structure to simulate the thermally coupled distillation column. In this work, the structural the conventional simple distillation is compared with the thermally coupled configuration where a three column is used to relace simple column. These columns were made to separate alcohol mixtures of ethanol, propalon, 1- and n- propanol. The equilibrium computation and inclusion of operational variables was implemented in Hysys.

**Methodology:**

The four component feed used for thermally coupled distillation simulations for the separation of a mixture of alcohols is listed in (Table 1). In the following table feed composition and relative volatilities are listed.

<table>
<thead>
<tr>
<th>Components</th>
<th>Feed Composition</th>
<th>Relative Volatilities</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>0.25</td>
<td>7.5</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0.25</td>
<td>5.0</td>
</tr>
<tr>
<td>n-propanol</td>
<td>0.25</td>
<td>2.1</td>
</tr>
<tr>
<td>i-propanol</td>
<td>0.25</td>
<td>1.9</td>
</tr>
</tbody>
</table>
The Equation for the preferred Split:
The preferred split was represented as the case when all the intermediates are distributed to both rectifications. The recoveries of A is one in Equation (8) Where \( r_{AT} \) is the recovery of A.

**PAD:**
\[
[r_{AT}, r_{BT}, r_{CT}] = [1, r_{BT}, r_{CT}]
\]  
(8)

Since three unknown variables were in question, the vapour should permit, the recovery of B \( r_{BT} \), the recovery of C \( r_{CT} \). These recoveries were obtained by the solutions of the three equations which are Equations (9), (10) and (11) respectively.

**Aspen procedure:**
Aspen Plus is an outstanding simulation tool programming in the formulation of distillation. The Aspen procedure gives a direct result of its capability to obtain operating line including a number of iteration. Here the majority of the conditions utilized are exceptionally convoluted. Recall that it is difficult to unravel simulation by manual calculations because of human errors and time requirements. Simulations were carried out for column design having 55cm height and 20cm diameter. The product from the top column was obtained by designing connections. The mass flow rate was set at 100kgmol/hr and thermal energy was adjusted in degree centigrade. The total liquid fraction is specified as 1. Thus 1% was stated as the specifications of composition fraction impurity at every stage of the componential balance. The corresponding energy balance were remotely calculated by the thermal energy response was at 75°C (Errico et. al., 2009a; Errico et. al., 2009b) with the implementation of the run command, the solid model was used simulated to reproduce the distillation process and control of the design to represent the natural process plant. Each procedure had its procedure model ranging from feed line to product and bottom lines. The flow sheet was prepared by addition of the working temperature and pressure to the included columns, reboiler, connecting tubes, a top column and bottom column in order to determining the distillate and bottom flow. Hysys gave the full detailed product streams which are Methanol, having 60% and ethanol having 40%. The advantage observed in the simulation of the distillation is the that it predicts the product and computes the effectual changes due to the variation of the parameter. A list of the components of the distillate stream is provided in Table 2 and 3 and the unit of flow when the simulation is finished. This means the flow sheet model the whole framework. The flow sheet clearly presents the whole streams going into the main column.

**Optimum structural design:**
The entire distillation column was optimized before defining the following stage. Each of the columns were optimized in details to enable simulation of the vapour flow and liquid flow phase. All the units of the entire process were specified with flow rate data and temperature which are ruxed into the primary column. More than one degree of freedom is required for a thermally coupled distillation unit therefore an iterative calculation was completed to optimize M in the Equation (12) where \( j \) is the iterative term from 1 to \( n \)

\[
P_n = \left[ \frac{2(M-1)\cdot(1-n)}{M(M-2)} \right] \cdot \left[ \sum_{j=1}^{M-3} \frac{(M-1)!}{j![M-2-j]!} \right] + 1
\]  
(12)

Where M is number of component separation the number of simple column sequences (Pn) can be predicted with Condition 1 for reproduction to acquire an ideal structure. At the initial, a perfect introductory structure was gone into the Hysys condition, next the operational factors were indicated for Ethanol, Propanol n-propanol and I-propanol. The sustain rate were specified as 25% each and the product of the distillation were reproduced. A trial structure was over and again made until the point that the ideal section configuration was reached. The perfect structure of the base plate configuration was utilized to plan the down to earth section framework. This plate circulation was gotten from the harmony refining line. This line has no blending at the sustain plate and no remixing of the middle of the road parts to augment the thermodynamic proficiency of the section.
Results and Discussion:-
The optimum structure chosen from the iteration is provided in Figure 2.

The solutions to the simulated equation in the procedure. The three equations gave the recoveries as stated below. 

\[ V_{T_{\min}} = 0.5791 \text{ and } r_{B,T} = 0.5390, \text{ and } r_{C,T} = 0.1891 \]

After obtaining the recoveries of B and C, the equation below was used to calculate the recovery of D using Equation (13)

\[
\frac{D}{F} = x_f_A + r_{B,T}x_f_B + r_{C,T}x_f_C = 0.4291
\] (13)

If the recoveries of B and C at the top column are \( r_{B,T} \) and \( r_{C,T} \) respectively, the ratios of D to F define the operating points, the underwood equation was utilized and the value of each possible binary combination was obtained. The results are provided in Table 2.

<table>
<thead>
<tr>
<th>Operating Point</th>
<th>( P_{AB} )</th>
<th>( P_{BC} )</th>
<th>( P_{CD} )</th>
<th>( P_{AC} )</th>
<th>( P_{BD} )</th>
<th>( P_{AD} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>D/F</td>
<td>0.249</td>
<td>0.490</td>
<td>0.749</td>
<td>0.359</td>
<td>0.569</td>
<td>0.392</td>
</tr>
<tr>
<td>( V_{T}/F )</td>
<td>0.907</td>
<td>1.049</td>
<td>1.196</td>
<td>0.692</td>
<td>0.790</td>
<td>0.490</td>
</tr>
</tbody>
</table>

The hysys continued with iterative calculation and streamlined technique yielded the ideal structure (Table 2) optimized for the distillation. The fractionation forms the separation of the alcohols from different stream. The favourable position is that it is conceivable to obtain a preparing volume which is abundantly contrasted with the straightforward arrangement. The computation of cost for plate and section by the thermally coupled configuration is brought down and compared with the convensional simple column configuration and about 35% of cost for simple configuration was saved. The energy requirement in the convensional configuration was first calculated next the equivalent energy necessity for the thermally coupled configuration was and the energy saved was calculated. Upto 65% as much as the energy for the conventional configuration was saved. This is a significant change in the thermodynamic prerequisite of the distillation procedure.

Structural Design:-
The procedures followed in the Hysys for the re-enactment of distillation have constraining factors for the estimations of plate numbers and fluid stream are explained in this section. These two factors are the essential for the column design. These two variables initiated the optimum design from the liquid. Here, a design strategy starting with the simple column structure was embraced for the simulation of thermally coupled column. In all, the reflux state, the required number of column plate is the determined by the alcohol in distillate. This indicates that the thermodynamic proficiency of the column is either perfect or not. At the point when the structure of a bottom fraction is gotten from the base plate section, the exceptionally proficient fraction is yielded. In this multicomponent distillation, the liquid fraction of the column gave up each distillate due to volatilities reached. A high
thermodynamic effectiveness was obtained since there is neither mixing at the top column nor remixing of middle of the road segments. The profile of build-up mixture is from pure component, and the bottom column structure has a similar profile of distilling line. In this manner, a functional section outlined from the bottom column has high effectiveness. Keeping in mind the end goal to wipe out top column mixing, which lessens the segment proficiency fundamentally, this is in line with Kin’s work (Kim, 2002). It is expected that the main column will be equivalent to enrich formation of the fraction in the bottom column. Additionally, the structure has perfect plate effectiveness, where the vapour synthesis of a phase is same as the liquid arrangement of one phase above. Henceforth, the plan of the fundamental segment starts with the enriched formulation and the liquid structures of the plate over the main column are assessed from balance connection in organize to-arrange computational way.

The cases with the parts were indicated in Aspen and the most reasonable liquid bundle. Additionally, we have to set the number of stages, the weight in the section and two different phases.

From the Hysys procedure, for the thermally coupled, we used 10 plate, that implies that the Distillate product (D) and the vapour flow rate in the top column (V_T) are obtained and the outcomes are presented in Table 3.

<table>
<thead>
<tr>
<th>Operating Point</th>
<th>P_{AB}</th>
<th>P_{BC}</th>
<th>P_{CD}</th>
<th>P_{AC}</th>
<th>P_{BD}</th>
<th>P_{AD}</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>23.49</td>
<td>49.9</td>
<td>69.51</td>
<td>35.03</td>
<td>59.00</td>
<td>42.950</td>
</tr>
<tr>
<td>V_T</td>
<td>109.90</td>
<td>108.00</td>
<td>111.00</td>
<td>70.00</td>
<td>80.01</td>
<td>58.01</td>
</tr>
</tbody>
</table>

Comparing Table 2 and Table 3, the V-min were evaluated for each component. The Underwood equations were used and the hysys simulation was carried out. The results in Table 4 shows a perfect agreement and the distillations of the mixtures results into pure components of methanol as 64%, and 36%ethanol in the stream of the top column. While the liquid of i-propanol and n-propanol where 50% each in the stream of the bottom column.

<table>
<thead>
<tr>
<th>Components</th>
<th>Top Composition</th>
<th>Recovery</th>
<th>Bottom Composition</th>
<th>Recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>0.64</td>
<td>0.4917</td>
<td>0.00</td>
<td>0.4917</td>
</tr>
<tr>
<td>Ethanol</td>
<td>0.36</td>
<td>0.4990</td>
<td>0.00</td>
<td>0.4990</td>
</tr>
<tr>
<td>n-propanol</td>
<td>0</td>
<td>0.6592</td>
<td>0.50</td>
<td>0.6592</td>
</tr>
<tr>
<td>i-propanol</td>
<td>0</td>
<td>0.0592</td>
<td>0.50</td>
<td>0.0592</td>
</tr>
</tbody>
</table>

Another remark about the thermally coupled is the advantage of utilizing it. In the traditional section remixing happens caused by reusing of the condenser and reboiler items, so in the finishes of the segment the piece drops in light of remixing. Rather, in the thermally coupled sections there is no remixing, so the arrangement does not change from stage to organize.

**Conclusion:**
Thermally coupled refining segments were utilized as another technique to save energy for partitions of multicomponent blends. In this report, the conventional distillation configurations were compared with the thermally coupled configuration. For this reason, distillation systems with less than N-1 columns were examined. First, considering the simple distillation columns in series arrangement and after that, the thermally coupled configuration.
References:
3. Errico M; Tola G.; Rong B.G, Demurtas D.; Turunen I. Energy saving and capital cost evaluation in distillation column sequences with a divided wall column. Chemical Engineering research and design (2009a)
5. Errico M; Tola G.; Rong B.G, Demurtas D.; Turunen I. Energy saving and capital cost evaluation in distillation column sequences with a divided wall column. Chemical Engineering research and design (2009)