

Determination of θ Acceptance Range in the Distillation Columns Design by θ Method of Convergence

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Abstract. Distillation tower design is considered an important part in chemical engineering; Different ways mentioned to design multi-component distillation towers Such as θ method of convergence. Exact determination of θ in this way is very important, but the equations that determine θ such a manner that is associated with try and error and θ can be any positive value. This paper tries to solve the mathematical equations governing the distillation of acceptance range for θ set. this paper shows that efforts was used to determine a range for θ resulted to estimate θ with an less than ten percent error, which could used as appropriate initial guess in determining θ and the calculations will be reduced.

Keywords: Distillation, Tower, θ method.

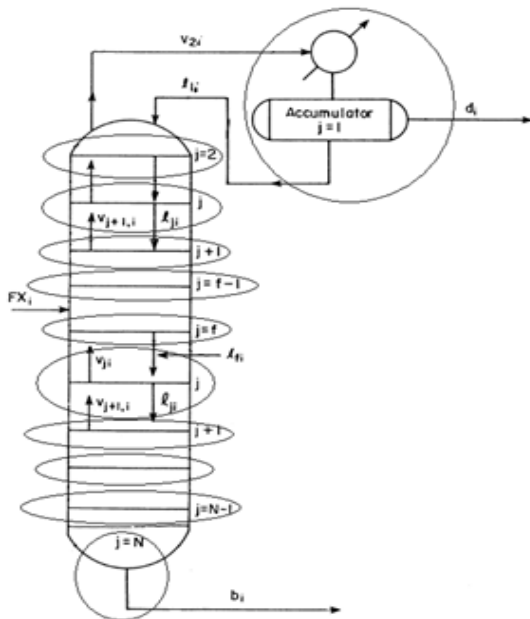
1. Introduction

Distillation is a method to separate a solution components which is based on the distribution of materials between liquid and gas phases is strong and therefore it is used in cases in which all components are included in both phases. In distillation operation, the new phase is obtained from the primary product through evaporation and condensation rather than from inserting a new material into the solution to create a second phase processes, such as what is performed in absorption and expulsion processes [1]. The distillation operation can be carried out in two main methods, first method is based on steam production and in that method, the liquid mixture which should be isolated, will be boiled and the obtained steam will get condensed with no liquid returned to the Distiller (instantaneous distillation). The second method is based on returning a part of the condensed liquid to the Distiller, so that this returned liquid contacts well with the steams which are entering the condenser [2]. The distillation column is composed of a number of trays in each one of which liquid and vapor are balanced. In this column, products are respectively separated in terms of boiling range, so that the lightest materials are obtained from the top of the column and middle distillate products from the lateral parts of the column. Currents egresses from the distillation column are steam like and will be turned to liquid after crossing the condensers. Some parts of this liquid are received as distillation product and the other part will be returned to the distillation column as Reflux. The aim of the reflex is to separate and regulate the column temperature better, because most of reflex will be evaporated again upon getting to the distillation column and will remove the thermal necessary for evaporation from materials in trays and consequently, more condensed materials in the steam which are ready to leave the column will be turned to liquid again and will flow towards the lower trays. Thus, the fluid phase which flows down enriched with heavier components continuously, due to impact of the mass and thermal transfer, while steam phase absorbs lighter components as gradually goes to the higher trays [3].

2. Distillation column Design

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One of the widely used methods for designing multi-component distillation columns is θ method of convergence, which will be analyzed in this paper. A conventional distillation column is defined with a feed and two Distillates (D) and Bottoms (B) stream. Schematic of Such a column can be seen in Figure 1. By performing material balance on each balance stage including condenser, column trays and Reboiler, we reach to equations 1 in which where d_i is flow rate of i component in the top product of column, b_i is flow rate of i component in bottom product of the column, and l_{ji} , v_{ji} are flow rate of i component on the j tray in the liquid and vapor phase respectively. By defining absorption coefficient A_{ji} in accordance with equation 2, material balance equations can be combined with balanced relations of absorption coefficient and equations category 3 can be obtained. In these equations, l_{Fi} , v_{Fi} are flow rate of i component in feed in liquid and vapor phases respectively, and f indicates the feed tray. In equation 2, L_j , V_j are also molar flow rate logged off the tray j in the liquid and vapor phases respectively. By calculating the absorption coefficients for the various components using k equilibrium values, equations 3, will have N equations and N unknowns which can be easily solved using matrix methods. The mentioned matrix can be shown as equation 4. By solving matrix equations, all the flows rates, including vapor flow rate, column top product and column bottom product will be obtained and by using absorption coefficients of equation 2, all flow rates of liquid in the column will be calculated. As specified in equation 2, absorption coefficients are a function of flow rate of vapor and liquid phases and k_{ji} equilibrium data which in itself represents the distribution of vapor phase to the liquid phase for i component, but at the beginning of solving the problem, none of these data are determined. As an initial guess to determine the flow rates of liquid and vapor phase within the column, it would be assumed that these flows do not change over the distillation column, so they can be achieved by having feed flow rates, column top product, column bottom product and the reflux ratio from the condenser to the column. In the second stage, it is possible to determine k_{ji} equilibrium data using Equations of state provided that all trays temperature and the column total pressure is specified, However, given that the distillation columns generally work at low close to atmosphere pressures, , so the impact of the temperature is very important in determining these equilibrium data and considering the lack of working temperature of the column trays at the beginning of the design, the temperature of the column trays would be conjectured as the second guess, thus the absorption coefficients, used as a key parameter in determining the flow intensity of components within the column, is associated with two initial assumptions. At this stage, it will be seen that the values of the column top and bottom products derived for i component will not apply for the overall column materials balance (Equation 5) and this is due to the two wrong assumptions which were performed for determining absorption coefficients and θ method of convergence are used to rectify the values obtained.



$$Eq.1 \begin{cases} -l_{2i} - d_i + v_{2i} = 0, (j = 1) \\ l_{2i} - v_{2i} - l_{3i} + v_{3i} = 0, (j = 2) \\ l_{j-1,i} - v_{ji} - l_{ji} + v_{j+1,i} = 0, (j = 3, 4, \dots, f-2) \\ l_{f-2,i} - v_{f-1,i} - l_{f-1,i} + v_{fi} = -v_{fi}, (j = f-1) \\ l_{f-1,i} - v_{fi} - l_{fi} + v_{f+1,i} = -l_{fi}, (j = f) \\ l_{j-1,i} - v_{ji} - l_{ji} + v_{j+1,i} = 0, (j = f+1, f+2, \dots, N-1) \\ l_{N-1,i} - v_{Ni} - b_i = 0, (j = N) \end{cases}$$

$$Eq.2 \begin{cases} A_{ji} = \frac{L_j}{k_{ji} V_j} \end{cases}$$

$$Eq.3 \begin{cases} -(A_{2i} + 1)d_i + v_{2i} = 0, (j = 1) \\ A_{2i}d_i - (A_{3i} + 1)v_{2i} + v_{3i} = 0, (j = 2) \\ A_{j-1,i}v_{j-1,i} - (A_{ji} + 1)v_{ji} + v_{j+1,i} = 0, (j = 3, 4, \dots, f-2) \\ A_{f-2,i}v_{f-2,i} - (A_{f-1,i} + 1)v_{f-1,i} + v_{fi} = -v_{fi}, (j = f-1) \\ A_{f-1,i}v_{f-1,i} - (A_{fi} + 1)v_{fi} + v_{f+1,i} = -l_{fi}, (j = f) \\ A_{j-1,i}v_{j-1,i} - (A_{ji} + 1)v_{ji} + v_{j+1,i} = 0, (j = f+1, f+2, \dots, N-1) \\ A_{N-1,i}v_{N-1,i} - (A_{Ni} + 1)v_{Ni} = 0, (j = N) \end{cases}$$

Fig. 1: Schematic of conventional distillation column

$$A_i = \begin{bmatrix} -\rho_{1i} & 1 & 0 & 0 & \dots & \dots & \dots & 0 \\ A_{1i} & -\rho_{2i} & 1 & 0 & \dots & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & A_{f-2,i} & -\rho_{f-1,i} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{f-1,i} & -\rho_{fi} & 1 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & 0 & A_{N-2,i} & -\rho_{N-1,i} & 1 \\ 0 & \dots & \dots & \dots & 0 & 0 & A_{N-1,i} & -\rho_{Ni} \end{bmatrix} \quad (4)$$

$$v_i = [d_i \quad v_{2i} \quad v_{3i} \quad \dots \quad v_{f-1,i} \quad v_{fi} \quad \dots \quad v_{N-1,i} \quad v_{Ni}]^T$$

$$\xi_i = [0 \quad 0 \quad \dots \quad 0 \quad v_{fi} \quad l_{fi} \quad 0 \quad \dots \quad 0]^T$$

$$\rho_{ji} = (A_{ji} + 1)$$

Logic of this approach is that if we multiply the ratio of flow rate of the column bottom product to the Column top Product computed for i component by a constant coefficient such as θ , this ratio will be revised and apply in overall balancing of the column (Equation 6), $g(\theta)$ convergence function can be defined from combining equations 5 and 6 (Equation 7). In this equation, θ must be determined so that the function result would be zero $g(\theta)=0$, which is usually determined through numerical and try and error methods. Having determined θ , new temperatures will be calculated for different balanced stages of the column by having flow rates of the column top and bottom product modified for the i component through k_b method and new liquid and vapor flow rates will also be obtained by enthalpy balance within the column. Now, having these new values, new absorption coefficients will be obtained again and this repetition continues. The obtained data would be accepted for the column provided that θ is equal to one [4].

3. Calculating Acceptance Range to Determine θ

As observed in the previous section, determining the numerical value of θ is an important parameter in designing the column by θ method of convergence, but according to the type of convergence function, determining it is by numerical methods and associated with many tries and errors. Given that the value of flow rates of Column product cannot be negative or zero, so θ is positive and non-zero. Figure 2 shows the chart of convergence function in the $\theta > 0$ region which is of interest. The closer temperatures of Column equilibrium stages and liquid and vapor flow rates within the column to the real values, the closer θ will get to one. In determining θ by numerical methods, no specific initial guess is specified which is along with numerical analysis and mathematical logic of the problem and is usually assumed to be zero initially, which increases the mathematical calculations in try and error operations in itself. In this section, attempt will be done to obtain ranges for values of θ so that through this method, mathematical calculations to determine would be reduced.

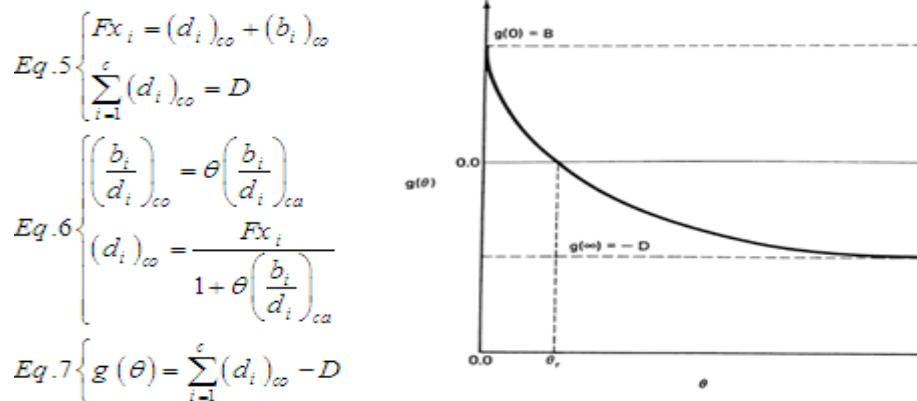


Fig.2: Convergence function

First, we consider a_i positive numbers as follow to determine θ range. There is a relationship between Arithmetic and adaptive intermediary of a_i positive numbers by using which we will reach to a significant inequality.

$$a_i = \frac{Fx_i}{1 + \left(\frac{b_i}{d_i}\right)\theta} \quad \text{And } \sum a_i = D$$

$$\frac{1}{\frac{1}{a_1} + \frac{1}{a_2} + \dots + \frac{1}{a_n}} \leq \frac{a_1 + a_2 + \dots + a_n}{n} \rightarrow \frac{nFx_1 \dots Fx_n}{\sum_{i=1}^n \left(1 + \left(\frac{b_i}{d_i}\right)\theta\right) \prod_{j=1, j \neq i}^n Fx_j} \leq \frac{D}{n} \rightarrow \frac{\sum_{i=1}^n \left(1 + \left(\frac{b_i}{d_i}\right)\theta\right) \prod_{j=1, j \neq i}^n Fx_j}{nFx_1 \dots Fx_n} > \frac{n}{D}$$

$$\rightarrow \sum_{i=1}^n \prod_{j=1, j \neq i}^n Fx_j + \sum_{i=1}^n \left(\frac{b_i}{d_i}\right)\theta \prod_{j=1, j \neq i}^n Fx_j > \frac{n^2 \prod_{i=1}^n Fx_i}{D} \rightarrow \theta > \frac{\frac{n^2 \prod_{i=1}^n Fx_i}{D} - \sum_{i=1}^n \prod_{j=1, j \neq i}^n Fx_j}{\sum_{i=1}^n \left(\frac{b_i}{d_i}\right)\theta \prod_{j=1, j \neq i}^n Fx_j} \quad (8)$$

Now we prove following inequality. We reach to the desired relationship using indirect Argument:

$$\theta < \frac{\frac{n^2 \prod_{i=1}^n Fx_i}{D}}{\sum_{i=1}^n \left(\frac{b_i}{d_i}\right)\theta \prod_{j=1, j \neq i}^n Fx_j} \quad (9)$$

$$\theta > \frac{\frac{n^2 \prod_{i=1}^n Fx_i}{D}}{\sum_{i=1}^n \left(\frac{b_i}{d_i}\right)\theta \prod_{j=1, j \neq i}^n Fx_j} \rightarrow \frac{n^2 \prod_{i=1}^n Fx_i}{D} < \theta \left(\sum_{i=1}^n \left(\frac{b_i}{d_i}\right) \prod_{j=1, j \neq i}^n Fx_j \right) \rightarrow \frac{n^2 \prod_{i=1}^n Fx_i}{D} < \theta \left(\sum_{i=1}^n \left(\frac{b_i}{d_i}\right) \right) \prod_{i=1}^n Fx_i$$

$$\rightarrow \frac{n^2}{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right)} < \theta$$

Now, we will multiply unequal sides by $\left(\frac{b_i}{d_i}\right)$ and we will have:

$$\left(\frac{b_i}{d_i}\right)\theta > \frac{n^2 \left(\frac{b_i}{d_i}\right)}{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right)} \rightarrow 1 + \left(\frac{b_i}{d_i}\right)\theta > 1 + \frac{n^2 \left(\frac{b_i}{d_i}\right)}{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right)} \rightarrow \frac{Fx_i}{1 + \left(\frac{b_i}{d_i}\right)\theta} < \frac{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right) Fx_i}{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right) + n^2 \left(\frac{b_i}{d_i}\right)}$$

Then we will have:

$$\sum_{i=1}^n \frac{Fx_i}{1 + \left(\frac{b_i}{d_i}\right)\theta} < \sum_{i=1}^n \frac{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right) Fx_i}{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right) + n^2 \left(\frac{b_i}{d_i}\right)}$$

We will get to the important relation which is issue contradiction from the above Inequality:

$$\frac{1}{\sum_{i=1}^n \left(\frac{b_i}{d_i}\right)} < \sum_{i=1}^n \frac{Fx_i}{D \sum_{i=1}^n \left(\frac{b_i}{d_i}\right) + n^2 \left(\frac{b_i}{d_i}\right)}$$

So θ always holds true in the following inequality.

$$\frac{\frac{n^2 \prod_{i=1}^n Fx_i}{D} - \sum_{i=1}^n \prod_{j=1, j \neq i}^n Fx_j}{\sum_{i=1}^n \left(\frac{b_i}{d_i}\right) \theta \prod_{j=1, j \neq i}^n Fx_j} < \theta < \frac{\frac{n^2 \prod_{i=1}^n Fx_i}{D}}{\sum_{i=1}^n \left(\frac{b_i}{d_i}\right) \theta \prod_{j=1, j \neq i}^n Fx_j} \quad (10)$$

4. Result and Discussion

Inequality obtained from equation 10 shows a reception range for θ , the smaller range makes it easier to determine θ , Therefore, to check accuracy and precision of this inequality studied five different case was investigated the results are summarize in Table 1. The second column from the table is shown solution of the exact equation of real convergence θ ; Third column is shown the minimum range for θ obtained from equation 8 and the fourth column is shown the maximum range for θ obtained from equation 9. It is not only obvious accuracy the values obtained from Inequality equation 10 it is also shows the range and set the small interval for θ . the mean value of lower and above bound of θ in the fourth column of Table 1 is shown very close to the actual value of θ in such a way that the mean value calculated error value of less than ten percent of the actual value of θ . The exact amount of error is shown in the fifth column in Table 1, so the efforts applied to determine a range for θ resulted to estimate with an error of less than ten percent which can be used as accurate initial guess in determining an appropriate θ and certainly will reduce the calculations.

Table 1. Case study for θ determination

tem	θ	Min.	Max.	Ave.	Error %
Case1	11.89563	7.434634	14.86927	11.15195	6.25
Case2	3.687276	2.272036	4.544071	3.408053	7.57
Case3	0.978866	0.611497	1.222995	0.917246	6.29
Case4	1.00046	0.624903	1.252498	0.9387	6.17
Case5	0.286716	0.175335	0.35067	0.263003	8.27

5. References

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