

## New calculation of the tray numbers for Debutanizer Tower in BIPC

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**Abstract:** Today numerous software programs are available to calculation and designing of distillation towers. All these software programs are made simplify by the mathematical models relations to design the equipment and plants. Not only there are limitations for each relation and mathematical model with the new design method, but also the software behaves like only a black box that input the numbers and displays the results. As to whether these answers are reliable, it is necessary to know how the mathematical modelings are used. With regards to utmost importance to the application of mathematical model relation, this article try to calculate the number of trays by utilizing two methods of Montross and Under wood by applying the empirical data. As a result, it was specified that by use of Montross and Under wood methods, the Debutanizer tower was 18.5% and 48.5% oversized respectively.

**Key words:** Debutanizer tower, Montross, Underwood, oversized

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### I. Introduction

Distillation is a process that separates two or more components into an overhead distillate and bottoms. The bottoms product is almost exclusively liquid, while the distillate may be liquid or a vapor or both. The separation process requires three things. First, a second phase must be formed so that both liquid and vapor phases are present and can contact each other on each stage within a separation column. Secondly, the components have different volatilities so that they will partition between the two phases to different extent. Lastly, the two phases can be separated by gravity or other mechanical means. There are limitations in these columns such as azeotropes, solids, optimum pressure and optimum temperature differences in reboilers and condensers. But besides these limits distillation is the least expensive means of separating mixtures of liquids [1]. Distillation towers are one of the most important equipment in oil and petrochemical industries. Efficient and economical performance of distillation equipment is vital to many processes. Although the art and science of distillation has been practiced for many years, studies still continue to determine the best design procedures for multicomponent, azeotropic, batch, multidraw, multifeed and other types. Though construction and development of petrochemical industries have been started only a few decades ago, nevertheless sufficient knowledge was not obtained to design and construct the distillation tower yet. Perhaps one of the factors that unable we to gain adequate knowledge for designing equipment such as tower are the lack of recognition on how to utilize the mathematical modeling by software for designing. Current design techniques using computer programs allow excellent prediction of performance for complicated multicomponent systems such as azeotropic or high hydrogen hydrocarbon as well as extremely high purity of one or more product streams. Of course, the more straightforward, uncomplicated systems are being predicted with excellent accuracy also. The use of computers provides capability to examine a useful array of variables, which is invaluable in selecting optimum or at least preferred modes or conditions of operation. Commercially available software to be able simulation of entire chemical plants for the purposes of design, optimization and control. The technique of these software is based on Equilibrium, thermodynamic, mass and heat transfer basic Considerations [2]. It is essential to calculate, predict or experimentally determine vapor-liquid equilibrium and in order to adequately perform distillation calculations. These data need to relate composition, temperature, system pressure and type of system (ideal or nonideal). There are many mathematical relation for calculation of designing parameters for example minimum reflux, minimum tray, theoretical trays at actual reflux, overhead composition and represented by Underwood equations, Fenske equation, Gilliland correlation, Amundson-Pontinen method, Montross equation and etc. Also there are alternate short-cut method to design distillation column. For example the Fenske and Underwood equation together with the Gilliland correlation provide a short cut design method for distillation columns [3]. Some of these short-cut equations provide a good practical solution method for most distillation problems. But assumptions are required to use of them. Softwares are based on these equations and assumptions and don't show how use of them. Efforts are made here to present on how to use the mathematical model relation to calculate the number of trays of debutanizer tower.

## 1.1. Methods

### 1.1.1. Montross method (Constant or variable volatility)

This method allows a direct approximate solution of the average multicomponent system with accuracy of 1-8% average. If the key components are less than 10% of the feed, the accuracy is probably considerably less than indicated. If a split key system is considered, Montross reports fair accuracy when the split components going overhead are estimated and combined with the light key, the balance considered with the heavy key in the L/D relation [4].

$$\left(\frac{L}{D}\right)_{min} = \frac{1}{X_{IF} + \sum X_{FL}} [X_{IF} \cdot R' + (X_{hF} + \sum X_{FH}) \sum \frac{X_{FH}}{\alpha_H - 1} + \sum \frac{X_{FL}}{\alpha_L} (1 + \frac{\alpha_L}{\alpha_L})] \quad (1)$$

Pseudo minimum reflux ( $R'$ ) given by follow equation:

$$(R') = \frac{x_{i0}}{(\alpha_i - 1)x_i} - \frac{(1 - x_i)(\alpha_i - 1)}{(1 - x_{i0})\alpha_i} \quad (2)$$

mol fraction liquid at intersection of operating lines at minimum reflux given by Eq.(3):

$$(x_{it}) = \frac{(\alpha_i - 1)(1 + m) \left(\frac{X_{IF}}{X_{IF} + X_{hF}}\right)^{-\alpha_i - m}}{2m(\alpha_i - 1)} \pm \left\{ \frac{\sqrt{[(\alpha_i - 1)(1 + m) \left(\frac{X_{IF}}{X_{IF} + X_{hF}}\right)^{-\alpha_i - m}]^2}}{2m(\alpha_i - 1)} + \frac{\sqrt{4m(\alpha_i - 1)(1 + m) \left(\frac{X_{IF}}{X_{IF} + X_{hF}}\right)}}{2m(\alpha_i - 1)} \right\} \quad (3)$$

The proper value for  $x_{it}$  is positive and between zero and one. Actually this is fairly straightforward and looks more difficult to handle than is actually the case. Pseudo ratio of liquid to vapor in feed ( $m$ ) given by Eq.(4):

$$m = \frac{x_L - \sum X_{FH}}{x_V - \sum X_{FL}} \quad (4)$$

### 1.1.2. Minimum Number of Trays ( Total Reflux and Constant volatility)

The minimum theoretical trays at total reflux can be determined by the Fenske relation:

$$S_{min} = N_{min} + 1 = \frac{\log \left( \frac{X_{DL}}{X_{Dh}} \right) \left( \frac{X_{Bh}}{X_{Bl}} \right)}{\log \alpha_{ave}} \quad (5)$$

Note that  $N_{min}$  is the number of trays in column and does not include the reboiler. When  $\alpha$  varies considerably through the column, the results will not be accurate using the  $\alpha_{avg}$  and the geometric means is used in these cases [5].

$$\alpha_{avg} = (\alpha_t \cdot \alpha_b)^{1/2} \quad (6)$$

### 1.1.3. Underwood method (constant $\alpha$ in overall column)

This system for evaluating multicomponent adjacent key systems, assuming constant relative volatility and constant molal overflow, has proven generally satisfactory for many chemical and hydrocarbon applications. It gives a rigorous solution for constant molal overflow and volatility, and acceptable results for most cases which deviate from these limitations [6].

The major equation represent by underwood:

$$1 - q = \sum \frac{\alpha_i \cdot x_{Fi}}{\alpha_i - \theta} \quad (7)$$

$$\left(\frac{L}{D}\right)_{min} + 1 = \sum \frac{(\alpha_i \cdot x_i)_D}{\alpha_i - \theta} \quad (8)$$

Eq.(7) expressing  $\theta$  and  $q$  evaluate  $\theta$  by trial and error, noting that  $\theta$  will have a value between the  $\alpha$  of the heavy key and the  $\alpha$  of the light key evaluated at or near pinch temperatures, or at  $\alpha_{ave}$ .

### 1.1.4. Underwood method (variable $\alpha$ ):

For varying  $\alpha$ , the following procedure is suggested:

1. Assume  $\left(\frac{L}{D}\right)_{min}$  and determine the pinch temperature by Colburn's method [4].
2. At this temperature, evaluate  $\alpha$  at pinch and  $\alpha$  at overhead temperature, obtaining a geometric average  $\alpha$ .

- Determine Underwood's  $\theta$  value, using the average  $\alpha$  value.
- Calculate  $(\frac{L}{D})_{min}$  and compare with assumed value of (1) above. If check is satisfactory,  $(\frac{L}{D})_{min}$  is complete; if not, reassume new  $(\frac{L}{D})_{min}$  using calculated value as basis, and repeat (1) through (4) until satisfactory check is obtained.

## II. Computations

### 1.2. Montrossmethod

Butane tower has the following feed, overhead and bottoms composition data given Table 1:

Table 1: overhead and bottoms composition data

Component	Feed	Mol%	Over Head	Product	Bottom	Mol%
	Flow (Kg.mol <sup>-1</sup> .hr <sup>-1</sup> )		Flow	Mol%	Flow	
Propane	9.26	0.55	9.26	0.902	-----	-----
I-Butane	309.60	18.400	309.28	30.154	0.03	<b>0.004</b>
n-Butane L	702.07	41.725	700.08	66.191	1.99	<b>0.304</b>
I-Pentane H	199.18	11.837	7.21	0.702	191.47	<b>29.205</b>
n- Pentane	209.82	12.470	0.53	0.051	209.30	<b>31.906</b>
Hexane	140.67	6.360			140.07	<b>21.444</b>
Heptane	48.72	2.895			48.72	<b>7.427</b>
Octane	31.23	1.850			31.33	<b>4.760</b>
nonane	21.05	1.251			21.05	<b>3.208</b>
Decane plus	11.03	0.650			11.03	<b>1.682</b>
$\Sigma = 1682.63$ $\Sigma = 100\%$ Temperature (°C) T = 183.92°F Pressure (Kg.cm <sup>-2</sup> ) P = 6.2 Kg.cm <sup>-2</sup>			$\Sigma = 1026.66$ $\Sigma = 100\%$ T=131.72°F P=6.0Kg.cm <sup>-2</sup>		$\Sigma = 655.99$ $\Sigma = 100\%$ T=243.86°F P=6.4Kg.cm <sup>-2</sup>	

Light Key → n-Butane, Heavy Key → I-Pentane

Relative volatility calculation for heavy components given Table 2:

Table 2: vapor pressure and relative volatility data for compounds

Component	Feed T=160°F P <sub>i</sub> = Vapor Pressure (psig)	$\alpha_i = \frac{P_i}{P_h}$	Overhead	Bottom
Propane	400	7.19	9.26	-----
I-Butane	159.5	2.87	304.28	0.03
n-Butane L	118.5	2.13= $\alpha_l$	700.08.	1.99
I-Pentane H	55.6	1= $\alpha_h$	7.21	191.97
n-pentane	45.57	0.82	0.53	209.30
Hexane	16	0.29	$\Sigma 1026.66$	140.07
Heptane	6	0.12		48.72
Octane	2.4	0.043		31.33
Nonane	1	0.018		21.05
Decane Plus	0.45	0.0084		11.03
				$\Sigma = 655.99$

Calculation of minimum reflux ratio:

T=183.92°F, P=6.2 kg.cm<sup>-2</sup>

As a calculation results:

X<sub>L</sub>=0.365, X<sub>V</sub> = 0.635

$\Sigma X_{FL} = 0.1894, \Sigma X_{FH} = 0.27476$

Pseudo minimum reflux (R') and Pseudo ratio of liquid to vapor in feed (m) calculated by Eqs. (2), (4):

(R')= 1.59169 , m=0.203

$$X_{Lo} = X_{lO} / (X_{lO} + X_{hO}) = 0.9848$$

Mole fraction liquidat intersection of operating line calculated by Eq (3):

$$X_{lt} = 0.54622$$

$(\frac{L}{D})_{min}$ , calculated by Eq (1) :

$$(\frac{L}{D})_{min} = 0.798$$

Calculation of tray numbers by using of Van Winkle curve [7]:

$$(\frac{L}{D})_{min} = 0.798, (\frac{L}{D}) = 1.5 (\frac{L}{D})_{min} = 1.198, D = 0.61 \frac{\text{Mol Product}}{\text{Mol feed}}$$

$$(\frac{L}{V})_{min} = \frac{1}{1 + (\frac{D}{L})_{min}}, (\frac{L}{V})_{min} = 0.444, (\frac{L}{D})_{min} = 0.798, L_{min} = 0.798D, L_{min} = 0.4868 V_m = 1.096,$$

$$q = 0.822, F(\text{Feed}) = 1, L_s = L_r + q.F, L_s = 1.3088$$

$$V_s = V_r - F(1 - q) = 0.918$$

Operating values:

$$(\frac{L}{D})_{min} = 0.798, \frac{L}{D} = 1.5 (\frac{L}{D})_{min} = 1.197, L_r = 0.7302$$

$$\frac{L}{V} = \frac{\frac{L}{D}}{\frac{D}{L} + 1} = 0.422, \frac{L}{V} = 0.422, V_r = 1.73, L_s = L_r + q.F = 1.5522$$

$$V_s = V_r - (1 - q) = 1.3742, A = \frac{[(\frac{L}{V})_s (\frac{V}{L})_r - 1]^{0 \rightarrow \text{Theoretical}}}{[(\frac{L}{V})_s (\frac{V}{L})_r - 1]_{min \rightarrow \text{min. Reflux}}} = 0.78$$

The composition of over head and Bottom given in Table 3:

Table 3: composition of over head and Bottom product

Component	Over Head Product				Bottom Product			
	Flow	Mol%	k	y=k.y	Flow	Mol%	k	y = k.x
<b>Propane</b>	4.26	0.902	2.9	0.026	-----	-----	-----	-----
<b>I-Butane</b>	309.28	30.154	1.32	0.398	0.03	0.004	3.5	0.00014
<b>n-Butane L</b>	700.08	68.191	0.98	0.668	1.99	0.304	2.6	0.0079
<b>I-Butane H</b>	7.21	0.702	0.956	0.0032	191.97	29.265	1.5	0.439
<b>n-pentane</b>	0.53	0.051	0.36	0.008	209.30	31.908	1.25	0.399
<b>Hexane</b>				$\Sigma y = 1.09$	140.07	21.444	0.44	0.094
<b>Heptane</b>					48.72	7.427	0.32	0.024
<b>Octane</b>					31.33	4.760	0.18	0.0086
<b>Nonane</b>					21.05	3.208	0.052	0.0017
<b>Decane Plus</b>					11.03	1.682	0.036	0.00061
								$\Sigma y = 0.975$

$$\alpha_l(\text{Top}) = 2.15, \alpha_l(\text{Bottom}) = 1.733, \alpha_{ave} = 1.93$$

Minimum Stages at Total Reflux calculated by Eq.(5):

$$S_m = 13.87$$

From fig .1.[4] by operating reflux and stages corretated with minimum these results can be obtained:

$$A = 0.78 \rightarrow \frac{\text{over}}{\text{curve}} \rightarrow \frac{S_o}{S_m} = 1.8, S_m = 13.87, \frac{S_o}{S_m} = 1.8, S_o = 24.966$$

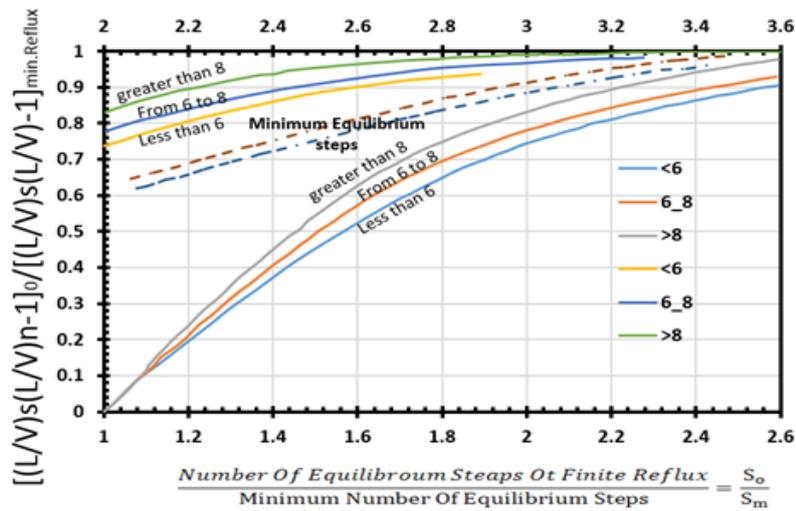


Fig.1. Operating reflux and stages corretated with minimum reflux and stage

### 2.2. Underwood method

Vapor pressure and relative volality data for compounds are given in Table4.

$T_{top} = 131.72^{\circ}\text{F}$  ,  $T_{Feed} = 160^{\circ}\text{F}$  ,  $T_{Bottom} = 243.86^{\circ}\text{F}$

Assumption of  $2/3 T = 169.4^{\circ}\text{F}$  , Assumption of  $1/3 T = 206.4^{\circ}\text{F}$

Table 4: vapor pressure and relative volality data for compounds

Component	Flow	T=169.4°F		$p_i$	$\alpha_i = P_i / P_h$	$\alpha_{ave}$
		$P_i = \text{Vapor pressure}$				
		$P_i$	$\alpha_i = P_i / P_h$			
<b>Propane</b>	9.26	420	6.9	600	5.71	6.28
<b>I-Butane</b>	309.60	190	3.11	240	2.29	2.67
<b>n-Butane L</b>	702.07	140	2.95	210	2.0	2.4
<b>I-Pantane H</b>	199.18	61	1.0	105	1.0	1.0
<b>n-pentane</b>	209.82	50	0.819	80	0.762	0.79
<b>Hexane</b>	140.67	18	0.295	32	0.30	0.297
<b>Heptane</b>	48.72	7	0.114	14	0.13	0.122
<b>Octane</b>	31.23	2.9	0.05	6	0.057	0.053
<b>Nonane</b>	21.05	1.25	0.02	2.8	0.0266	0.023
<b>Decaneplus</b>	11.03	0.52	0.0085	1.4	0.013	0.011

From Eq. (7):  $\theta = 1.14$

$\alpha_h^{1/2} \text{Top} = 2.15, \alpha_h^{1/2} \text{Botton} = 1.33, \alpha_{ave} = 1.93$

Minimum stages at total reflux calculated by Eq.(5):

$S_m = 13.87$

Calculation of minimum reflux ratio ( $L/D$ ) from Eq.(8) resulted that :

$$\left(\frac{L}{D}\right)_{min} = 0.249$$

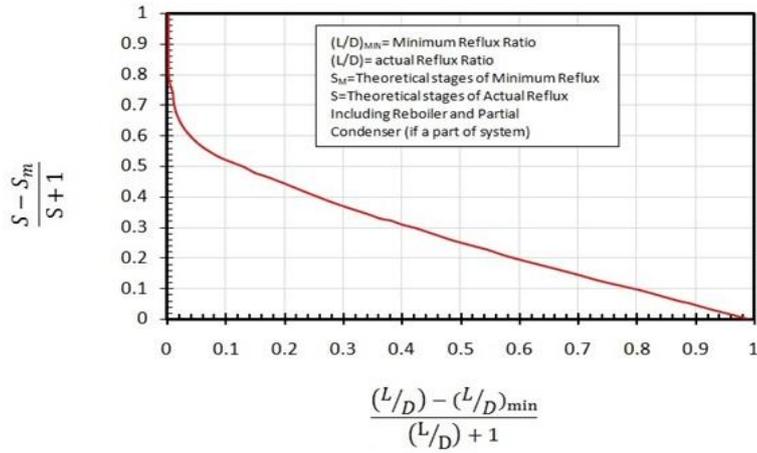


Fig .2. Correlation of theoretical plates with reflux ratio

As mention from Fig.2.[4]:  $(\frac{L}{D}) = 1.35$  ,  $S_o = 21$

**Tray Efficiency**

Use average column temperature of 187.8°F and feed analysis, the viscosity data given by Table5:

Table 5: The composition and viscosity data of compounds

Component			$\mu \cdot X_{iF}$
Propane	0.0055	0.1	<b>0.00055</b>
I-Butane	0.184	0.1	<b>0.0184</b>
n-Butane	0.41725	0.1	<b>0.041725</b>
I-Pentane	0.11837	0.14	<b>0.017</b>
n-Pentane	0.1247	0.14	<b>0.0175</b>
Hexane	0.0836	0.18	<b>0.015</b>
Heptane	0.02895	0.25	<b>0.0072</b>
Octane	0.01850	0.29	<b>0.0054</b>
Nonane	0.0125	0.35	<b>0.0044</b>
Octane	0.00650	0.42	<b>0.0027</b>

$E_0$  values may be calculated from empirical correlations of overall efficiencies for fractionation and absorption [8 ].

**2. Results and analyses**

**2.1. Calculation of actual number of trays by calculation of hydrocarbons viscosity**

At T=187.8 °F

$$T_{ave} = \frac{(T_{Top} + T_b)}{2}$$

As a  $\mu=0.134825$  cp and by using of Drickmer and Bradford curve [9] the tower efficiency was about 70%, at  $\mu=0.135$  cp with Drickmer correlation efficiency was 71% and by Combell correlation this value is 81%.

Actual number of trays illustrated in Fig. 3, also calculated by equations given in this section.

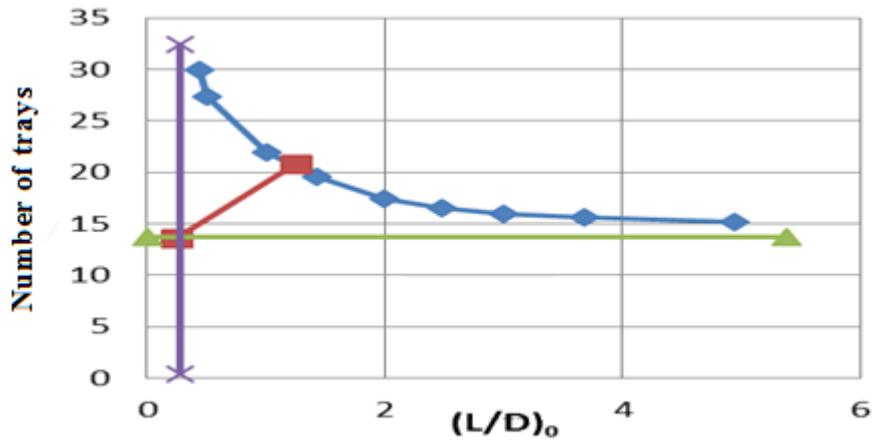


Fig. 3. Calculation of actual number of trays

### 3.1.1 Actual number of trays from Montross method

(Theoretical tray numbers)  $S_0 = 24.966$

Debutanizer has a reboiler and a total condenser so that:

$$S_0 = N_0 + 1 \rightarrow N_0 = S_0 - 1 = 23.966, N_{act} = \frac{N_0}{E_0} \Rightarrow N_{ac} = 33.75$$

### 3.1.2 Actual number of trays from Underwood method

$$S_0 = 21, S_0 = N_0 + 1 \rightarrow N_0 = 20, N_{act} = \frac{N_0}{E_0} = 28.169, N_{ac} = 28.169$$

Actual debutanizer tray numbers at BIPC:

By the use of Montross method:

$$N_{ac} = 40$$

By the use of Underwood method:

$$\text{Over Design\%} =$$

$$\text{Over Design\%} =$$

## IV. Conclusion

As a result, it was specified that by use of Montross and Underwood methods, the debutanizer tower at BIPC was 18.5% and 48.5% oversized respectively.

### Subscripts

h = heavy key

l = light key

t = top

b = bottom

o = Initial conditions; or operating condition

F = feed

### Nomenclature

B = bottoms flowrate, mol/h

D = distillate flowrate, mol/h

F = flowrate of feed, mol/h

L = liquid flowrate, mol/h

$\alpha$  = relative volatility  
 l = light key  
 h = heavy key  
 $x_{hF}$  = mol fraction heavy key in feed  
 $\alpha_l$  = relative volatility of light key to heavy key at feed  
 $\alpha_H$  = relative volatility of components heavier than heavy key at feed tray temperature  
 $\alpha_L$  = relative volatility of components lighter than light key at feed tray temperatures  
 $x_{it}$  = mol fraction liquid at intersection of operating lines at minimum reflux. (Calculated or from graph)  
 $x_{io}$  = mol fraction light key in overhead expressed as fraction of total keys in overhead.  
 $x_L$  = mol fraction of feed as liquid  
 $x_V$  = mol fraction of feed as vapor  
 $F_L$  = mols of liquid feed  
 $F_V$  = mols of vapor feed  
 $\sum F_H$  = total mols of components heavier than heavy key  
 $\sum F_L$  = total mol of components lighter than light key in in feed  
 $\sum X_{FL}$  = sum of all mol fractions lighter than light key in feed  
 $\sum X_{FH}$  = sum of all mol fractions heavier than heavy key in feed  
 $L_r$  = Liquid flowrate down rectifying section of distillation tower  
 $L_s$  = Liquid flowrate down stripping section of distillation tower  
 $q = q_F$  = Thermal condition of feed, approximately amount of heat to vaporize one mol of feed at feed tray conditions divided by latent heat of vaporization of feed.  
 $L/V$  = Internal reflux ratio  
 $L/D$  = Actual external reflux ratio  
 $(L/D)_{min}$  = Minimum external reflux ratio  
 $V_r$  = Vapor flowrate up rectifying section of tower  
 $V_s$  = Vapor flowrate up stripping section of tower  
 $S_m$  = Minimum Stages at Total Reflux  
 $S_o$  = Theoretical stages at a finite operating reflux  
 $N_o$  = Theoretical trays at the operating reflux

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