

ENGINEERING DESIGN SEMINAR

SEPTEMBER 6, 1994 – NOVEMBER 11, 1994

MULTICOMPONENT DISTILLATION

Comp	α	mol/hr		
		Feed	OVHD	BTM
A	6	40	40	
B-LK	2	20	20	
C-LK	1	20	-	
D	0.5	20	-	20
		<u>100</u>	<u>60</u>	<u>20</u>
				80

Binning approx.

B.p feed - perfect sep.

$$Y/F = \frac{1}{\alpha-1} = \frac{1}{2-1} = 1$$

$$L = 100 \times 1 = 100 \text{ mole/hr.}$$

High
Limit

$$Y/F = \frac{1}{(\alpha-1)} [\alpha_{LK} + \alpha_{HK}]$$

$$= 1 (0.2 + 0.2) = 0.4$$

Low
Limit

$$L = 100 \times 0.4 = 40 \text{ mole/hr.}$$

Underwood.

1st equation

$$\sum_{i=1}^n \frac{(d_i x_i)_F}{\alpha_i - \phi} = 1 - \theta$$

$$\sum_{i=1}^n \frac{(d_i x_i)_D}{\alpha_i - \phi} = \left(\frac{L}{D}\right)_{\min} + \theta$$

1st equation,

$$\frac{(6)(0.4)}{(6 - \phi)} + \frac{(2)(0.2)}{(2 - \phi)} + \frac{(1)(0.2)}{(1 - \phi)} + \frac{(0.5)(0.2)}{(0.5 - \phi)} = 1 - 0.8$$

MIN REFLUX.

Approx. Bin. analog

Max. possible reflux rate.

= Binary value.

Min. possible reflux rate

$$= \text{Binary value} \times (x_{LK} + x_{HK})$$

mole fraction in total feed.

Correct reflux ratio is between these limits

Example for bubble point feed.

imperfect separator

1) High Limit

$$C/D_m = \frac{1}{\alpha - 1} \left(\frac{x_D}{x_F} - \frac{\alpha (1 - x_D)}{(1 - x_F)} \right)$$

2) Low Limit

$$(C/F)_m = \frac{1}{\alpha - 1} (x_{LK} + x_{HK})_{\text{Feed}}$$

Min. Reflux.

Underwood method.

Assump.

constant molar overflow
const α .

$$a) \sum_{i=1}^n \frac{\alpha_i x_i F}{\alpha_i - \theta} = 1 - q$$

$$b) \sum_{i=1}^n \frac{(\alpha_i x_i)_D}{\alpha_i - \theta} = (L/D)_{min} + 1$$

All possible roots of equation a line between the α 's of the feed components

Substitution of these roots into b yields simultaneous equations whose solutions give $(L/D)_{min}$ and $x_{i,D}$ (non key components)

COMPONENT DISTRIBUTION

WHY VALUABLE?

- To estimate column material balance
- To start a tray to tray calculation
- To simplify a min. reflux calculation.

Approximate method.

Component are:

Lighter than light key $\rightarrow$ OVPD

Heavier than heavy key $\rightarrow$ BTMS

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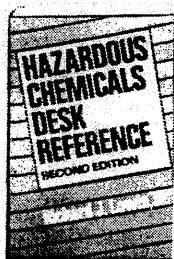
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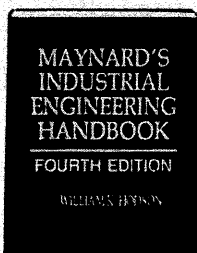
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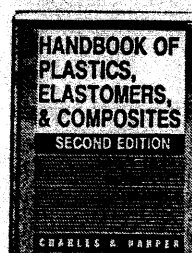
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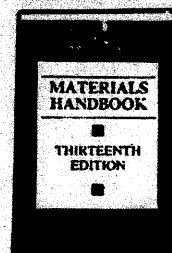
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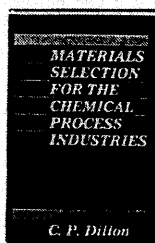
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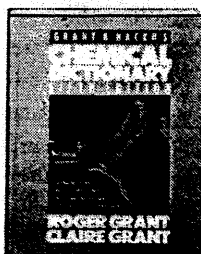
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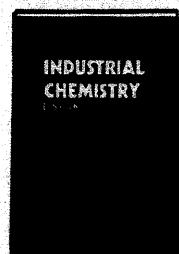
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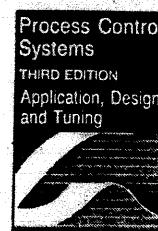
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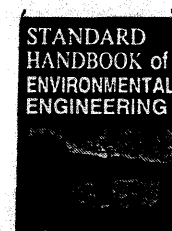
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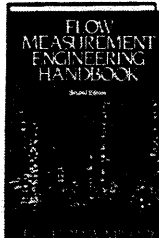
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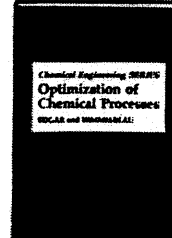
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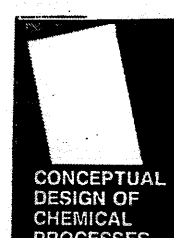
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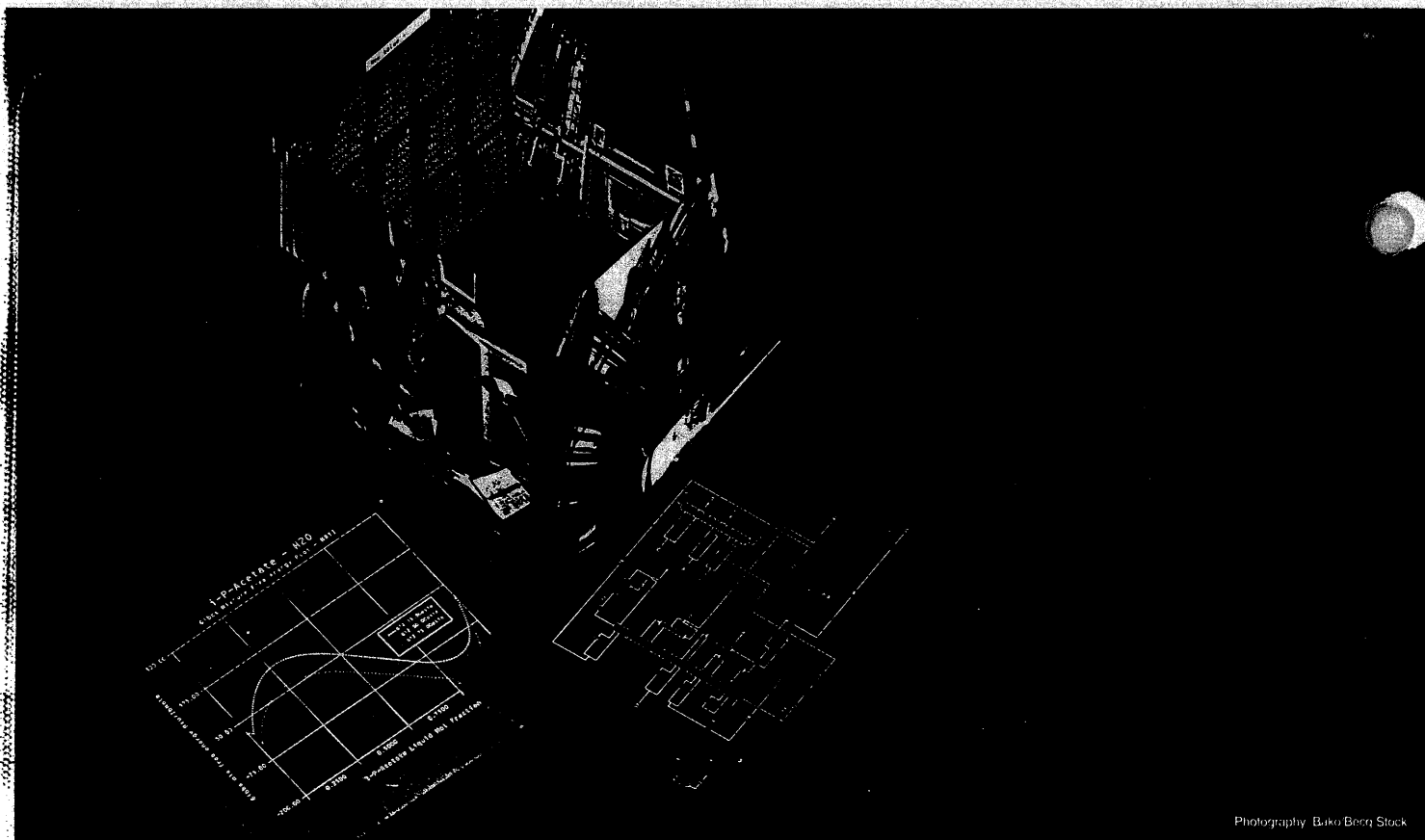
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HYSIM 24 HR Run

Hard to believe that any sane people would want to run for 24 hours, but, who said these people were sane. In late June, a team of Hyprotech employees (including a couple of the principals) and friends participated in the **Labatts Lite 24 hour relay**. This event raises money for Camp Horizon, a camp for disabled children.



This is a big event here in Calgary, with over 2,000 people on 120 teams taking part. This year raised over \$500,000, which was a record. Our Hyprotech team did themselves proud, finishing 20th in distance covered and 40th in total money raised.

Special congratulations to those who were fortunate (?) enough to draw the midnight shifts, at which time the skies decided it was an opportune time to open.

HYPROP/DIPPR Interface

HYPROP Version 1.50 provided an interface to the Dortmund Data Base, which proved immensely useful for importing pure component information, or locating experimental data that can be automatically imported for regression. The Dortmund Data Base contains over 13000 sets of VLE data and over 3000 sets of LLE data.

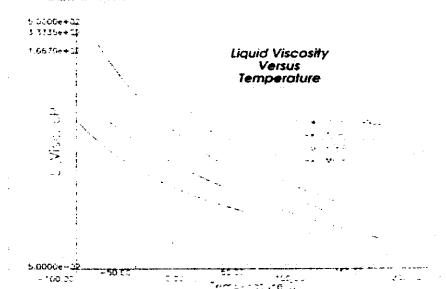
For version 2.10 of HYPROP, available shortly after Version 2.1 of HYSIM, the software interface to the DIPPR data base has been completed. This provides access to over 1400 pure components. Although many of the components are identical to those in HYSIM, the DIPPR data base contain information on properties not carried with HYSIM's components, such as: flammability limits, auto ignition temperatures, and second virial coefficients. Also, temperature dependant properties are provided in DIPPR as coefficients of an expression, for example a fourth order polynomial.

DIPPR is sponsored by the AIChE. All data is critically evaluated and provides an excellent pure component reference.

Experimental sources and data accuracy are provided for every listed physical property.

The **Tabular Property Package** in Version 2.1 of HYSIM, when combined with HYPROP and its link to the DIPPR data base, will allow you to have the coefficients (and the associated equation) used directly in HYSIM for calculating the temperature dependant properties.

Additional utilities allow printing of the data tables, plotting the properties as a function of temperature (or as a function



of another property - like T_c versus molecular weight for a number of components) as well as search routines.

For information on the DIPPR data base, contact:

TDS Numerica
(212) 245-0044
247-0587 (fax)

or

**National Institute of
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(301) 975-2208 or 926-0416 (fax)
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HYPROTECH HEADQUARTERS

(Hysim)
400, 119 14th St. N.W.
Calgary, Alberta, T2N-1Z6
Phone: 403-283-7710
Hotline: 1-800-661-8696
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EUROPEAN HEADQUARTERS

Hyprotech S.L.
Caspé 127 2nd Floor, #4
Barcelona, Spain
Phone: 011-34-3-447-2852
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REGIONAL OFFICES

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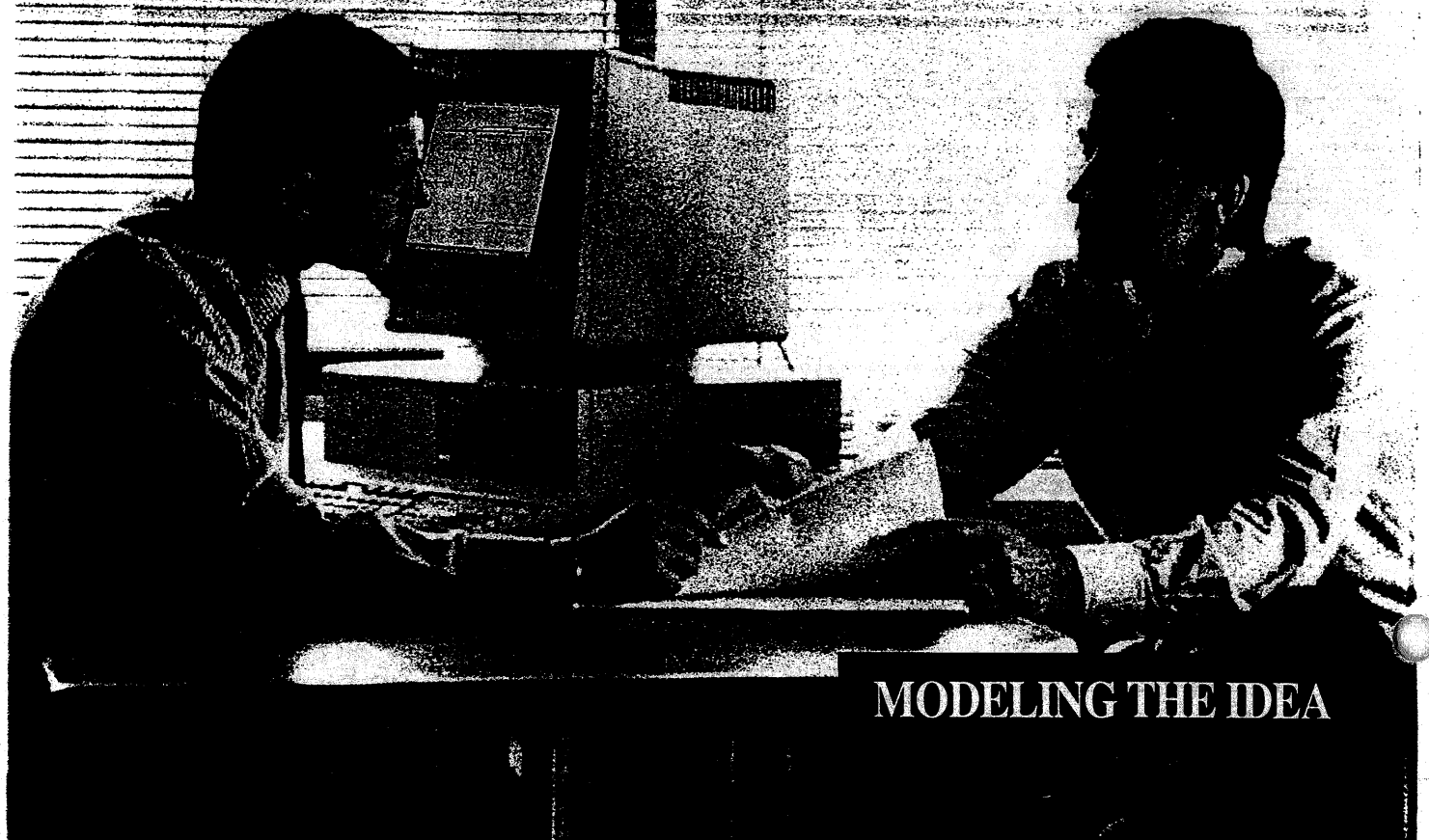
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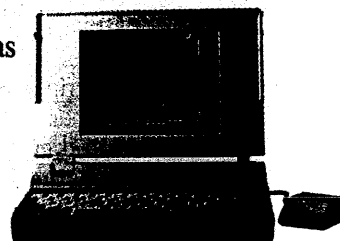
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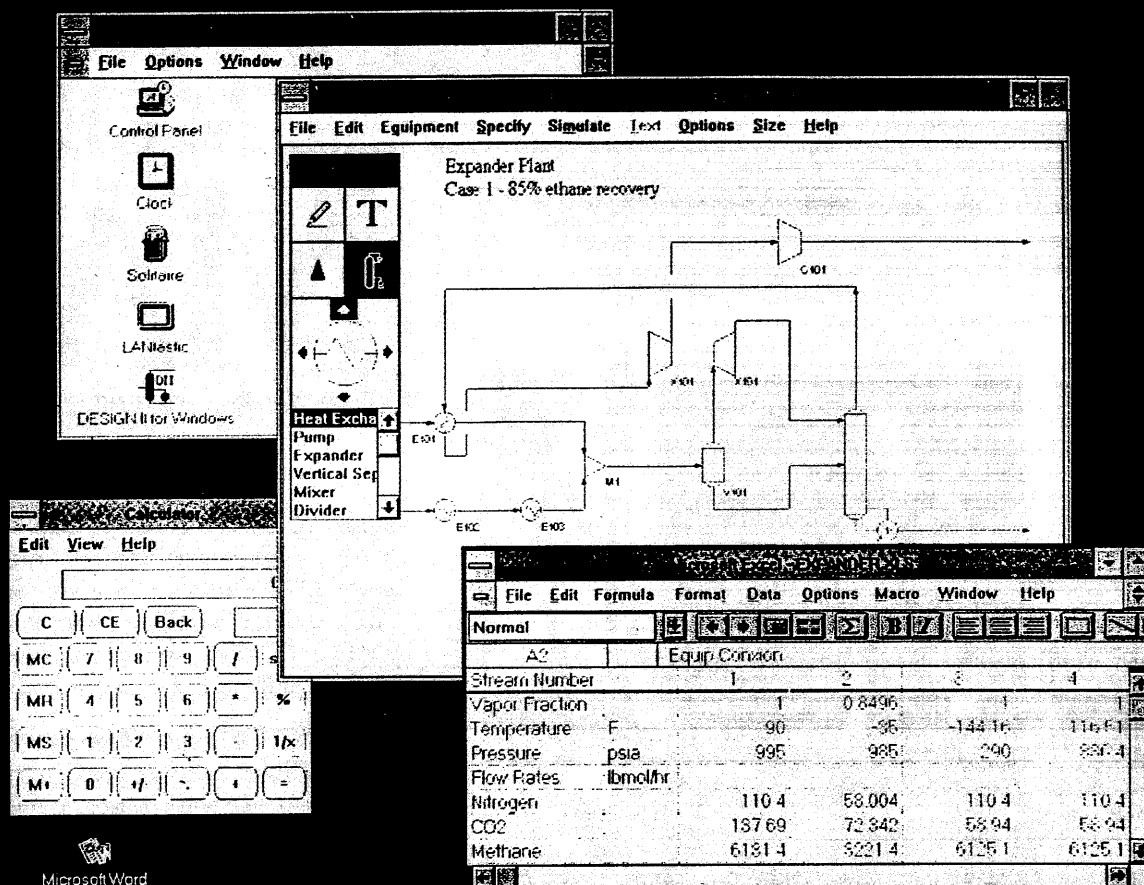
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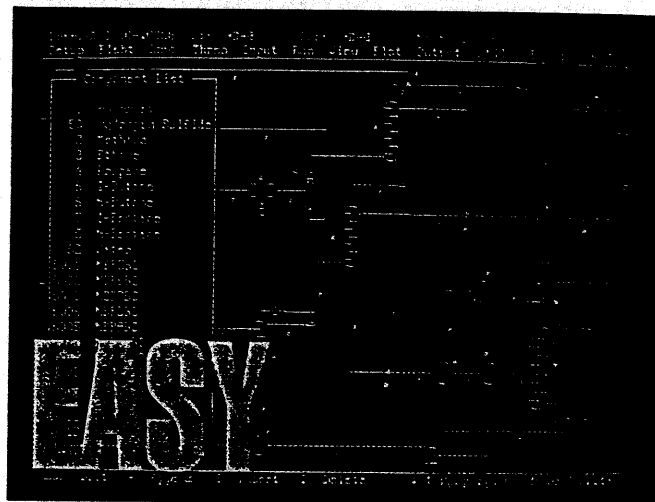
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the valve body. Minor deviations in the height of each part can greatly affect the critical amount of gasket compression needed to prevent internal leakage between parts. Too little compression, and leakage will occur. Too much, and a thermal spike can crush gaskets resulting in leakage or in permanent part deformation, potentially causing a sticking action as the valve strokes. Once internal leakage begins, rapid failure often results.

Parts from sources other than the OEM are typically reverse engineered. Because of this, they can pose one significant risk: tolerances and dimensions may vary from OEM specifications. These parts typically "will fit" into an OEM valve and appear equal to the OEM specifications. However, laboratory testing and evaluations have revealed many dimensions and tolerances well outside OEM design requirements.

Parts that deviate from OEM specifications may significantly impact process control, and may require laborious documentation to comply with OSHA 1910.119.

Don't be misled. *Will fit* parts, as they are frequently called, are not new. Nearly all OEMs have to contend with parts manufactured by nonauthorized sources. These parts, which are typically sold as equals, may be produced by the repair shop next door or may be manufactured and distributed worldwide by larger, replacement part operations. In either case, keep a few points in mind before considering such parts.

- The valve manufacturer cannot be responsible for improper valve and/or process operation if *will fit* parts have been used.

- Non-OEM parts may cause a significant process



The author

Bruce L. Quernemoen is the parts marketing manager for Fisher Controls International, Marshalltown, Iowa. He holds a BA degree in accounting and finance from Moorhead State University. Previously he worked at FMC Corp. His recent assignments at Fisher Controls included working as a worldwide quality director and as a worldwide parts marketing manager, where he is involved in developing and implementing strategies for Fisher's replacement parts business.

change.

- Only the OEM can provide proper documentation for its valves and parts to help you comply with OSHA's 1910.119.

- No one can reverse-engineer replacement parts that meet or exceed OEM specifications.

Don't be misled by non-OEM parts and repair sources who claim their parts meet or exceed OEM specifications. Instead, ask yourself these questions:

- Am I jeopardizing my safety and also the safety of other employees or the entire plant?
- Am I affecting equipment life or the total cost of operation?
- Am I altering the original process flow design?
- Am I complying with OSHA 1910.119?
- Is it worth the risk?

These are some hard questions that need well-thought answers before you replace.

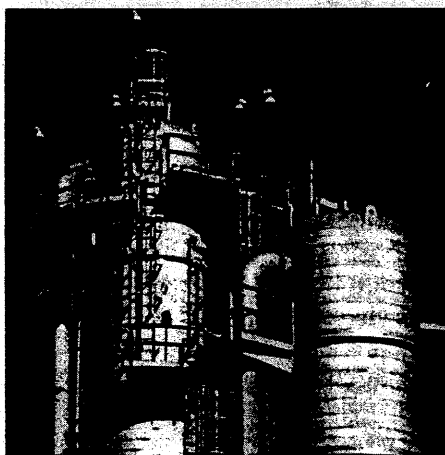
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- ¹ *Process Safety Management of Highly Hazardous Chemicals* (29 CFR 1910.119).
- ² *Quality Assurance*, 29 CFR 1910.119(j)(6)(iii).

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MULTICOMPONENT DISTILLATION

Introduction

The fundamental relationships – heat balances, mass balances, and equilibrium relationships – are used to analyze and solve multicomponent distillation problems.

The primary problem is computational – developing mathematical approaches and calculation procedures to apply these relationships in designing fractionators.

Most questions regarding multicomponent distillation can be answered with adequate accuracy by various "shortcut", approximate design methods. Preliminary design investigations, many economic studies, feasibility of using an existing fractionation system, etc., fall into this category. The bulk of our discussion will be on such methods. Rigorous, exact methods are only necessary in a final design mode.

In the general case, exact solutions are obtained through two mathematical approaches, both of which are trial-and-error.

Simultaneous Equations Approach

Appropriate equations describing the fundamental relationships are written for each tray. Since such equations are non-linear complex functions, initial assumptions must be made concerning temperature profile, composition profile, etc., before such set of equations can be solved (by numerical methods). The solution then is the basis for the next estimated profiles upon which the next solution to the equations is obtained. This trial-and-error process is continued until convergence criteria of heat balance, mass balance, composition change, etc., tolerances are met. This approach is popular where large digital computers are available, but is not practical for hand calculations or simple computers.

Tray-to-Tray Calculation Approach

In this approach, a composition is assumed for a theoretical tray in a column. The next tray's parameters either up or down from that tray are determined by applying the fundamental relationships. The process is continued with trays being calculated and recalculated including the originally assumed tray or trays until the convergence criteria are met. Again, a completely rigorous solution is only possible utilizing large digital computers.

However, with simplifying assumptions, this approach can be adapted to hand calculation or simple computers/programmable calculators; this approach will be discussed in depth.

For exact solutions, column pressure, reflux, theoretical trays in each column section and criteria of component separations are specified. If a change in any of these parameters is desired, the entire trial-and-error solution must be repeated. For multicomponent distillation, the direct determination of required trays (for a chosen reflux rate) is not possible in the general case as is possible in binary distillation via the McCabe-Thiele diagram approach.

It is helpful in multicomponent distillation to designate two components in the feed as key components. There are usually components whose recoveries are specified in advance and are thought of as the components between which the "split" or "cut" is made. That is, all components lighter than the light key appear mostly in the overhead and all components heavier than the heavy key appear mostly in the bottoms. The key components need not be adjacent in terms of order of relative volatility. If there are components between key components, they are usually called distributed components.

Our discussion will be limited to simple fractionators – one feed and two products.

Many approximate design methods are available. The simplified Kremser approach as applied to absorbers and strippers is a popular method and will be discussed.

Minimum Reflux and Trays

A very simple method of estimating minimum reflux is to treat the keys as binary and use techniques developed for binary distillation. For a minimum reflux value which is conservative, one can assume the entire feed consists of the keys ($x_{LK} + x_{HK} = 1.0$). More accurately, the minimum reflux ratio is related to the mol fraction in the feed of the selected keys. For example, with a bubble point feed, the minimum reflux is:

All cases (high limit):

$$(L/D)_{min} = \frac{1}{\alpha - 1} \left[\frac{x_D}{x_F} - \frac{\alpha(1 - x_D)}{1 - x_F} \right]$$

Mol fractions relative to key components

All cases (low limit):

Same as above times $(x_{lk} + x_{hk})_{Distillate}$

Perfect separation (high limit):

$$(L/F)_{min} = \frac{1}{\alpha - 1}$$

Perfect separation (low limit):

$$(L/F)_{min} = \frac{1}{\alpha - 1} (x_{lk} + x_{hk})_{Feed}$$

The most popular, more exact method for multicomponent minimum reflux estimation is that developed by Underwood. This method does assume constant molal overflow and constant relative volatility.

Underwood Equations Summary:

$$\sum_{i=1}^n \frac{(a_i x_i)_F}{\alpha_i - \phi} = 1 - q$$

$$\sum_{i=1}^n \frac{(a_i x_i)_D}{\alpha_i - \phi} = \left(\frac{L}{D} \right)_{min} + 1$$

ϕ = Underwood Parameter

α = Relative Volatility

x = Mol Fraction

q = Feed Thermal Condition

$\left(\frac{L}{D} \right)_{min}$ = Minimum Molal Ratio of Internal Reflux to Distillate Product

Subscripts:

i = Any Component

F = Feed

D = Distillate Product

In the general case, there are i possible values (roots) of ϕ ; and to begin with, the mol fractions of all components in the distillate product are not known. The general solution involves solving sets of simultaneous equations to determine which root of ϕ gives real values for the distillate compositions. This requires computer aid.

Where there are no distributed components, the correct root (ϕ) is between the relative volatility of the key components enabling a relatively easy solution.

To estimate minimum trays, the Fenske equation as applied to the chosen keys can be used.

Design Parameters

Column Material Balance

With feed and product specifications known (determined by customer and process constraints), the composition and quantity of products can be estimated. Readjustment due to results of fractionation calculations is not usually justified.

Considerations in Determining Operating Pressure

Since alpha's for hydrocarbons increase with decreasing pressure, the lowest pressure gives the lowest utilities. Optimum pressure is considered to be the lowest pressure obtainable for a reasonable temperature difference between process (overhead product bubble point, or receiver temperature) and conventional cooling sources (air or water).

Exceptions to the practice of using lowest possible pressure are:

Vacuum columns are usually only employed where a temperature degradation problem exists. Disadvantages of vacuum operation are low tray efficiency and low turndown, high capital cost due to large diameter column and piping which results from low vapor density and process oxygen contamination possibility.

Routing of gas product to destination without compression.

Minimizing loss of valuable components in gas products sent to fuel gas or disposal.

Increasing pressure to where the temperature increase allows column heat removal via external exchange against process or utility streams can have an attractive payout. Total column heat input increases and capital costs are usually significantly higher.

Design Reflux and Trays

As in binary distillation, an operating reflux must be selected. In setting design reflux rates, flexibility and accommodations for future column feed changes in rate and composition should be considered. Design for a reflux rate higher than optimal is often prudent as the incremental increase in capital costs is minimal. The Gilliland relation can also be used for multicomponent distillation to estimate the theoretical trays for design reflux rate.

Component Distribution

To complete an estimated column material balance, to start a tray-to-tray calculation or to simplify a minimum reflux calculation, a procedure to estimate the distribution of all feed components into the column products is needed.

A simplification which is often made is to put all of the components lighter than the light key in the overhead and all of the components heavier than the heavy key in the bottoms. This obviously will not give a rigorous result, but usually gives a good enough answer if those components have an α far removed from the key components.

Where this simplification is not possible, a method based on the Fenske equation can be used. This procedure is to apply the Fenske equation to the key components to determine minimum trays, then apply it to one key and each of the other components one at a time using the number of trays calculated from the key components and the α between the one key and the component in question.

This method assumes that the distribution of components between distillate and bottoms is the same at finite reflux ratio as at infinite reflux ratio. Not a bad assumption.

Illustrative example:

Nomenclature:

- F = Feed
- D = Distillate
- B = Bottoms
- X = Mols (Or Mols/H) of Any Component
- lk = Light Key Component
- hk = Heavy Key Component
- i = Component Lighter Than Heavy Key
- r = Ratio of Component Distribution in Distillate or Bottoms Relative to Some Reference Component – Usually the Heavy Key
- R = Ratio of Distillate Distribution to Bottoms Distribution
- α = Relative Volatility
- n = Minimum Trays (Fenske)
- $\ln$ = Logarithm

Fenske Equation for minimum trays:

$$n = \ln(r_D/r_B) / \ln \alpha$$

Using r and α relative to the heavy key ($\alpha = 1.0$):

$$r_D = X_{lkD}/X_{hkD} \text{ and } r_B = X_{lkB}/X_{hkB}$$

For any component (i) lighter than the heavy key component:

$$r_{iD} = X_{iD}/X_{hkD} \text{ and } r_{iB} = X_{iB}/X_{hkB}$$

To solve for any X_{ID} :

Let:

$$R_I = r_{ID}/r_{IB}$$

$$R_I = \frac{X_{ID}}{X_{hkD}} \frac{X_{hkB}}{X_{IB}}$$

$$R_I X_{hkD} X_{IB} = X_{ID} X_{hkB}$$

Since:

$$X_{IB} = X_{IF} - X_{ID}$$

Then:

$$R_I X_{hkD} (X_{IF} - X_{ID}) = X_{ID} X_{hkB}$$

$$R_I X_{hkD} X_{IF} - R_I X_{hkD} X_{ID} = X_{ID} X_{hkB}$$

$$X_{ID} (X_{hkB} + R_I X_{hkD}) = R_I X_{hkD} X_{IF}$$

$$X_{ID} = \frac{R_I X_{hkD} X_{IF}}{X_{hkB} + R_I X_{hkD}}$$

For small values at X_{IB} :

$$X_{IB} = X_{IF} X_{hkB} [X_{hkB} + R_I X_{hkD}]$$

Given a feed of components A through H with a limit of 3.0 mol/h of C in the bottoms and 0.1 mol/h of N in the distillate:

1 Comp	2 α	3 $\ln \alpha$	4 $\ln r_D/r_B$	5 r_D/r_B	6 X_F	7 X_D	8 X_B
A	1.650	0.501	13.126	501822	196.1	195.8	0.3
C(k)	1.490	0.399	10.452	34604	122.6	119.6	3.0
E	1.445	0.368	9.642	15398	95.8	90.7	5.1
G	1.188	0.172	4.506	91	68.4	6.5	61.9
M	1.140	0.131	3.432	31	86.8	2.8	84.0
N(hk)	1.000	0.000	0.000	1	86.9	0.1	86.8

Having set the concentration of component *N* in the distillate and component *C* in the bottoms and establishing *C* and *N* as the key components, calculate the ratios r_D and r_B .

$$r_D = 119.6/0.1 \quad r_B = 3.0/86.8$$

$$r_D/r_B = 34604$$

$$\ln r_D/r_B = 10.452$$

For this specified degree of fractionation, calculate the minimum trays from the Fenske Equation.

$$n = \ln(r_D/r_B) / \ln \alpha$$

This value for n , once fixed by the distribution of components *C* and *N*, the light and heavy keys, will be the same for all components with respect to the established feed composition, F .

$$D_i = (r_D/r_B) F_i D_H / C_B$$

Thus:

$$n = \ln 34604 / \ln 1.490$$

$$= 10.452 / 0.399$$

$$= 26.2 \text{ trays}$$

Now all the other values in Column 4 can be calculated by multiplying each value in Column 3 ($\ln \alpha$) by 26.2 (n).

Having the values of Column 4, the values of Column 5 are readily obtained, and from the r_D/r_B ratio, values for X_{ID} can be calculated from the equation derived above.

Alternative Method (more suitable for Graphical Solution):

$$\ln(X_{ID}/X_{IB}) = n \ln \alpha + \ln(X_{hkD}/X_{hkB})$$

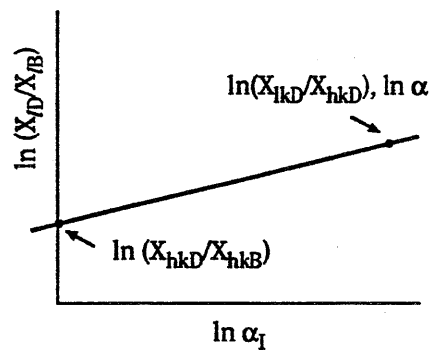
Determine (X_{ID}/X_{IB}) by graph or equation

Then:

$$X_{IB} = X_{IF} [1 + X_{ID}/X_{IB}]$$

$$X_{ID} = X_{IF} - X_{IB} \quad \text{or for small } X_{ID}$$

$$X_{ID} = X_{IF} + \left[1 + \left(\frac{X_{ID}}{X_{IB}} \right)^{-1} \right]$$



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Tray-to-Tray Calculation

The calculation can be started at each end of the column and worked toward the feed tray. It is also possible to start at either the top or bottom and work all the way through the column, but this technique is usually more difficult. Plate-to-plate calculations are seldom started at the feed tray because no simple relationship exists between feed tray composition and feed composition.

The method will consist of calculating the liquid compositions on each tray in the top section of the column by running the dew points on the vapor leaving the tray, starting from the distillate. The vapor composition rising from each tray is, in turn, obtained by material balance on the top section envelope. To get the vapor composition on each tray in the bottom section, bubble points are run on the liquids leaving each tray. In like manner, the liquid composition is calculated from the bottom section envelope as shown. Making these material balances, without writing heat balances, is only possible if constant internal reflux can be assumed, otherwise it is necessary to make heat balances on each tray as well.

We will limit this discussion to the technique of starting at both ends and working toward the feed tray. The feed tray is reached when the feed is added to a tray and the compositions of the vapor and liquid entering and leaving the feed tray match the compositions calculated from both ends of the column. In addition, the heat balance around the feed tray must close.

To converge mathematically to a feed plate match, all components' concentrations must be determined in the feed and bottoms even though those concentrations may be ridiculously small. Now we see why a rigorous plate-to-plate calculation gets the name tedious. Many trials are needed to correct the guessed overhead and bottoms compositions.

A simplification that makes a hand calculation solution possible is to assume the feed tray liquid key component ratio is the same as the key component ratio in the feed. This means we calculate down the column from the top until the key ratio is the same as in the feed, then calculate up from the bottom until the key ratio again is the same

as in the feed. Thus, the number of theoretical trays in the top and bottom section of the column can be determined.

This assumption of feed plate match criteria comes from binary distillation where, for a bubble point feed, the optimal feed tray is that tray having the same liquid composition as the feed.

Figure 1 is a sketch of a typical simple fractionator, and the following pages outline the tray-to-tray calculation procedure.

Distillation Column Nomenclature


$$L_0 = \text{External Reflux Rate, Mols/h}$$

Constant Molal Overflow Procedure

To calculate trays in top section, calculate the dew point of vapor leaving each tray. This gives composition of liquid leaving tray. To get vapor entering tray, use material balance.

$$V_{m+1} = L_m + D + V_0 \quad (\text{Refer to Figure 1})$$

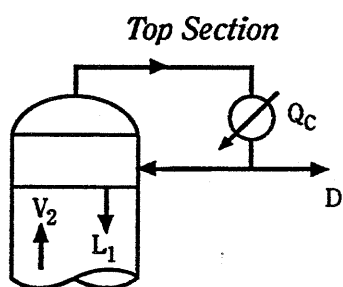
To calculate trays in bottom section, calculate the bubble point of liquid leaving each tray. This gives composition of vapor leaving tray. To get liquid entering tray, use material balance.

$$L_{n-1} = V_n + B \quad (\text{Refer to Figure 1})$$

Procedure with Heat Balance

Where constant molal overflow is not assumed, heat balance must also be done.

Liquid Composition Known:



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- a. Estimate a liquid rate
- b. Find vapor rate by material balance

$$V_2 = L_1 + D + V_o(\text{if any})$$

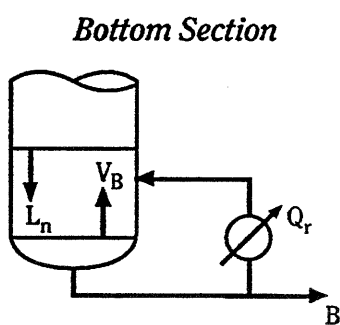
- c. Calculate dew point on vapor and find vapor enthalpy.

- d. Check heat balance:

$$L_1 H_{L_1} + D H_D + Q_c = V_2 H_{V_2}$$

- e. Repeat above steps until a satisfactory heat balance is obtained. Note vapor dew point calculation gives liquid composition to next tray down.

Vapor Composition Known:



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- a. Estimate a vapor rate.
- b. Find liquid rate by material balance.

$$L_n = V_B + B$$

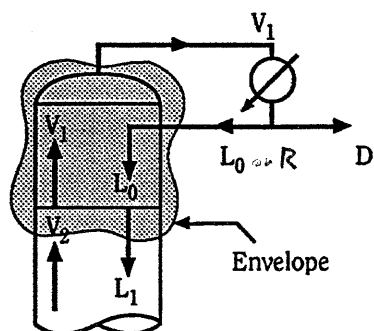
- c. Calculate bubble point on liquid and find liquid enthalpy.

- d. Check heat balance:

$$V_B H_{V_B} + B H_B = L_n H_{L_n} + Q_R$$

- e. Repeat above steps until a satisfactory heat balance is obtained. Note liquid bubble point calculation gives vapor composition to next tray up.

External/Internal Reflux Relationships



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Internal reflux material and heat balance:

$$L_0 + V_2 = V_1 + L_1 \quad \text{mass}$$

$$L_0 H_{L_0} + V_2 H_{V_2} = V_1 H_{V_1} + L_1 H_{L_1} \quad \text{Heat}$$

Additional Material Balances:

TRAY 1 BALANCES

$$V_1 = L_0 + D$$

$$V_2 = L_1 + D$$

If $H_{V_2} = H_{V_1}$, it may be shown that:

$$L_1 = \frac{L_0 (H_{V_1} - H_{L_0})}{(H_{V_1} - H_{L_1})}$$

latent heat for pure component

Note: the denominator can be considered a latent heat.

Example Problem – Tray-to-Tray Calculation

Example problem: a Deethanizer.

The overhead condenser will be refrigerated and the overhead product will be a vapor with no liquid product. The overhead receiver temperature will be 0°F and its pressure will be 300 psig. The following assumptions will be made:

Constant molal internal reflux.

All methane and lighter will be in the overhead; all butane and heavier will be in the bottom.

Key components are C₂ and C₃.

No liquid phase non-ideality and H₂ does not affect vapor phase fugacity.

Constant pressure on all trays.

We want only 1.0 mol/h C₂ in bottoms and only enough C₃ in overhead to make reflux. Design column for external reflux of 275.3 mol/h.

The sketch of the simple fractionator as shown in Figure 1 applies to this problem.

	Vapor Feed mol/h	Liquid Feed mol/h	Total Feed mol/h	Net Overhead (As Gas) mol/h	Bottoms mol/h
H ₂	13.1	1.1	14.2	14.2	
C ₁	7.4	5.0	12.4	12.4	
LK C ₂	7.0	24.1	31.1	30.1	1.0
HK C ₃	13.1	104.4	117.5	4.1	113.4
iC ₄	2.0	42.9	44.9		44.9
nC ₄	1.9	67.6	69.5		69.5
iC ₅	0.4	50.5	50.9		50.9
nC ₅	0.2	32.2	32.4		32.4
iC ₆	0.1	9.7	9.8		9.8
	45.2	337.5	382.7	60.8	321.9

Assume no heavier component present.

At 300 psig and 0°F, calculate the amount of C₃ required in the overhead vapor product in order to get liquid reflux.

	Y Vapor mol/h	K @ 315 psia 0 °F	Y/K	Vapor mol/h	External Reflux Y/K
H ₂	14.2	74.5	0.2	14.2	0.2
C ₁	12.4	4.0	3.1	12.4	3.1
C ₂	30.1	0.79	38.1	30.1	38.1
C ₃	Z	0.21	Y/0.21	4.1	19.4
	56.7 + Z		41.4 + Z/0.21	60.8	60.8

unknown

$$56.7 + Z = 41.4 + Z/0.21$$

$$Z = 4.1$$

Calculation of top tray temperature and composition of internal reflux leaving first tray.

Try 60°F.

	Net Overhead V ₀	Reflux L ₀	V ₁ = V ₀ + L ₀	K @ 315 psia 60 °F	V ₁ /K
H ₂	14.2	0.9	15.1	63.9	0.2
C ₁	12.4	14.0	26.4	5.50	4.8
C ₂	30.1	172.6	202.7	1.317	153.9
C ₃	4.1	87.8	91.9	0.486	189.1
	60.8	275.3	336.1		348.0

Close enough

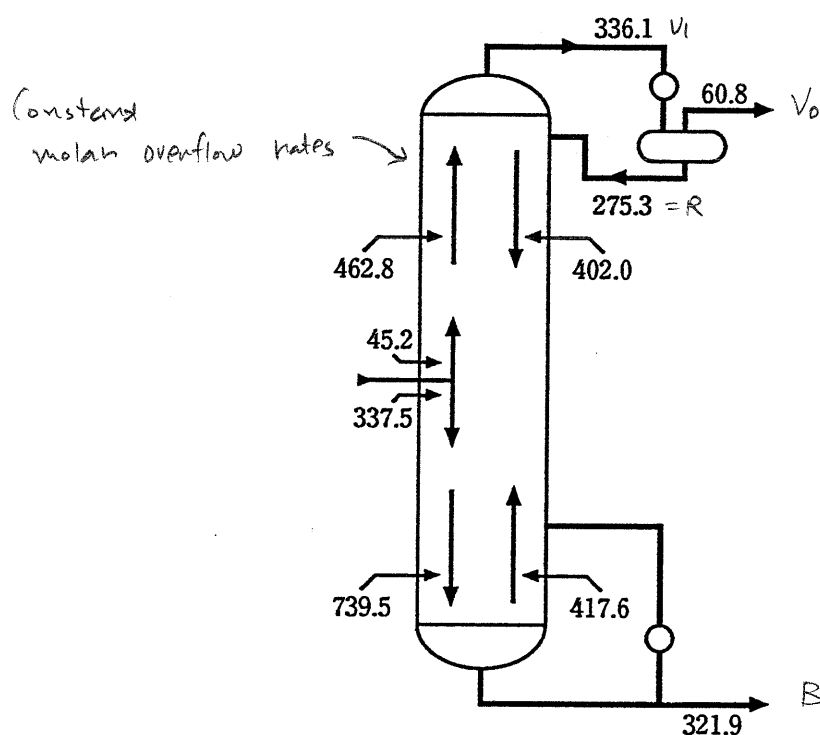
Internal Reflux

Assume $V_2 = V_1$; with V_1 and L_0 compositions known along with their temperatures, the molal enthalpies can be determined. Thus, internal reflux can be computed.

$$L_1 = 275.3 \times \frac{8500 - 3300}{8500 - 4950} = 402.0$$

R_{D1} V_1 at 60°F R at 0°F
 Molar Enthalpies L_1 at 60°F

Assuming constant internal reflux, draw a sketch for the column flow rates. *Can use later heat of A product with same m.w. as V_1*



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Example of tray-to-tray calculation:

Deethanizer, constant internal reflux.

Top section, $L = 402.0$, $V = 462.8$

	Net Overhead Gas V_0	External Reflux L_0	$V_0 + L_0 = V_1$	K 315 psia 60°F	V_1/K	L_1	$V_0 + L_1 = V_2$	K 315 psia 90°F	V_2/K
H ₂	14.2	0.9	15.1	63.9	0.2	0.2	14.4	59.2	0.2
C ₁	12.4	14.1	26.5	5.5	4.8	5.5	17.9	6.75	2.6
C ₂	30.1	172.5	202.6	1.32	153.9	177.8	207.9	1.52	137.0
C ₃	4.1	87.8	91.9	0.486	189.1	218.5	222.6	0.65	342.5
	60.8	275.3	336.1		348.0	402.0	462.8		482.3

$$L_1 = (402/348.0)(V_1/K)$$

C₂/C₃ 7.34

1.96

0.815

Close enough

	L_2	$V_0 + L_2 = V_3$	K 315 psia 105°F	V_3/K	L_3	$V_0 + L_3 = V_4$	K 315 psia 115°F	V_4/K	L_4
H ₂	0.2	14.4	57.0	0.3	0.3	14.5	55.5	0.3	0.3
C ₁	2.2	14.6	7.25	2.0	1.7	14.1	7.61	1.9	1.6
C ₂	114.1	144.2	1.77	81.5	69.3	99.4	1.85	53.7	46.0
C ₃	285.5	289.6	0.745	388.7	330.7	334.8	0.81	413.3	354.1
	402.0	462.8		472.5	402.0	462.8		469.2	402.0

C₂/C₃ 0.400

0.210

0.130

Comparisons to this point.

	Feed	Feed Vapor	Feed Liquid	L_0	L_1	L_2	L_3	L_4
C ₂ /C ₃	0.264	0.534	0.231	1.96	0.815	0.400	0.210	0.130
Temp °F				0	60	90	105	115

The C_2/C_3 ratio in L_3 is 0.210, which is less than the 0.231 of the feed liquid. This reflects the ethane enrichment sought in this section of the column and indicates that 3 trays are sufficient for the enrichment required.

$$\text{Liquid to Feed Tray} = L_2 + L_F$$

$$C_2 = 114.1 + 24.1 = 138.3 \text{ mol/h}$$

$$C_3 = 285.5 + 104.4 = 389.9 \text{ mol/h}$$

$$C_2/C_3 = 138.2/389.9 = 0.354$$

Since L_2 is richer in C_2 than the feed liquid, we must conclude that 2 trays are not enough to do the required separation.

C_2/C_3 in feed vapor	0.534
in feed liquid	0.221
in total feed.	0.264

Therefore, about 3 trays are

Deethanizer – Bottom Section

$$L_n = L_F + \text{Internal Reflux} = 337.5 + 402.0 \text{ mol/h} = 739.5 \text{ mol/h}$$

$$V_B = L_n - L_B = 739.5 - 321.9 = 417.6 \text{ mol/h}$$

	Bottoms B	K 315 psia 230°F	KL _B	V _B	L _n = V _B + L _B	K 315 psia 200°F	KL _n	V _n
C ₂	1.0	3.56	3.6	4.3	5.3	3.04	15.9	9.1
C ₃	113.4	1.64	186.0	224.3	337.7	1.35	455.9	262.4
iC ₄	44.9	1.03	46.2	55.7	100.6	0.870	87.5	50.3
nC ₄	69.5	0.895	62.2	75.0	144.5	0.732	105.8	60.8
iC ₅	50.9	0.570	29.0	35.0	85.9	0.444	38.1	21.9
nC ₅	32.4	0.500	16.2	19.5	51.9	0.380	19.7	11.3
iC ₆	9.8	0.332	3.2	3.8	13.6	0.236	3.2	1.8
	321.9		346.4	417.6	739.5		726.1	417.6

$$C_2/C_3 \quad 0.0088$$

$$0.0157$$

	L _{n-1} = V _n + L _B	K 315 psia 190°F	KL _{n-1}	V _{n-1}	L _{n-2} = V _{n-1} + L _B	K(*) 315 psia 190°F	KL _{n-2}	V _{n-2}
C ₂	10.1	2.88	29.1	16.7	17.7	2.88	51.0	28.2
C ₃	375.8	1.29	484.8	278.2	391.6	1.29	505.2	279.1
iC ₄	95.2	0.819	78.0	44.8	89.7	0.819	73.5	40.6
nC ₄	130.3	0.682	88.9	51.0	120.5	0.682	82.2	45.4
iC ₅	72.8	0.405	29.5	16.9	67.8	0.405	27.5	15.2
nC ₅	43.7	0.344	15.0	8.6	41.0	0.344	14.1	7.8
iC ₆	11.6	0.210	2.4	1.4	11.2	0.210	2.4	1.3
	739.5		727.7	417.6	739.5		755.9	417.6

$$C_2/C_3 \quad 0.0269$$

$$0.0452$$

(*) Note that, when T changes but little per tray, using the same K as for previous tray gives a satisfactory result.

	$L_{n-3} = V_{n-2} + L_B$	K 315 psia 180°F	KL_{n-3}	V_{n-3}	$L_{n-4} = V_{n-3} + L_B$	K 315 psia 170°F	KL_{n-4}	V_{n-4}
C ₂	29.2	2.72	79.4	44.4	45.4	2.58	117.1	67.6
C ₃	392.5	1.23	482.8	270.3	383.7	1.17	448.9	259.3
iC ₄	85.5	0.762	65.2	36.5	81.4	0.71	57.8	33.4
nC ₄	114.9	0.631	72.5	40.6	110.1	0.58	63.8	36.8
iC ₅	86.1	0.367	31.6	17.7	68.6	0.332	22.8	13.2
nC ₅	40.2	0.309	12.4	6.9	39.3	0.277	10.9	6.3
iC ₆	11.1	0.186	2.1	1.2	11.0	0.164	1.8	1.0
	739.5		746.0	417.6	739.5		723.1	417.6

C₂/C₃ 0.074

0.118

	$L_{n-5} = V_{n-4} + L_B$	K 315 psia 170°F	KL_{n-5}	V_{n-5}	$L_{n-6} = V_{n-5} + L_B$
C ₂	68.6	2.58	177.0	96.7	97.7
C ₃	372.7	1.17	436.1	238.4	351.8
iC ₄	78.3	0.71	55.6	30.4	75.3
nC ₄	106.3	0.58	61.6	33.7	103.2
iC ₅	64.1	0.332	21.3	11.6	62.5
nC ₅	38.7	0.277	10.7	5.8	38.2
iC ₆	10.8	0.164	1.8	1.0	10.8
	739.5		764.1	417.6	739.5

C₂/C₃ 0.184

0.277

(end of calculation)
(C₂/C₃ in feed liquid = 0.231)

Summary:

External R/F = 0.719

Internal R/F = 1.050

Number of theoretical trays in column

top 3

bottom 7

Note: Reboiler and condenser are each a theoretical stage.

Absorbers and Strippers – Simplified Kremser Approach

The Kresmer absorption or stripping factor approach—assume V/L and K for each component is constant.

Absorbers:

$$\text{Define } A = \frac{L}{VK} = \text{absorption factor}$$

Fraction of component in gas absorbed (assuming no component in lean oil):

$$f(A) = (A^{n+1} - A) / (A^{n+1} - 1)$$

Where:

n = theoretical trays

Note

*Liquid phase nonideality
corrections are usually*

Strippers:

$$\text{Define } S = \frac{VK}{L} = \text{stripping factor}$$

Fraction of component in liquid stripped (assuming no component in lean gas):

$$f(S) = (S^{n+1} - S) / (S^{n+1} - 1)$$

A graphical solution of these equations is shown on page 27.

Notes:

For absorbers, want low K – hence operation favors high pressure + low temperature.

For strippers, want high K – hence operation favors low pressure + high temperature.

Where A or S is ≤ 0.8 and $n = \geq 5$, fraction of component absorbed (stripped) = $A(S)$.

Absorber or stripper with components in lean oil or stripping gas:

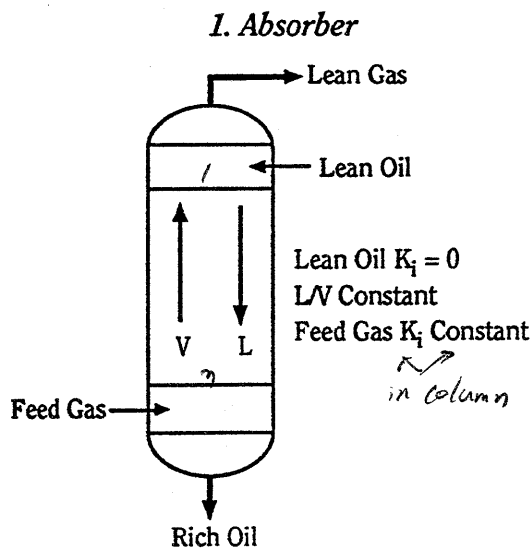
$$D = F \left\{ \frac{(S^{n+1} - S)}{(S^{n+1} - 1)} \right\} + G \left\{ \frac{(A - 1)}{(A^{n+1} - 1)} \right\}$$

$$D = F \{f(S)\} + G \{1 - f(A)\}$$

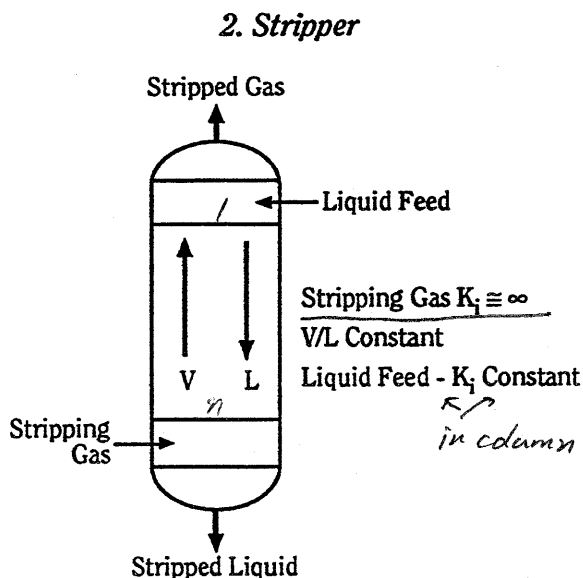
D = Component in Vapor from Top Tray

F = Component in Liquid to Top Tray

G = Component in Vapor to Bottom Tray



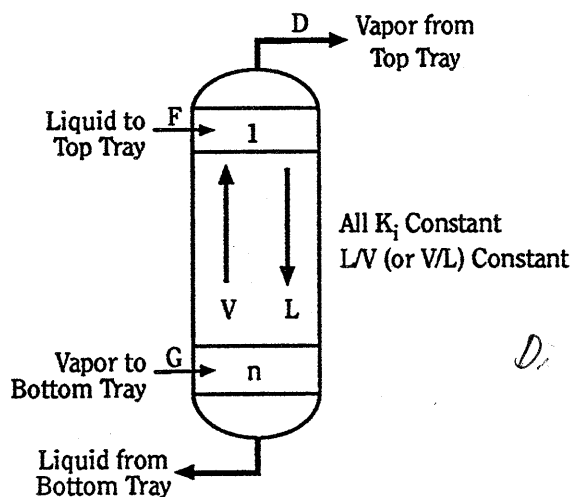
EDS-R00-2507



EDS-R00-2508

Define $A = L/VK$
↑ absorption factor.

3. Absorber or Stripper - General Case



EDS-R00-2509

$$D_i = F_n [f(G_i)]$$

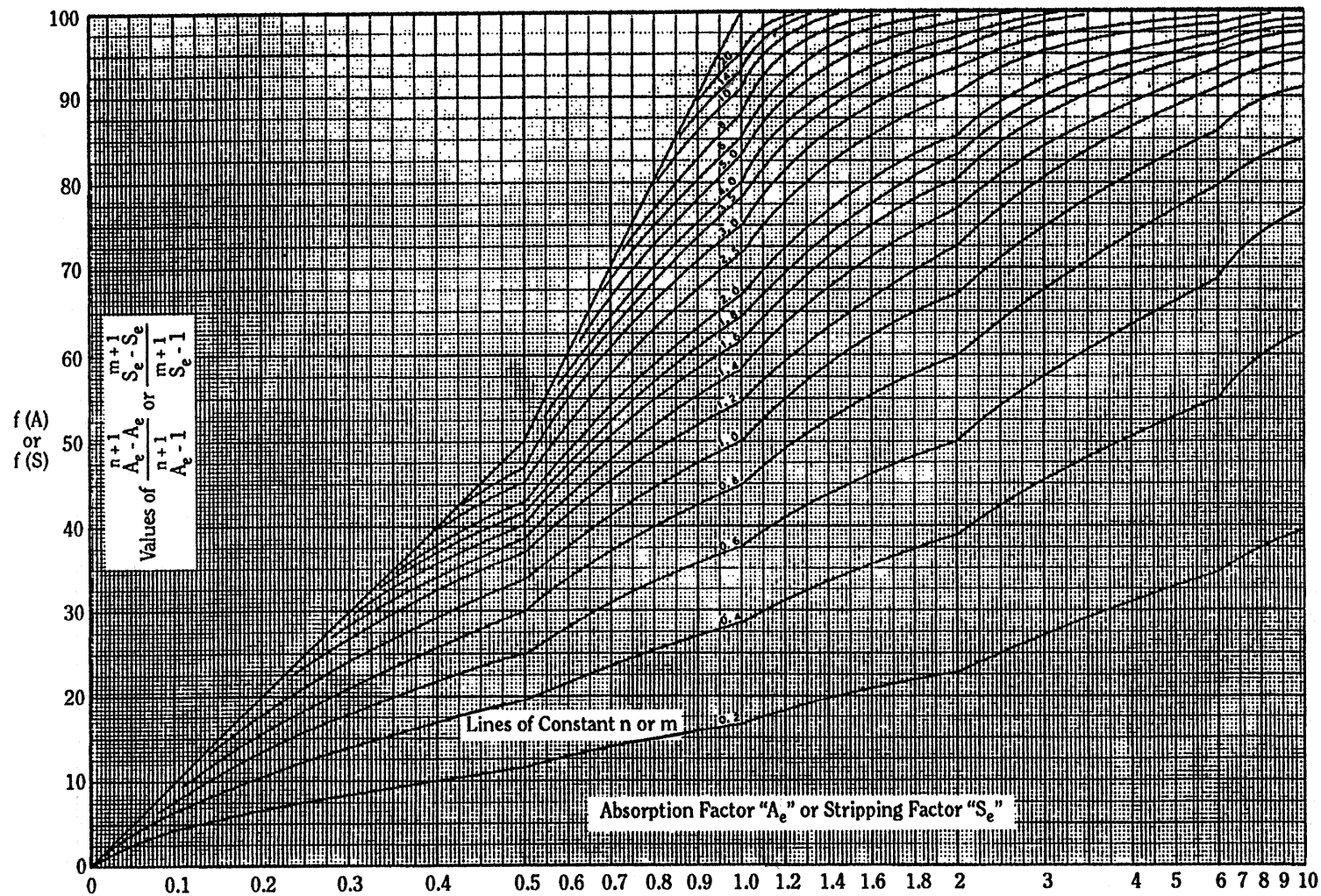
Notes:

Liquid phase non-ideality corrections are significant for absorbers.

For average L/V , external top and bottom streams are usually used; however, internal streams average is more accurate (especially for reboiled strippers)

GP54

Kremser Chart



Example – Simple Absorber

When the percent recovery of one component is specified, along with the number of theoretical trays used, the recoveries of all the other components will be fixed. For this calculation, we use the Kremser chart. The following example is to illustrate the use of this chart.

Gas is available at 250 psia and 100°F. Design this absorber to recover 90 percent of the propane and show the compositions of the streams around the absorber. Tray efficiencies in absorbers are very low. For this example, use 6 theoretical trays. Find the required absorption oil rate. The temperature of the oil will rise due to the heat of absorption, so we will plan to use intercoolers and an average absorption temperature of 125°F.

use for average pressure

use intercoolers *FOR 90% PROPANE RECOVERY*
COMPLETE ABSORBER *MATERIAL BALANCE*

1 Comp.	2 Gas to Abs (R + V ₀)	3 K	4 $\frac{L}{KV}$	5 Percent Absorbed	6 Absorbed Material R	7 Off Gas V ₀
H ₂	172	68.2	0.017	1.7	3	169
N ₂	151	12.5	0.093	9.3	14	137
C ₁	339	9.26	0.126	12.6	43	296
C ₂	361	2.437	0.479	47.9	173	188
C ₃	95	1.029	1.135	90.0	86	9
iC ₄	52	0.558	2.093	100.0	52	
nC ₄	61	0.434	2.691	100.0	61	
iC ₅	42	0.222	5.261	100.0	42	
nC ₅	18	0.178	6.562	100.0	18	
nC ₆	16	0.0728	16.0	100.0	16	
	1307				508	799

$$[\text{Average } L/V = 1.168 = (1.135)(1.029)]$$

Column 1 Component

Column 2 Pound mols per hour of each component

Column 3 Look up $K\pi$ for all components and get K by dividing by 250. We prefer to tabulate $K\pi$ rather than make K curves because $K\pi$ does not change much with pressure.

24.130

Column 4 For 90 percent C_3 recovery, read $L/KV = 1.135$ from Kremser chart for 6 theoretical trays. From $K = 1.029$ for C_3 , get $L/V = (1.135)(1.029) = 1.168$. This is total liquid divided by total vapor. Divide L/V by each K to get L/KV for each component.

Column 5 Look up percent absorbed for each component at 6 theoretical trays from Kremser chart. Notice that when L/KV becomes small, 6 trays approaches infinite trays and the fraction of component absorbed approaches L/KV . Also notice that when L/KV becomes around 2.0 and over, the recovery is 100 percent.

Column 6 Calculate mols/h of absorbed material by multiplying Column 2 by Column 5.

Column 7 Subtract Column 6 from Column 2 for lean gas from absorber. The lean oil rate to the absorber is calculated by this equation:

$$\text{Define average } L/V = (L_o + R/2)/(V_o + R/2)$$

where:

L_o = lean oil, mol/h

V_o = lean gas, mol/h

R = total amount absorbed

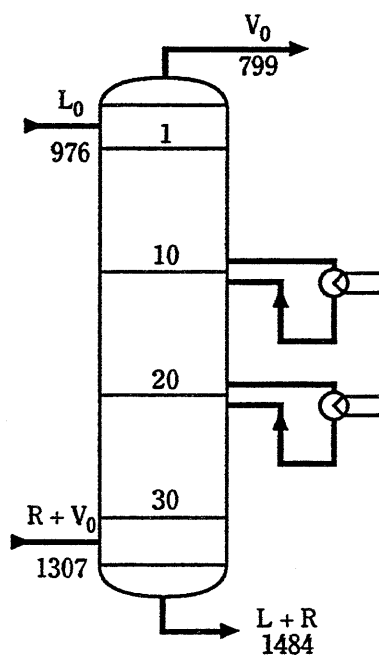
The absorption oil rate, L_o , is calculated:

$$L_o = \frac{(L/V)(2V_o + R) - R}{2}$$

$$L_o = \frac{(1.168)[(2)(799) + 508] - 508}{2}$$

$$L_o = 976 \text{ mols/h}$$

Estimating a tray efficiency of 20 percent, use 30 trays.



EDS-R00-2511

PROBLEMS

Distillation Problems

Page 14-19

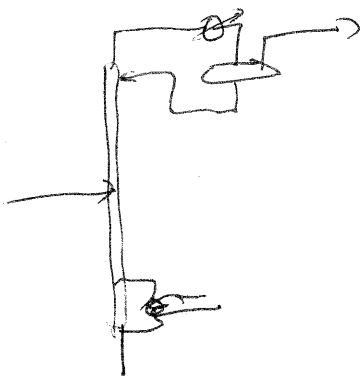
For the Deethanizer example problem, use K at 315 psia and 150°F for relative volatilities and calculate:

- Minimum reflux – high and low limits for perfect separation and bubble point feed. (page 4)
- Minimum reflux by Underwood method.
(Page 4)
- Component distribution. (Page 7 & 8)
Internal → (Page 4)
- For the reflux used in the example problem, estimate theoretical tray requirement by the Gilliland method – use results of b and c.
page 7 & 8 → Since no distribution

Do tray-to-tray calculations for bottom 5 trays of a fractionator. Pressure is 150 psia for all trays. Use ideal fugacity K's. Use V/L of 0.9 for all trays. Net bottoms are listed:

iC ₄	0.1
nC ₄	9.0
iC ₅	18.0
nC ₅	24.0
nC ₆	300.0
nC ₇	599.9
	951.0

Calculate Reboiler
as Done on page 18



$$\sum \frac{d_i P_{iF}}{\alpha_i - \phi} = 1 - q$$

Page 14
q = liquid mole fraction

Absorption and Stripping Problems

A stripper is designed to remove 98 percent of the C_2 from the following liquid. Use 220°F average temperature and 250 psia. Use 14 theoretical trays. Use ideal fugacity K's. Determine the split of the other feed components.

*Kermers Chart
on equation Page 20-12*

	Stripper Feed mol/h	K @ 220°F 250 psia	$\frac{KY}{L}$	Fraction Stripped	Stripped Vapor	Bottoms
C_1	21					
C_2	132					
C_3	157					
iC_4	211					
nC_4	413					
iC_5	512					
nC_5	814					
nC_6	1210					

Design absorber to recover propane at 150 psia and average temperature of 120°F. Use 7 theoretical trays. For 1500 mol/h of absorber oil equimolar in toluene and metaxylene, what is column material balance? Consider L/V to be average of top and bottom values. Trial-and-error solution is required. Use ideal fugacity K's.

*not
on page 20-15*

	Gas to Absorber mol/h
H_2	150
N_2	20
C_1	35
C_2	15
C_2	65
C_3	138
C_3	250
iC_4	50
nC_4	110
iC_5	16
nC_5	28
2MP	8
	885

*Guess y_i
Calculate y_i
Reguess y_i
Plot Grand Calculated
 y_i vs. Calculated y_i
on Log-Log paper
to minimize trials*

MULTICOMPONENT DISTILLATION

- Introduction**
- Minimum Reflux**
- Minimum Trays**
- Design Parameters**
- Component Distribution**
- Tray-to-Tray Calculation Description**
- External versus Internal Reflux**
- Tray-to-Tray Calculation Example Problem**
- Absorbers and Strippers Using Kremser Method**

INTRODUCTION

Fundamental Relations

- Heat Balance
- Material Balance
- Equilibrium

Shortcut Methods

- Fenske Equation
- Underwood Equation
- Gilliland Graph

Exact Methods

- Simultaneous Equations
- Top Down/Bottom Up
- Trays are Always Specified

Approximate Design Methods

- Kremser for Absorbers and Strippers
- Naphtha Fractionation

PLATFORMATE SPLITTER

Overhead to Sulfolane and Bottoms to Isomar-Parex

	Component	nbp, °F	Feed mol/h	Overhead mol/h	Bottoms mol/h
Non Distributed	n-C ₄	31	4	4	—
	n-C ₅	97	100	100	—
	n-C ₆	156	140	140	—
	MCP	161	2	2	—
	Bz	176	104	104	—
	n-C ₇	209	200	200	—
	MCH	214	3	3	—
Light Key	Tol	231	559	553	6
Distributed	n-C ₈	258	150	149	1
Distributed	ECH	269	10	9	1
Heavy Key	EB	277	129	0.1	128.9
Non Distributed	p-Xyl	281	132	—	132
	m-Xyl	282	307	—	307
	o-Xyl	292	300	—	300
	n-C ₉	303	11	—	11
			2151	1264.1	886.9

MINIMUM REFLUX

Approximate Binary Analogy

Maximum possible reflux ratio = binary value.

Minimum possible reflux ratio = *(binary value)* $(x_{LK} + x_{HK})_{Feed}$

Where:

x_{LK} = Mol fraction of light key in feed

x_{HK} = Mol fraction of heavy key in field

Correct reflux ratio is between these limits.

Example for bubble point feed:

Imperfect separation:

High limit:

$$(L/D)_{min} = \frac{1}{\alpha - 1} \left[\frac{x_D}{x_F} - \frac{\alpha(1 - x_D)}{(1 - x_F)} \right]$$

Low limit:

$$\alpha(x_{LK} + x_{HK})_{Distillate}$$

Perfect Separation:

High Limit:

$$(L/F)_{min} = \frac{1}{\alpha - 1}$$

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Overhead to Sulfolane and Bottoms to Isomar-Parex

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Imperfect separation:

High limit:

293 M 493 J93 MB 494

$$(L/D)_{min} = \frac{1}{\alpha - 1} \left[\frac{x_D}{x_F} - \frac{\alpha(1 - x_D)}{(1 - x_F)} \right]$$

Low limit:

$$\frac{1}{\alpha - 1} \left[\frac{x_D}{x_F} - \frac{\alpha(1 - x_D)}{(1 - x_F)} \right] (x_{LK} + x_{HK})_{Distillate}$$

~~$\alpha(x_{LK} + x_{HK})_{Distillate}$~~

page break

Perfect Separation:

High Limit:

$$(L/F)_{min} = \frac{1}{\alpha - 1}$$

Low Limit:

$$(L/F)_{min} = \frac{1}{\alpha - 1} (x_{LK} + x_{HK}) \left[\frac{x_D}{x_F} - \frac{\alpha(1-x_D)}{(1-x_F)} \right]$$

Underwood's Method

Assumptions:

Constant molal overflow

Constant α :

$$\sum_1^i \frac{(\alpha_i x_i)_F}{\alpha_i - \phi} = 1 - q$$

$$\sum_1^i \frac{(\alpha_i x_i)_D}{\alpha_i - \phi} = (L/D)_{min} + 1$$

- x = Mol fraction in total stream
- ϕ = Underwood parameter
- q = Feed thermal condition
- i = Any component

All possible roots of the first equation lie between the α 's of the feed components.

Substitution of these roots into the second equation yields simultaneous equations whose solutions give $(L/D)_{min}$ and $(x_i)_D$ (non-key components).

Component	α	mol/h		
		Feed	Overhead	Bottoms
A	6	40	40	—
B-LK	2	20	20	—
C-HK	1	20	—	20
D	0.5	20	—	20
		100	60	40

Binary approximation:

Boiling point feed – perfect separation

High Limit:

$$L/F = \frac{1}{\alpha - 1} = 1$$

$$L = 100 \times 1 = 100 \text{ mol/h}$$

Low Limit:

$$L/F = \frac{1}{\alpha - 1} (x_{LK} + x_{HK}) = 1(0.2 + 0.2) = 0.4$$

$$L = 100 \times 0.4 = 40 \text{ mol/h}$$

UNDERWOOD

First Equation

$$\frac{(\alpha x_F)_A}{\alpha_A - \phi} + \frac{(\alpha x_F)_B}{\alpha_B - \phi} + \frac{(\alpha x_F)_C}{\alpha_C - \phi} + \frac{(\alpha x_F)_D}{\alpha_D - \phi} = 1 - q$$

Since feed is at boiling point, $q = 1$.

Then:

$$\frac{(6)(0.4)}{6 - \phi} + \frac{(2)(0.2)}{2 - \phi} + \frac{(1)(0.2)}{1 - \phi} + \frac{(0.5)(0.2)}{0.5 - \phi} = 1 - 1 = 0$$

$$\alpha_{HK} \leq \phi \leq \alpha_{LK}$$
$$1 \leq \phi \leq 2$$

By trial-and-error, $\theta = 1.2267$.

Second Equation

$$\frac{(\alpha x_D)_A}{\alpha - \theta} + \frac{(\alpha x_D)_B}{\alpha - \theta} = \frac{6\left(\frac{40}{60}\right)}{6 - 1.2267} + \frac{2\left(\frac{20}{60}\right)}{2 - 1.2267} = \frac{L}{D} + 1 = 1.700$$

$$\frac{L}{D} = 0.700$$

$$L = (0.7)(60) = 42.0 \text{ mol/h}$$

$$\text{High Limit} = 100.0 \text{ mol/h}$$

$$\text{Low Limit} = 40.0 \text{ mol/h}$$

COMPONENT DISTRIBUTION

Why Valuable?

- To estimate column material balance
- To start a tray-to-tray calculation
- To simplify a minimum reflux calculation

Approximate method:

Components that are:

- Lighter than light key $\rightarrow$ all to overhead
- Heavier than heavy key $\rightarrow$ all to bottoms

Only valid if non-key component α 's are considerably different than α of keys.

Method based on Fenske equation:

$$n = \frac{\ln(r_D/r_B)_K}{\ln \alpha_K}$$

1 Component	2 α	3 $\ln \alpha$	4 $\ln(r_D/r_B)$	5 r_D/r_B	6 X_F	7 X_D	8 X_B
A	1.65	0.501	13.126	501821	196.1	195.8	0.3
B-LK	1.49	0.399	10.452	34604	122.6	119.6	3.0
C	1.445	0.368	9.641	15383	95.8	90.7	5.1
D	1.188	0.172	4.506	91	68.4	6.5	61.9
E	1.14	0.131	3.432	31	86.8	3.0	83.8
F-HK	1.0	0.000	0.000	1	86.9	0.1	86.8

$$r_D/r_B = (119.6/0.1)/(3.0/86.8) = 34604$$

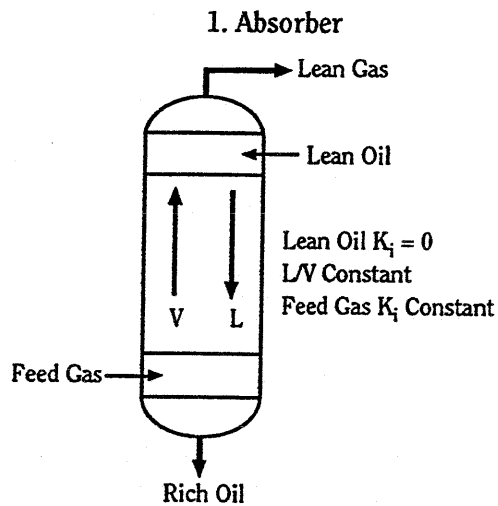
$$n = \ln(r_D/r_B)/\ln \alpha = 10.451/0.399 = 26.20$$

$$\ln(r_D/r_B) = (n)(\ln \alpha)$$

$$x_{DI} = (r_{DI}/r_{BI})x_{FI}x_{HD}/[x_{HB} + (r_{DI}/r_{BI})x_{HD}]$$

$$x_{BI} = x_{FI} - x_{DI}$$

KREMSER



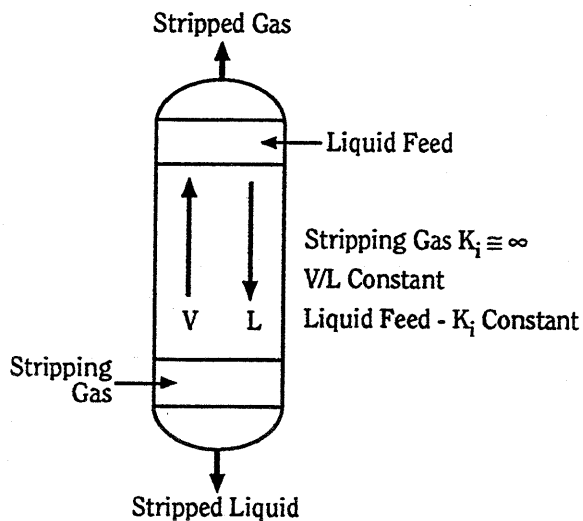
EDS-R00-2507

Define $A = L/VK = \text{Absorption Factor}$

$$\text{Fraction of gas component absorbed} = f(A) = \frac{(A^{n+1} - A)}{(A^{n+1} - 1)}$$

Note: Liquid phase non-ideality corrections are usually significant for absorbers.

2. Stripper

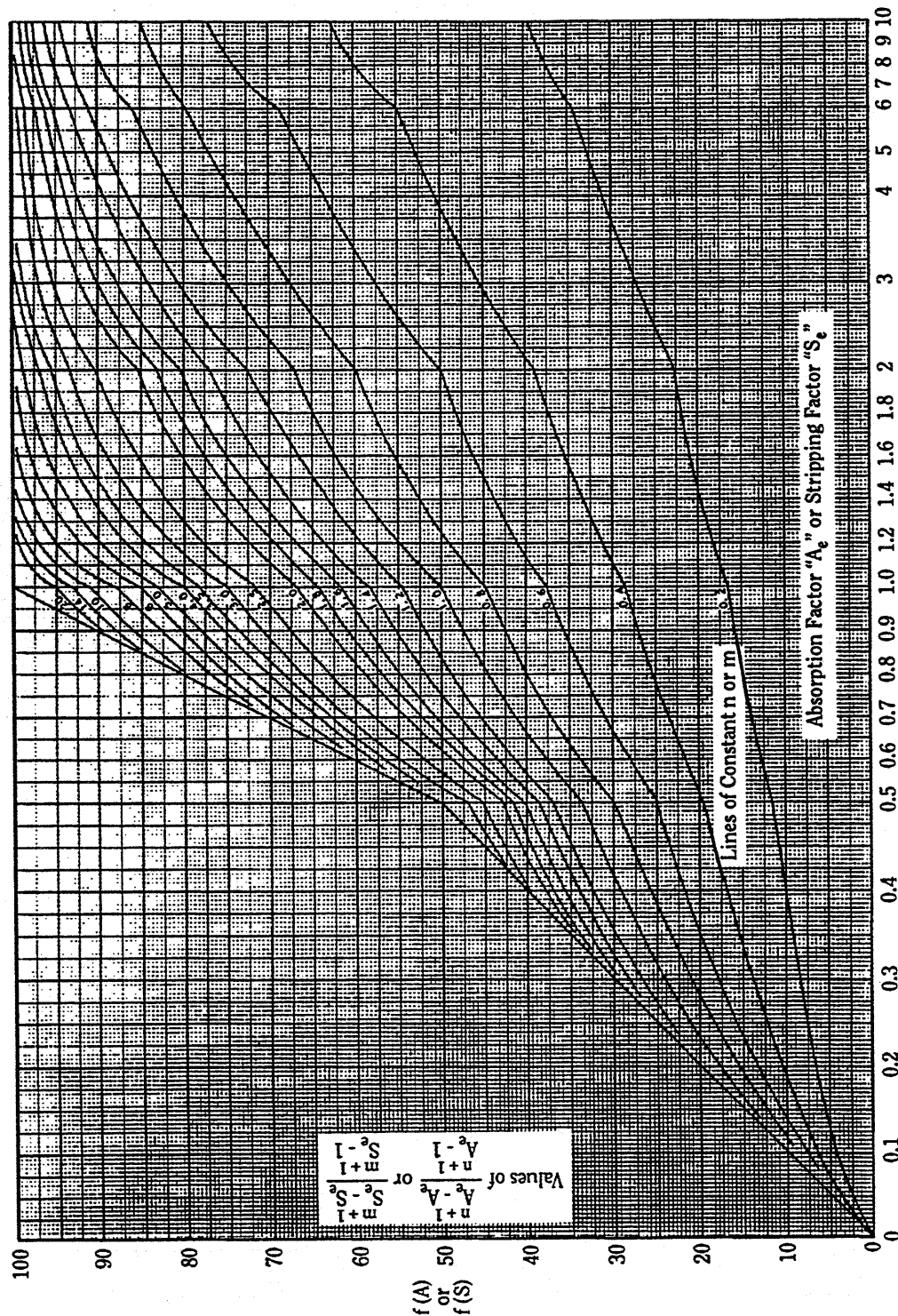


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Define $S = VK/L = \text{Stripping Factor}$

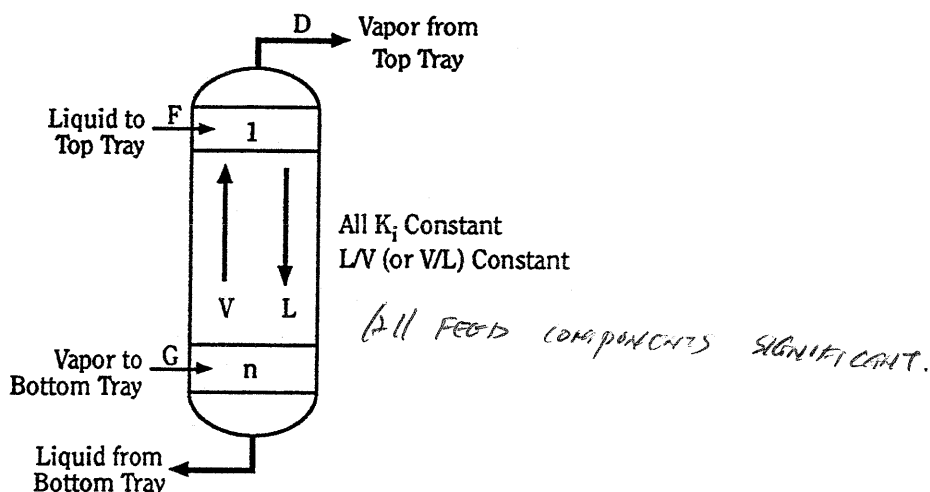
$$\text{Fraction of liquid component stripped} = f(S) = \frac{(S^{n+1} - S)}{(S^{n+1} - 1)}$$

Kremser Chart



EDS-R00-2510

3. Absorber or Stripper - General Case



EDS-R00-2509

$$D_i = F_i[f(S_i)] + G_i[1 - f(A_i)]$$

Note: For average L/V , external top and bottom streams are usually used; internal stream averages give greater accuracy. All feed components are significant.

Tray Efficiency

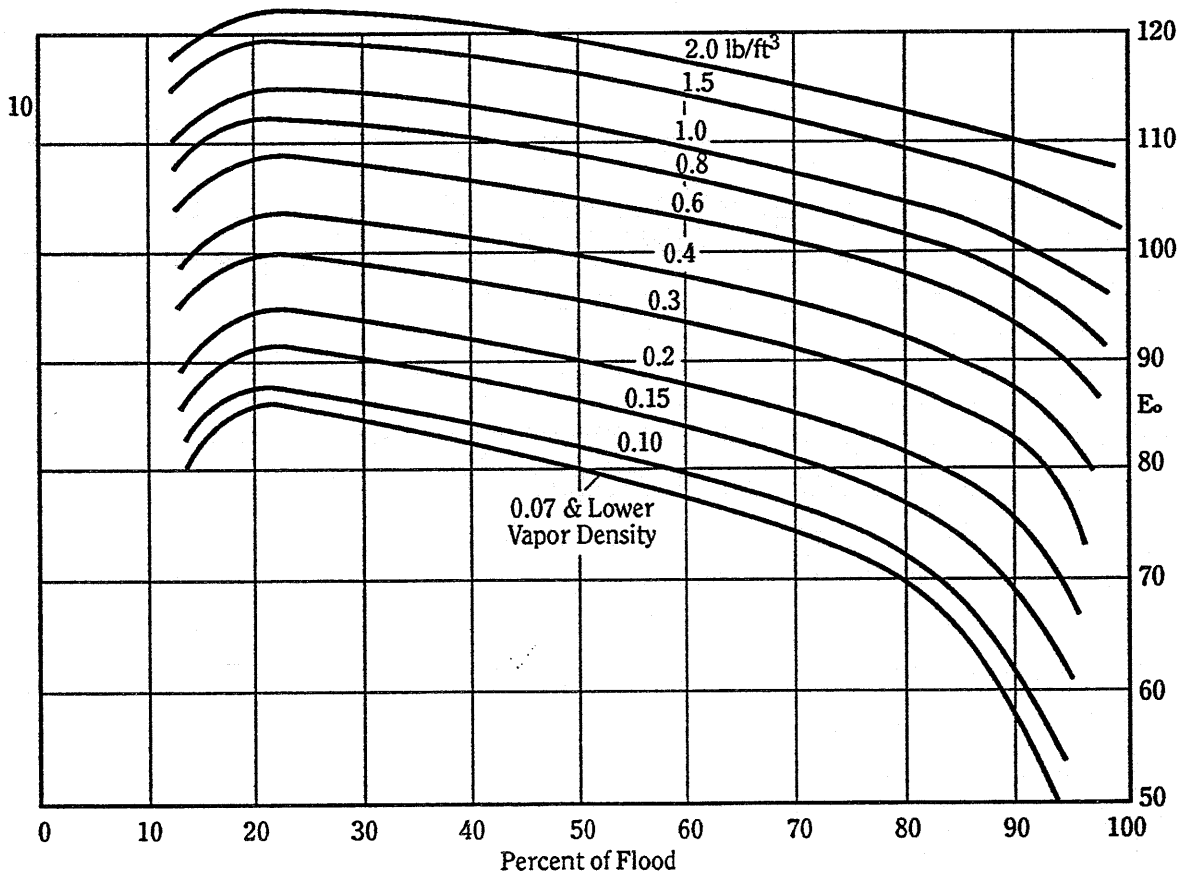
Figure 12 shows a plot of overall tray efficiency of the V-1 Ballast tray obtained in a 4 feet-0 inch diameter fractionating column on the isobutane/n-butane and cyclohexane/n-heptane systems at several pressures. The results of these tests are described fully in Glitsch Bulletin No. 160.

This figure may be used as a guide in selecting tray efficiency for design of commercial columns for similar systems. However, the usual practice has been to establish the number of trays required to obtain the desired separation with bubble cap or sieve trays and to use the same number of Ballast trays. The V-4 Ballast tray has been used to separate the ethylbenzene-styrene system in a single column without having an excessive bottom tray pressure.

Large size V-2 Ballast units have been used to replace bubble cap and riser assemblies in existing columns. The efficiency and capacity of the installations have exceeded that of the original bubble cap tray.

Extra trays to compensate for mislocation of the feed tray and instrumentation swings should be considered when the number of trays is established.

*V-1 Ballast Tray
Overall Tray Efficiency
vs
Vapor Density & Load
Experimental Data at Total
Reflux 2" Weir Height, 30" FPL*

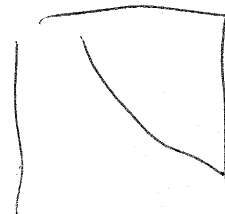


EDS-R00-0245

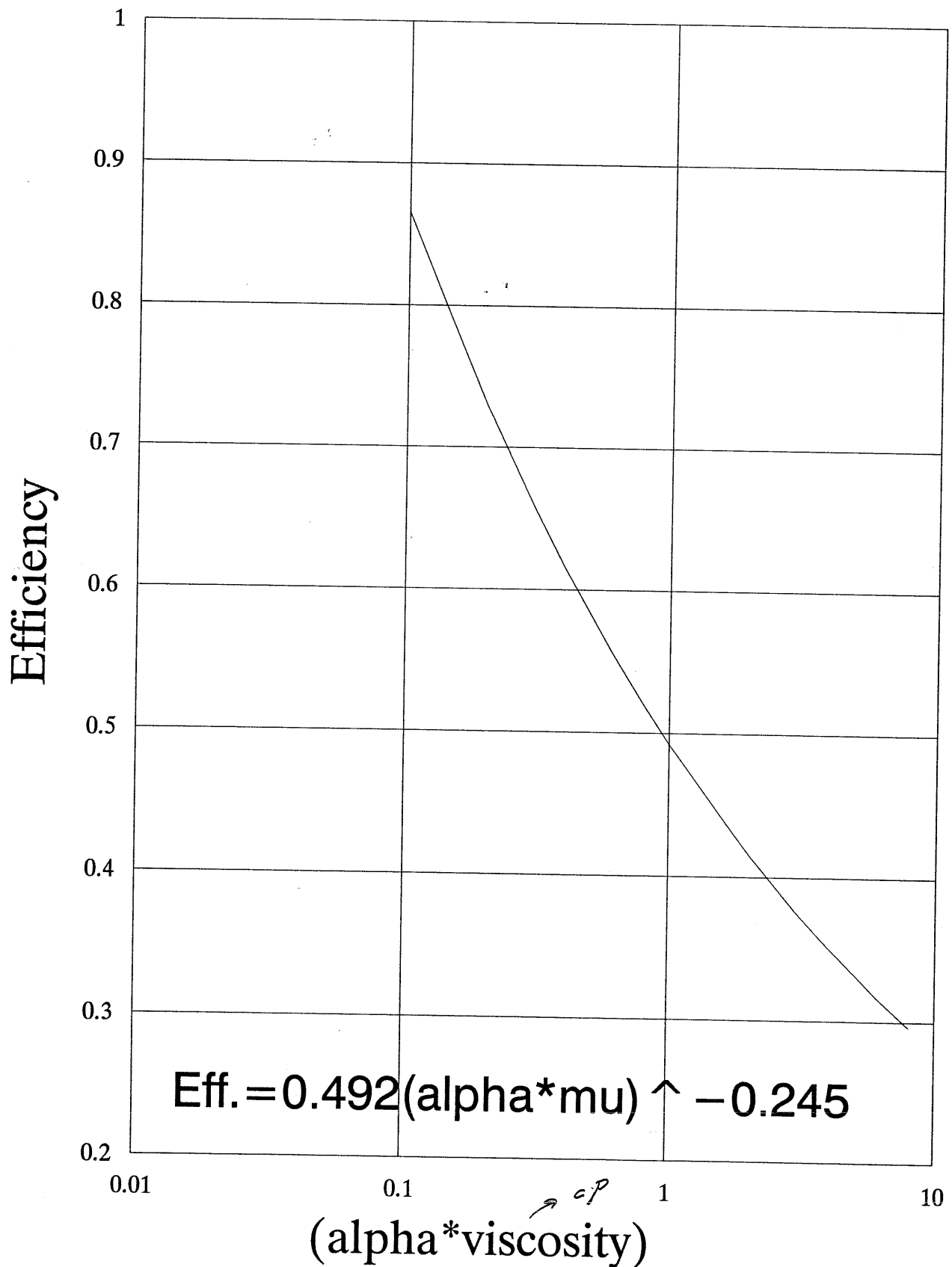
O'Connell Efficiency

$$E_f = 0.492 (K \cdot m)^{-0.295}$$

Eff



O'Connel Efficiency



$$\frac{1}{N_{OG}} = \frac{1}{N_G} + \frac{mG}{L} \frac{1}{N_L}$$

$$\frac{mG}{L} = \lambda$$

Point Efficiency:

$$E_{OG} = 1 - e^{-NOG}$$

Murphree Tray Efficiency: For Lewis case 1

$$E_{mG} = (L/mG) \left(e^{(E_{OG})(mG/L)} - 1 \right)$$

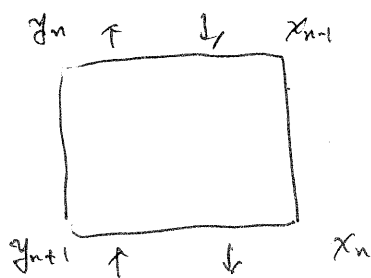
Overall Efficiency:

assume: $\lambda = \text{const.}$

$$E_O = \frac{\ln[1 + E_{mG}(\lambda - 1)]}{\ln \lambda}$$

Murphree Tray Efficiency:

$$y_n^* = f(x_n)$$



$$E_{mD} = \left(\frac{y_n - y_{n-1}}{y_n^* - y_{n-1}} \right)$$

DESIGNING A COLUMN

- **Define Feed**
- **Define Product Specification**
- **Set Column Pressure**
- **Optimize Column Design**
- **Calculate Tray Loads**
- **Size Trays**
- **Set Composition Control**

DEFINE FEED

- Composition
- Flow Rate
- Temperature
- Pressure
- Enthalpy

DEFINE PRODUCT SPECIFICATIONS

- Receiver Temperature
- Product Purities and Recoveries
- Zero Purity Specification is Not Acceptable
- Does Customer Have a Good Definition of the Desired Purities and Recoveries
- Determine Effects of Other Streams Internal to Unit or Complex
Consult with PDC's and project manager for
- Determine the Highest Purities that the Column Ever Has to Produce

Process design Coordinator

SET COLUMN PRESSURE

- Maximize Alpha Value
- Minimize Column Cost
- Keep Flare Material Out of Overhead
- Totally Condense Overhead Products
- Prevent Need for Net Gas Compression
- Minimize Net Overhead Vapor
- Use Condenser as Heat Source
- Use Bottoms as Hot Oil
- Limit Bottom Temperature

Cracking

Polymerization

Approach to Critical

OPTIMIZE COLUMN DESIGN

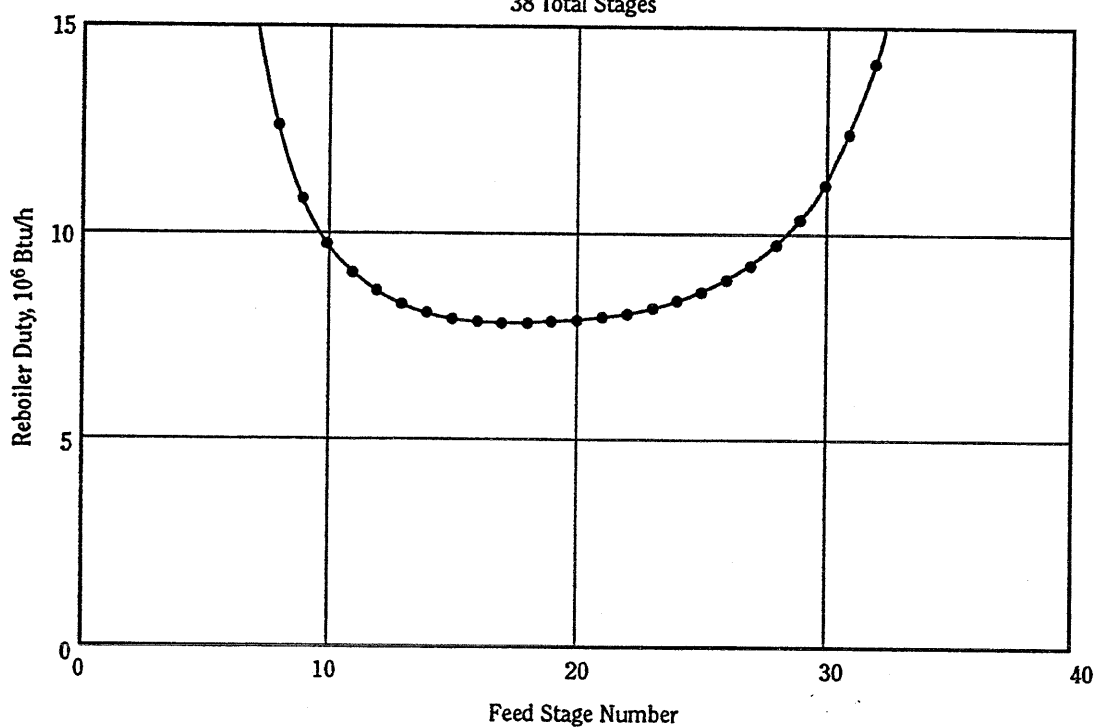
- Best Trays Versus Reboiler
- Best Feed Tray Location
- Feed Preheat

BEST FEED TRAY LOCATION

C₃/IC₄ Splitter
38 Total Stages

Feed Stage	Reboiler Duty 10 ⁶ Btu/h	Feed Stage	Reboiler Duty 10 ⁶ Btu/h	Feed Stage	Reboiler Duty 10 ⁶ Btu/h
1	288.701	14	8.141	27	9.309
2	148.546	15	8.008	28	9.785
3	83.707	16	7.929	29	10.417
4	49.136	17	7.891	30	11.277
5	30.807	18	7.885	31	12.480
6	21.036	19	7.908	32	14.223
7	15.723	20	7.957	33	16.847
8	12.720	21	8.032	34	20.964
9	10.944	22	8.134	35	27.665
10	9.840	23	8.269	36	38.831
11	9.130	24	8.442	37	57.548
12	8.660	25	8.663	38	88.681
13	8.348	26	8.945		

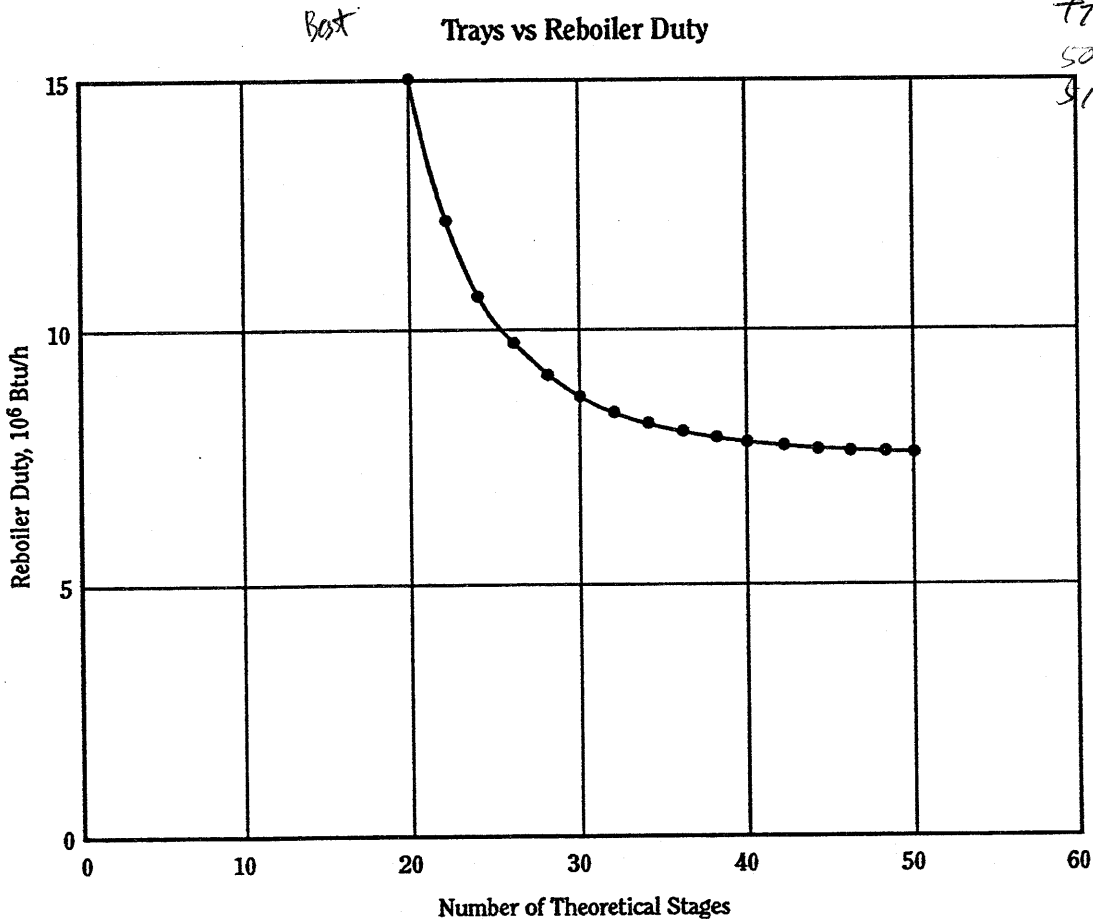
Best Feed Tray
38 Total Stages



EDS-R00-2513

TRAYS VERSUS REBOILER DUTY SELECTION

Feed Stage	Total Stages	Reboiler 10 ⁶ Btu/h	Percent Delta Reboiler/Theo Tray	Feed Stage	Total Stages	Reboiler 10 ⁶ Btu/h	Percent Delta Reboiler/Theo Tray
25	50	7.582	0.18	15	30	8.689	2.38
24	48	7.609	0.21	14	28	9.102	3.28
23	46	7.641	0.31	13	26	9.699	4.74
22	44	7.689	0.36	12	24	10.619	7.17
21	42	7.744	0.43	11	22	12.141	11.70
20	40	7.811	0.61	10	20	14.982	22.66
19	38	7.907	0.77	9	18	21.771	72.92
18	36	8.028	0.99	8	16	53.521	770.88
17	34	8.187	1.28	7	15	466.104	
16	32	8.397	1.74	7	14	Will not solve	



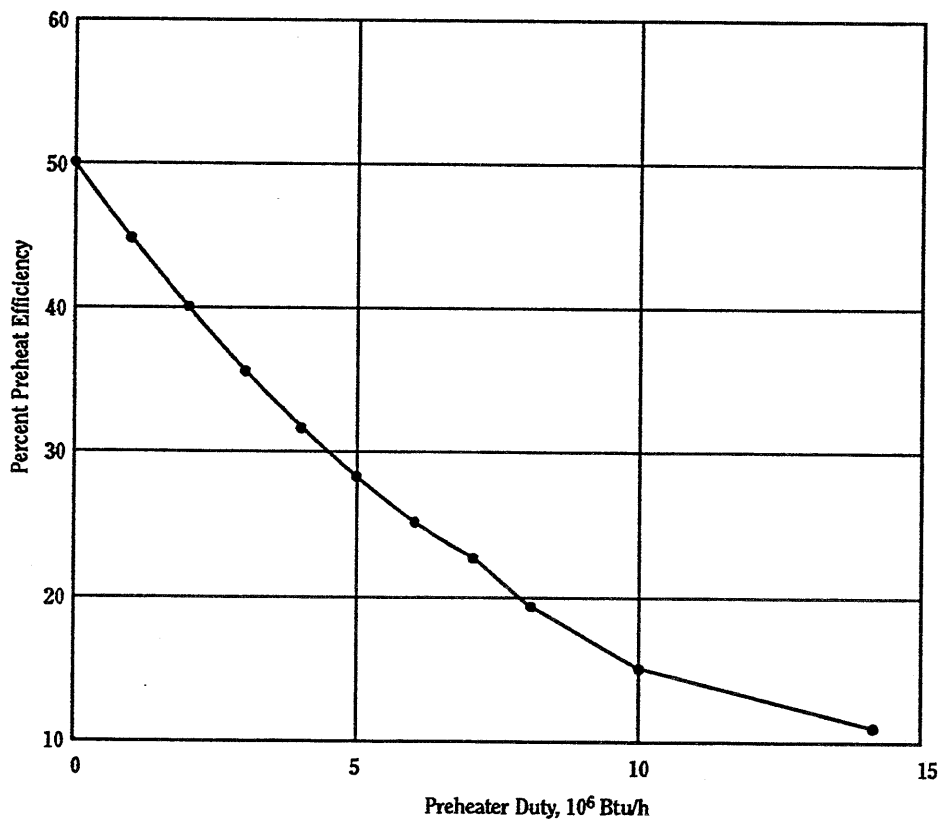
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FEED PREHEAT

Preheater Duty 10 ⁶ Btu/h	Feed Vapor Fraction	Reboiler Duty 10 ⁶ Btu/h	Preheat Efficiency Percent
0	0	8.741	50.5
1	0	8.236	45.1
2	0.0084	7.785	40.2
3	0.2363	7.383	35.7
4	0.4645	7.026	31.7
5	0.6932	6.709	28.2
6	0.9227	6.427	25.3
7	1	6.174	22.8
8	1	5.946	19.6
10	1	5.555	15.2
14	1	4.947	11.0
20	1	4.289	

?
possible
reasonable
approach

Feed Preheat Efficiency



EDS-R00-2515

Naphtha Stripper Preheat Efficiency

Feed Temp., °F	340	350	360	370	380
Feed Enthalpy, 10 ⁶ Btu/h	98.810	103.300	107.950	112.91	117.980
Reflux/Feed	0.562	0.605	0.650	0.70	0.752
Reboiler, 10 ⁶ Btu/h	86.670	84.990	83.372	81.68	80.110

Preheat efficiency is the delta reboiler duty divided by the delta feed enthalpy.

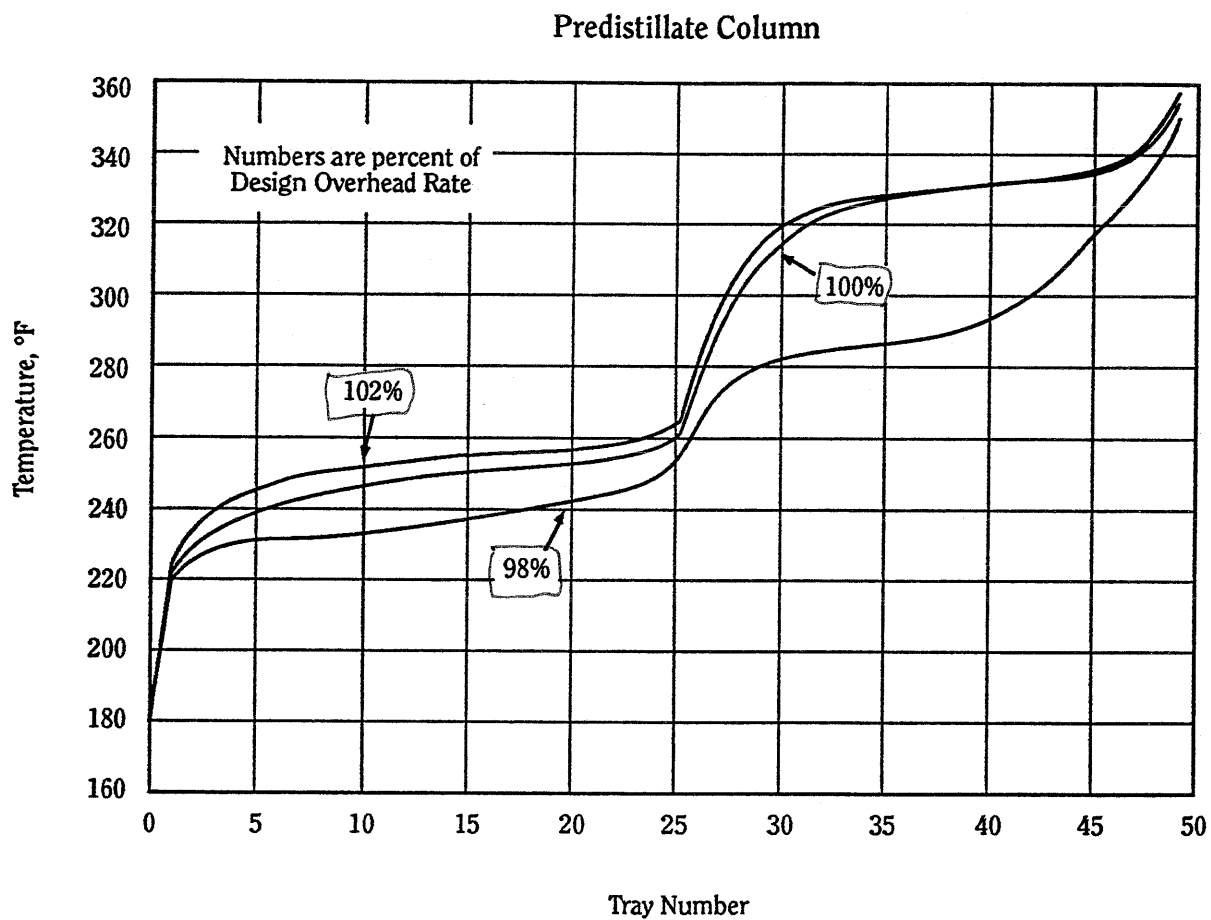
Delta Temperature	Preheat Efficiency, Percent
340→350	37.4
350→360	34.8
360→370	34.1
370→380	31.1

Feed Temp., °F	275	285	305	315
Feed Enthalpy, 10 ⁶ Btu/h	69.7	73.46	94.21	106.82
Reflux/Feed	0.6	0.63	0.828	0.97
Reboiler, 10 ⁶ Btu/h	74.19	72.41	64.38	60.82

Delta Temperature	Preheat Efficiency, Percent
275→285	47.3
285→305	38.7
305→315	28.2

Duty Stripper Splitter
 0 50 20
 ↓ 60 30
 30 40

PREDISTILLATION COLUMN



EDS-R00-2516

Toluene - Xylene Fractionation.

MULTICOMPONENT DISTILLATION

Distillation Problem 1.a

Minimum Reflux – High and Low Limits.

(From $K\pi$, 315 psia, 150 °F)			
↓			
Component	α	x_F	x_D
H ₂	47.740	0.0371	0.234
C ₁	7.734	0.0324	0.204
C ₂	2.185	0.0813	0.495
C ₃	1.000	0.3069	0.067
iC ₄	0.587	0.1170	
nC ₄	0.472	0.1820	
iC ₅	0.262	0.1330	
nC ₅	0.216	0.0847	
iC ₆ (2MP)	0.123	0.0256	
Total		1.0000	1.000

Keys → C₂ and C₃

Perfect separation

Boiling point feed

High Limit:

$$(R/F)_m = \frac{1}{\alpha - 1} = \frac{1}{1.185} = 0.844$$

Low Limit:

$$(R/F)_m = (x_{LK} + x_{HK}) \left(\frac{1}{\alpha - 1} \right) = (0.081 + 0.307)(0.844) = 0.327$$

Distillation Problem 1.b

Minimum R/D by Underwood:

$$q = 337.5/382.7 = 0.882 \text{ (feed liquid mol fraction)}$$

$$\sum_{i=1}^I \frac{\alpha_i x_i}{\alpha_i - \phi} = 1 - q, \text{ Correct } \phi \text{ between } 1.0 \text{ and } 2.185 (\alpha_K).$$

$$\frac{1.771}{(47.74 - \phi)} + \frac{0.2506}{(7.734 - \phi)} + \frac{0.1776}{(2.185 - \phi)} + \frac{0.3070}{(1.0 - \phi)} + \frac{0.0689}{(0.587 - \phi)} + \frac{0.0857}{(0.472 - \phi)}$$

$$+ \frac{0.0348}{(0.262 - \phi)} + \frac{0.0183}{(0.216 - \phi)} + \frac{0.0032}{(0.123 - \phi)} = 1 - q = 1 - 0.882 = 0.118$$

High and low limits in terms of R/D for boiling point feed:

High limit – mol fraction relative to keys:

$$R/D = \frac{1}{\alpha - 1} \left[\frac{x_D}{x_F} - \alpha \frac{(1 - x_D)}{(1 - x_F)} \right] = \frac{1}{1.185} \left[\frac{0.495}{0.0813} - 2.185 \frac{1 - 0.881}{1 - 0.209} \right] = 3.271$$

$\begin{matrix} 0.495 \rightarrow .881 \\ 0.495 + 0.067 \\ 0.0813 \\ 0.0813 + 0.3069 \\ \rightarrow .209 \end{matrix}$

$$R/F = (R/D)(D/F) = R/D \left[\frac{x_F - x_B}{x_D - x_B} \right]$$

$$x_B = \frac{1.0}{1.0 + 113.4} = 0.009$$

$$R/F = (3.271)(0.230) = 0.752$$

$$\left(\frac{.209 - .009}{.881 - .009} \right)$$

Distillation Problem 1.b (continued)

Low limit:

$$R/D = (R/D)_{BI} (x_{LK} + x_{HK})_D = 3.271(0.495 + 0.067) = 1.84$$

$$R/F = (R/D)(D/F) = (1.84)(0.159) = 0.292$$

↑
Total mol basis

For $q = 0.118$ Binary $R/D = 3.62$

ϕ	A	B	C	D	E	F	G	H	I	$\Sigma(+118)$
1.70	38	42	366	-439	-62	-70	-28	-18	-2	-173
1.90	39	43	623	-341	-52	-60	-24	-11	-2	+215
	$\Delta = -(215 - 118) / (215 + 173)(1.90 - 1.70) + 1.90 = 1.850$									
1.850	39	43	530	-361	-55	-62	-25	-11	-2	96
	$\Delta = 1.90 - (215 - 118) / (215 - 96)(1.90 - 1.85) = 1.8592$									
1.8592	39	43	545	-357	-54	-62	-25	-11	-2	116

↑
OK

$$\sum_{i=1}^I \frac{\alpha_i x_i}{(\alpha_i - \phi)} = L/D + 1$$

$$\frac{47.74(0.234)}{(47.74 - 1.859)} + \frac{7.734(0.204)}{(7.734 - 1.859)} + \frac{2.185(0.495)}{(2.185 - 1.859)}$$

$$+ \frac{1.0(0.067)}{(1.0 - 1.859)} = 0.243 + 0.269 + 3.318 + (-0.078) = 3.752 = L/D + 1$$

$$L/D = 2.752$$

$$D/F = 60.8/382.9 = 0.159$$

$$L/F = (2.752)(0.159) = 0.437$$

Distillation Problem 1.c

Component Distribution

Component	α	$\ln \alpha$	$\ln(r_D/r_B)$	r_D/r_B	F_i x_F	D_i x_D	B_i x_B
H ₂	47.740	3.866	33.26	$2.78 \cdot 10^{14}$	14.2	14.2	$1.41 \cdot 10^{-12}$
C ₁	7.734	2.046	17.60	$4.40 \cdot 10^7$	12.4	12.39	$7.80 \cdot 10^{-6}$
C ₂	2.185	0.782	6.72	$8.33 \cdot 10^2$	31.1	30.1	1.00
C ₃	1.000	0.000	0.00	1.00	117.5	4.1	113.40
iC ₄	0.587	-0.533	-4.58	$1.02 \cdot 10^{-2}$	44.9	0.02	44.88
nC ₄	0.472	-0.751	-6.46	$1.57 \cdot 10^{-3}$	69.5	0.003	69.497
iC ₅	0.262	-1.339	-11.52	$9.90 \cdot 10^{-6}$	50.9	$1.82 \cdot 10^{-5}$	50.9
nC ₅	0.216	-1.532	-13.18	$1.88 \cdot 10^{-6}$	32.4	$2.20 \cdot 10^{-6}$	32.4
2MP	0.123	-2.096	-18.03	$1.48 \cdot 10^{-8}$	9.8	$5.24 \cdot 10^{-9}$	9.8

Fenske Equation:

$$n = \ln(r_D/r_B) / \ln \alpha$$

For ethane:

$$n = 6.72 / 0.782 = 8.603$$

Once "r" is known, calculate:

$$\ln(r_D/r_B) = (n)(\ln \alpha)$$

$$x_D = (r_D/r_B) \left(\frac{F_i}{x_F} \right) \left(\frac{x_{FD}}{x_{FB} + (r_D/r_B) x_{FD}} \right)$$

$$x_B = \left(\frac{F_i}{x_F} \right) \left(\frac{x_{FB}}{x_{FB} + (r_D/r_B) x_{FD}} \right)$$

Distillation Problem 1.d

Gilliland Relation

Find operating trays for a reflux of 402.0 mol/h

$$L/D = 402.0/60.8 = 6.61$$

$$X = (R - R_m)/(R + 1)$$

$$Y = \overset{.213}{\underset{.213}{.213}} \text{ (From Gilliland Graph)}$$

$$Y = (N - N_m)/(N + 1)$$

$$0.213 = (N - 8.6)/(N + 1)$$

$$N = 11.2$$

MINIMUM AND TOTAL REFLUX CALCULATIONS

uop

25 East Algonquin Road
Des Plaines, Illinois
60017-5017

Engineering Design Seminar
Distillation Problem

Feed Thermal Condition, (q) 0.882
Number of Components 9
Light Key in Distillate, Mols 30.100
Heavy Key in Distillate, Mols 4.100

Component Name	Feed (Mols)	Component Distribution (Mols)				Equilibrium Data	Relative Volatility (Calc)	Roots of Underwood Equation
		Minimum Reflux		Total Reflux				
		Dist.	Bott.	Dist.	Bott.			
H ₂	14.20	14.20	0.00	14.20	0.00	47.740	47.740	
C ₁	12.40	12.40	0.00	12.40	0.00	7.734	7.734	35.6972
LK C ₂	31.10	30.10	1.00	30.10	1.00	2.185	2.185	6.5197
HK C ₃	117.50	4.10	113.40	4.10	113.40	1.000	1.000	1.8591
i-C ₄	44.90	0.00	44.90	0.02	44.88	0.587	0.587	0.7009
n-C ₄	69.50	0.00	69.50	0.00	69.50	0.472	0.472	0.5250
i-C ₅	50.90	0.00	50.90	0.00	50.90	0.262	0.262	0.2978
n-C ₅	32.40	0.00	32.40	0.00	32.40	0.216	0.216	0.2256
2MP	9.80	0.00	9.80	0.00	9.80	0.123	0.123	0.1255
Totals:	382.70	60.80	321.90	60.82	321.88			

Theoretical Plate Requirements (Gilliland Correlation)

Internal Reflux/Distillate	Theoretical Plates	Internal Reflux/Distillate	Theoretical Plates
2.75	Infinite	4.36	14.39
2.95	22.71	6.50	11.80
3.03	21.08	11.51	10.19
3.17	19.61	17.76	9.58
3.69	16.46	Infinite	8.60

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MULTICOMPONENT DISTILLATION

Problem 2

	x_1	K @ 150π 250°F	ΣKx	K @ 150π 340°F	ΣKx	K @ 150π 360°F	ΣKx
iC ₄	0.1	2.05	0.2	3.25	0.3	3.56	0.4
nC ₄	9.0	1.75	15.8	2.90	26.1	3.18	28.6
iC ₅	18.0	1.05	18.9	1.88	33.8	2.10	37.8
nC ₅	24.0	0.929	22.3	1.73	41.5	1.95	46.8
nC ₆	300.0	0.499	149.7	1.06	318.0	1.21	363.0
nC ₇	599.9	0.266	159.6	0.659	395.4	0.772	463.2
Total	951.0		366.5		815.1		939.8

Acceptable

Use 360°F

$$V/L = 0.9, L = V + 951.0, D/L = 951.0, L = 9510.0, V = 8559.0$$

	(By Ratio) V ₁	$x_1 + V_1$ L ₂	K @ 150π 350°F	ΣKL_2	(By Ratio) V ₂	$x_2 + V_2$ L ₃	K @ 150π 340°F	ΣKL_3
iC ₄	3.6	3.7	3.40	12.6	10.9	11.0	3.25	35.8
nC ₄	260.5	269.5	3.04	819.3	708.6	717.6	2.90	2081.0
iC ₅	344.3	362.3	1.99	721.0	623.6	641.6	1.88	1206.2
nC ₅	426.2	450.2	1.84	828.4	716.4	740.4	1.73	1280.9
nC ₆	3305.9	3605.9	1.13	4074.7	3524.0	3824.0	1.06	4053.4
nC ₇	4218.5	4818.4	0.714	3440.3	2975.5	3575.4	0.659	2356.2
Total	8559.0	9510.0		9896.3	8559.0	9510.0		11013.5

OK

	K @ 150π 330°F	ΣKL_3	K @ 150π 310°F	ΣKL_3	K @ 150π 320°F	ΣKL_3	V ₃
iC ₄	3.10	34	2.82	31	2.96	33	29.4
nC ₄	2.77	1988	2.52	1808	2.64	1894	1684.7
iC ₅	1.78	1142	1.57	1007	1.67	1071	952.7
nC ₅	1.63	1207	1.44	1066	1.53	1133	1007.8
nC ₆	0.987	3774	0.851	3254	0.917	3507	3119.5
nC ₇	0.607	2170	0.507	1813	0.555	1984	1764.9
Total		10315		8979		9622	8559.0

OK

L_1

		$L_1 + V_3$ L_4	K @ 150π 290°F	ΣKL ₄	K @ 150π 280°F	ΣKL ₄
iC ₄	0.1	29.5	2.56	76	2.44	72
nC ₄	9.0	1693.7	2.26	3828	2.13	3608
iC ₅	18.0	970.7	1.39	1349	1.30	1262
nC ₅	24.0	1031.8	1.25	1290	1.17	1207
nC ₆	300.0	3419.5	0.723	2473	0.663	2267
nC ₇	599.9	2364.8	0.416	984	0.368	870
Total	951.0	9510.0		10000		9286

OK

	V ₄	$L_1 + V_4$ L_5	K @ 150π 250°	ΣKL ₅	$L_1 + V_5$ L_6	Tray	nC ₄ /iC ₅	°F
iC ₄	66.4	66.5	2.05	136	119.1	1	0.5	360
nC ₄	3325.5	3334.4	1.75	5835	5088.8	2	0.744	350
iC ₅	1163.2	1181.2	1.05	1240	1097.4	3	1.12	320
nC ₅	1112.5	1136.5	0.929	1055	942.3	4	1.75	280
nC ₆	2089.5	2389.5	0.499	1192	1337.2	5	2.83	250
nC ₇	801.9	1401.8	0.266	373	924.2	6	4.64	
Total	8559.0	9510.0		9831	9510.0			

OK

V_5
 118.4
 5080.0
 1079.6
 918.5
 1037.8
 324.7
8559.0

118.5
 5089.0
 1097.6
 942.5
 1337.8
 924.6

Handout Example Problem – Bottoms

	L_0	$K\pi$ @ 300 psia 230°F	$L_0K\pi$	V_0	$K\pi$ @ 300 psia 210°F	$L_0K\pi$	V_0
C ₂	1.0	1097	1097	4.2	994	994	4.2
C ₃	113.4	517	58628	223.8	469	53185	227.8
iC ₄	44.9	328	14727	56.2	292	13110	56.1
nC ₄	69.5	283	19668	75.1	248	17236	73.8
iC ₅	50.9	180	9162	35.0	154	7839	33.6
nC ₅	32.4	159	5152	19.7	133	4309	18.5
iC ₆	9.8	103	1009	3.9	84	823	3.5
Total	321.9		109443	417.9		97496	417.5

Shows temperature change has small effect on composition because α changes little with temperature.

Delete

MULTICOMPONENT DISTILLATION

Absorption and Stripping – Problem 1

	mol/h	$K\pi$ @ 250 psia 220°F	K	KV/L	Fraction Stripped	Overhead	Bottom
C ₁	21	3171	12.684	3.555	1.000	21.0	0.0
C ₂	132	1032	4.128	1.157	0.980	129.4	2.6
C ₃	157	474	1.896	0.531	0.531	83.4	73.6
iC ₄	211	289	1.156	0.324	0.324	68.4	142.6
nC ₄	413	247	0.988	0.277	0.277	114.4	298.6
iC ₅	512	151	0.604	0.169	0.169	86.7	425.3
nC ₅	814	132	0.528	0.148	0.148	120.5	693.5
nC ₆	1210	69.8	0.2792	0.078	0.078	94.7	1115.3
Total	3470					718.5	2751.5

Kremser Equation:

$$\text{Fraction Stripped} = (S^{n+1} - S) / (S^{n+1} - 1)$$

where:

$$S = KV/L$$

$$n = 14$$

C₂ stripping required is 98 pct.

From Kremser Chart or Kremser Equation:

$$(KV/L)_{C_2} = 1.157$$

The V/L value is calculated by dividing the $(KV/L)_{C_2}$ by the K_{C_2} value.

$$V/L = 1.157/4.128 = 0.280$$

MULTICOMPONENT DISTILLATION

Absorption and Stripping – Problem 2

$$D_i = F_i[f(S_i)] + G_i[1 - f(A_i)]$$

$$S_i = K_i V/L \quad A_i = L/K_i V$$

$$\text{Fraction Stripped} = f(S_i) = (S_i^{n+1} - S_i)(S_i^{n+1} - 1)$$

$$\text{Fraction Absorbed} = f(A_i) = (A_i^{n+1} - A_i)(A_i^{n+1} - 1)$$

	Mol/h G_i	$K\pi$ @ 150 psia 120°F	K_i	Try $L/V=3$ $L/K_i V$	Fraction Absorbed	D_i Overhead	Bottom
H ₂	150	17270.000	115.133	0.026	0.026	146.1	3.9
N ₂	20	3061.500	20.410	0.147	0.147	17.1	2.9
C ₁	35	2223.300	14.822	0.202	0.202	27.9	7.1
C ₂	15	761.490	5.077	0.591	0.585	6.2	8.8
C ₃	65	559.810	3.732	0.804	0.762	15.4	49.6
C ₄	138	244.960	1.633	1.837	0.993	0.9	137.1
C ₅	250	214.410	1.429	2.099	0.997	0.7	249.3
iC ₄	50	108.250	0.722	4.157	1.000	0.0	50.0
nC ₄	110	83.067	0.554	5.417	1.000	0.0	110.0
iC ₅	16	40.072	0.267	11.230	1.000	0.0	16.0
nC ₅	28	31.815	0.212	14.144	1.000	0.0	28.0
2MP	8	16.114	0.107	27.926	1.000	0.0	8.0
Total	885					214.3	670.7
	F_i	$K_i \pi$	K_i	$K_i V/L$	Fraction Stripped	D_i Overhead	Bottom
Toluene	750	2.6706	$1.78 \cdot 10^{-2}$	$5.93 \cdot 10^{-3}$	$5.93 \cdot 10^{-3}$	4.5	745.5
m-X	750	1.0309	$6.87 \cdot 10^{-3}$	$2.29 \cdot 10^{-3}$	$2.29 \cdot 10^{-3}$	1.7	748.3
Total	1500					6.2	1493.8
Define $(L/V)_{\text{average}} = [F/D + (F - D + G)/G]/2$							D=220.5
Calculated $(L/V)_{\text{average}} = 4.62$							4.62 > 3.2 ∴ try greater L/V

Absorption and Stripping – Problem 2

$$D_i = F_i[f(S_i)] + G_i[1 - f(A_i)]$$

$$S_i = K_i V/L \quad A_i = L/K_i V$$

$$\text{Fraction Stripped} = f(S_i) = (S_i^{n+1} - S_i)(S_i^{n+1} - 1)$$

$$\text{Fraction Absorbed} = f(A_i) = (A_i^{n+1} - A_i)(A_i^{n+1} - 1)$$

	Mol/h G_i	$K\pi$ @ 150 psia 120°F	K_i	Try $L/V=6$ $L/K_i V$	Fraction Absorbed	D_i Overhead	Bottom
H ₂	150	17270.000	115.133	0.052	0.052	142.2	7.8
N ₂	20	3061.500	20.410	0.294	0.294	14.1	5.9
C ₁	35	2223.300	14.822	0.405	0.404	20.8	14.2
C ₂	15	761.490	5.077	1.182	0.935	1.0	14.0
C ₃	65	559.810	3.732	1.608	0.986	0.9	64.1
C ₄	138	244.960	1.633	3.674	1.000	0.0	138.0
C ₅	250	214.410	1.429	4.198	1.000	0.0	250.0
iC ₄	50	108.250	0.722	8.314	1.000	0.0	50.0
nC ₄	110	83.067	0.554	10.835	1.000	0.0	110.0
iC ₅	16	40.072	0.267	22.460	1.000	0.0	16.0
nC ₅	28	31.815	0.212	28.289	1.000	0.0	28.0
2MP	8	16.114	0.107	55.852	1.000	0.0	8.0
Total	885					179.0	706.0
	F_i	$K_i \pi$	K_i	$K_i V/L$	Fraction Stripped	D_i Overhead	Bottom
Toluene	750	2.6706	$1.78 \cdot 10^{-2}$	$2.97 \cdot 10^{-3}$	$2.97 \cdot 10^{-3}$	2.2	747.8
m-X	750	1.0309	$6.87 \cdot 10^{-3}$	$1.15 \cdot 10^{-3}$	$1.15 \cdot 10^{-3}$	0.9	749.1
Total	1500					3.1	1496.9
Define $(L/V)_{\text{average}} = [F/D + (F - D + G)/G]/2$							D=182.1
Calculated $(L/V)_{\text{average}} = 5.36$							5.36 < 6.0 ∴ try smaller LV

ENGINEERING DESIGN SEMINAR

SEPTEMBER 6, 1994 – NOVEMBER 11, 1994

BINARY FRACTIONATION

Mr. Paul Steacy

122 3000, 20, 2500

Example X_{1D} means mols per hour of light component in the distillate. Since we are talking about binary distillation, we can skip the 1 – 2 subscripts if we wish and always understand that we refer to the light component when we say, for example x . Then $(1-x)$, of course, means mol fraction of heavy component.

Sometimes the following superscripts are utilized

$1, 2, 3 \dots n, n+1 = \text{tray numbers}$

Tools for Distillation Analysis

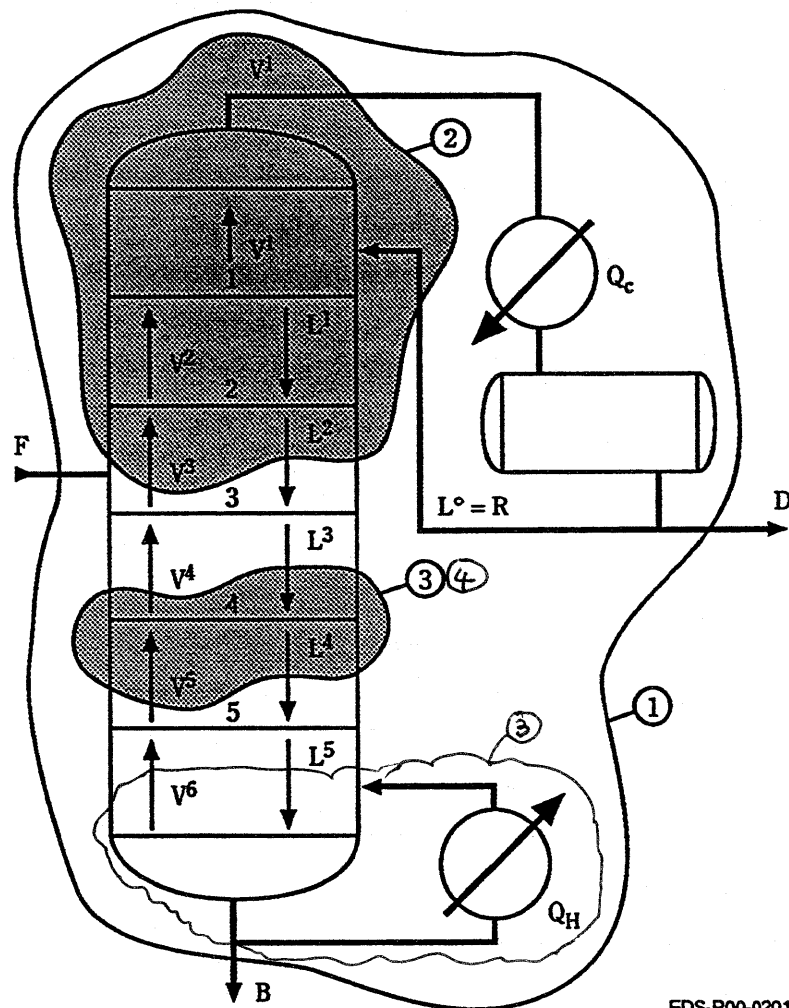
Tools to analyze and solve distillation problems are:

Material Balances

Heat Balances

Equilibrium Relationships

Figure 1



EDS-R00-0201

Envelope Technique

As an aid to developing these relationships, the "envelope technique" is used. On a sketch of a fractionator or portion thereof, envelopes are drawn around which material and heat balances can be written.

Let us consider a simple fractionator (one feed and just top and bottom products) with five trays with the overhead product being all liquid and the reflux is not subcooled. We will write material and heat balances around three possible envelopes. Each tray will be defined a theoretical tray where the liquid and vapor phases leaving each tray are in equilibrium (V^1 with L^1 , V^2 with L^2 , etc.).

Envelope 1

Mass Balance

In = Out

$$F = B + D$$

$$x_i^F F = x_i^D D + x_i^B B$$

Heat Balance

In = Out

$$FH_F + Q_H = DH_D + BH_B + Q_C$$

Envelope 2

Mass Balance

In = Out

$$V^3 + L^0 = V^1 + L^2$$

Heat Balance

In = Out

$$V^3 H_{V^3} + L^0 H_{L^0} = V^1 H_{V^1} + L^2 H_{L^2}$$

Envelope 3

Mass Balance

In = Out

$$V^5 + L^3 = V^4 + L^4$$

Heat Balance

In = Out

$$V^5 H_{V^5} + L^3 H_{L^3} = V^4 H_{V^4} + L^4 H_{L^4}$$

Envelope 4

$$\text{Mass balance} \rightarrow V^{n+1} = V^n + L^n - L^0$$

$$\text{Heat Balance} \rightarrow Q_{V^n} V^n + Q_{L^n} L^n - Q_{V^{n+1}} V^{n+1} - Q_{L^0} L^0 + Q_{L^0} = Q_{V^n} V^n + Q_{L^n} L^n$$

$$L^n = L^0 = \text{constant}$$

Assume

- sensible heat change only by the
- Molal heats of vaporization are constant

BINARY DISTILLATION MATERIAL BALANCES

Binary Concept

We now simplify the system by defining the feed to consist of two components. The liquid and vapor mol fraction of the light component will be designated x and y .

Example: Material Balance for Envelope 1 for The Light Component

$$F x_F = D x_D + B x_B$$

Constant Molal Overflow Concept

In distillation calculations, the simplifying concept of constant molal overflow eliminates the need for heat balances except around the feed tray. Constant molal overflow means that in a section of the column, the vapor and liquid molal flows do not change. A section is defined as a portion of the fractionator between two adjacent entering and/or exit streams.

For our simple fractionator, there are only two sections: a top or rectifying section and a bottoms or stripping section. Therefore, $V^3 = V^2 = V^1$ and $L^1 = L^2$; also $V^4 = V^5$ and $L^3 = L^4 = L^5$.

Commercial fractionation such as benzene/toluene, isobutane/n-butane, ethylbenzene/styrene and propylene/propane can be considered binary distillations with constant molal overflow.

Constant molal overflow occurs when:

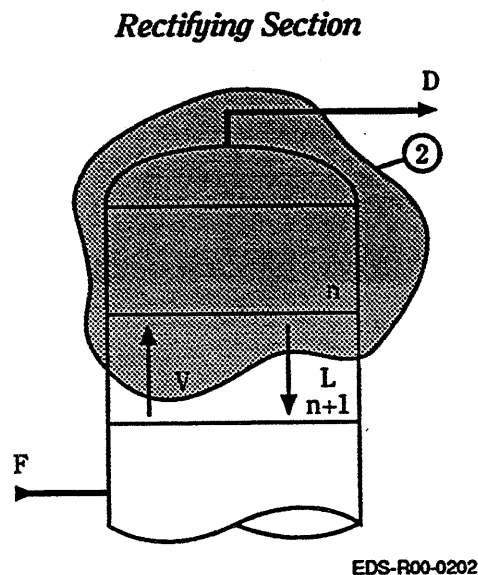
Molal latent heats of both components are similar (at tray temperatures)

Sensible heat changes (from tray to tray) are negligible in comparison with latent heats.

Rectifying and Stripping Sections

Now let us consider the fractionator not to be limited in trays and derive material balances for each section of the column.

Figure 2



Light Component Mass Balance

$$In = Out$$

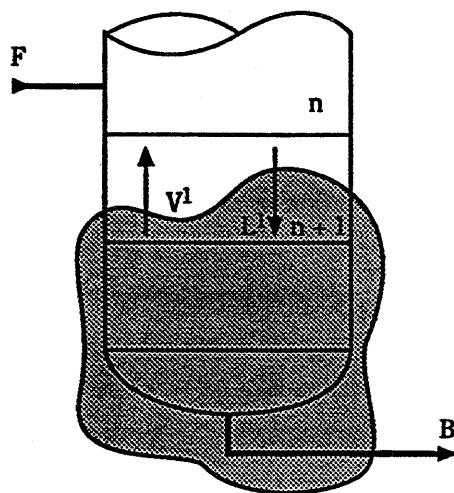
$$Vy^{n+1} = LX^n + DX_D$$

(a)
$$y^{n+1} = (L/V)x^n + (D/V)X_D$$

Tray above Feed.

Figure 3

Stripping Section



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Light Component Mass Balance

$$V'y^{n+1} = L'X^n - BX_B$$

(b)
$$y^{n+1} = (L'/V')X^n - (B/V')X_B$$

Tray below Feed

Feed Tray Balances

The relationship between L , V and L' , V' is determined by material and heat balances around the feed tray.

Let us define a thermal property of the feed, q , such that

$$(c) \quad L' = L + qF \text{ and hence } V' = V + (q-1)F$$

Where the molal latent heats of both components are the same on both the feed tray and in the feed:

$$(d) \quad q = \frac{H_F^V - H_F}{\lambda}$$

q is the total heat required to convert a mol of feed to saturated vapor divided by the molal latent heat of vaporization.

This convenient definition of q eliminates the need for feed tray heat balances. It also allows the development of a relationship (equation) giving the conjunction of the rectifying and stripping material balance relationships. Graphically, this is the locus (y^{n+1}) of the intersection of the lines representing the material balance equations. Inserting the definitions in (c) into equations (a) and (b) and eliminating L and V results in:

$$(e) \quad y^{n+1} = [q/(q-1)]x^n - [1/(q-1)]x_F$$

Summary of Equations

(a) Rectifying Section Operating Line

$$y^{n+1} = (L/V)x^n + (D/V)x_D$$

(b) Stripping Section Operating Line

$$y^{n+1} = (L'/V')x^n - (B/V')x_B$$

(c)
$$L' = L + qF$$

(d)
$$q = \frac{H_F^V - H_F}{\lambda}$$

(e) q Line

$$y^{n+1} = [q/(q-1)]x^n - [1/(q-1)]x_F$$

EQUILIBRIUM

Concept

A vapor and a liquid in a system containing two components quickly come into equilibrium when mixed or agitated. At this condition of fixed temperature and pressure, molecules of either component in the vapor are condensing at the same rate as molecules of these components in the liquid are evaporating. The composition of each phase is then constant forever, as long as the temperature and pressure do not change.

The more light material there is in the liquid, the more light material there will be in the vapor. This is common sense. We can say that y is proportional to x :

$$y_1 = K_1 x_1 \quad y_2 = K_2 x_2$$

In binary distillation, K_2 is always less than 1.0 on all trays, and K_1 is always greater than 1.0. When $K_1 = K_2$, an azeotrope occurs and then separation by distillation is impossible. Another useful concept is relative volatility or α (alpha). This is simply K_1/K_2 and its use has the advantage that it remains nearly constant over a rather wide variation of temperature and pressure. For some binaries where the boiling points are very close to each other, it is not a bad approximation to use the same value of α all

the way from the top to the bottom of the column. But, more important, it is the best single criterion of the **difficulty** of separation. Difference in boiling point is not always a good indicator. For instance, if two materials boil close together, the relative volatility will be much greater if the binary pair are low-boiling, compared to a high-boiling pair. For instance, it is much easier to fractionate a pair boiling at 30°F and 40°F, respectively, than it is to fractionate a pair at 320°F and 330°F. The α for the first pair is about 1.27 and for the second pair is about 1.10. It can be shown that the reflux ratio is approximately inversely proportional to $(\alpha-1)$, thus the relative reflux rate for the high-boiling pair will be nearly three times greater than for the low-boiling pair. For hydrocarbons belonging to the same family, that is, the same general molecular structure, the mixtures behave nearly ideally.

Then these relationships hold

$$K_1 = \frac{P_1^o}{\pi} \quad \alpha = \frac{P_1^o}{P_2^o}$$

Equilibrium Line Equations

(a)

$$y_1 = K_1 x_1$$

$$K_1 x_1 = 1 - y_2$$

$$K_1 x_1 = 1 - K_2 x_2$$

$$K_1 x_1 = 1 - K_2 (1 - x_1)$$

$$K_1 x_1 = 1 - K_2 + K_2 x_1$$

$$K_1 x_1 - K_2 x_1 = 1 - K_2$$

$$x_1 (K_1 - K_2) = 1 - K_2$$

$$x = \frac{(1-K_2)}{(K_1-K_2)}$$

(defines x and y as a function of temperature and pressure)

$$y = K_1 x$$

(b)

$$y_1 = K_1 x_1$$

$$y_2 = K_2 x_2$$

$$y_1/y_2 = (K_1/K_2)(x_1/x_2) = \alpha(x_1/x_2)$$

$$y_2 = 1 - y_1 \quad x_2 = 1 - x_1$$

$$y_1/(1 - y_1) = \alpha x_1/(1 - x_1)$$

$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$

(defines relationship between x and y if α is constant over the temperature range)

(c)

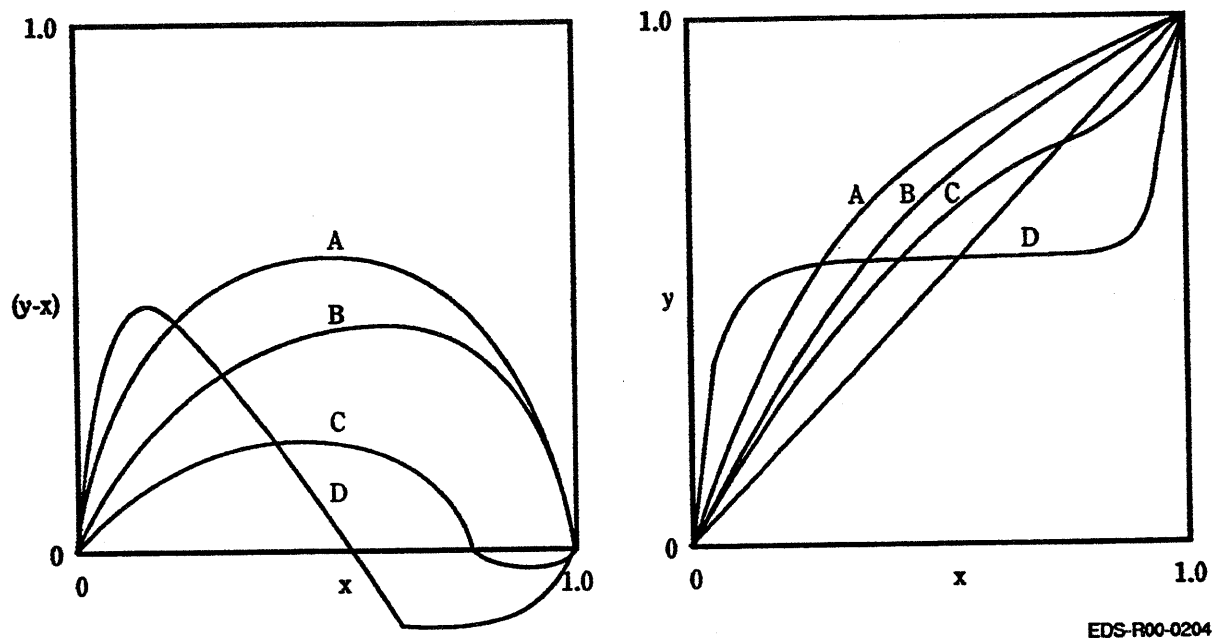
$$\alpha = K_1/K_2$$

Non-Ideal Systems

Certain binary systems exhibit equilibrium phenomena wherein the equilibrium curve crosses the 45° line (the azeotropic composition). In such systems (e.g. ethanol-water) where the two components are fully miscible over the entire composition range, it is not possible to obtain two products of compositions which fall on opposite sides of the azeotropic composition. In such systems (e.g. propane-water) where the two components are only partially miscible, separation can be achieved provided two fractionators are used connected via a common receiver. The receiver provides

mechanical separation of the two liquid phases and each can then be separately stripped of the soluble impurity.

Figure 4



Ideal and Non-Ideal Systems

- A – Ideal (Symmetrical)
- B – Non-Ideal (Unsymmetrical)
- C – Non-Ideal (Azeotrope)
- D – Non-Ideal (Partially Miscible Mixtures)

McCABE-THIELE DIAGRAM

Introduction

Given feed rate and composition, product specifications and with pressure set to condense the overhead product, the typical fractionation problem can be solved in two ways:

For a reflux or boil up rate, find theoretical trays required (easiest approach, often used for design).

For a fixed number of theoretical trays, find reflux or boil up rate required (more difficult approach, used for design when a computer is available, necessary for rating an existing column).

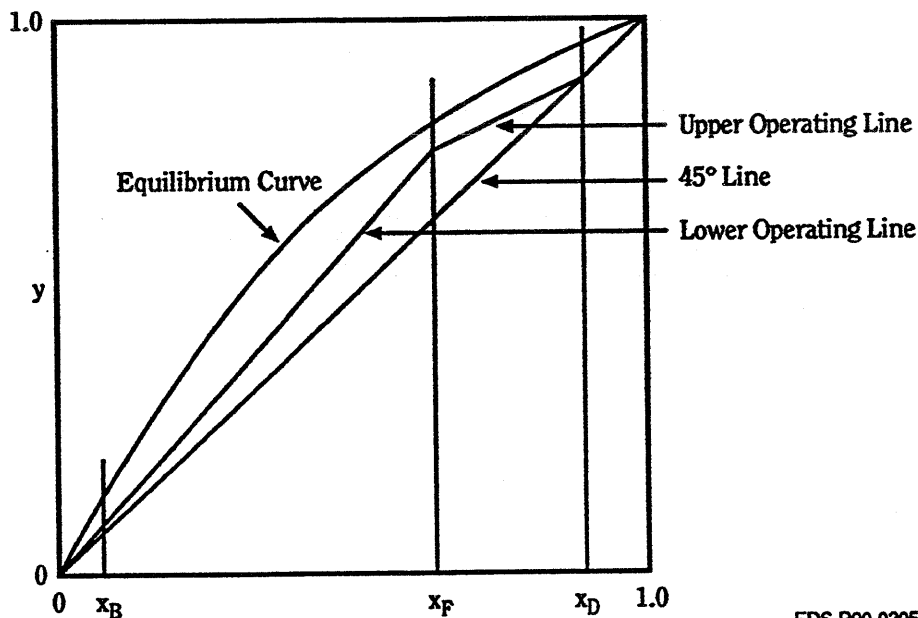
Since all relationships have been defined quantitatively, an analytical solution is possible. However, a graphical technique – The McCabe-Thiele diagram – can be a useful tool for solving fractionation problems and also for understanding fractionation parameter relationships.

As with any graphical method, any coordinate system can be chosen. Most problems are solved with rectangular coordinates and, unless otherwise noted, this will be the system described in the following discussion.

The material balance relationships are plotted (these are usually called operating lines) along with the equilibrium relationship as mol fraction (0.0 to 1.0) y and x of the light component. The 45° line is also automatically plotted.

Below is a typical plot.

Figure 5



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Binary distillation calculations are easy to do rapidly. Many systems in our business actually are binaries or can be treated as such. Learning binary distillation and the McCabe-Thiele diagram is one of the most profitable and productive of all of the techniques we have. McCabe-Thiele diagrams are the most useful for fractionation problem analysis, for troubleshooting, for arguing the effect of various variables, for setting up instrumentation of columns, for discussing instrumentation, and for such deliberations as to whether you should raise the feed nozzle or lower it. The McCabe-Thiele diagram is the only simple technique which shows clearly what the terms "minimum reflux ratio" and "minimum trays" and "tray efficiency" mean. The McCabe-Thiele diagram also shows, most clearly, the effect of "feeding on the wrong tray," how much benefit can be gained by increasing the reflux and what is gained by adding trays. Also, it is excellent in studying azeotropes and other non-ideal systems.

Equilibrium Curve

The equilibrium curve is a plot of y_1 against x_1 . At a given pressure for every value of x_1 , there is only one value for y_1 and the temperature is thereby fixed. Of course, this follows Gibbs' phase rule. Each tray temperature is the bubble point of the liquid (or dew point of the equilibrium vapor). The x - y curve is constructed using the following steps:

Determine the pressure. This is dictated by the composition of the desired distillate, available coolant temperature, and whether the distillate should be a vapor or liquid. In binary distillation, the distillate is almost never taken off as a vapor.

Find the temperature when $K_1 = 1.00$. This will be very nearly the top temperature of the column if the distillate is nearly pure.

Find the temperature where $K_2 = 1.00$. This will be very nearly the bottom temperature.

Make a column of temperatures lying between these two temperatures with some conveniently chosen increment of temperature.

Make two columns of equilibrium constants (K_1 and K_2) to correspond with the column of temperatures.

Make column for x ; calculate x using equation (a), page 11.

Make column for y ; calculate y using equation (b), page 11.

On suitable graph paper, plot y against x . Of course the curve will terminate at $x = y$ at both ends going through (0,0) and (1,1).

In certain instances, a plot of the temperature (from step d) against x on the same paper will prove useful when plate temperatures are required.

Example, for the Binary n-Butane – I-Pentane

For 140 °F reflux, 100 psia receiver:

Temp. °F	K_1 nC ₄	K_2 iC ₅	α	$x = \frac{(1 - K_2)}{(K_1 - K_2)}$	$y = K_1 x$
*140	0.942	0.460			
150	1.050	0.524	2.00	0.905	0.950
160	1.164	0.593	1.96	0.713	0.830
170	1.284	0.667	1.93	0.540	0.693
180	1.409	0.746	1.89	0.384	0.541
190	1.540	0.829	1.86	0.240	0.370
200	1.677	0.918	1.83	0.108	0.182
*210	1.820	1.011			

*outside operating range as $K_1 < 1$ or $K_2 > 1$

Operating Lines

After the equilibrium curve is plotted, it is necessary to plot, on the same paper, the operating lines. First, it is convenient to draw the 45° line ($x = y$) from $x_1 = 0$ to $x_1 = 1$. Then the feed and product purities at both ends are shown as verticals from the 45° line.

The equations for the operating lines are linear and hence will plot as straight lines on rectangular coordinates. A straight line can be drawn with two points or one point and a slope. Note that for the rectifying section operating line (equation (a), page 8), when $x^n = x_D$, $y^{n+1} = x_D$. Therefore, this line always passes through the coordinates x_D, y_D .

Similarly note that, for the feed q operating line (equation (e), page 9), when $x^n = x_F$, $y^{n+1} = x_F$. Therefore, this line always passes through the coordinates x_F, y_F . Finally, for the stripping section operating line (equation (b), page 9), when $x^n = x_B$, $y^{n+1} = x_B$. Therefore, this line always passes through the coordinates x_B, y_B . The simplest method for plotting these lines is to first draw a straight line with slope = L/V through the point x_D, y_D ; second, draw a straight line with slope = $q/q-1$ through the

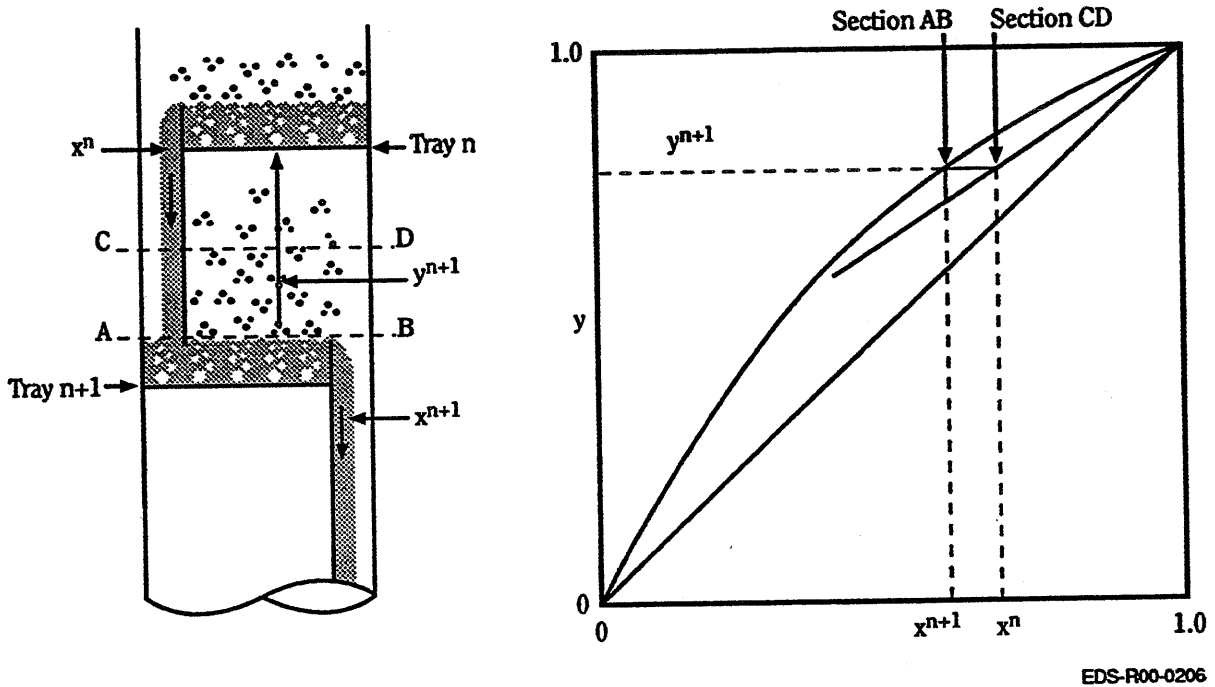
point x_F, y_F and third, draw a straight line through the point x_B, y_B and the point of intersection of the first and second lines.

Physical Meaning of Points on McCabe-Thiele

At this point, it may be well to back up and briefly describe the process of separation of two components to a high degree of purity by distillation to get an insight as to how it works. When the feed is introduced into the column, the more volatile component will be in somewhat higher concentration in the vapor from the feed tray. As the vapor rises through the tray above the feed, the heavier component tends to condense first, the vapor being contacted intimately with the colder internal reflux from above. This enrichment is directly related to the relative volatility, α , and to the internal reflux ratio. An equivalent amount of enrichment occurs successively on each tray as we proceed in a similar manner up the column.

At each tray, if perfect mixing takes place, the vapor rising from that tray is at its dew point, and the liquid leaving that tray is at its bubble point. For a perfect tray, a horizontal plane A-B drawn through the vapor-liquid interface represents the x and y values corresponding to a point on the equilibrium curve. A horizontal plane C-D drawn through the space between the trays represents the x and y values corresponding to a point on the operating line.

Figure 6



Feed Conditions

The line connecting the intersection of the operating lines and the intersection of $x = y$ at $x = x_F$ is called the q-line in most texts. The equation for it is:

$$y^{n+1} = [q/(q-1)]x^n - [1/(q-1)]x_F$$

The value of q is characterized as follows:

If Feed Is:	Then q is:
Superheated Vapor	< 0
Saturated Vapor	$= 0$
Partly Vapor	$= \text{Mol Fraction Liquid}$
Saturated Liquid	$= 1$
Subcooled Liquid	> 1

Absorption and Stripping – Problem 2

$$D_i = F_i[f(S_i)] + G_i[1 - f(A_i)]$$

$$S_i = K_i V/L \quad A_i = L/K_i V$$

$$\text{Fraction Stripped} = f(S_i) = (S_i^{n+1} - S_i)(S_i^{n+1} - 1)$$

$$\text{Fraction Absorbed} = f(A_i) = (A_i^{n+1} - A_i)(A_i^{n+1} - 1)$$

	Mol/h G_i	$K_i \pi$ @ 150 psia 120°F	K_i	Try $L/V = 5.23$ $L/K_i V$	Fraction Absorbed	D_i Overhead	Bottom
H ₂	150	17270.000	115.133	0.045	0.045	143.2	6.8
N ₂	20	3061.500	20.410	0.256	0.256	14.9	5.1
C ₁	35	2223.300	14.822	0.353	0.353	22.7	12.3
C ₂	15	761.490	5.077	1.030	0.888	1.7	13.3
C ₃	65	559.810	3.732	1.401	0.971	1.9	63.1
C ₄	138	244.960	1.633	3.203	1.000	0.0	138.0
C ₅	250	214.410	1.429	3.659	1.000	0.0	250.0
iC ₄	50	108.250	0.722	7.247	1.000	0.0	50.0
nC ₄	110	83.067	0.554	9.444	1.000	0.0	110.0
iC ₅	16	40.072	0.267	19.577	1.000	0.0	16.0
nC ₅	28	31.815	0.212	24.658	1.000	0.0	28.0
2MP	8	16.114	0.107	48.684	1.000	0.0	8.0
Total	885					184.4	700.6
	F_i	$K_i \pi$	K_i	$K_i V/L$	Fraction Stripped	D_i Overhead	Bottom
Toluene	750	2.6706	$1.78 \cdot 10^{-2}$	$3.40 \cdot 10^{-3}$	$3.40 \cdot 10^{-3}$	2.6	747.4
m-X	750	1.0309	$6.87 \cdot 10^{-3}$	$1.31 \cdot 10^{-3}$	$1.31 \cdot 10^{-3}$	1.0	749.0
Total	1500					3.6	1496.4
Define $(L/V)_{\text{average}} = [F/D + (F - D + G)/G]/2$							D=187.9
Calculated $(L/V)_{\text{average}} = 5.23 = \text{assumed } L/V \therefore \text{correct}$							

It is seen that a highly vaporized feed often requires more trays, or alternatively, more reflux. For a given number of trays, the feed tray location generally needs to be lowered as feed vaporization increases until a "pinch" occurs between the lower Operating Line and the Equilibrium Curve. Usually, this crossover occurs when the feed vapor rate equals the distillate rate. At this point, further feed vaporization necessitates raising the feed tray location. A further phenomenon that occurs is that, for a given number of trays, increasing feed vaporization necessitates increased reflux ratio for the specified product quality. The increase in reflux requirement can result in an increase in reboiler duty despite the higher heat content of the feed.

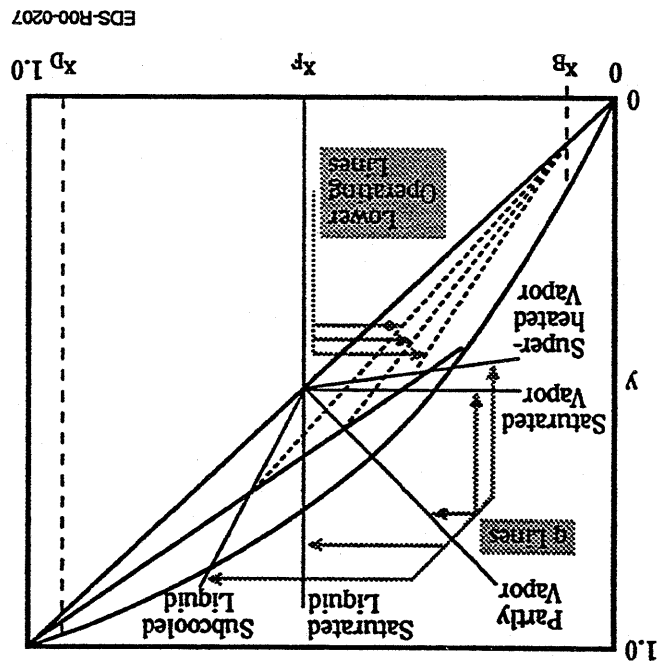


Figure 7