

Çok Komponentli Distilasyon İçin Yeni Bir Software Paket

A New Software Package for The Calculation of Multicomponent Distillation

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Bu makalede yazar tarafından geliştirilen ve yazılan, Çok Komponentli Distilasyon Hesaplamaların da başarıyla uygulaması yapılan yeni bir FORTRAN IV programı tanıtılacaktır. Söz konusu komputer programı ile ideal ve ideal olmayan çok komponentli distilasyon hesaplamaları «Değiştirilmiş Tridiagonal Matris (Modified Tridiagonal Matrix) ve Rilaksasyon (Modified Relaxation) metodları kullanılarak yapılmaktadır. Hesaplamalara esas alınan verilerde, buhar basıncı - temperatur ilişkileri için Antoine denklemi, sıvı ve buhar fazı denge şartları için Wilson ve Margules denklemleri kullanılmaktadır. Program azeotrop ve ekstraktif distilasyon problemlerini az bir hesaplama zamanı içinde büyük güvenirlilikle çözebilmekte ve birden fazla besleme akımı ve yan akım ihtiva eden kompleks distilasyon kolonlarına kolaylıkla uygulanabilmektedir.

Programın ana özellikleri ve uygulama esasları verildikten sonra bir uygulama çalışması Su - Etanol - Metanol azeotrop sistemi için yapılmıştır.

In this paper has been introduce a FORTRAN IV computer program for the calculation of multicomponent distillation which was de-

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veloped and written by the author. The proposed computer program uses the methods of the Modified Tridiagonal Matrix and Relaxation for the calculation of ideal and nonideal multicomponent distillation processes. The data of calculation are based on Antoine equation for vapor pressure - temperature relations, and Wilson and Margules equations for the conditions of vapor - liquid equilibrium. The proposed program can be applied easily to the complex distillation columns which have multi - feeds and side - cut streams and solves the problem of Extractive and Azeotropic distillation in a small computation time with a big accuracy.

After giving the main feature and principles of application, an application work is illustrated by Water - Ethanol - Methanol, azeotrope system.

Introduction and A Brief Survey on The Multicomponent Distillation

The multicomponent distillation has been most rapidly developed subject in chemical engineering science and its importance is apparent from the tremendous number of papers written on this subject. It is clear such as accumulated literature has several calculation procedures for multicomponent distillation. Those calculation procedures can be classified into four groups namely a) Stage - by - stage, b) Short - cut, c) Iteration and d) Relaxation procedures.

The first realistic and practical method of solving separation problems was stage - by - stage analysis shown by Sorel in 1893 (*La rectification de l'alcool*, Paris, 1893). The general method of stage - by - stage calculation for multicomponent systems was first shown by Lewis and Matheson [*Ind.Eng.Chem.*24.,494 (1932)] and by Underwood [*Trans. Inst. Chem. Engr. (London)* 10, 112, (1932)]. The method of Lewis and Matheson was further improved by Robinson and Gilliland [*Elements of Fractional Distillation*, 4th Ed. Mc. Graw - Hill New York, 1950].

The short - cut methods which allow determination of the number of theoretical plates as a function of reflux ratio, minimum plates, and minimum reflux are commonly used to study the effect of reflux ratio on investment and operating costs with a minimum of tedious and extensive calculations. The Colborn [*Trans. A. I. Ch. E.*, 37, 805 (1941)]. and Underwood [*Chem. Eng. Progr.* 44, 603 (1948)] minimum reflux methods are used for more accurate calculation of minimum reflux while the Brown - Martin [*Trans. A. I. Ch. E.*, 35, 679 (1939)] method can be used for safe approximations.

Iteration methods are best - suited for solution of almost the reverse problem for which stage - by - stage can be used. Iteration solutions were first proposed by Thiele and Geddes [Ind. Eng. Chem. 24, 289 (1933)]. Amundson and Potinen [Ind. Eng. Chem. 50, 730 (1958)], have proposed a general method of solution through matrices. Edmister [A. I. Ch. E. Journal 3, 165 (1957)] has solved the equations through development of a series expression relating the amount of a component at a stage to the amount in a product. The Smith [A. I. Ch. E. Journal 6, 451 (1960)], [Design of Equilibrium Stage Processes Mc. Graw - Hill, New York, 1963] and Hanson et al. [Computation of Multistage Separation Processes, Reinhold, New York, 1962] have solved the equations by a method which assumes the amount of a component in a product and calculates to the other end of the column, tracking the error made in the assumed amount can be calculated and precise corrections applied at each stage. The Lyster et al. [Pet. Ref., 38, No. 6, 221 (1959), Pet. Ref. 38, No. 7, 151 (1959), Pet. Ref. 38, No. 10, 139 (1959)] and Holland [Multicomponent Distillation, Prentice - Hall Englewood Cliffs., New Jersey, 1963] have developed correction methods to improve the calculated product compositions for complicated columns, and have worked extensively on convergence techniques, Yamada and Sugie [Studies on the Multicomponent Distillation, Bulletin of Nagoya Institute of Technology, vol. 19, pp - 517 - 528, (1967)] have proposed the Modified Successive Approximation Method, Successive Perturbation and Successive Iteration Methods.

Relaxation solutions are conceptually the most simple methods of solution for any multistage separation process. They were first proposed by Rose et al. [Ind. Eng. Chem. 50, 737 (1958)] and Duffin [Solution of Multistage Separation Problems by Using Digital Computers. Ph. D. Thesis, University of California, Berkeley, 1959]. Extension of the relaxation method to include heat balance was proposed by Hanson et al. [Computation of Multistage Separation Processes, Reinhold, New York 1962].

The above mentioned methods of calculation of multicomponent distillation processes can be programmed to the any near computer. But, the basic methods of calculation have not been improved to take adequate advantage of the rapidity and accuracy of the computing devices. Therefore, the principal advantage lies in the ability of the computer (when correctly programmed) to solve complex trial - and - error iterative calculations with ease in a short time. Generally, proposed com-

puter methods of calculation of multicomponent distillation fall into two categories which utilize the equations and approach previously described. One method involves the assumption of the component distribution in the distillate and bottoms product, the feed plate location, and the reflux ratio, and computation is carried out plate to plate from the top of the column toward the feed plate and from the bottom of the column toward the feed plate until the composition ratios or composition calculated from both directions match within designated limits in the vicinity of the feed location. The other method involves the assumption of the reflux ratio, number of plates, and the temperature profile and, starting from the feed compositions, the calculation is carried out plate to plate for the number of stages specified in the rectifying section. By repeatedly modifying the assumed temperature on each plate and repeating the calculations, the bubble or dew-point temperature for the liquid or vapor at each plate is matched. The calculation proceeds in a similar manner for the number of stages specified in the stripping section to obtain the bubble point or dew point of the vapor and liquid at each plate. If the first trial does not converge, a different number of plates, reflux ratio, or temperature profile is assumed and the calculation is repeated. (Distillation, M. V. Winkle, Mc Graw - Hill Book Company, 1967)

The Application Procedure of DISTHB Computer Program

In the design of a fractionating column essentially required information are the determination of the number of plates (or packed height) and the column diameter. The determination of the parameters of actual design is required a theoretical design which are needed following column specifications.

- Quantity, composition and thermal condition of the feed,
- Column pressure,
- Type of overhead condenser,
- Reflux ratio or (V_1 or L_0),
- Quantity of distillate and composition.

In general case the number of theoretical stages is defined by DISTHB computer program in the way of calculation as a trial and error procedure. In each trial calculation, a number of theoretical stages is assumed for the given condition of the problem which in the above mentioned data.

If the first trial does not converge, a different number theoretical stages is assumed and the application of DISTHB is repeated.

In the other cases, the DISTHB computer program can be applied to define the optimal feed conditions, reflux ratio and feed stages which are described by user as a trial specification.

The Main Feature of the Proposed Computer Program.

The main feature of the proposed computer program is written in FORTRAN IV, and called DISTHB. The main feature of the DISTHB is given by following computer output.

```

C
C .....*.....
C *
C *
C *          A NEW CALCULATION SYSTEM
C *
C *          FOR
C *
C * AN IDEAL AND A NON-IDEAL MULTICOMPONENT DISTILLATION COLUMNS *
C *
C *          WITH
C *
C *          ANY NUMBER OF SIDE-CUT STREAMS AND FEEDS
C *
C .....*.....
C
C----- THE METHOD USED IN THIS PROGRAM ARE THE MODIFIED TRIDIAGONAL
C MATRIX METHOD AND THE MODIFIED RELAXATION METHOD.
C METHOD=1 REFERS TO THE MODIFIED TRIDIAGONAL MATRIX METHOD
C WHICH IS GOOD FOR GENERAL COMPLEX COLUMNS.
C METHOD=2 REFERS TO THE MODIFIED RELAXATION METHOD WHICH IS
C GOOD FOR GENERAL COMPLEX COLUMNS, EXTRACTIVE DISTILLATION
C COLUMNS, AND AZEOTROPIC DISTILLATION COLUMNS.
C
C----- THE VAPOR-LIQUID EQUILIBRIUM RELATIONSHIPS USED IN THIS PROGRAM
C ARE THOSE OF WILSON AND MARGULES.
C NVL=1 REFERS TO THE WILSON'S METHOD.
C NVL=2 REFERS TO THE MARGULES'S METHOD.
C
C----- THE DEFENCE OF THE COVERAGE OF THIS PROGRAM-----
C THIS PROGRAM IS DESIGNATED FOR A GENERAL COMPLEX DISTILLATION
C COLUMN. THEREFORE, SOME SPECIAL COLUMNS, WHICH MAY NOT BE
C REGARDED AS A GENERAL COMPLEX COLUMN, COULD NOT BE SOLVED.
C IF SUCH OCCASION APPEARS, THE USER SHOULD REFER TO THE OTHER PROGRAM
C DEVELOPED FOR THE SPECIAL COLUMN.
C
C***** NOMENCLATURE OF INPUT DATA, *****
C
C TITLE=THE TITLE OF YOUR CALCULATION. IT SHOULD BE WRITTEN
C WITHIN 80 CHARACTERS.
C
C M=NUMBER OF COMPONENTS
C
C N=TOTAL NUMBER OF STAGES
C THE FIRST STAGE REFERS TO THE CONDENSER AND THE LAST(N-TH)
C STAGE REFERS TO THE REBOILER.
C
C NVL=PARAMETER WHICH SELECTS THE VAPOR-LIQUID EQUILIBRIUM EQUATION,
C TAKING THE VALUE OF ONE OR TWO
C
C V(1)=MOLAR FLOW RATE OF VAPOR LEAVING FROM THE CONDENSER

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The Nomenclature of Input Data for DISTHB

DISTHB computer program are composed a main program and 29 subprograms which are shown by Figure 1. The subprograms contain three types of subroutines namely a) Subprograms for reading b) Subprograms for calculation c) Subprograms for printing.

```

C
C   R=REFLUX RATIO AT THE COLUMN TOP
C
C   PAI=TOTAL PRESSURE OF THE COLUMN
C
C   F(J)=FEED MOLES AT THE J-TH STAGE
C
C   TFEED(J)=FEED TEMPERATURE AT THE J-TH STAGE
C
C   Q(J)=THERMAL FACTOR OF THE COLUMN FEED AT J-TH STAGE
C
C   Z(I,J)=FEED MOLAR COMPOSITION OF I-TH COMPONENT AT J-TH STAGE
C   WHEN F(J) IS ZERO, THE VALUES OF TFEED(J),Q(J),AND Z(I,J) ARE
C   AUTOMATICALLY SET TO ZERO. THEREFORE, THE DATA FOR TFEED(J),Q(J),
C   AND Z(I,J) ARE NECESSARY, ONLY WHEN F(J) IS NON-ZERO.
C   THE I-TH COMPONENT IS DESIGNATED AS THE ONE WHICH HAS
C   THE HIGHEST BOILING TEMPERATURE, AND THE M-TH (THE LAST)
C   IS DESIGNATED AS THE ONE WHICH HAS THE LOWEST BOILING
C   TEMPERATURE.
C
C   W(J)=MOLAR FLOW RATE OF VAPOR SIDE-CUT AT THE J-TH STAGE
C
C   U(J)=MOLAR FLOW RATE OF LIQUID SIDE-CUT AT THE J-TH STAGE
C
C   U(1)=MOLAR FLOW RATE OF LIQUID LEAVING FROM THE CONDENSER
C
C   U(N)=MOLAR FLOW RATE OF LIQUID LEAVING FROM THE REBILER
C
C   TB(I)=BOILING POINT TEMPERATURE OF THE I-TH COMPONENT
C
C   NAME=COMPOSITION NAME WHICH SHOULD BE WRITTEN WITHIN 16 CHARACTERS
C
C   MW(I,J)=CONSTANTS OF THE WILSON EQUATION OR THE MARGULES EQUATION
C   THE IDEAL MIXTURES MAY BE TREATED BY SETTING THESE CONSTANTS TO
C   UNITY FOR THE WILSON EQUATION AND TO ZERO FOR THE MARGULES EQUATION.
C
C   A(I)*B(I)*C(I)=CONSTANTS IN THE ANTOINE EQUATION
C
C----- THIS PROGRAM TERMINATES WHEN THERE IS NO DATA CAPD FOR THE READING
C   OF THE INPUT DATA. IF YOU HAVE SOME PROBLEMS TO BE SIMULTANEOUSLY
C   SOLVED, PUT THE SETS OF THE INPUT DATA TOGETHER IN ORDER.
C   THE PROBLEMS WILL BE SOLVED ONE BY ONE ACCORDING TO THE ORDER
C   OF THE INPUT DATA SET.
C
C*** THE DIMENSION SIZE IS TENTATIVELY GIVEN FOR UP TO TWENTY COMPONENTS
C   AND TWO HUNDRED STAGES. IF THE AVAILABLE MEMORIES ARE NOT
C   ENOUGH, OR IF THE PROBLEM UNDER CONSIDERATION EXCEEDS THIS LIMITATION,
C   THE APPROPRIATE CHANGE OF THE DIMENSION SIZE IS NECESSARY. ***
C
1   MMAX=20
2   MMAX=200
3   COMMO=ONE/PAI

```

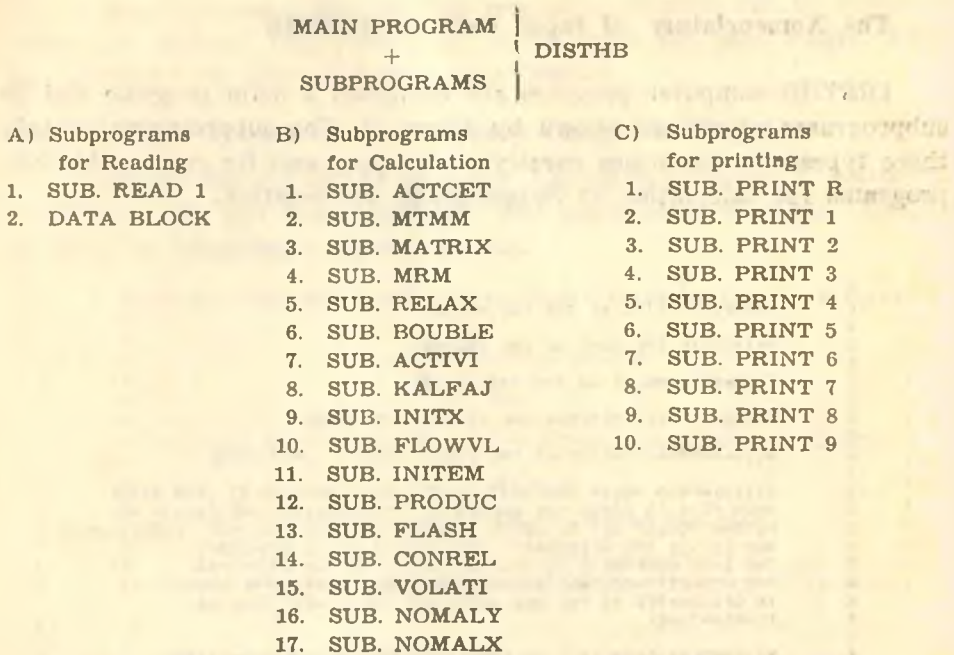


Fig. 1. The Subprograms of DISTHB computer program.

The Handling of DATA for DISTHB Computer Program

DISTHB computer program can be applied to the any digital computer which has a FORTRAN IV compiler. The organization of the DATA DECK is depends on the feature of used computer machine. The DISTHB has a organization of control card as any optimization program. It is never need special control card. But, the data can be punched into cards using the EBCDIC code: In this section the format of cards punched in EBCDIC code will be described.

In all cases, there are two types of cards in the data file:

- 1) Control cards, which are specified by computer machine,
- 2) Data cards, which contain the actual data values.

Notes on Input Data

- 1) The all integer numbers of data cards are defined by FORMAT (I5).

2) The all non - integer numbers of data cards are defined by **FORMAT (F10.3)**.

3) Only, the type of used method and the equation of vapor - liquid equilibrium relationships, and the number of components and theoretical stages are defined in integer form. The other variables are defined in non - integer form.

4) The title of searching problem and the name of components (which is discribed of composition of liquid and vapor) of data cards can be composed by alphameric and special characters.

5) The names of all components which are appearing in llth group of data cards must be composed of from 1 to 16 alphameric and special characters.

6) This program terminates when there is no data card for the reading of the input data. If, it had have been some problems to be simultaneously solved, put the sets of the input data together in order. The problems will be solved one by one according to the order of the input data set.

7) The dimension size is tetatively given for up to twenty components and two hundred stages. If, the available memories are not enough, or the problem under consideration exceeds this limitation, the appropriate change of the dimension size is necessary.

8) In this program, the measurement of design variables are defined by metric system as follows; the amount of stream (vapor and liquid) with [Kg mol], temperature with centigrate [$^{\circ}\text{C}$] and pressure with [mm Hg]

The Organization of the DATA DECK

1) A **TITLE** card is always the first card, and an **ENDATA** card is always the last card of a data deck. The **TITLE** card gives a user - specified name to the data deck. It has the following format:

	Field 1
Columns	1 — 80
Type of contents	Name assigned by user
Nomenclature	TITLE

The **TITLE** may contains from one to eighty of the following characters, in any order: A to Z, 0 (zero) to 9, . (period).

2) The **METHOD** card is always the second card and it contains 1 or 2. [1] indicates MTMM (Moddified Tridiagonal Matrix Method), [2] indicates MRM (Modifed Relaxation Method). It has the following format:

	Field 1
Columns	1 — 5
Type of contents	1 or 2
Nomenclature	METHOD

3) The **EQUATION** card is the third card and it contains 1 or 2. [1] indicates Wilson Equation, [2] indicated Margules Equation. It has the following format:

	Field 1
Columns	1 — 5
Type of contents	1 or 2
Nomenclature	EQUATION (NVL)

4) The group of fourth card contains the number of the components and the stages. It has the following format :

	Field 1	Field 2
Columns	1 — 5	6 — 10
Type of contents	number of components	number of stages
Nomenclature	M	N

5) The fifth card of data cards contains the molar flow rate of vapor which is leaving from the condenser, the reflux ration at the top of column and the total pressure of the column. It has the following format:

	Field 1	Field 2	Field 3
Columns	1 — 10	11 — 20	21 — 30
Type of contents	Molar flow rate of vapor which is leaving from condenser	Reflux ratio at the top of column	Total pressure of column
Nomenclature	V (1)	R	PAI

6) The sixth group of data is *not one card*. It depends on the number of stage. This group of data cards contain the feed moles at the each stage. If there is no feed into any stage it will be contain empty field. It has the following format and it is illustrated for three feeds.

	Field 1	Field 2	Field 3
Columns	1 — 10	11 — 20	21 — 30
Type of contents	feed moles at first stage	feed moles at second stage	feed moles at third stage
Nomenclature	F (1)	F (2)	F (3)

7) The seventh group of data cards contain the temperature of feeds, termal factor of the column feeds and molar composition of feeds. It has the following format:

The below mentioned format is illustrated for one feed and three components. When $F(J)$ is zero, the values of $TFEED(J)$, $Q(J)$, and $Z(I, J)$ are automatically set to zero. Therefore, the data for $TFEED(J)$, $Q(J)$, and $Z(I, J)$ are necessary, only when $F(J)$ is non-zero. The 1-st component is designated as the one which has the highest boiling tem-

perature, and the M - th (the last) is designated as the one which has the lowest boiling temperature.

	Field 1	Field 2	Field 3	Field 4	Field 5
Columns	1 — 10	11 — 20	21 — 30	11 — 40	41 — 50
Type of contents	Feed temperature of J-th stage	Termal factor of the columns feed at J-th stage	Feed molar composition of 1 - st component at J-th stage	Feed molar composition of 2 - nd component at J-th stage	Feed molar composition of 3 - rd component at J-th stage
Nomenclature	TFEED (J)	Q (J)	Z (1, J)	Z (2, J)	Z (3, J)

8) The 8 - th group of data cards contain the molar flow rate of vapor side-cut at the J - th stage. It has the following format, and it is illustrated for three side-cut streams.

	Field 1	Field 2	Field 3
Columns	1 — 10	11 — 20	21 — 30
Type of contents	Molar flow rate of vapor side-cut at 1 - th stage	Molar flow rate of vapor side-cut at 2 - nd stage	Molar flow rate of vapor side-cut at 3 - rd stage
Nomenclature	W(1)	W(2)	W(3)

Notice : The first stage is condenser and the last stage is reboiler.

9) The 9 - th group of data cards contain the molar flow rate of liquide side-cut at the J - th stage. It has the following format; and it is illustrated three liquid side-cut streams.

	Field 1	Field 2	Field 3
Columns	1 — 10	11 — 20	21 — 30
Type of contents	Molar flow rate of liquid side - cut 1 - st at 1 - st stage	Molar flow rate of liquid side - cut 2 - nd at 2 - nd stage	Molar flow rate of liquid side - cut 3 - rd at 3 - rd stage
Nomenclature	U (1)	U (2)	U (3)

10) The tenth card of data cards contain the boiling temperature of the components from 1. to M. It has the following format:

	Field 1	Field 2	Field 3
Columns	1 — 10	11 — 20	21 — 30
Type of contents	Boiling temp. of 1 - st component	Boiling temp. of 2nd. component	Boiling temp. of 3 rd. component
Nomenclature	TB (1)	TB (2)	TB (3)

11) The 11 - th group data contains the name of component which should be written within 16 characters. It has following format:

	Field 1	Field 2	Field 3
Columns	1 — 16	17 — 32	33 — 48
Type of contents	name of component of 1 - th	name of component of 2 - nd	name of component of 3 - rd
Nomenclature	Name assigned by user	Name assigned by user	Name assigned by user

12) The 12 - th group data of data cards contains the constants of the Wilson equation or the Margules equation. The ideal mixtures may be treated by setting these constants to unity for the Wilson equation and to zero for the Margules equation. If, it is used three suffix constants for the Wilson and Margules equations and each card uses for a component. It has following format:

for the first component			
	Field 1	Field 2	Field 3
Columns	1 — 10	11 — 20	21 — 30
Type of contents	1 - st constant of used equation	2 - nd constant of used equation	3 - rd constant of used equation
Nomenclature	WW(1, 1)	WW(1, 2)	WW(1, 3)

13) The 13 - rd group data of data cards contains the constants in the Antoine equation with (—B). It has following format and can be used up 80 columns of each card. The following illustration is for the first component and other components can take places in the same data cards.

	Field 1	Field 2	Field 3
Columns	1 — 10	11 — 20	21 — 30
Type of contents	1 - st constant of Antoine Eq. for 1 - st component	2 - nd constant of Antoine Eq. for 1 - st component	3 - rd constant of Antoine Eq. for 1 - st component
Nomenclature	A(1)	A(2)	A(3)

The Handling of the Required Information of the DISTHB Computer Program for Applications

The above mentioned 13 groups data are classified into three classes namely a) to determine the name of illustrated problem, used equations and methods which are 1, 2, 3, and 11, of data, b) to determine the given parameters of distillation column which are 4, 5, 6, 7, 8, 9 and 10 groups of DATA c) to determine the constant of used equations which are 12 and 13 groups of DATA.

The first classe of the groups of DATA is indicated by the distillation type, such as azeotropic, extractive distillation etc. The second classe is indicated by the column conditions, the third classe is indicated by the constants of the used equations and methods. Therefore some parts of DATA can be determine by given problem, other parts must be handling from the data books which are THE THERMAL FACTOR of FEEDS of COLUMN, CONSTANTS of ANTOINE, WILSON and MARGULES.

The determination of the thermal factor of feeds of column, and constants of Antoine, Wilson and Margules

The thermal factor of feeds of column can be calculated by using following three equations, those equations are driven by using «The principec of constant rate of molar vaporisation of the Mc. Cabe-Thiele.

- a) driven based on the amount of liquid phase

$$q = \frac{L - L}{F} \quad (1)$$

- b) driven based on the amount of vapor phase

$$q = 1 - \frac{V - \bar{V}}{F} \quad (2)$$

- c) driven based on the enthalpy of the liquid and vapor phase

$$q = \frac{H_f - h_f}{H_v - h_v} \quad (3)$$

The nomenclature of the used symbol in Eq. (1), (2), (3)

q : Thermal factor in DISTHB program Q

L : Molar amounts of liquid which is coming into feed stage,

\bar{L} : Molar amounts of liquid which is going down from feed stage

F : Feed stream

V : Molar amounts of vapor which is going up from feed stage

\bar{V} : Molar amounts of vapor which is coming into feed stage

H_f : Enthalpy of vapor which is going up from feed stage

h_f : Enthalpy of liquid which is coming into feed stage

h_f : Enthalpy of feed stream

Figure 2 are shown the condition of feeds in five cases as the following,

a) Feed is liquid at boiling point $q=1$

b) Feed is cold liquid $q>1$

c) Feed is saturated vapor $q=0$

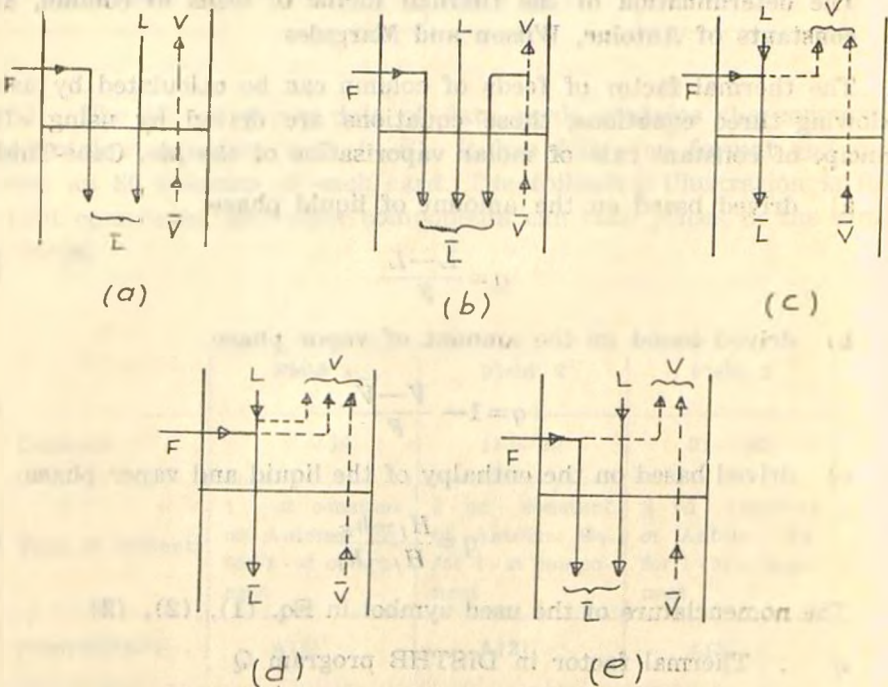


Fig. 2. Illustration of condition of feeds

d) Feed is superheated vapor $q < 0$ and negative

e) Feed is mixture of liquid and vapor $0 < q < 1$

Three illustrations are given by the following examples.

Example 1: (for the *b* case) Calculate the thermal factor of feed for the given conditions.

C_p : 30 Btu/(lb - mol) (°F)

λ_v : 900 Btu/lb mol (latent heat)

T_F : 400°F

$$q = \frac{C_p T_F + \lambda_v}{\lambda_v} = 1 + \frac{C_p T_F}{\lambda_v} = 1 + \frac{30 \times 40}{900} = 1.13$$

Example 2: (for the *d* case) Calculate the thermal factor of feed for the given conditions.

C_p : 14 Btu/(lb mol) (°F)

T_F : 50°F

λ_v : 900 Btu/lb mol

$$q = \frac{C_p (-T_F)}{\lambda_v} = \frac{(14)(-50)}{900} = -0.078$$

Example 3: (for the *e* case) calculate the thermal factor of feed for the given condition.

Condition : Feed includes 40% liquid and 60% vapor

$$q = \frac{\bar{L} - L}{F} \quad \bar{L} - L = F \times 0.40, \quad q = \frac{F \times 0.40}{F} = 0.40$$

Notice : in such as condition q is always equal to liquid %

Determination of Reflux Ratio :

The reflux ratio is determined by $R = \frac{L_0}{D}$

R : Reflux ratio on top of column

D : Moles of top product (mol kgr)

L_0 : Moles of reflux stream (mol kgr)

Determination of the constants of Antoine Equation

Vapor pressure and temperature are commonly related by means of the Antoine Equation [Compt. Rend. Acad. Sci., Paris, 107: 681, 836, 1143 (1888) |

$$\text{Log } P = A - \frac{B}{C + t}$$

where, A, B, and C are constants for a particular compound over a relatively narrow temperature range (usually not over 100°C). Values of these constant for various compounds and families of compounds and the temperature ranges for which the constants apply appear in a number of references. Dreisbach [Physical Properties of Chemical Compounds I, II and III. Am. Chem. Soc. Advan. chem. ser., nos 15(1955); 22(1959); 29(1961)], API Project Report No. 44 [«Selected values of physical and Thermodynamic Properties of Hydrocarbons and Related compounds,» Carnegie Press, Pittsburgh, 1953]. Perry [Chemical Engineers' Handbook, 3 rd. ed., Mc Graw-Hill, 1950], and others present either the Antoine constants, tabular vapor pressure data, or both.

An example : Determine of the constants of Antoine Equ. for ethylbenzene,

Solution : The three points of data permit the direct solution for a set of Antoine constants by algebraic means. An alternative method described in Dreisbach can be used. The constant C is solved for first by the empirical formula :

$$C = 239 - 0.19 t_n$$

Pressure, mm Hg	Temperature, °C	
	Ethylbenzene	Ethyl cyclohexane
760	136.19	131.78
100	74.1	69.04
30	46.7	41.50

where t_n is the normal boiling points. The three linear equations can then be solved for the best values of A and B.

For ethylbenzene,

$$\log P = A - \frac{B}{t + C}$$

$$C = 239 - 0.19(136.19) = 213.12$$

$$B_{12} = \frac{\log(P_2/P_1)}{(1/(t_1 + C)) - 1/(t_2 + C)} = \frac{0.52288}{1/259.82 - 1/287.22} = 1424.1$$

$$B_{11} = 1423.7 \quad B_{21} = 1423.3 \quad B_{av} = 1423.7$$

substituting directly for A,

$$A_1 = 6.95668 \quad A_2 = 6.95683 \quad A_3 = 6.95656 \quad A_{av} = 6.9567$$

For ethyl cyclohexane the solution is identical

Tabulated Results for Ethylbenzene

Source or method	Antoine constants		
	A	B	C
Direct algebraic solution	9.093	3007.6	384.722
Dreisbach's method	9.9567	1423.7	213.12
Published values	6.95719	1424.255	213.206

Determination of the constants of Margules and Wilson Equations:

The values of these constants for various compounds and families of compounds and the temperature and pressure ranges for which the constants apply appear in a number of references.

It can be recommended the following references for the handling of the constants of Margules Equation.

- 1 — J.H. Perry, Chemical Engineers' Handbook section 13-6, Table 13-4, 1963 4 th Edition
- 2 — Joffe, J., Ind. Eng. Chem. 47:2553 (1953)
- 3 — E. Hála, I. Wichterle, J. Polák and T. Boublik «Vapour - Liquid Equilibrium Data at Normal Pressures Pergamon Press Ltd. 1968.
- 4 — Null, R.H., Phase Equilibrium in Proces Design Wiley-Interscience, 1970

It can be recommended the following references for the handling of the constants of Wilson Equation.

- 1 — Wilson, A and Simms, E.D., Ind. Eng. Chem., 44, 2214 (1952)
- 2 — Null, R.H., Phase Equilibrium in Process Design, Wiley-Interscience, 1970
- 3 — Winkle, V.M., Distillation, Mc - Graw - Hill 1967
- 4 — Frank C., Radice Jr., Analysis of Some Modeling Equations used in the Prediction of Multicomponent Equilibrium Data, Univ. of R.I. Prof. Harold N. Knickle 368 pp. On file Univ. of R.I. Loan copi available Univ. Microfilm

The Type of Applications of DISTHB Computer Program

- 1 — For the design of any kind of distillation columns
 - a) Ideal systems
 - b) non-ideal systems
 - c) Azeotropic distillation
 - d) Extractive distillation
 - e) Some special distillation
- 2 — Re - design of any working distillation columns
- 3 — Design of Distillation systems for solvent recovery

The sample problem : A continous fractionating column operating at 760 mm Hg is to be designed to separate 1 mol kgr/hr of a solution of water, ethanol and methanol, containing 0.50 mole fraction water, 0.30 mole fraction ethanol, and 0.20 mole fraction methanol. The top product will be 0.50 mol kgr/hr. A reflux ratio of 3.0 mol kgr of reflux per mol kgr of product is to be used. The feed will be liquid at its boiling point, and the reflux will be returned to the column containing 0.5 mol kgr vapor at boiling point. The theoretical stage number is 11 include condenser and reboiler.

- a) Determine the stage variables
- b) Calculate the composition of top and bottom products
- c) Determine the liquid composition profile
- d) Determine the vapor composition profile
- e) Determine the relative volatility profile

The Handling DATA by a Special Form

The data sheet of DISTHB computer program is prepared within three pages which are illustrated as a following;

The first page of data sheet contains TITLE, METHOD, NVL, M, N, V(1), R, PAI, and F(J), TFEED (J) and Q(J)

The second page of data sheet contains W(J), U(J), Z(I, J) and TB

The third page of data sheet contains the constants of Antoine Equ. and Margules or Wilson Equ.

SHEET of DATA
(Distillation)

TITLE	Case 1, Water - Ethanol - Methanol		
METHOD	2	Modified Relaxation Method	
NVL	2	Margules equation	
M =	3	N = 11	
V (1) =	0.5	R = 3	PAI = 760 mmHg

(J)	F (J)	TFEED (J)	Q (J)
6	1 mol kgr/mm	75 °C	1

J	1	11
Akım		
W (J)	0.5	0
U (J)	0	0.5

I Z(I, J)	1	2	3	4	5	6	7	8	9	10
Z(1, 6)	0.5									
Z(2, 6)		0.2								
Z(3, 6)			0.3							
TB	100.	78.	64.							

Vapor pressure Antoine equ. $\text{LOG}(P) = A + B/(T + C)$

Gempr No.	A	B	C
1	7.967	-1668.210	228.00
2	8.045	-1554.300	222.65
3	7.879	-1473.110	230.00

Activity Coefficient

J J	1	2	3
1	0.0	0.421	0.231
2	0.778	0.0	0.0
3	0.378	0.0	0.0

CASE NO-1

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.....
.  CALCULATION OF DISTILLATION  .
.      FOR                      .
.  GENERAL COLUMN COLUMNS    .
.  AND                         .
.  EXTRACTIVE DISTILLATION    .
.  COLUMNS                    .
.  BY                           .
.  MODIFIED TRIANGULAR MATRIX  .
.  METHOD OR                     .
.  MODIFIED RELAXATION METHOD  .
.....

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THIS PROGRAM IS DESIGNATED FOR THE CALCULATION OF A MULTICOMPONENT DISTILLATION COLUMN WITH ANY NUMBER OF SIDE-CUT STREAMS AND FEEDS.

THE METHOD USED IN THIS PROGRAM IS THE MODIFIED TRIANGULAR MATRIX METHOD WHICH IS DEVELOPED FOR EXTENDING THE APPLICABILITY OF THE ORIGINAL METHOD TO THE NON-IDEAL MIXTURES BY USING THE PRINCIPLES OF THE PERTURBATION.

THE VAPOR-LIQUID EQUILIBRIUM RELATIONSHIPS USED IN THIS PROGRAM ARE THOSE OF WILSON AND MARGULES. NVL=1 REFERS TO THE WILSON EQUATION. NVL=2 REFERS TO THE MARGULES EQUATION.

THE IDEAL DISTILLATION COLUMN MAY BE REGARDED AS A SPECIAL CASE OF THE NON-IDEAL DISTILLATION COLUMN. THE SOLUTION MAY BE OBTAINED BY SETTING THE VALUES OF THE CONSTANTS OF THE WILSON EQUATION AND THE MARGULES EQUATION TO UNITY AND ZERO RESPECTIVELY.

COMPONENT	NO.	% A * E
	1	WATER
	2	ETHANOL
	3	METHANOL

THE CONVERGENCE CRITERIA IS SET BY THE FOLLOWING CONDITION.

THE RELATIVE VOLATILITIES AND THE TEMPERATURE ON EACH STAGE CONVERGE FROM THE INITIAL VALUES TO THE FINAL SOLUTIONS USING THE PRINCIPLES OF THE PERTURBATION. THE MEAN SQUARE TEMPERATURE FLUCTUATION SHOULD BE LESS THAN 0.01. FURTHERMORE, THE ABSOLUTE PERCENTAGE PERTURBED VALUES OF THE RELATIVE VOLATILITIES ON ALL STAGES SHOULD BE LESS THAN 2 %.

CASE NO.1

*** INPUT DATA ***

TOTAL NUMBER OF STAGES 11
 TOP PRODUCT AMOUNT 0.500000 (KG-MOL/HR)
 BOTTOM PRODUCT AMOUNT 0.500000 (KG-MOL/HR)
 REFLUX RATIO 3.000000
 TOTAL PRESSURE 160.000000 (MM-HG A)

FEED

FEED STAGE NO.	COMP. NO.	MOL FLOW	MOL FRACTION	FEED CONDITION
	1	0.3000	0.3000	1.000
	2	0.2000	0.2000	
	3	0.3000	0.3000	
	TOTAL	1.0000	(AG=MOL/HR)	

CASE NO.1

COMP. NO.	ANTOINE CONSTANTS		
	A	B	C
1	0.7966810E 03	-0.1668210E 04	0.2280000E 03
2	0.8064940E 03	-0.1558300E 04	0.2226500E 03
3	0.7878630E 03	-0.1473110E 04	0.2300000E 03

COMP. NO.	ACTIVITY COEFFICIENTS		
	1	2	3
1	0.0	0.210000E 00	0.2310000E 00
2	0.7780000E 00	0.0	0.0
3	0.3780000E 00	0.0	0.0

CASE NO.1

1-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	75.0	75.0	75.0	75.0	75.0	75.0	75.0	75.0	75.0	75.0
X(1,J)	J=2	0.282	0.309	0.324	0.332	0.337	0.413	0.413	0.414	0.414	0.414
X(1,J)	J=3	0.274	0.272	0.270	0.268	0.266	0.235	0.235	0.235	0.235	0.235
X(1,J)	J=3	0.444	0.419	0.406	0.400	0.397	0.352	0.351	0.351	0.351	0.351
2-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	72.3	72.7	72.9	73.0	73.1	74.0	74.0	74.0	74.0	74.0
X(1,J)	J=2	0.183	0.203	0.215	0.222	0.229	0.267	0.268	0.268	0.268	0.268
X(1,J)	J=3	0.269	0.288	0.298	0.304	0.301	0.258	0.258	0.258	0.258	0.258
X(1,J)	J=3	0.548	0.509	0.487	0.474	0.431	0.375	0.375	0.374	0.374	0.287
3-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	70.7	71.2	71.5	71.7	72.4	73.5	73.5	73.5	73.5	74.0
X(1,J)	J=2	0.124	0.140	0.150	0.166	0.248	0.352	0.352	0.352	0.381	0.456
X(1,J)	J=3	0.244	0.275	0.295	0.314	0.309	0.264	0.264	0.264	0.305	0.310
X(1,J)	J=3	0.632	0.588	0.556	0.500	0.443	0.384	0.384	0.384	0.313	0.234
4-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	69.5	70.1	70.5	71.3	72.2	73.3	73.3	73.3	74.2	75.5
X(1,J)	J=2	0.084	0.098	0.133	0.180	0.246	0.349	0.349	0.366	0.396	0.473
X(1,J)	J=3	0.213	0.250	0.290	0.312	0.308	0.264	0.264	0.308	0.343	0.334
X(1,J)	J=3	0.702	0.653	0.576	0.507	0.446	0.387	0.387	0.326	0.262	0.193
5-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	68.5	69.1	70.1	71.2	72.1	73.2	73.2	74.0	74.9	76.1
X(1,J)	J=2	0.057	0.090	0.132	0.183	0.247	0.349	0.361	0.378	0.407	0.486
X(1,J)	J=3	0.182	0.241	0.286	0.304	0.306	0.263	0.304	0.344	0.313	0.395
X(1,J)	J=3	0.760	0.670	0.582	0.508	0.447	0.388	0.335	0.278	0.220	0.159
6-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	67.7	68.4	70.1	71.2	72.1	73.2	73.9	74.6	75.5	76.6
X(1,J)	J=2	0.052	0.040	0.134	0.183	0.247	0.359	0.371	0.387	0.414	0.497
X(1,J)	J=3	0.173	0.236	0.283	0.308	0.305	0.299	0.334	0.370	0.398	0.371
X(1,J)	J=3	0.775	0.674	0.584	0.509	0.448	0.382	0.291	0.238	0.166	0.132
7-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	67.5	68.4	70.1	71.1	72.1	73.4	74.5	75.2	75.9	77.0
X(1,J)	J=2	0.052	0.041	0.134	0.183	0.259	0.365	0.378	0.394	0.422	0.505
X(1,J)	J=3	0.169	0.234	0.281	0.307	0.341	0.321	0.357	0.391	0.412	0.378
X(1,J)	J=3	0.779	0.676	0.585	0.510	0.441	0.314	0.265	0.215	0.166	0.117
8-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	67.5	68.4	70.1	71.1	72.7	74.2	74.8	75.5	76.2	77.2
X(1,J)	J=2	0.052	0.041	0.134	0.195	0.266	0.370	0.383	0.399	0.427	0.512
X(1,J)	J=3	0.167	0.232	0.280	0.340	0.364	0.335	0.374	0.403	0.421	0.382
X(1,J)	J=3	0.780	0.677	0.586	0.465	0.370	0.296	0.247	0.199	0.152	0.107
9-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	67.5	68.4	70.1	71.7	73.1	74.4	75.0	75.7	76.4	77.4
X(1,J)	J=2	0.052	0.041	0.145	0.203	0.271	0.373	0.380	0.402	0.431	0.518
X(1,J)	J=3	0.166	0.231	0.311	0.364	0.381	0.344	0.380	0.411	0.427	0.383
X(1,J)	J=3	0.783	0.678	0.584	0.432	0.348	0.282	0.239	0.187	0.143	0.100
10-TH ITERATION											
TEMPERATURE											
X(1,J)	J=1	67.5	68.4	70.1	72.1	73.4	74.6	75.4	75.9	76.5	77.5
X(1,J)	J=2	0.052	0.100	0.153	0.209	0.275	0.376	0.389	0.405	0.434	0.523
X(1,J)	J=3	0.166	0.258	0.335	0.383	0.393	0.352	0.387	0.417	0.431	0.383
X(1,J)	J=3	0.782	0.642	0.512	0.408	0.332	0.272	0.224	0.178	0.136	0.095

THE TOTAL ITERATIONS= 81

CASE NO.1

*** SOLUTION ***

***** STAGE VARIABLES *****

STAGE	TEMP.	LIQUID	VAPOR
1(COND)	70.039	0.15000E 01	0.0
2	71.663	0.15000E 01	0.20000E 01
3	72.863	0.15000E 01	0.20000E 01
4	73.737	0.15000E 01	0.20000E 01
5	74.437	0.15000E 01	0.20000E 01
6	75.230	0.25000E 01	0.20000E 01
7	75.837	0.25000E 01	0.20000E 01
8	76.435	0.25000E 01	0.20000E 01
9	77.091	0.25000E 01	0.20000E 01
10	78.306	0.25000E 01	0.20000E 01
11(REB)	84.456	0.0	0.20000E 01

CASE NO.1

***** PRODUCT AMOUNTS *****

STAGE	COMP	MOL FLOW	MOL FR.
1(TOP PRODUCT)			
	1	0.050340	0.1006797
	2	0.160706	0.3214112
	3	0.288955	0.5779091
11(BOTTOM PRODUCT)			
	1	0.449459	0.8989178
	2	0.039487	0.0789750
	3	0.011054	0.0221072

CASE NO.1

***** LIQUID COMPOSITION PROFILE *****

COMP.	1	2	3
STAGE			
1 (COND)	0.100680E 00	0.321411E 00	0.277909E 00
2	0.146735E 00	0.398286E 00	0.454978E 00
3	0.190361E 00	0.442740E 00	0.566899E 00
4	0.235948E 00	0.456971E 00	0.507031E 00
5	0.293467E 00	0.440246E 00	0.266267E 00
6	0.388445E 00	0.378512E 00	0.233043E 00
7	0.401759E 00	0.409676E 00	0.188565E 00
8	0.419513E 00	0.432825E 00	0.147663E 00
9	0.457059E 00	0.432471E 00	0.110470E 00
10	0.598206E 00	0.330307E 00	0.714861E-01
11 (REB)	0.898918E 00	0.789750E-01	0.221072E-01

***** VAPOR COMPOSITION PROFILE *****

COMP.	1	2	3
STAGE			
1 (COND)	0.641120E-01	0.240380E 00	0.695510E 00
2	0.100680E 00	0.321412E 00	0.277910E 00
3	0.135221E 00	0.379067E 00	0.485713E 00
4	0.167940E 00	0.412407E 00	0.419654E 00
5	0.202168E 00	0.423080E 00	0.374754E 00
6	0.245284E 00	0.410535E 00	0.344181E 00
7	0.260725E 00	0.453490E 00	0.285785E 00
8	0.277367E 00	0.492446E 00	0.230187E 00
9	0.299559E 00	0.521380E 00	0.179060E 00
10	0.346487E 00	0.520934E 00	0.132568E 00
11 (REB)	0.522894E 00	0.393196E 00	0.838310E-01

***** RELATIVE VOLATILITY PROFILE *****

COMP.	1	2	3
STAGE			
1 (COND)	0.100000E 01	0.117446E 01	0.188996E 01
2	0.100000E 01	0.117614E 01	0.185125E 01
3	0.100000E 01	0.120531E 01	0.186367E 01
4	0.100000E 01	0.126821E 01	0.192073E 01
5	0.100000E 01	0.139509E 01	0.204319E 01
6	0.100000E 01	0.171763E 01	0.233890E 01
7	0.100000E 01	0.170572E 01	0.233542E 01
8	0.100000E 01	0.172080E 01	0.235777E 01
9	0.100000E 01	0.183938E 01	0.247307E 01
10	0.100000E 01	0.272235E 01	0.320133E 01
11 (REB)	0.100000E 01	0.855614E 01	0.651755E 01

***** PROBLEM SOLVED *****