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A computer program for the design of packed extraction columns

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A COMPUTER PROGRAM FOR THE
DESIGN OF PACKED EXTRACTION COLUMNS

BY

GEORGE P. GACCIONE

A THESIS

PRESENTED IN PARTIAL FULFILLMENT OF

THE REQUIREMENTS FOR THE DEGREE

OF

MASTER OF SCIENCE IN CHEMICAL ENGINEERING

AT

NEWARK COLLEGE OF ENGINEERING

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Newark, New Jersey

June, 1970

APPROVAL OF THESIS

A COMPUTER PROGRAM FOR THE
DESIGN OF PACKED EXTRACTION COLUMNS

BY

GEORGE P. GACCIONE

FOR

DEPARTMENT OF CHEMICAL ENGINEERING
NEWARK COLLEGE OF ENGINEERING

BY

FACULTY COMMITTEE

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ABSTRACT

A computer program for the design of packed extraction columns has been developed. This program can operate with a minimum of data of the type that can easily be determined or estimated. The program can be used to investigate design alternates during the preparation of project cost estimates and for the final design of extraction columns.

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INTRODUCTION

The objective of the work summarized in this presentation is the development of a computer program for the design of a packed extraction column. A computer program was developed, since the calculations necessary for the specification of a packed extraction column are lengthy and tedious, especially if a number of design parameters must be estimated and if alternative designs are investigated. The program developed will simplify the investigation of design alternates and will allow the study of the effect of variations in the basic parameters on column design.

Much work has been done on the development of calculation procedures for the design of packed columns. Treybal (13) has summarized these and suggested which equations are the most useful. He has also reviewed the empirical and theoretical correlations for the estimation of the parameters needed in the design equations, if these parameters have not been determined experimentally. The equations and calculation methods given in his book are the basis for the work presented in the section covering the development of the design equations, pages 5 to 43.

Calculation procedures for the estimation of the following

parameters have been included:

1. The equilibrium slope; equations (1) to (35), pages 6 to 10.
2. The extract diffusion coefficient; equation (85), page 30.
3. The mass transfer coefficient for the extract; equations (86) and (87), page 35.
4. The raffinate diffusion coefficient; equation (84), page 30.
5. The mass transfer coefficient for the raffinate; equations (91) to (93), page 36.

The equations used for calculations are based on three major assumptions. The first of which is that a ternary system is involved. The second is that the two solutions associated with the ternary are dilute. The third and final assumption is that the extract is the dispersed phase.

The computer program developed, allows the design of a column from the data input shown in Table 15, page 116. The allowed variations in the type of input are given in the discussion of data input on pages 47 to 50.

The program calculates a column design for solvent flows of 1.2 to 3.0 times the minimum solvent rate, in increments of 0.2. This is done for each packing size greater than the critical packing size and gives ten runs for each size of packing. A typical computer print out for 0.75 inch Raschig Rings is given in Table 10, page 111.

In addition to the development of a computer program, several runs were made to determine the effect of parameters such as solvent rate, etc., on column design. The results of these runs are discussed in detail on pages 55 to 58, and are plotted in Figures (6) through (14), pages 96 to 104.

The major conclusions reached from the above runs were:

1. For a given ratio of extract to raffinate flow, the height of a transfer unit and the number of transfer units are independent of packing size.
2. The tower cost drops off rapidly, with increasing ratios of extract to raffinate flows, until the ratio of extract flow to minimum extract flow is 1.6; then

the cost begins to level. Therefore, ratios larger than 1.6, should not be used for design purposes.

3. Variations in raffinate viscosity and the mutual solubility of the extracting solvent and raffinate solvent have no significant effect on column design.
4. The column cost decreases with decreasing solvent viscosity or interfacial tension.
5. The column cost also decreases with increasing density difference between the extract and raffinate phases.

EQUATION DEVELOPMENT

The equations used for design calculations can be divided into three categories; equations developed by Treybal (13); equations developed from correlations presented by Treybal in the form of a graph, and equations derived by the author for use in the program.

No attempt will be made to derive the equations suggested by Treybal, since their derivations are presented in his book. However, the limitations placed on the design program by the assumptions made in their derivations will be detailed.

The major equations developed for use in the design program include the equations for the conversion of concentration to a weight fraction basis from a mole fraction basis (equations (36) - (37), page 10); the equation for the determination of the minimum solvent rate (equation (41), page 13); the equation for the calculation of the extract composition (equation (49), page 14), and the equations for the calculation of the cost of a packed extraction column (equations (104) - (111), pages 40 to 42).

Estimation of Distribution Coefficient

The first value to be determined is the distribution coefficient. If the distribution coefficient for the ternary system under study has not been determined experimentally, it can be estimated from the mutual solubility data for the three binary pairs of the ternary mixture. First, equations (1) through (27) are used to calculate the constants for the two suffix van laar equations (14) of activity coefficients, for each of the binary pairs.

The following equations are used for the calculation a-b binary constants.

$$Y_1 = x_{aa1} / x_{ba} + x_{ab} / x_{bb1} \quad (1)$$

$$Y_2 = \text{Log}(x_{ab} / x_{aa1}) / \text{Log}(x_{ba} / x_{bb1}) \quad (2)$$

$$Y_3 = 2 x_{aa1} x_{ab} \text{Log}(x_{ab} / x_{aa1}) \quad (3)$$

$$Y_4 = x_{ba} x_{bb1} \text{Log}(x_{ba} / x_{bb1}) \quad (4)$$

$$\frac{A_{ab}}{A_{ba}} = (Y_1 Y_2 - 2) / (Y_1 - Y_3 / Y_4) \quad (5)$$

$$Y_5 = \text{Log}(x_{ab} / x_{aa1}) \quad (6)$$

$$Y_6 = (1 + (A_{ab} x_{aa1} / A_{ba} x_{ba}))^2 \quad (7)$$

$$Y_7 = (1 + (A_{ab} x_{ab} / A_{ba} x_{bb1}))^2 \quad (8)$$

$$A_{ab} = Y_5 / (1/Y_6 - 1/Y_7) \quad (9)$$

The equations for the b-c binary constants are obtained by applying the rotation principle, i. e., substituting b for a and c for b, in equations (1) through (9).

$$Y_8 = x_{bb2} / x_{cb} + x_{bc} / x_{cc1} \quad (10)$$

$$Y_9 = \text{Log}(x_{bc} / x_{bb2}) / \text{Log}(x_{cb} / x_{cc1}) \quad (11)$$

$$Y_{10} = 2 x_{bb2} x_{bc} \text{Log}(x_{bc} / x_{bb2}) \quad (12)$$

$$Y_{11} = x_{cb} x_{cc1} \text{Log}(x_{cb} / x_{cc1}) \quad (13)$$

$$\frac{A_{bc}}{A_{cb}} = (Y_8 Y_9 - 2) / (Y_8 - Y_{10} / Y_{11}) \quad (14)$$

$$Y_{12} = \text{Log}(x_{bc} / x_{bb2}) \quad (15)$$

$$Y_{13} = (1 + (A_{bc} x_{bb2} / A_{cb} x_{cb}))^2 \quad (16)$$

$$Y_{14} = (1 + (A_{bc} x_{bc} / A_{cb} x_{cc1}))^2 \quad (17)$$

$$A_{bc} = Y_{12} / (1/Y_{13} - 1/Y_{14}) \quad (18)$$

The equations for the a-c binary constants are obtained by substituting c for a and b for c, in equations (10) through (18).

$$Y_{15} = x_{cc2} / x_{ac} + x_{ca} / x_{aa2} \quad (19)$$

$$Y_{16} = \text{Log}(x_{ca} / x_{cc2}) \text{Log}(x_{ac} / x_{aa2}) \quad (20)$$

$$Y_{17} = 2 x_{cc2} x_{ca} \text{Log}(x_{ca} / x_{cc2}) \quad (21)$$

$$Y_{18} = x_{ac} x_{aa2} \text{Log}(x_{ca} / x_{aa2}) \quad (22)$$

$$\frac{A_{ca}}{A_{ac}} = (Y_{15} Y_{16} - 2) / (Y_{15} - Y_{17} / Y_{18}) \quad (23)$$

$$Y_{19} = \text{Log}(x_{ca} / x_{cc2}) \quad (24)$$

$$Y_{20} = (1 + (A_{ca} x_{cc2} / A_{ac} x_{ac}))^2 \quad (25)$$

$$Y_{21} = (1 + (A_{ca} x_{ca} / A_{ac} x_{aa2}))^2 \quad (26)$$

$$A_{ca} = Y_{19} / (1/Y_{20} - 1/Y_{21}) \quad (27)$$

Once the binary constants are determined, they are substituted into equations 28 through 32. These equations are used because of the length of the ternary Van Laar equation (equation (33)) for the solute activity coefficient, given by Treybal (15).

$$Y_{22} = x_a A_{ca} (A_{ac} / A_{ca})^2 \quad (28)$$

$$Y_{23} = x_b A_{cb} (A_{bc} / A_{cb})^2 \quad (29)$$

$$Y_{24} = x_a x_b (A_{ac} / A_{ca}) (A_{bc} / A_{cb}) \quad (30)$$

$$Y_{25} = A_{ca} + A_{cb} - A_{ba} (A_{cb}/A_{bc}) \quad (31)$$

$$Y_{26} = (x_c + x_a (A_{ac}/A_{ca}) + x_b (A_{bc}/A_{cb}))^2 \quad (32)$$

$$\text{Log } \gamma_c = (Y_{22} + Y_{23} + Y_{24} + Y_{25})/Y_{26} \quad (33)$$

Treybal has shown (16) that, if dilute solutions are assumed, equation (33) and the mutual solubility data for the a-b binary can be used to calculate the distribution coefficient (m'). The assumption of dilute solutions is the basis for the equations used in the design program.

If the solute concentration (x_c) is set equal to zero, the mutual solubility data for the a-rich layer of the a-b binary can then be substituted into equation (33) and $\text{Log } \gamma_{ca}$ calculated. The substitution of the data for the b-rich layer will give $\text{Log } \gamma_{cb}$. Equation (34) below is then used to calculate the distribution coefficient.

$$m' = 10^{(\text{Log } \gamma_{ca} - \text{Log } \gamma_{cb})} \quad (34)$$

The distribution coefficient calculated using (34) is on a mole fraction basis. Since all the calculations performed in the design program are on a weight fraction basis, the distribution coefficient must be converted to that basis. This is accomplished

simply if it can be assumed that extract solvent (b-component) and the raffinate solvent (a-component) are relatively insoluble. This is a valid assumption for most industrial systems since, if a significant solubility exists, a more expensive recovery system would be required. The following equation is used to convert the distribution coefficient calculated from equation (34) on the preceding page to a weight fraction basis (4).

$$m = m' M_a / M_b \quad (35)$$

Calculation of the Minimum Solvent Rate

Before the minimum solvent rate is calculated, the mole fractions of the components of the feed and solvent have to be converted to a weight fraction basis. Equation (36) will be used for the extract concentration and equation (37) for the raffinate concentration.

$$X_{ce} = x_{ce} M_c / (x_{ce} M_c + (1 - x_{ce}) M_b) \quad (36)$$

$$X_{cr} = x_{cr} M_c / (x_{cr} M_c + (1 - x_{cr}) M_a) \quad (37)$$

Another check is necessary before proceeding with the solvent calculations, since it is possible that the solvent proposed for a given

extraction process may already contain the solute it is desired to recover. As an absolute minimum, the solute concentration in the solvent should not be in equilibrium with the raffinate from the column. This will be checked with the following equation.

$$X_{ce2} \leq m X_{cr2} \quad (37A)$$

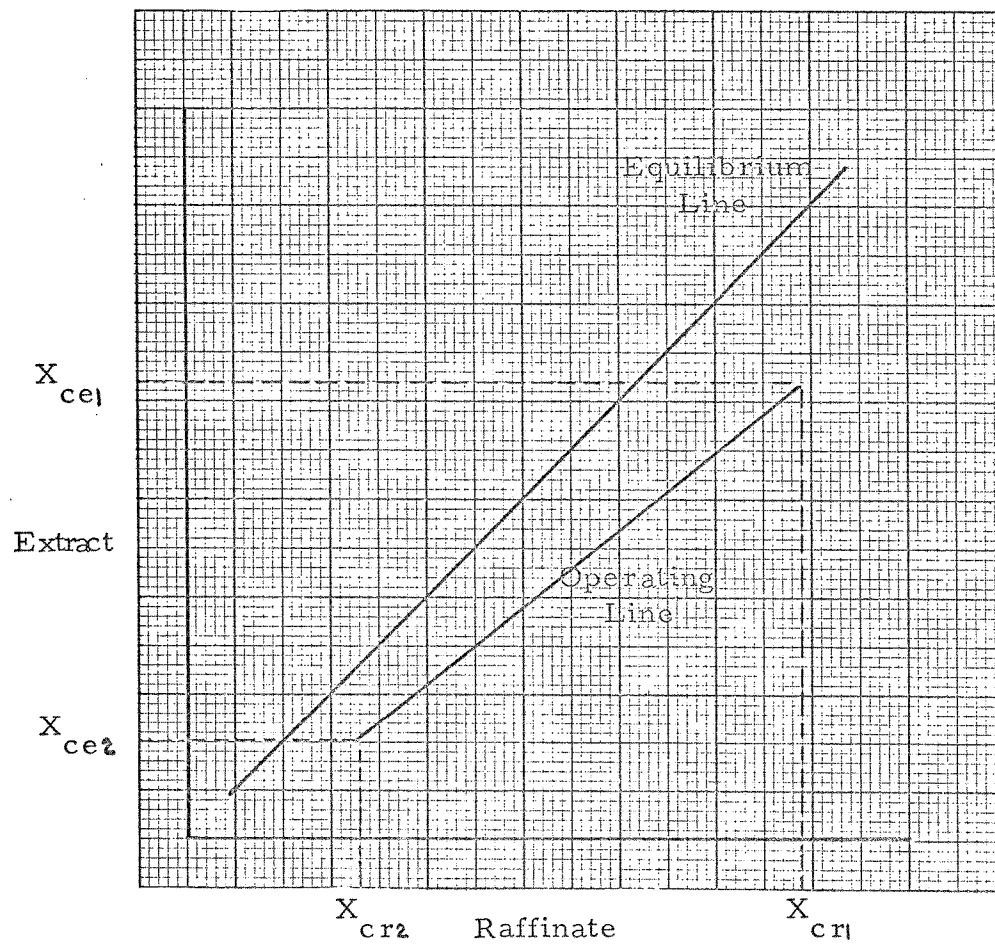
The minimum solvent rate must be determined, before the operating ratio of solvent to feed (E_2 / R_2) can be fixed. The operating line of Figure 1, page 12, gives the following material balance.

$$R_2 (X_{cr1} - X_{cr2}) = E_2 (X_{ce1} - X_{ce2}) \quad (38)$$

Since dilute solutions are assumed, the extract flow (E_2) and the feed to the column (R_2) can be used without causing a significant error. Both R_2 and E_2 do not vary appreciably throughout the column. R_2 and E_2 are also used, since the transfer units are normally concentrated at the dilute end. The slope of the operating line can be described as

$$R_2 / E_2 = (X_{ce1} - X_{ce2}) / (X_{cr1} - X_{cr2}) \quad (39)$$

FIGURE 1
OPERATING DIAGRAM FOR
CONTINUOUS COUNTERCURRENT EXTRACTION



The minimum solvent rate occurs when the operating line intersects the equilibrium line (see Figure 1, page 12). This determines the minimum solvent rate since at this point the extract flow from the column is in equilibrium with the feed. The following then holds.

$$X_{ce1} = m X_{cr1} \quad (40)$$

Equations (39) and (40) are combined to give the equation for the minimum solvent rate.

$$(E_2)_{\min} = R_2 / ((m X_{cr1} - X_{ce2}) / (X_{cr1} - X_{cr2})) \quad (41)$$

Calculation of Extract and Raffinate Rates

Once the minimum solvent rate has been determined, the ratio of actual extract flow to minimum extract flow (G_1) can be determined. A column would actually be designed for a flow greater than the minimum. The design program will investigate designs for ratios of 1.2 to 3.0 times the minimum. The ratio is described by

$$G_1 = E_2 / (E_2)_{\min} \quad (42)$$

The operating ratio of extract to raffinate (P) is then given by

$$P = G_1 (E_2)_{\min} / R_2 \quad (43)$$

The raffinate flow from the column (R_2) is calculated by,

$$R_2 = R_1 - (X_{cr1} - X_{cr2})R_1 \quad (44)$$

while the solvent feed (E_2) and extract (E_1) rates can be calculated from

$$E_2 = R_2 P \quad (45)$$

$$E_1 = E_2 + R_1 (X_{cr1} - X_{cr2}) \quad (46)$$

Also, once the solvent flow to the column has been calculated, the concentration of the extract leaving the column (X_{ce1}) can be determined by

$$Y_{27} = R_1 (X_{cr1} - X_{cr2}) + R_2 P X_{ce2} \quad (47)$$

$$Y_{28} = R_1 (X_{cr1} - X_{cr2}) + R_2 P \quad (48)$$

$$X_{ce1} = Y_{27} / Y_{28} \quad (49)$$

The next step in the calculations will be the determination of the critical packing size.

Critical Packing Size

For each combination of feed and extracting solvent, there exists a minimum packing diameter or critical packing size (19). For Raschig Rings and Berl Saddles, the following equation holds.

$$d_{fc} = 0.24 (\sigma / \Delta \rho)^{0.5} \quad (50)$$

Treybal (19), recommends that the packing size selected be greater than critical packing diameter (d_{fc}), since for packing diameters equal to or less than d_{fc} the mean drop diameter d_p of the dispersed phase droplets is dependent upon dispersed phase flow rate. The design program will calculate a column design for the packing sizes greater than d_{fc} up to a packing diameter of 3.0 inch.

Dispersed Phase Hold-up and Flooding Velocities

There are two related criteria to be concerned with when determining the diameter of a packed extraction column. The

first concerns dispersed phase hold-up (ϕ_d) and the second column flooding. Treybal (20) has indicated that for packing sizes greater than d_{fc} the diameter of the dispersed phase droplets is relatively independent of the dispersed phase flow rates. The dispersed phase hold-up increases linearly with flow rate, up to transition point where droplets begin to coalesce and hold-up begins to increase sharply. For design purposes, it is necessary that the dispersed phase hold-up be less than that at transition since efficient mass transfer cannot occur when the dispersed phase droplets coalesce. For packed columns, the hold-up at transition is given by (21),

$$\phi_{dt} = (((P_1)^2 + 8P_1)^{0.5} - 3P_1) / 4(1 - P_1) \quad (51)$$

The ratio of volumetric flow rates (P_1) in equation (51) above is calculated from

$$(V_r)_{av} = (R_1 + R_2) / 2\rho_r \quad (52)$$

$$(V_e)_{av} = (E_1 + E_2) / 2\rho_e \quad (53)$$

$$P_1 = (V_e)_{av} / (V_r)_{av} \quad (54)$$

Many correlations are available for the calculation of flooding velocities. Treybal (22) recommends two correlations for flooding calculations, with one being specific for cases where the continuous phase is water. The second correlation (3) which does not have this restriction will be used and is presented in Figure 2, page 18. The equations below represent the coordinates of Figure 2.

FA = Flooding Abscissa

$$= (V_{rf}^{0.5} + V_{ef}^{0.5})^2 \rho_r / a_f \mu_r \quad (55)$$

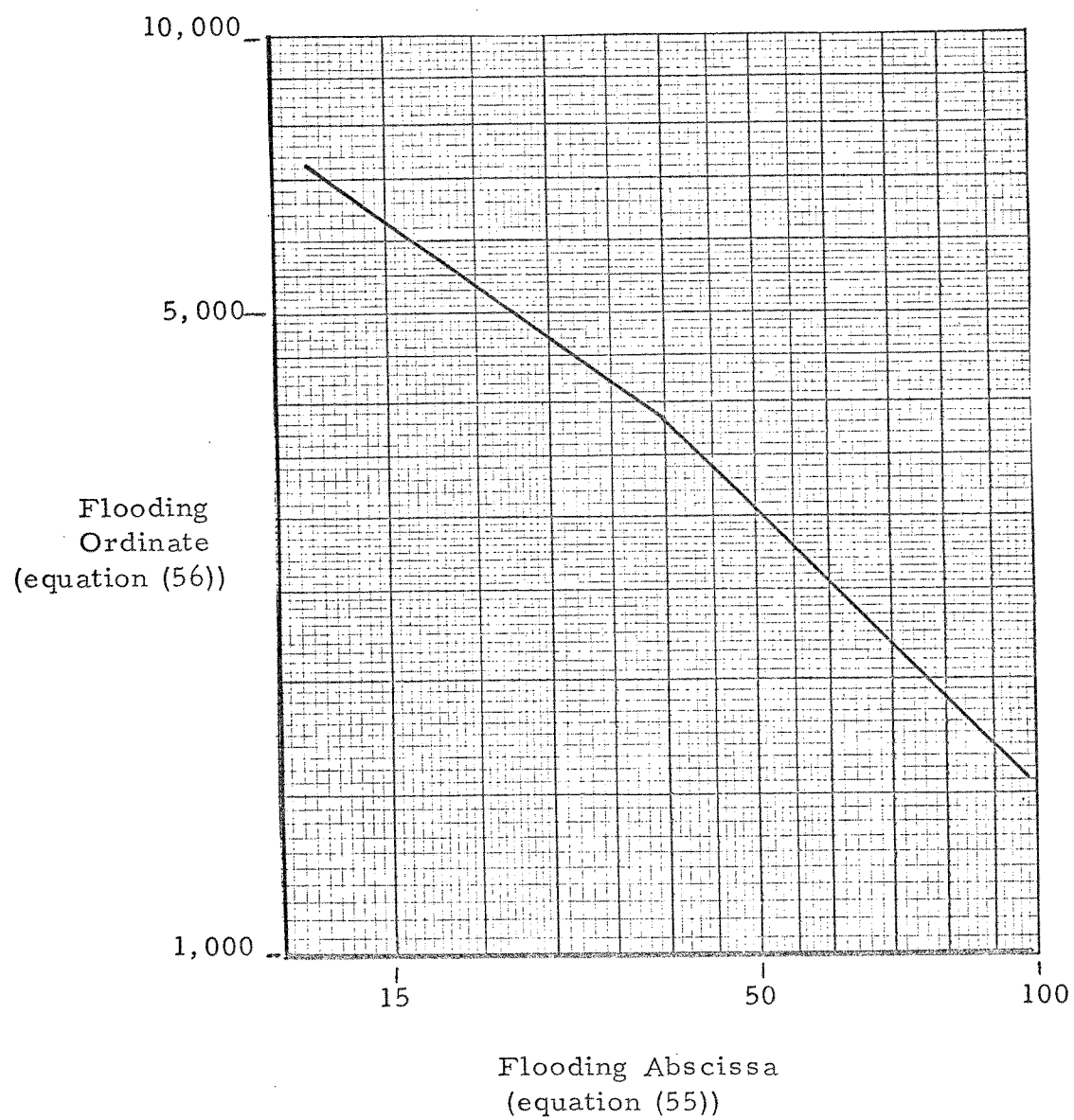
FO = Flooding Ordinate

$$= (28,700 / \rho_r)^{0.2} (2.42 \mu_r / \rho_r - \rho_e) (a_f / \epsilon)^{1.5} \quad (56)$$

The curved line of the original correlation was approximated by two straight lines, for which equations have been developed. Since Figure 2 is plotted on log-log paper, it is of the form

$$y = a x^b \quad (57)$$

FIGURE 2

FLOODING IN A PACKED TOWER (3)

The slope (b) and the y intercept (a) were calculated and the equations rearranged to give

$$FA = (140,000/FO)^{1.02} \quad \text{for } 160 \leq FO \leq 3,800 \quad (58)$$

$$FA = (54,000/FO)^{1.39} \quad \text{for } 3,800 < FO \leq 54,000 \quad (59)$$

Since the ratio of the flow rates of the raffinate and extract at flooding must equal the ratio of volumetric rates calculated in equation (54), the following relationship of flooding velocities holds

$$P_1 = V_{ef}/V_{rf} \quad (60)$$

Equation (55) and equation (60) were combined and rearranged to give the equation used for calculating the raffinate flooding velocity.

$$V_{rf} = (2.42 a_f \mu_r (FA)) / (1 + (P_1)^{0.5})^2 \rho_r \quad (61)$$

The extract flooding rate can be calculated from

$$V_{ef} = V_{rf} P_1 \quad (62)$$

The calculation method used is as follows:

- (a) FO is calculated from equation (56).
- (b) FA is calculated from equation (58) or equation (59).
- (c) The raffinate flooding velocity V_{rf} is calculated from equation (61).
- (d) The extract flooding velocity V_{ef} is then calculated from equation (62).

Once the flooding rates and the dispersed phase hold-up at transition have been determined, the calculation of tower diameter can proceed.

Calculation of Tower Diameter

Before the tower diameter can be calculated, design bases must be established. The design criteria to be established concern the allowable limits for both the dispersed phase hold-up and superficial velocities of the raffinate and extract.

The upper limit of dispersed phase hold-up has already been determined and is the hold-up at transition (equation (51)). The lower limit will be set arbitrarily at $\phi_d = 0.05$.

The extract superficial velocity will be set at between 45 and 60 percent of the extract flooding rate. The only limitation on the raffinate velocity will be that it be less than 60 percent of flooding. Design velocities for extraction columns are generally set lower than those for absorption towers, since the correlations for mass transfer in extraction columns are not as highly developed as those for absorption. The lower operating velocities will allow for design inaccuracies.

The method of calculation will be as follows:

- (a) To start with, a dispersed phase hold-up of

$$\phi_d = 0.15 \text{ will be assumed.}$$

- (b) The superficial velocities for extract (V_e) and raffinate (V_r) will then be computed and compared to the limits set above.

- (c) The dispersed phase hold-up will be increased, if V_e and V_r are too small, or decreased, if V_e and V_r are too large, in increments of 0.1.

- (d) The superficial velocities will then be calculated again.

This procedure will be repeated until V_e and V_r are within the

prescribed range. The dispersed phase hold-up values will also be limited to the range of variation previously set up for it. The detailed calculation procedures for the superficial velocities will be covered next.

Since the superficial velocities for the extract and raffinate must be in the same ratio (P_1) as the volumetric flow rates given by equation (54). The following then holds

$$P_1 = V_e / V_r \quad (63)$$

For values of dispersed phase hold-up less than that at transition the following relationship (23) holds

$$V_k (1 - \phi_d) = V_e / \epsilon \phi_d + V_r / \epsilon (1 - \phi_d) \quad (64)$$

Where V_k is defined as a limiting mean drop velocity at $V_r = 0$, for low values of V_e . Equations (63) and (64) can be combined to give

$$V_k / V_r = 1 / (\epsilon \phi_d (1 - \phi_d)) + 1 / (P_1 \epsilon (1 - \phi_d)^2) \quad (65)$$

To simplify subsequent calculations a new ratio will be defined as

$$P_2 = V_k / V_e \quad (66)$$

Once P_2 has been calculated, the mean drop diameter can be calculated from (24),

$$d_p = 0.00762 (\sigma' / \rho_r - \rho_e)^{0.5} (P_2 \epsilon \phi_d) \quad (67)$$

Next the dimensionless value P_3 (25) will be calculated from

$$P_3 = 1644 (\rho_r)^2 (\sigma')^3 / (\mu_r)^4 (\rho_r - \rho_e) \quad (68)$$

The terminal drop velocity (V_t) will be determined next. Treybal recommends using the Hu-Kintner (6) correlation for the calculation of V_t , which is then used to calculate the characteristic drop velocity (V_k). Once V_k has been calculated, the superficial velocities can then be calculated from equations (66) and (63) since P_2 and P_1 are known.

The correlation for V_t is the log-log plot shown in Figure 3, page 25. The curve of the original correlation can be approxi-

mated by three straight lines, without causing significant calculation errors. The ordinate of Figure 3 is

TVO = Terminal Velocity Ordinate

$$= 19,400 (\rho_r - \rho_e) d_p^2 (P_3)^{0.15} / \sigma \quad (69)$$

TVA = Terminal Velocity Abscissa

$$= V_t d_p \rho_r / 2.42 \mu_r (P_3)^{0.15} \quad (70)$$

The value of TVO calculated from equation (69) is then substituted into the appropriate equation developed from the correlation given in Figure 3, page 25. These equations are

$$TVA = 0.26 (TVO)^{1.25} \quad \text{for } 3.0 \leq TVO < 7.2 \quad (71)$$

$$TVA = 0.6 (TVO)^{0.8} \quad \text{for } 7.2 \leq TVO < 78.0 \quad (72)$$

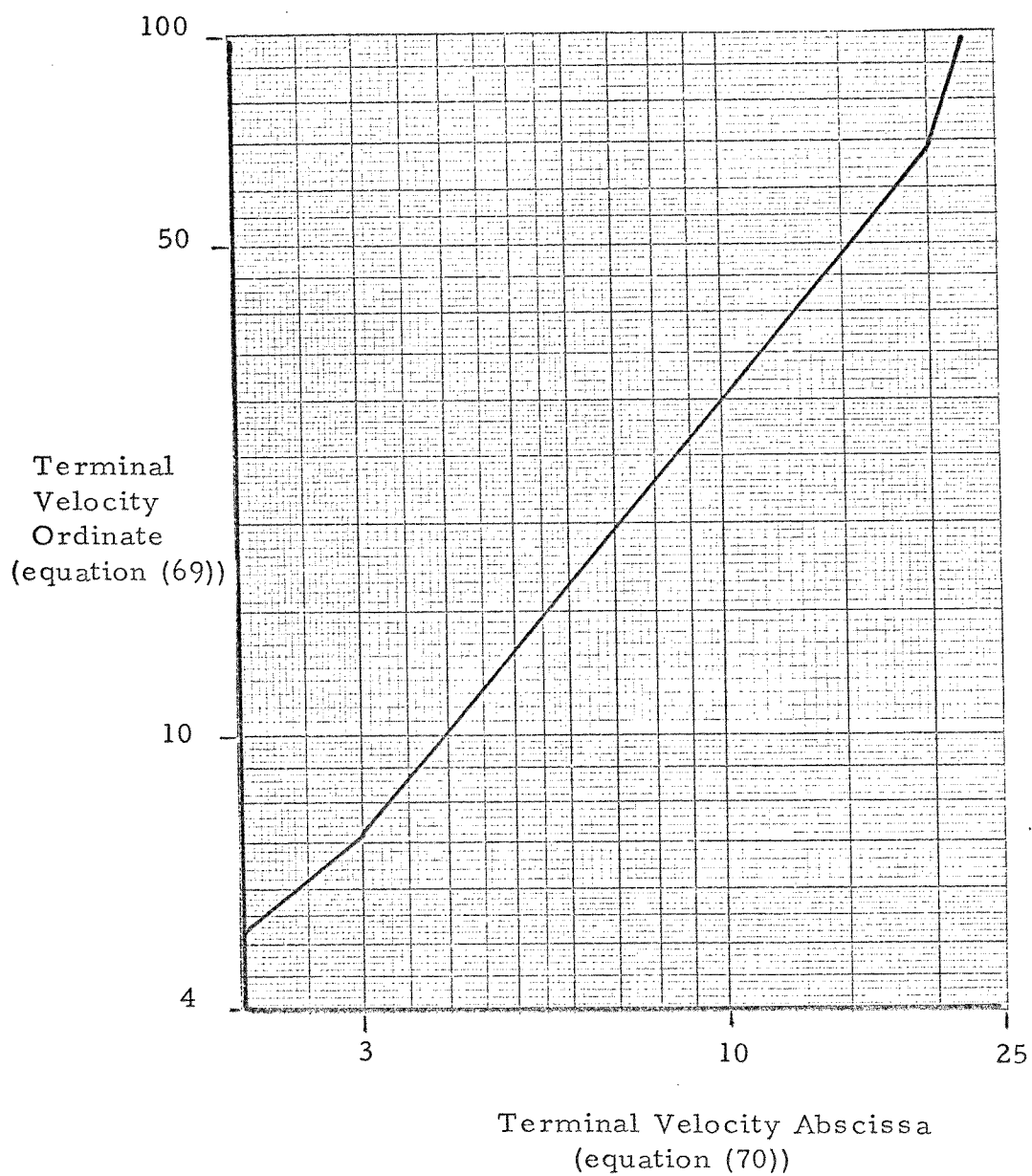
$$TVA = 3.4 (TVO)^{0.424} \quad \text{for } 78.0 \leq TVO \leq 1000.0 \quad (73)$$

Equation (70) can be rearranged and solved for V_t , which gives

$$V_t = 2.42 (TVA) \mu_r (P_3)^{0.15} / d_p \rho_r \quad (74)$$

FIGURE 3

TERMINAL VELOCITY CORRELATION FOR
LIQUID DROPS (6)



The value of TVA calculated is then substituted into equation (74) and V_t calculated.

Once the terminal drop velocity (V_t) has been calculated, the characteristic drop velocity (V_k) can be calculated. This is accomplished by means of the correlation (4) presented in Figure 4, page 28. The slightly curved line of the original correlation can be represented by a straight line, without any significant error. The ordinate of Figure 4 is given by,

$$Y_{29} = 4.18 \times 10^8 (\rho_r - \rho_e) / \rho_e V_t^2 \quad (75)$$

$$Y_{30} = (0.38 d_f - 7.62 \times 10^{-3}) (\sigma' / \rho_r - \rho_e)^{0.5} \quad (76)$$

$$V_k^0 = Y_{29} Y_{30} \quad (77)$$

While the abscissa is given by,

$$V_k A = (V_k / V_t) (1 - e^{-7.2T}) \quad (78)$$

For packed tower diameters (T) greater than 0.5 ft; the term $(1 - e^{-7.2T})$ in equation (78), can be neglected. Equation (78)

then becomes

$$V_k A = V_k / V_t \quad (79)$$

The correlation given in Figure 4, page 28, is in the form of a semi-logarithmic plot which is described by

$$y = a e^{cx} \quad (80)$$

The correlation given in Figure 4, when put in the form of equation (80) gives

$$V_k A = \ln(V_k 0 / 0.028) / 6.42 \quad (81)$$

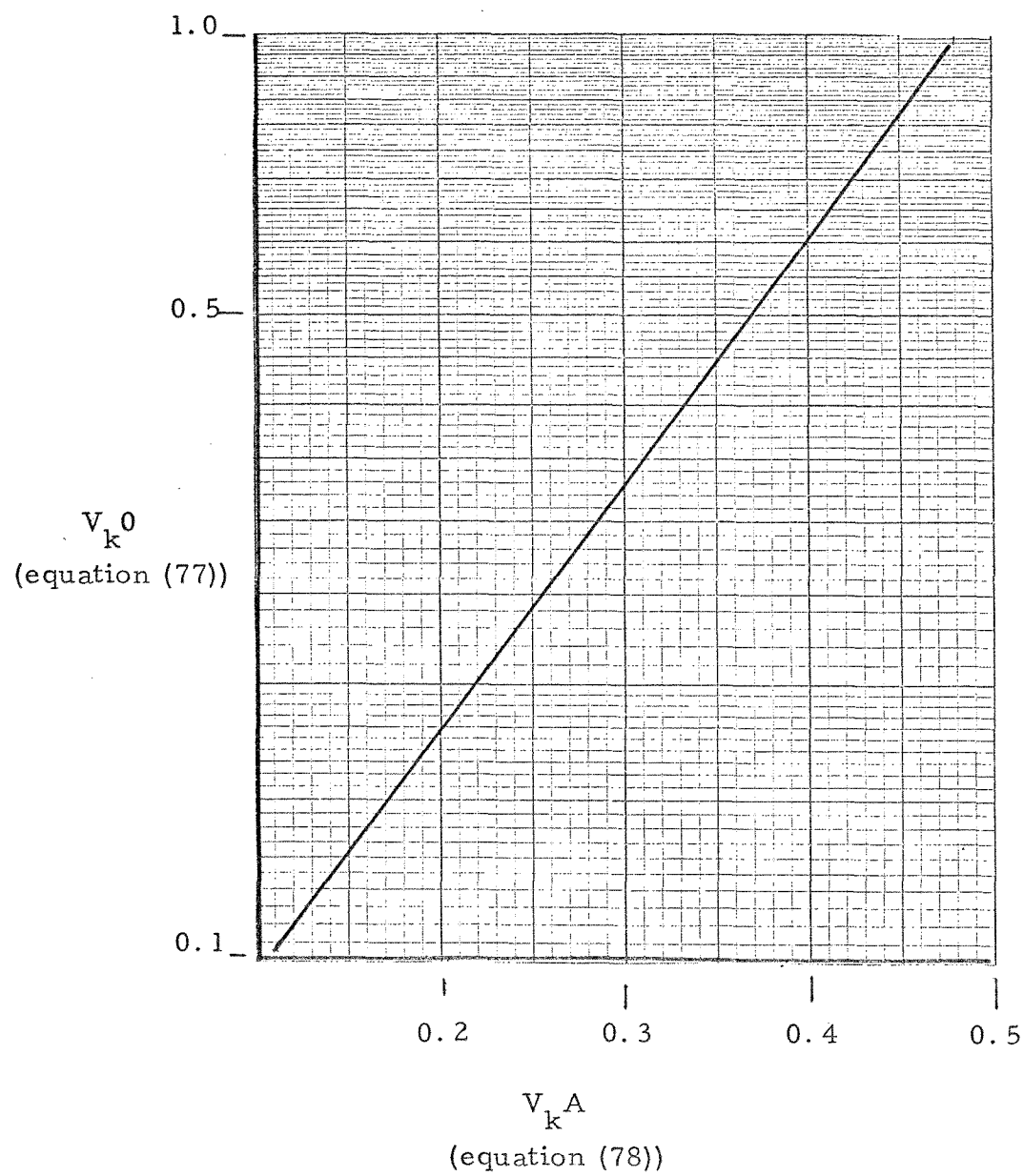
The value of $V_k 0$ calculated from equation (77) is then substituted into equation (81) for calculation of $V_k A$. Equation (79) can be rearranged to give

$$V_k = V_t (V_k A) \quad (82)$$

$V_k A$ is then substituted into equation (82) and V_k calculated.

Once the characteristic drop velocity (V_k) has been calculated, the extract superficial velocity (V_e) and the raffinate superficial

FIGURE 4
CHARACTERISTIC DROP VELOCITIES
FOR PACKINGS (4)



velocity (V_r) can be calculated from

$$V_e = V_k / P_2 \quad (83)$$

$$V_r = V_e / P_1 \quad (84)$$

Where P_2 is calculated from equation (66), page 23, and P_1 is calculated from equation (54), page 16, the superficial velocities calculated are then compared to the flooding velocities to see if they are within the previously prescribed limits (see page 20). If they are not, the dispersed phase hold-up (ϕ_d) value is adjusted and the superficial values recalculated. This process is repeated until the superficial velocities are within the prescribed range. The above, as stated before, is subject to the limits set on the dispersed phase hold-up ($0.05 \leq \phi_d < \phi_{dt}$).

Estimation of Diffusion Coefficient

Once the tower diameter has been calculated, the next variable to be determined is the height of packing required. In order to do this, the extract phase and raffinate phase mass transfer coefficients (k_e , k_r) must be calculated. Before the

mass transfer coefficients can be determined, the diffusion coefficient for the solute in the raffinate (D_{cr}) and the diffusion coefficient for the solute in the extract (D_{ce}) must be calculated.

Theoretical approaches to the problem of calculating diffusion coefficients have not succeeded, so Treybal (26) recommends the use of the following empirical correlation developed by Wilke and Chang (34, 35).

$$D_{ab} = 7.4 \times 10^{-8} (\varphi M_b)^{0.5} T_l / \mu (V_a)^{0.6} \quad (83)$$

The above gives diffusivities with units of sq cm/sec, which must be converted to the English system. After conversion to the English system and a change of subscripts to conform to previous usage, the diffusivity of the solute in the raffinate is given by

$$D_{cr} = 2.87 \times 10^{-7} (\varphi_a M_a)^{0.5} T_l / \mu_r V_c^{0.6} \quad (84)$$

The diffusivity of the solute in the extract is then

$$D_{ce} = 2.87 \times 10^{-7} (\varphi_b M_b)^{0.5} T_l / \mu_e V_c^{0.6} \quad (85)$$

The solvent association factor (φ) used in equation (84) and (85) can be found from Table 1, page 32. The molal volume (V_c) of the solute may be estimated by using Kopp's Law. This law states that the molal volume of a molecule at its normal boiling point is equal to the sum of the atomic volumes of its constituents. Table 2, page 33, is a list of atomic volumes and Table 3, page 34, is a list of molecular volumes. Both tables are used for the estimation of the solute molecular volumes.

Equations (84) and (85) may only be used for dilute solutions of solute, which is one of the basic assumptions of the design program. In addition, they cannot be used for solutions of electrolytes; where a chemical reaction occurs, or where complexes are formed.

Once the diffusion coefficients are estimated, the calculation of the mass transfer coefficient can proceed.

Calculation of Height of Dispersed Phase Transfer Unit

Treybal (27) recommends two correlations for the calculation of dispersed phase mass transfer coefficients, with the

TABLE 1
SOLVENT ASSOCIATION FACTORS (ψ)

<u>(ψ)</u>	<u>Solvent</u>
2.6	Water
1.9	Methyl Alcohol
1.5	Ethyl Alcohol
1.0	Benzene
1.0	Ethyl Ether
1.0	Heptane
1.0	For unassociated solvents such as Benzene, etc.

TABLE 2
ATOMIC VOLUMES FOR COMPLEX MOLECULES

	<u>Atomic Volume</u>		<u>Atomic Volume</u>
Bromine	27.0	Nitrogen, in secondary amines	12.0
Carbon	14.8	Oxygen (except as noted below)	7.4
Chlorine	24.6	Oxygen, in methyl esters	9.1
Hydrogen	3.7	Oxygen, in methyl ethers	9.9
Iodine	37.0	Oxygen, in higher ethers and esters	11.0
Nitrogen, double bonded	15.6	Oxygen, in acids	12.0
Nitrogen, in primary amines	10.5	Sulfur	25.6
For three-membered ring, as in ethylene oxide, deduct			0.6
For four-membered ring, as in cyclobutane, deduct			8.5
For five-membered ring, as in furan, thiophene, deduct			11.5
For pyridine, deduct			15
For benzene ring, deduct			15
For naphthalene ring, deduct			30
For anthracene ring, deduct			47.5

TABLE 3

MOLECULAR VOLUMES FOR SIMPLE SUBSTANCES

<u>Substance</u>	<u>Molecular Volume</u>	<u>Substance</u>	<u>Molecular Volume</u>
H ₂	14.3	N ₂ O	36.4
O ₂	25.6	NH ₃	25.8
N ₂	31.2	H ₂ O	18.9
Air	29.9	H ₂ S	32.9
CO	30.7	COS	51.5
CO ₂	34.0	Cl ₂	48.4
SO ₂	44.8	Br ₂	53.2
NO	23.6	I ₂	71.5
D ₂ O*	20.0		

*Estimated Value

basis for choosing between the two being the diameter of the dispersed phase droplets (d_p). For values of d_p greater than the transition size for terminal velocity (d_{pt}), the correlation of Handlos and Barron (5) will be used, with the substitution of $V_k (1 - \phi_d)$ for V_t .

$$k_e = 0.00375 V_k (1 - \phi_d) / (1 + \mu_e / \mu_r) \quad (86)$$

For values of $d_p < d_{pt}$, the correlation of Spells (12) will be used, where

$$k_e = 17.9 D_{ce} / d_p \quad (87)$$

In order to use equations (86) and (87), the transition drop size (d_{pt}) must be calculated. The following equation suggested by Treybal (28) will be used for calculation of d_{pt} .

$$d_{pt} = 0.006 (\sigma' / (\rho_r - \rho_e) P_3^{0.15})^{0.5} \quad (88)$$

Before the height of the dispersed phase transfer unit can be calculated, the interfacial liquid surface associated with free hold-up must be calculated from (29),

$$a = 6 \epsilon \phi_d / d_p \quad (89)$$

The height of a dispersed phase transfer unit is then calculated from (30, 10),

$$H_{te} = V_e / k_e a \quad (90)$$

Calculation of Height of Continuous Phase Transfer Unit

For the calculation of the continuous phase mass transfer coefficient, Treybal (31) recommends the following correlation of Ruby and Elgin (11), with $V_k (1 - \phi_d)$ replacing V_s .

$$Y_{31} = (d_p (1 - \phi_d) \rho_r / 2.42 \mu_r)^{-0.43} \quad (91)$$

$$Y_{32} = (2.42 \mu_r / \rho_r D_{cr})^{0.58} \quad (92)$$

$$k_r = 0.725 (Y_{31}) (Y_{32}) V_k (1 - \phi_d)^2 \quad (93)$$

The height of a continuous phase transfer unit is then calculated from (30, 10) the following

$$H_{tr} = V_r / k_r a \quad (94)$$

Once the raffinate and extract mass transfer coefficient are

determined, the height of an overall transfer unit can be calculated.

Calculation of Height of Overall Transfer Unit

The equation used for the calculation of the height of an overall transfer unit depends on which resistance is controlling, either the continuous or dispersed phase. In cases where the dispersed phase resistance is controlling, or $H_{te} < H_{tr}$, the following is used.

$$H_{toe} = H_{te} + (m V_e / V_r) H_{tr} \quad (95)$$

Conversely, in cases where the continuous phase resistance is controlling, or $H_{tr} < H_{te}$, the following is used.

$$H_{tor} = H_{tr} + (V_r / m V_e) H_{te} \quad (96)$$

No attempt has been made to correct equations (95) and (96) for axial mixing, since both Treybal (30) and Li and Ziegler (7) concur on the fact; that while a great deal of work has been done on axial mixing, no useful design correlations have been developed. Because of this, no attempt has been made to

correct the height of an overall transfer unit for axial mixing.

Calculation of the Number of Overall Transfer Units

Since the assumption of dilute solutions has been made, the number of overall transfer units can be calculated directly, without performing a graphical integration. The number of transfer units based on raffinate is calculated from

$$Y_{33} = (X_{cr1} - (X_{ce2}/m)) / (X_{cr2} - (X_{ce2}/m)) \quad (97)$$

$$N_{tor} = \ln (Y_{33}(1-1/F) + 1/F) / (1-1/F) \quad (98)$$

The number of transfer units based on the extract is calculated from

$$Y_{34} = (X_{ce1} - mX_{cr2}) / (X_{ce2} - mX_{cr2}) \quad (99)$$

$$N_{toe} = \ln (Y_{34}(1-F) + F) / (1-1/F) \quad (100)$$

The extraction factor (F) in equations (98) and (100) is calculated from

$$F = m P \quad (101)$$

The operating ratio of extract to raffinate flow rate (P) is obtained from equation (43), page 14.

Calculation of Packed Height

For cases where the dispersed phase resistance is controlling, the height of packing is given by

$$HOP = H_{toe} N_{toe} \quad (102)$$

Where the continuous phase resistance is controlling the height of packing is given by

$$HOP = H_{tor} N_{tor} \quad (103)$$

Calculation of Packed Tower Cost

In order to compare different design alternates, the tower cost for each alternate will be calculated. The first step is to calculate the cost of the packing. The unit cost of the packing can either be found in cost estimating information such as that presented by Peters (8) or may be obtained directly from a packing manufacturer such as U. S. Stoneware. The packed volume (PV) is

calculated as follows.

$$PV = 0.785 (\text{HOP}) T^2 \quad (104)$$

The packing cost (PC) is then calculated by

$$PC = PV (\text{dollars/cu ft}) \quad (105)$$

Since the main purpose of calculating the cost of the tower is the comparison of design alternates, as to effect on column cost, some simplifying assumption concerning the tower design will be made. First, it will be assumed that the wall thickness will be 0.375 inches and that this thickness will not vary with column height. Secondly, it will be assumed that the column has flat heads. The third assumption was that items such as nozzles, hand holes, and thermowells would add ten percent to the weight of the column. The fourth assumption was the allowance of three feet of column before and after the packed section. The density of metal used is 488 lbs per cu ft. The weight of the heads is calculated as follows

$$\begin{aligned} \text{Heads (lbs)} &= \text{No. Heads} \times \text{Thickness} \times \text{Density} \times \text{Area} \times 1.1 \\ &= 26.4 T^2 \end{aligned} \quad (106)$$

The weight of the shell is calculated from

$$\begin{aligned} \text{Shell (lbs)} &= \text{Shell Cross Section} \times \text{Column Ht.} \times \text{Density} \times 1.1 \\ &= 421 (\text{HOP} + 6) ((T + 0.0313)^2 - T^2) \end{aligned} \quad (107)$$

The weight of the column is given by

$$\begin{aligned} \text{Tower Weight} &= \text{TW} \\ &= 26.4T^2 + 421 (\text{HOP} + 6) ((T + 0.0313)^2 - T^2) \end{aligned} \quad (108)$$

The fabrication cost of the column can be calculated from the costs presented by Peters (9). These costs are based on the year 1969. They were up-dated to a 1969 basis using the Marshall and Stevens Index as follows

$$1969 \text{ Cost} = 1957 \text{ Cost} (1969 \text{ Index}/1957 \text{ Index}) \quad (109)$$

$$1969 \text{ Cost} = 1957 \text{ Cost} (285/217) = 1957 \text{ Cost} (1.31)$$

The cost data is plotted in Figure 5, page 42, and is in the form of a log-log plot. The equation developed from Figure 5 is

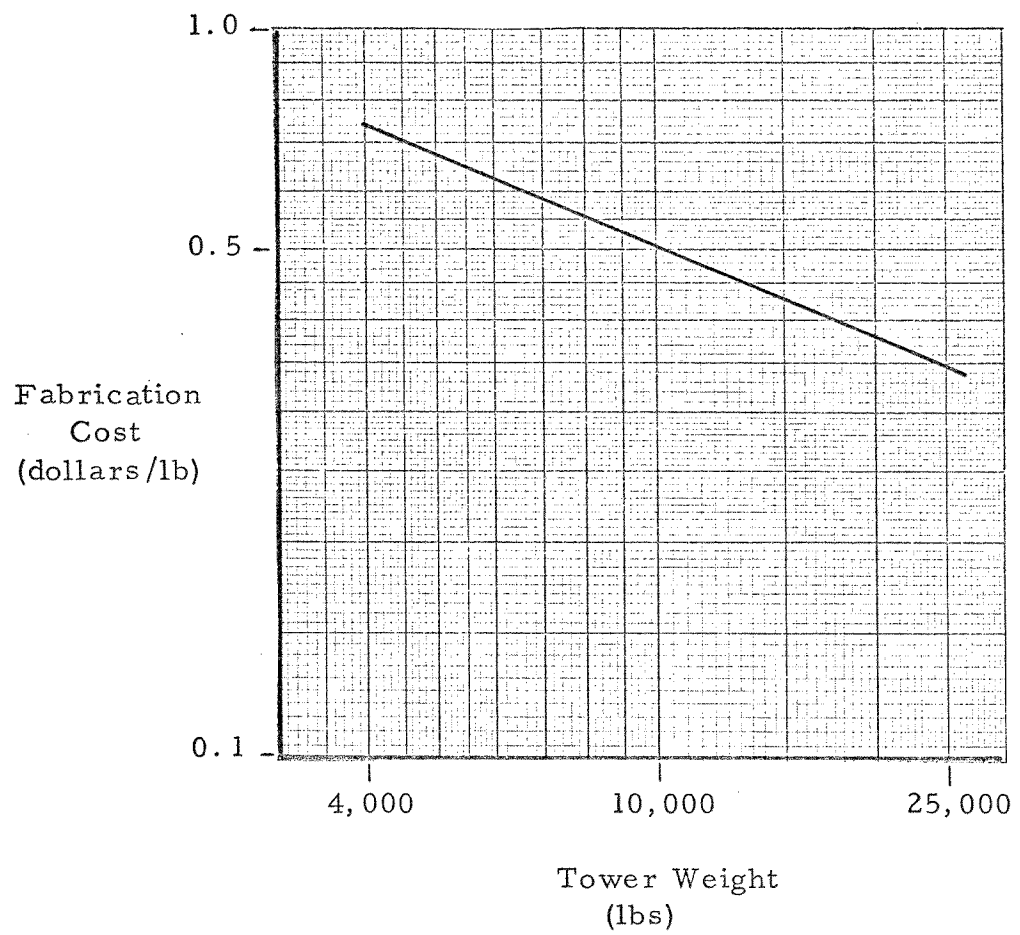
$$\text{Fabrication Cost} = \text{FC} = 19.1 \text{ TW}^{0.607} \quad (110)$$

The tower cost (TC) is then calculated from

$$\text{Tower Cost} = TC = FC + PC \quad (111)$$

FIGURE 5

FABRICATION COST FOR
CARBON STEEL COLUMNS (9)



PROGRAM ORGANIZATION

The computer program developed for the design of packed extraction columns requires a minimum of input data. This is desirable, since in the early stages of plant design, a minimum of data is available. This lack of data normally makes preliminary costs estimates highly inaccurate, since usually there is insufficient time available for the lengthy calculations associated with the estimation of the equilibrium slope and other system variables. The program can be used to calculate a column size for different extracting solvent rates, different solvents, and different packings. It will also calculate an estimated column purchase cost for each alternate.

During the latter stages of plant design more data is usually available. The program has been designed to accept this data and to by-pass the portion of the program used to estimate it. Again, different operating conditions can be investigated.

What follows is a general description of the computer program and its operation. The program organization is given in detail in Block Diagrams 1 through 21 (pages 69 to 89).

Program Design Bases

The equations presented in the Equation Development, pages 5 to 43, have been developed into a computer program for the design of packed extraction columns. This program is coded in Fortran IV, in accordance with the Fortran IV Reference Manual (70-00-604-1; July 1968), for the Radio Corporation of America, Spectra-70, digital computer. Although the limitations of the design equation used have already been discussed during their development, they will be summarized again in order to emphasize them. These assumptions are:

1. Both the raffinate and extract solutions are considered dilute.
2. The extract phase is the dispersed phase and the raffinate the continuous phase.
3. It has been assumed that no chemical reactions occur.
4. The packing used can either be Berl Saddles or Raschig Rings.

The computer program is limited to the two packings given in (d) above, since the equation used (equation (50), page 15) for

the determination of the critical packing diameter is applicable only to Berl Saddles and Raschig Rings. If another type of packing were used, the equation for the calculation of its critical packing diameter would have to be substituted for the one presently included in the design program.

Program Variable Names

The definition of the variable names used in the computer program can be found in the listing of equation and program nomenclature given on pages 60 to 68. The program variables are defined in terms of the nomenclature used in the equations presented in the section on equation development. The definitions of the equation variables are also given in this listing.

The basis used for the selection of the variable names was that the name selected should represent an abbreviation of its actual definition. For example, the program variable name RAFDEN represents the raffinate density. There were two limitations on the naming of program variables. The first was that the name could not be longer than six characters. The second was that the name of a floating point variable could not

begin with I, J, K, L, M, and N. Thus, while a logical abbreviation of the number of transfer units would be NTU(I), it had to be changed to XNTU(I).

Data Input

The format of the twelve data cards required is given in Table 15, page 116. The content of each card is listed in terms of the program variable names, along with the card columns associated to each variable.

Ten columns on each data card are assigned to each piece of data. The data may be punched in any position in the ten columns allowed for it, but the position of the decimal point must be shown correctly.

A value must be given to each of the variables given in Table 15, with the following exceptions:

1. If the equilibrium slope (SLOPE) is known, its value is punched in columns 11 - 20 of the second data card.

The mutual solubility data for the three binaries associated with the ternary system under study would

not be required, so blank cards are substituted for the third, fourth, and fifth data cards. Blank data cards are required since the position of the data cards is important for correct data input.

2. If the equilibrium slope is not known, columns 11 - 20 of the second data card are left blank. The mutual solubility data for the a, b binary is then punched on the third data card; the mutual solubility data for the b, c binary on the fourth data card; and the mutual solubility data for the c, a binary on the fifth data card. The mutual solubility data is punched in columns 1 - 40 according to the format of Table 15, page 116
3. If the distribution coefficients for the solute in the raffinate (DCR) and for the solute in the extract (DCE) are known, their values are punched in columns 1 - 10 and 11 - 20, respectively, of the sixth data card. No data is then needed for the solute molal volume (VOLMOL); for the column operating temperature (OPTEMF); for the extract solvent association factor (ASSOCE); and for the raffinate association factor (ASSOCR). The data positions allocated to the above are then left blank

(see Table 15, page 116), since this data is not needed for the estimation of the distribution coefficients.

4. If both distribution coefficients are not known, then columns 1 - 20 on the sixth data card are left blank. The data needed for the estimation of the distribution coefficients must then be supplied. The required data is listed in (3) on the preceding page and is punched in according to the format of Table 15.
5. If only one distribution coefficient is known, the data is punched in the proper position on the sixth data card. The solute molal volume, the column operating temperature and the solvent association factor, for the unknown distribution coefficient, must be then supplied.

The program is designed to handle calculations based on one type of packing at a time and requires packing data for six sizes of that packing. The number of packing sizes was based on the use of packing diameters of 0.5, 0.75, 1.0, 1.5, 2.0, and 3.0 inches. Packing is available in other sizes, such as 0.25, 0.75, and 1.25 inches, but since these sizes are not widely used, they were not included.

The packing data supplied for each packing diameter (PD(J)) are the void fraction (PE(J)); the surface area (PA(J)); the density of the packing (PDEN(J)); and the cost of the packing (PCOST1(J)). This data is punched on the seventh through twelfth data cards, according to the format of Table 15, page 116. The packing data is punched in order of increasing size starting with the data for the 0.5 inch packing punched on the seventh data card.

If packing data is not available for six sizes of packing, the specification for the DO loop given in statement 93, page 91, must be changed. The statement now reads, DO 14 J=1, 6, 1; so that the number six would be changed to reflect the number of packing sizes available.

Program Operation

The general sequence of calculations follows that presented in the equation development portion of this presentation (pages 5 to 43). The following variable limits are maintained during the program operation:

1. The value of the dispersed phase hold-up must be equal

to or greater than 0.05 and less than the hold-up at transition, as calculated by equation (51), page 16.

2. The superficial raffinate velocity must be equal to or less than 60 percent of its flooding velocity.
3. The superficial extract velocity must be equal to or greater than 45* percent of its flooding velocity. Also, the extract velocity must be less than or equal to 60 percent of its flooding velocity.

The first section of the program, statement numbers 23 to 102 (pages 90 to 92), calculates the variable values which are fixed for each run; such as the equilibrium slope (SLOPE 1) and the raffinate flow from the column (R2). The calculation of the variables which are subscripted and whose values change during a given program run is accomplished by statements number 103 to 244, pages 92 to 94.

For each packing size greater than the critical packing diameter (PDC), the program will design and calculate a purchase cost for a column to handle extract flows of from 1.2 to 3.0 times the minimum solvent flow, in increments of 0.2. This gives a total of ten runs for each packing diameter greater than the critical packing diameter.

Internal Error Checks

There are several error messages programmed into the operation of the calculation routines. These will be described now; they have been inserted to indicate problem areas which would be obvious to a person doing hand calculations, but which will cause the computer program to abort.

The first of these concerns the value of the equilibrium slope supplied to the computer. If this value is negative, the computer will print out an appropriate error message and stop the program (see Block Diagram 2, page 70). Also, if the solute concentration in the extracting solvent feed to the column is in equilibrium with the exit raffinate concentration, an error message will be printed and the program stopped (see Block Diagram 8, page 76).

An error message is also printed if the critical packing diameter (PDC) calculated is larger than any of the packing diameters in the data input to the computer. Again, the program will stop after printing an error message (see Block Diagram 9, page 77). If the flooding ordinate calculated from equation (56), page 17, is outside the range of equations (58) and (59), page 19, an error

message will be printed out, along with the value of the flooding ordinate and the value of the major program variables calculated up to that point (see Block Diagram 11, page 79). These values are printed out to simplify debugging.

If the value of the terminal velocity ordinate (TVO) calculated from equation (69), page 24, is outside the range of equations (71), (72), and (73) an error message will be printed out (see Block Diagram 13, page 81). The value of TVO and the major program values calculated up to that point will again be printed out.

Data Output

Tables 10 through 14, pages 111 to 115, are an example of the format for the data output. The data is punched out in the form of two tables, for each packing diameter larger than the critical packing diameter, with one page of output for each packing diameter.

For each packing diameter, the data output is based on extracting solvent to minimum extracting solvent ratios of 1.2 to 3.0, in increments of 0.2. Ten values are then printed for each output variable. The logical presentation of the data would have

been one table containing all the data, but, because of the number of variables printed out, two tables were set up.

The first table contains the dispersed phase hold-up; the percent of flooding for the extract; the percent of flooding for the raffinate; the ratio of actual to minimum solvent rate; and the concentration of the extract from the column. The data is presented in the above order.

The second table contains the solvent flow rate; the number of transfer units; the height of a transfer unit; the diameter of the extraction column; the height of packing required; and the estimated purchase cost for the column. Again, the data is presented in the order given above.

CONCLUSIONS

A computer run, for data given in Table 16, page 117, was made in order to check the program operation; determine the effect of packing size and the effect of the ratio of actual to minimum solvent rates on column design. The data used is synthetic, except for the packing data for Raschig Rings, which was obtained from U.S. Stoneware Co., Bulletin TP54R, 1963.

Tables 10 through 14, pages 111 to 115, are the computer print-outs of the data for the five packing sizes larger than the critical packing size. This data is the basis for Figures 12, 13, and 14, pages 102, 103, and 104.

Figure 14 is a plot of the height of an overall transfer unit ($HTU(I)$) and tower diameter ($T(I)$), versus the packing diameter ($PD(M)$), for a fixed solvent to feed ratio. The height of a transfer unit and the number of transfer units do not vary with packing size, while the tower diameter decreases with packing size. The most economical choice would be the largest packing size available, since the column diameter, for a given solvent to feed ratio, decreases with packing size. Treybal has established

a minimum packing size (19) but has made no mention of the effect of increasing packing size on column design.

Figure 13, page 103, is a plot of tower cost (TCOST(I)) and tower diameter (T(I)) verses the ratio of actual to minimum solvent feed rates (G1). The tower cost drops off rapidly until $G1=1.6$, then the cost begins to level. Figure 12, page 102, shows that the same effect is observed on the number of transfer units, while the height of a transfer unit shows a more constant decrease with increasing solvent rates. Based on the above, the ratio of actual to minimum solvent rate should be about 1.6, since higher rates would increase solvent recovery costs without significantly decreasing the column cost. In an actual design case, an economic balance between solvent recovery costs and extraction column costs would have to be made, in order to determine the actual ratio. The above result is not unique and has been predicted (32).

A number of runs, for 1.0 inch Raschig Rings and a ratio of actual to minimum solvent rates of 1.5, were made in order to determine the effect of various parameters on column design. The basic data used is found in Table 16, page 117. The results of

these runs are given in Tables 4 through 9, pages 105 to 110. The variation of two parameters had no significant effect on column design. They are the raffinate viscosity (Table 7, page 108) and the mutual solubility between extract and raffinate phases (Table 9, page 110).

Figure 6, page 96, and Figure 7, page 97, show the effect of increasing solvent density. These figures show that as the density difference between the solvent and raffinate increases, the column cost decreases. Therefore, for a given feed, a solvent whose density is much different than the feed should be used.

Figure 8, page 98, shows the effect of solvent viscosity. Based on this plot, a solvent with a low viscosity should be used in order to lower the column cost.

Figure 9, page 99, and Figure 10, page 100, shows the effect of raffinate density on column design. The same effect as was previously noted for extract density is true. That is, the greater the density difference, the more economical the column.

Treybal has noted (33) the effect of the extract viscosity and the difference in densities between the extract and raffinate. The results obtained above agree with his recommendations for selection of a solvent.

Figure 11, page 101, gives the effect on column design of interfacial tension. As the interfacial tension increases, the extraction column cost increases. This is because the height of a transfer unit increases. Treybal (33) discusses interfacial tension, but not in terms of its effect on column design.

RECOMMENDATIONS

One of the basic assumptions of this program is the assumption of dilute solutions. If this assumption is not made, new calculation procedures would be needed. This program could be modified to design a column where dilute solutions are not the case.

In addition to the modification mentioned above, there are many more that could be made in order to make the design program universally applicable for design. This would require a great deal more effort. The program presented herein is suitable for the design of simple ternary systems extraction columns and is a start in the development of an extraction column design program.

APPENDIX

EQUATION AND PROGRAM NOMENCLATURE

<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
a	A(I)	specific interfacial area, sq ft/cu ft, of active extractor volume.
a_f	PA(J)	surface area of packing: sq ft/cu ft.
A_{ab}	A2AB	limit of $\log \gamma_a$ as $x_a \rightarrow 0$, $x_b \rightarrow 1$.
A_{ba}	----	limit of $\log \gamma_b$ as $x_b \rightarrow 0$, $x_a \rightarrow 1$.
A_{ac}	----	limit of $\log \gamma_a$ as $x_a \rightarrow 0$, $x_c \rightarrow 1$.
A_{ca}	A2CA	limit of $\log \gamma_c$ as $x_c \rightarrow 0$, $x_a \rightarrow 1$.
A_{bc}	A2BC	limit of $\log \gamma_b$ as $x_b \rightarrow 0$, $x_c \rightarrow 1$.
A_{cb}	----	limit of $\log \gamma_c$ as $x_c \rightarrow 0$, $x_b \rightarrow 1$.
----	A1AB	A_{ab}/A_{ba}
----	A1BC	A_{bc}/A_{cb}
----	A1CA	A_{ca}/A_{ac}
D_{ce}	DCE	diffusivity for solute in extract: sq ft/hr.

EQUATION AND PROGRAM NOMENCLATURE (con't)

<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
D_{cr}	DCR	diffusivity for solute in raffinate: sq ft/hr.
d_f	PD(J)	packing diameter: ft.
d_{fc}	PDC	critical diameter for packing piece: ft.
d_p	DP	mean drop diameter: ft.
d_{pt}	DPT	mean drop diameter at transition: ft.
E_1	E1(I)	rate of flow of extract phase from column: lbs/hr.
E_2	E2(I)	rate of flow of extract phase to column: lbs/hr.
$(E_2)_{min}$	E2MIN	minimum rate of flow of solvent: lbs/hr.
F	F(I)	extraction factor, $m E_2/R_2$, dimensionless.
FA	FA	flooding abscissa, Figure 2.
FC	FC	fabrication cost: dollars.
FO	FO	flooding ordinate, Figure 2.
G_1	G1(I)	ration of actual to minimum solvent feed.

EQUATION AND PROGRAM NOMENCLATURE (con't)

<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
HOP	HOP(I)	height of packing: ft.
H_{tr}	HTE(I)	height of continuous-phase (raffinate) transfer unit: ft.
H_{te}	HTR(I)	height of dispersed-phase (extract) transfer unit: ft.
H_{tor}	HTU(I)	overall height of continuous-phase (raffinate) transfer unit: ft.
H_{toe}	HTU(I)	overall height of dispersed-phase (extract) transfer unit: ft.
k_e	XKE	extract mass transfer coefficient: lb moles/(hr) (sq ft) (lb moles/cu ft).
K_r	XKR	raffinate mass transfer coefficient: lb moles/(hr) (sq ft) (lb moles/cu ft).
M_a	FEEDMW	molecular weight of major component of feed.
M_b	SOLVMW	molecular weight of solvent.
M_c	SOLUMW	molecular weight of solute.
m	SLOPE1	equilibrium - distribution co- efficient, weight fraction basis.

EQUATION AND PROGRAM NOMENCLATURE (con't)

<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
m'	SLOPE	equilibrium - distribution co-efficient, mole fraction basis.
N_{tor}	XNTU(I)	number of overall transfer units based on continuous phase (raffinate).
N_{toe}	XNTU(I)	number of overall transfer units based on dispersed phase (extract).
P	P(I)	operating ratio, defined by equation (43).
P_1	P1	ratio of volumetric flow rates, $(V_e)_{av}/(V_r)_{av}$.
P_2	P2	ratio, V_k/V_e .
P_3	P3	dimensionless, defined by equation (68).
PC	PCOST2(I)	packing cost: dollars.
----	PCOST1(J)	packing cost: dollars/cu ft.
PV	PV	packing volume: cu ft.
R_1	R1	rate of flow of raffinate phase to column: lbs/hr.
R_2	R2	rate of flow of raffinate phase from column: lbs/hr.

EQUATION AND PROGRAM NOMENCLATURE (con't)

<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
T	T(I)	tower diameter: ft.
T_1	OPTEMK	temperature: $^{\circ}\text{K}$.
----	OPTEMF	temperature: $^{\circ}\text{F}$.
TC	TCOST(I)	tower cost: dollars.
TVA	TVA	terminal velocity abscissa, Figure 3.
TVO	TVO	terminal velocity ordinate, Figure 3.
TW	TW	tower weight: lbs.
V_c	VOLMOL	solute molal volume at normal boiling point: cu cm/g-mole.
V_e	VE(I)	extract phase superficial velocity: ft/hr.
$(V_e)_{av}$	VEAV(I)	extract phase volumetric rate: cu ft/hr.
V_{ef}	VEF	extract phase flooding velocity: ft/hr.
V_k	VK	characteristic velocity of drops: ft/hr.
V_k^A	VKA	characteristic drop velocity abscissa, Figure 4.

EQUATION AND PROGRAM NOMENCLATURE (con't)

<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
V_k^O	VKO	characteristic drop velocity ordinate, Figure 4.
V_r	VR(I)	raffinate phase superficial velocity: ft/hr.
$(V_r)_{av}$	VRAV(I)	raffinate phase volumetric rate: cu ft/hr.
V_{rf}	VRF	raffinate phase flooding velocity: ft/hr.
V_t	VT	terminal drop velocity: ft/hr.
x_{aa1}	XAA1	mole fraction of component a in a rich layer, A-B binary.
x_{aa2}	XAA2	mole fraction of component a in a rich layer, C-A binary.
x_{ab}	XAB	mole fraction of component a in b rich layer, A-B binary.
x_{ac}	XAC	mole fraction of component a in c rich layer, C-A binary.
x_{ba}	XBA	mole fraction of component b in a rich layer, A-B binary.

EQUATION AND PROGRAM NOMENCLATURE (con't)

<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
x_{bb1}	XBB1	mole fraction of component b in b rich layer, A-B binary.
x_{bb2}	XBB2	mole fraction of component b in b rich layer, B-C binary.
x_{bc}	XBC	mole fraction of component b in c rich layer, B-C binary.
x_{ca}	XCA	mole fraction of component c in a rich layer, C-A binary.
x_{cb}	XCB	mole fraction of component c in b rich layer, B-C binary.
x_{cc1}	XCC1	mole fraction of component c in c rich layer, B-C binary.
x_{cc2}	XCC2	mole fraction of component c in c rich layer, C-A binary.
x_{ce2}	CE2	mole fraction of component c in solvent feed.
x_{cr1}	CR1	mole fraction of component c in feed.
x_{cr2}	CR2	mole fraction of component c in raffinate.
X_{cel}	XCE1(I)	weight fraction of component c in extract.

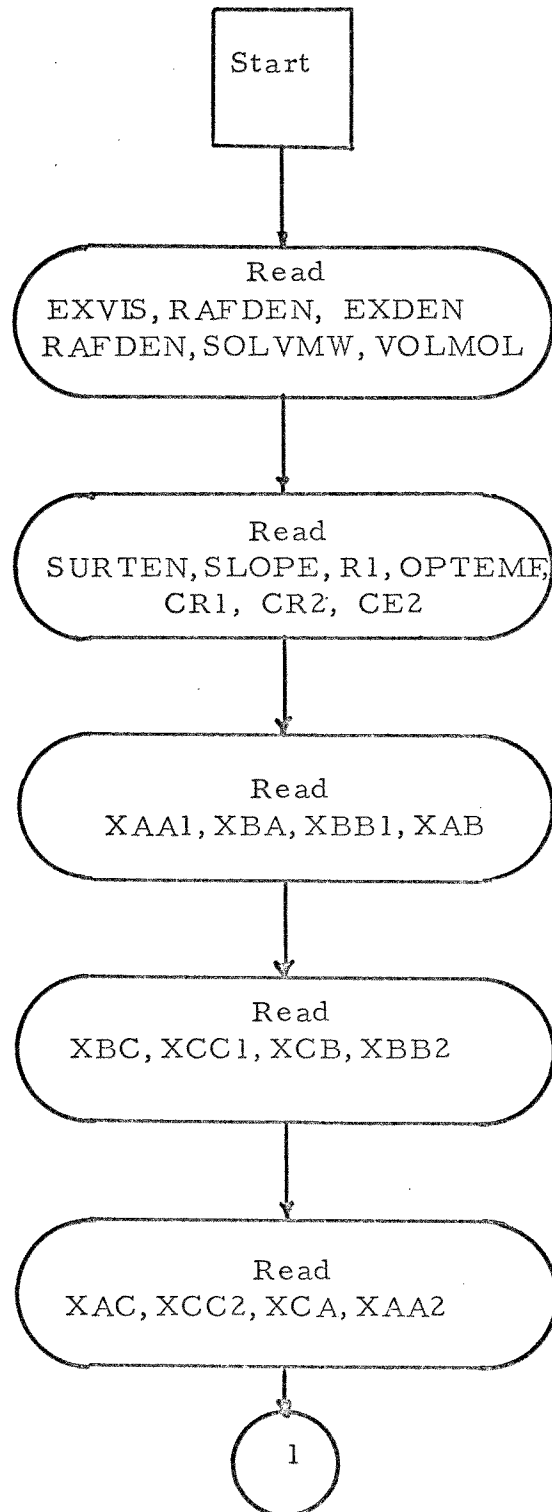
EQUATION AND PROGRAM NOMENCLATURE (con't)

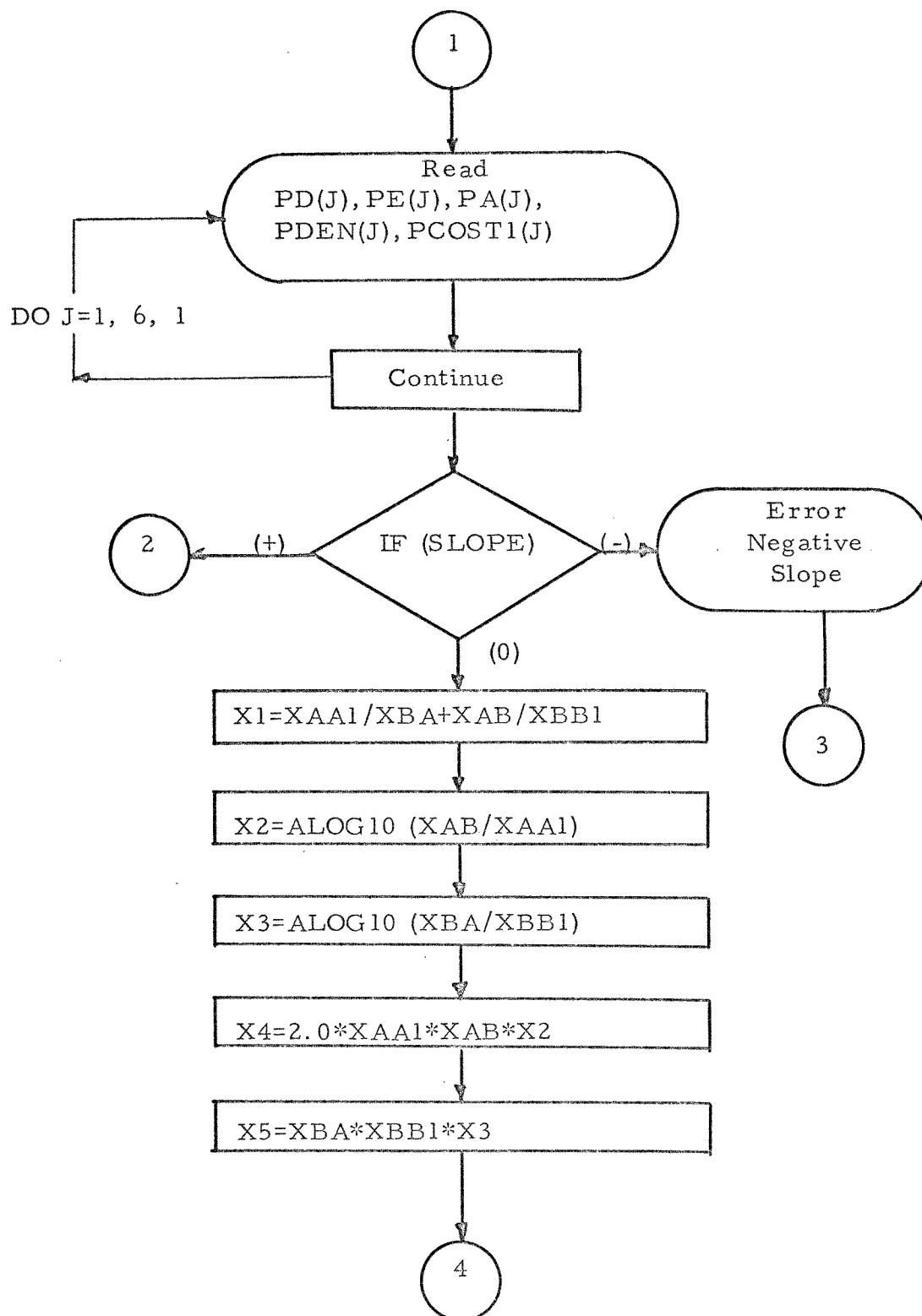
<u>SYMBOL</u>	<u>PROGRAM CODE</u>	<u>DESCRIPTION</u>
X_{ce2}	XCE2	weight fraction of component c in solvent feed.
X_{cr1}	XCR1	weight fraction of component c in feed.
X_{cr2}	XCR2	weight fraction of component c in raffinate.
γ	----	activity coefficient.
ϵ	PE(J)	voids in packed section, volume fraction.
μ_e	EXVIS	extract viscosity: centipoise.
μ_r	RAFVIS	raffinate viscosity: centipoise.
ρ_e	EXDEN	extract density: lbs/cu ft.
ρ_r	RAFDEN	raffinate density: lbs/cu ft.
σ	SURTEN	interfacial tension: dynes/cm.
ϕ_d	HOLDUP(I)	dispersed phase holdup, volume fraction void space in extractor.
φ_b	ASSOCE	association factor for extracting solvent.
φ_a	ASSOCR	association factor for feed solvent.

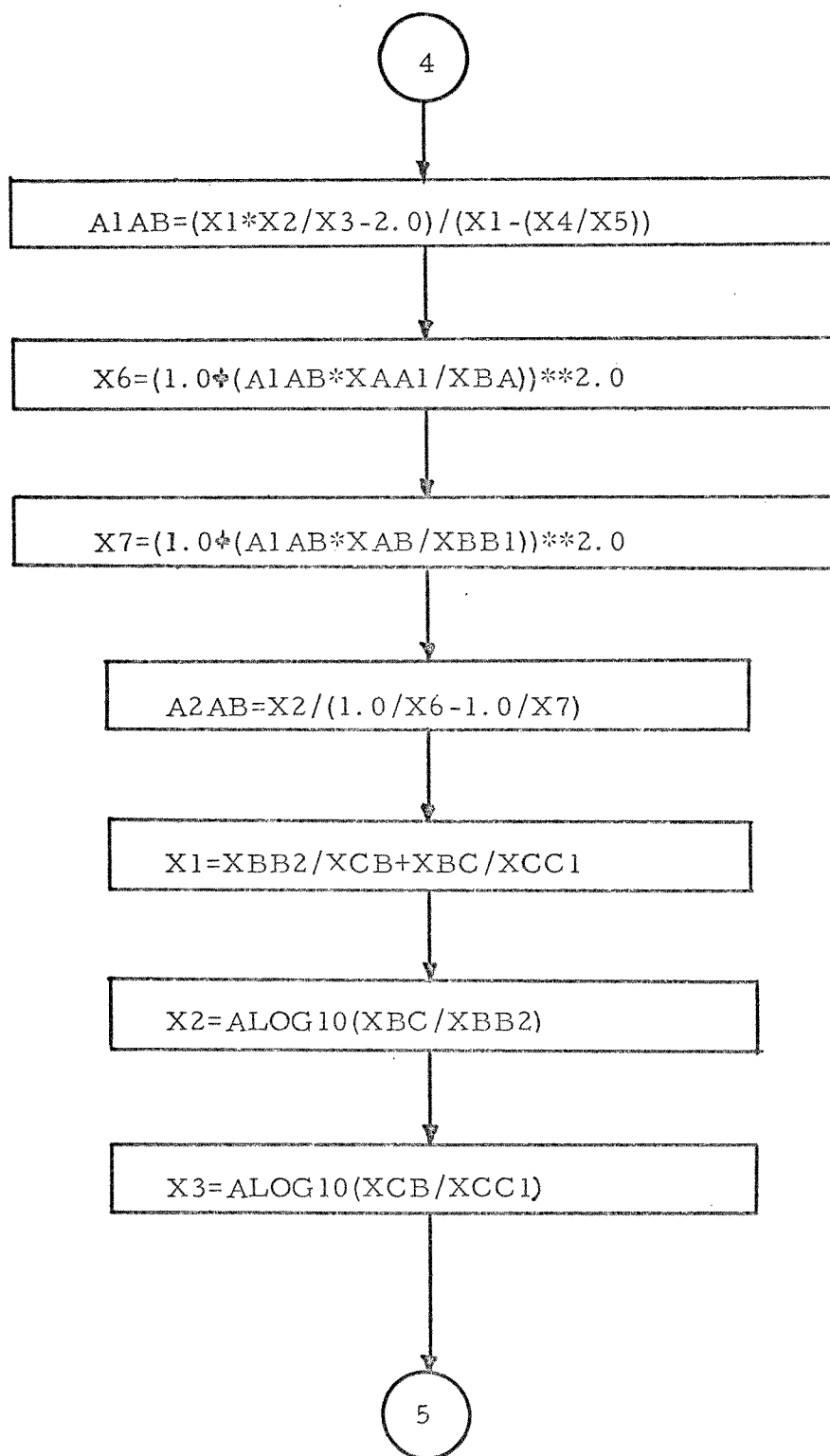
EQUATION AND PROGRAM NOMENCLATURE (con't)SUBSCRIPTS

a	=	major component of feed solution.
av	=	average.
b	=	extracting solvent.
c	=	solute.
d	=	dispersed phase.
e	=	extract.
e1	=	extracting solvent from column.
e2	=	extracting solvent to column.
f	=	flooding.
r	=	raffinate.
r1	=	raffinate phase to column.
r2	=	raffinate phase from column.

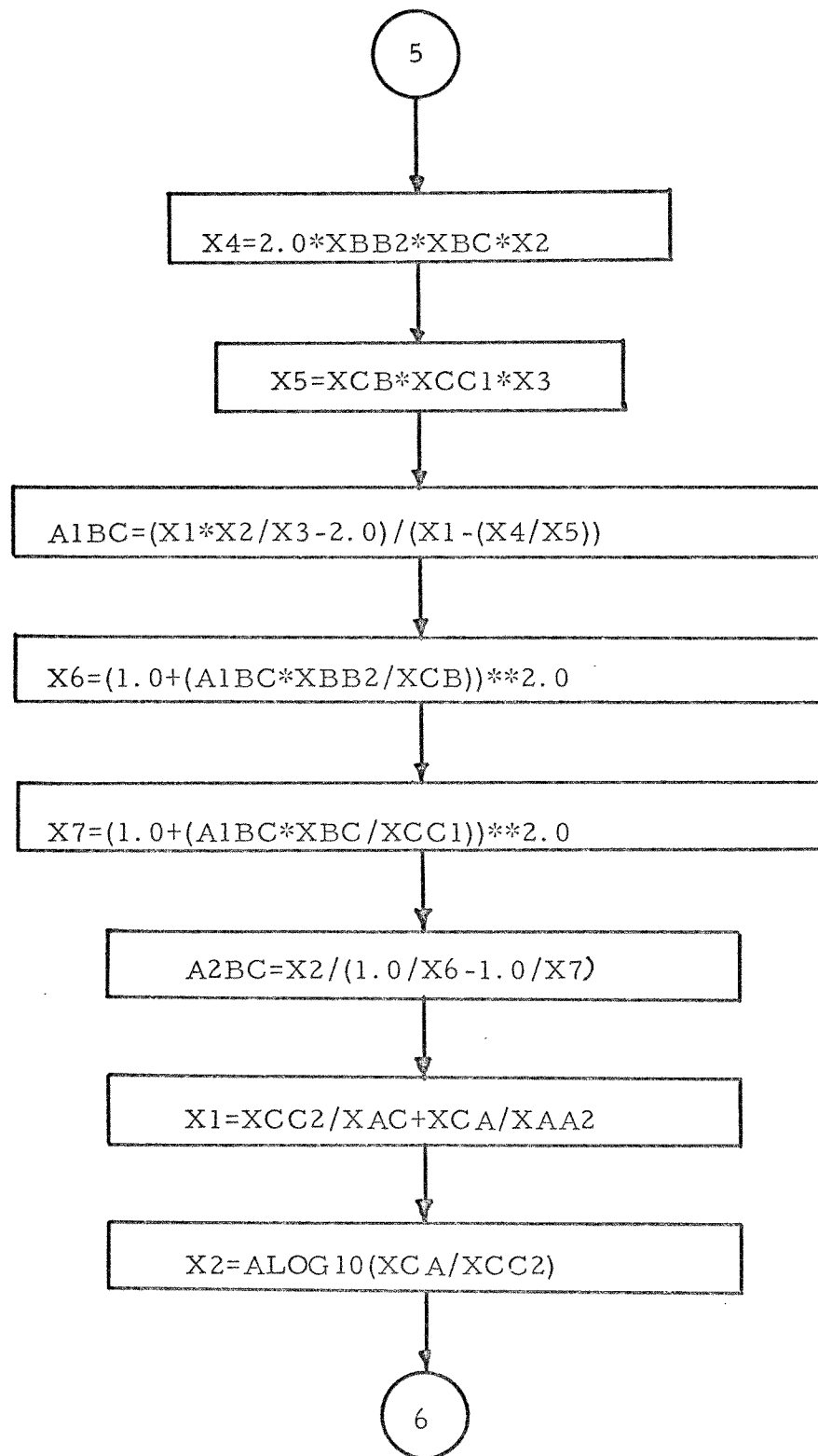
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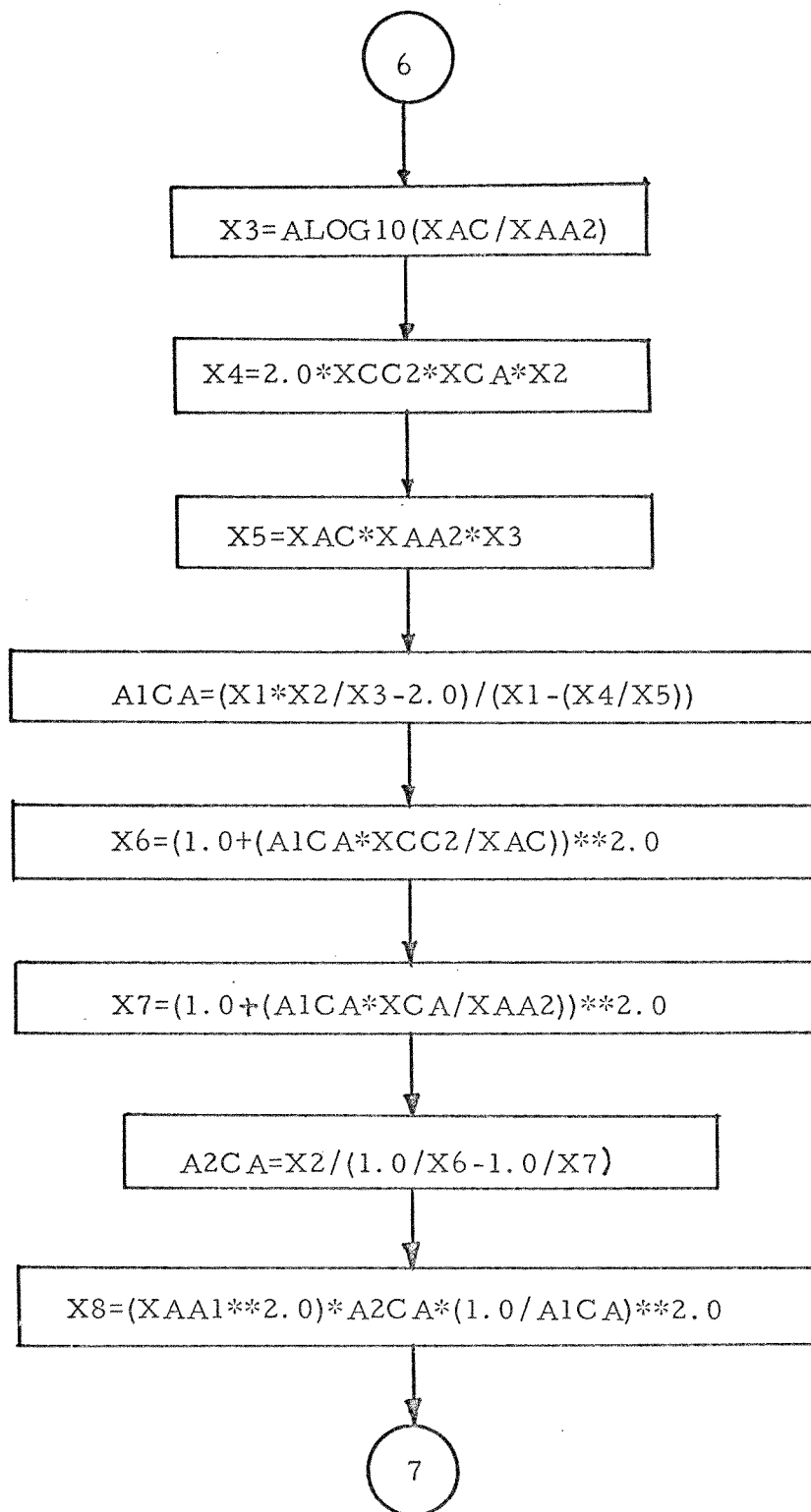
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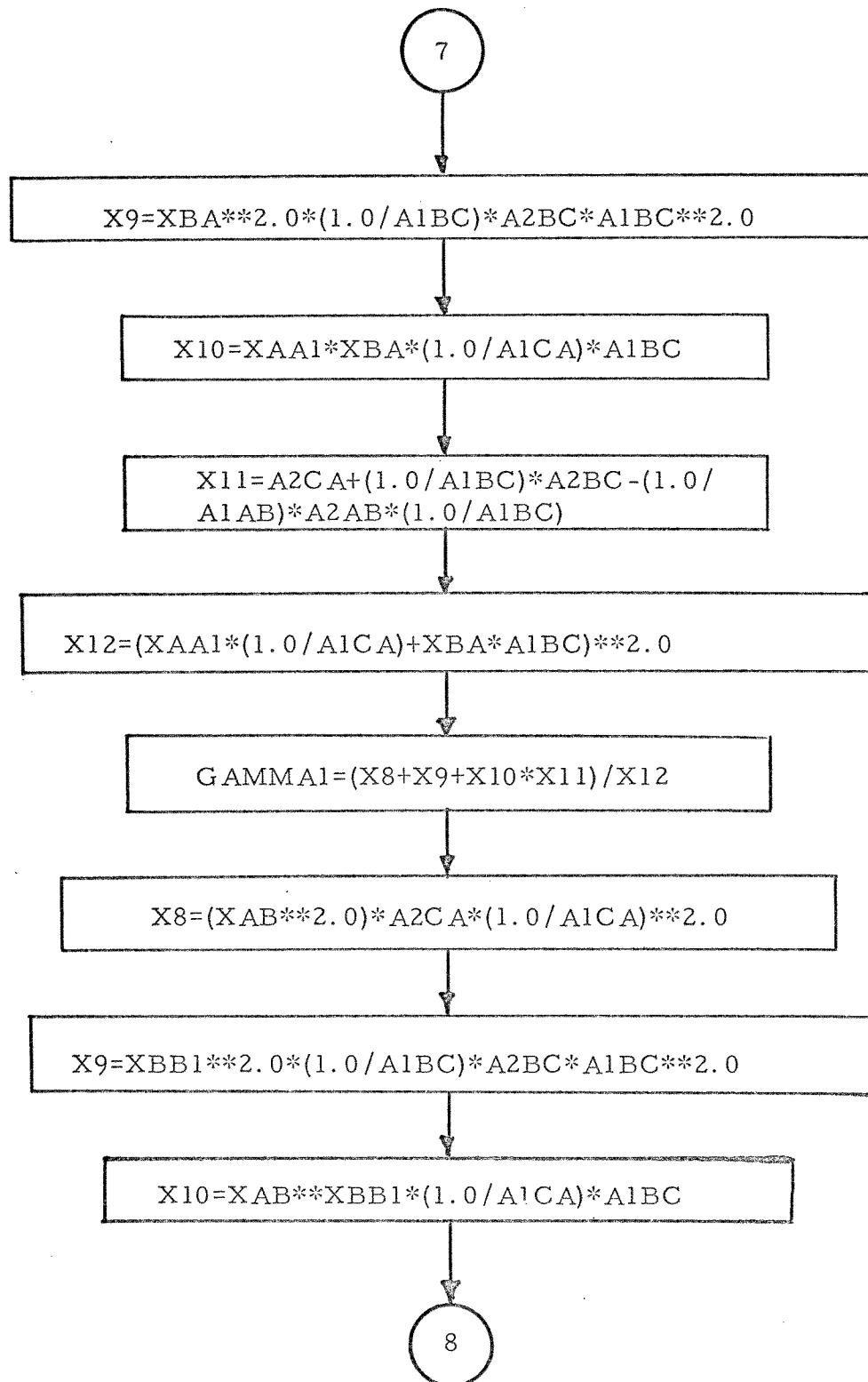
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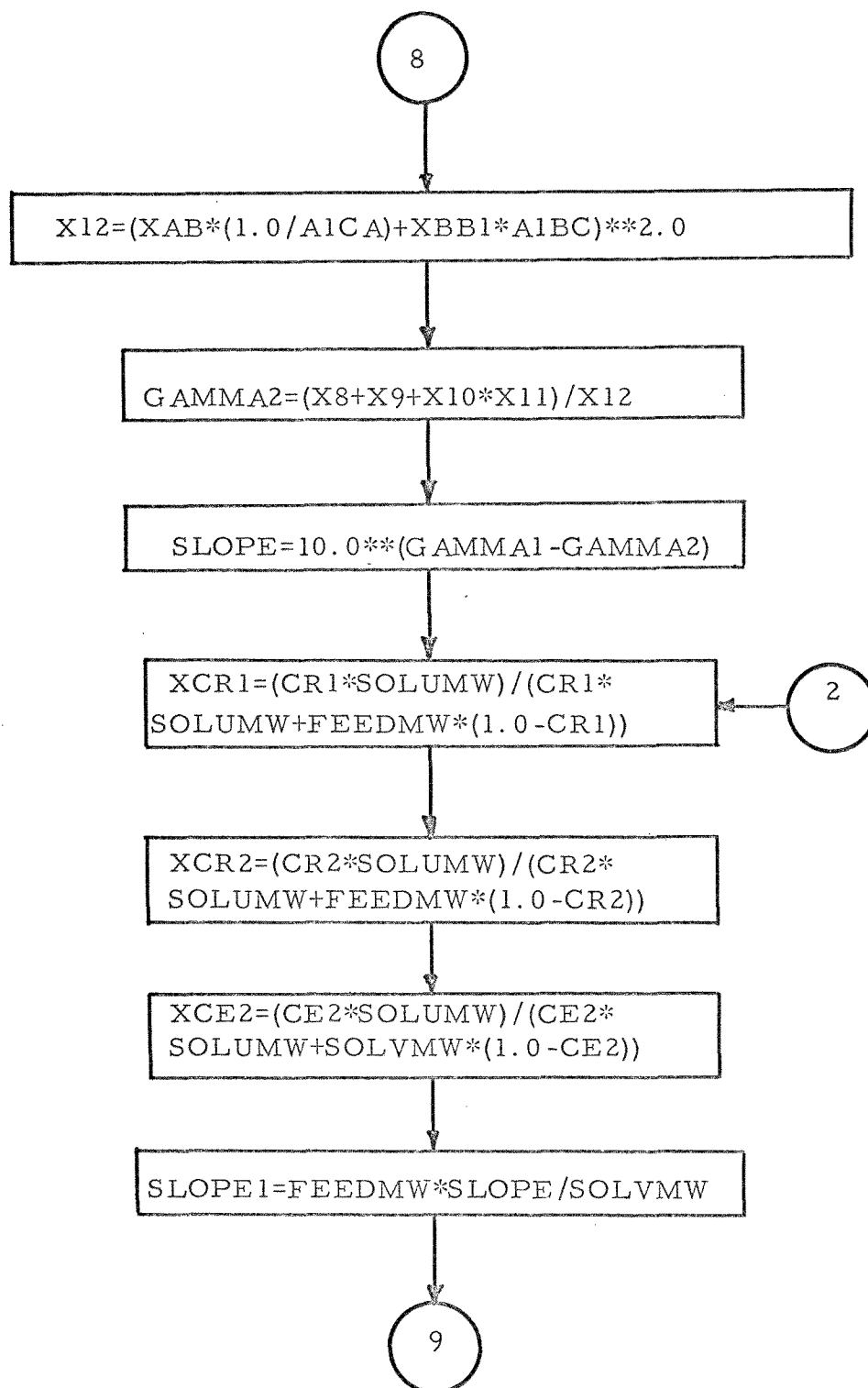


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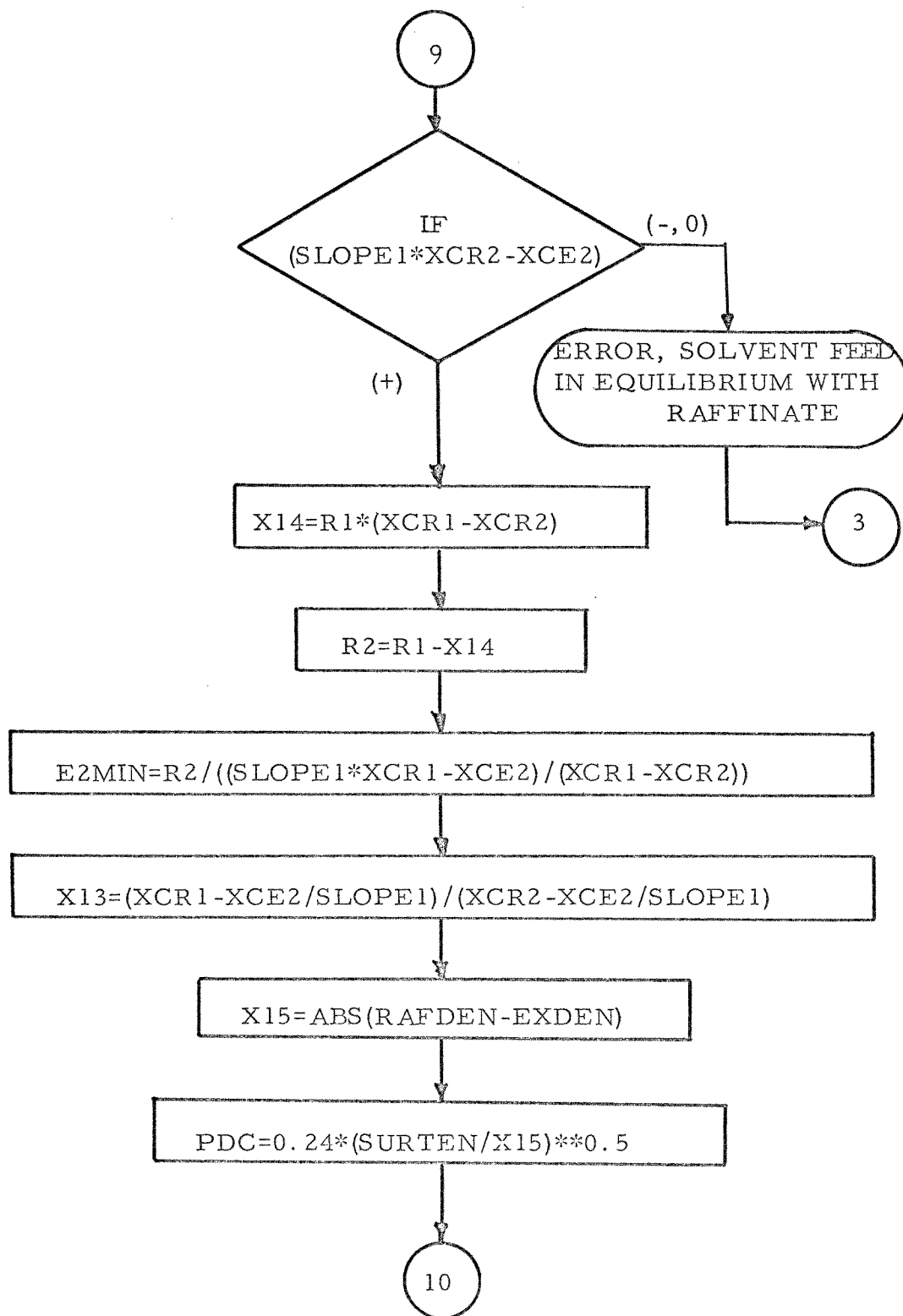
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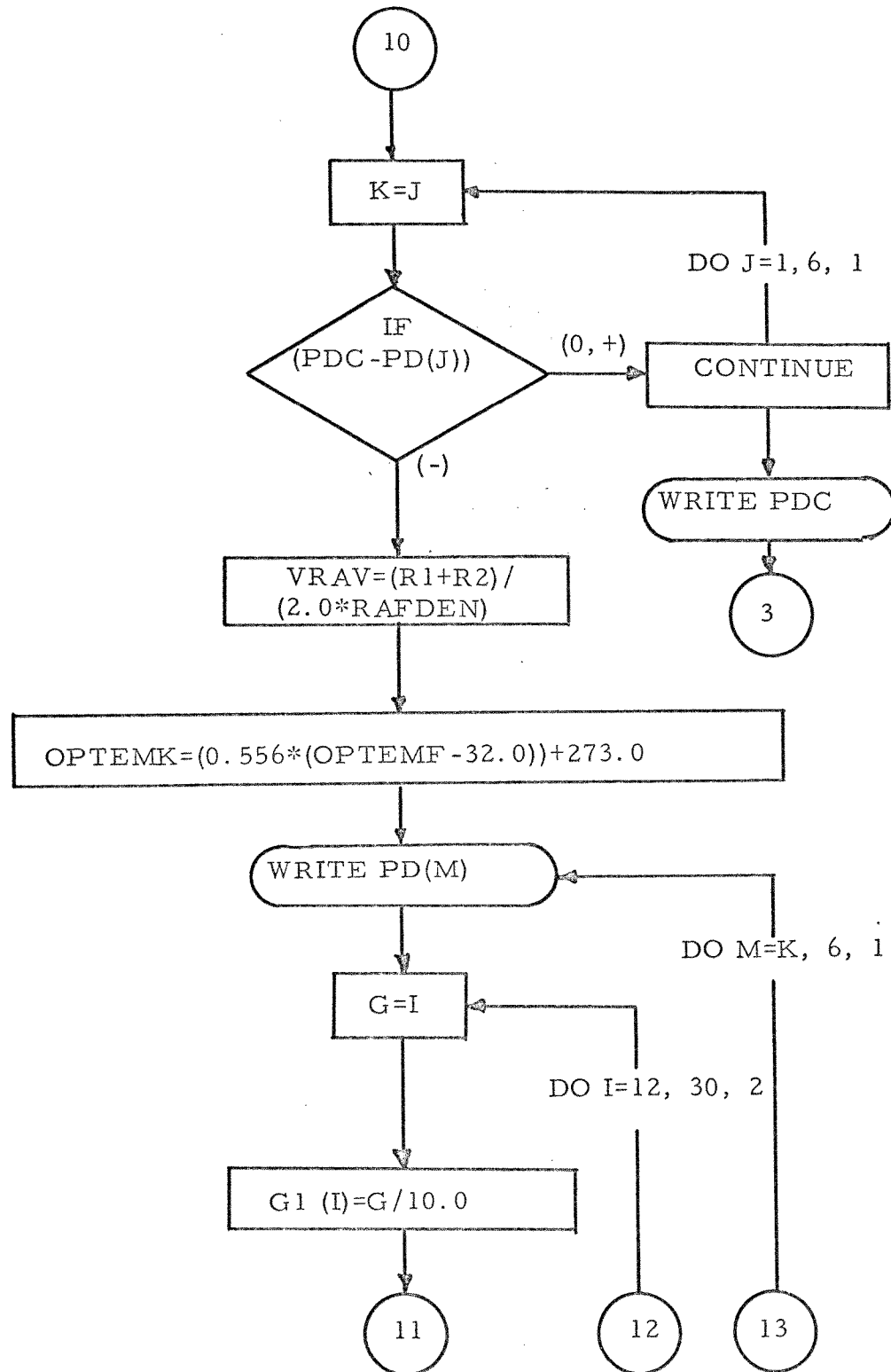


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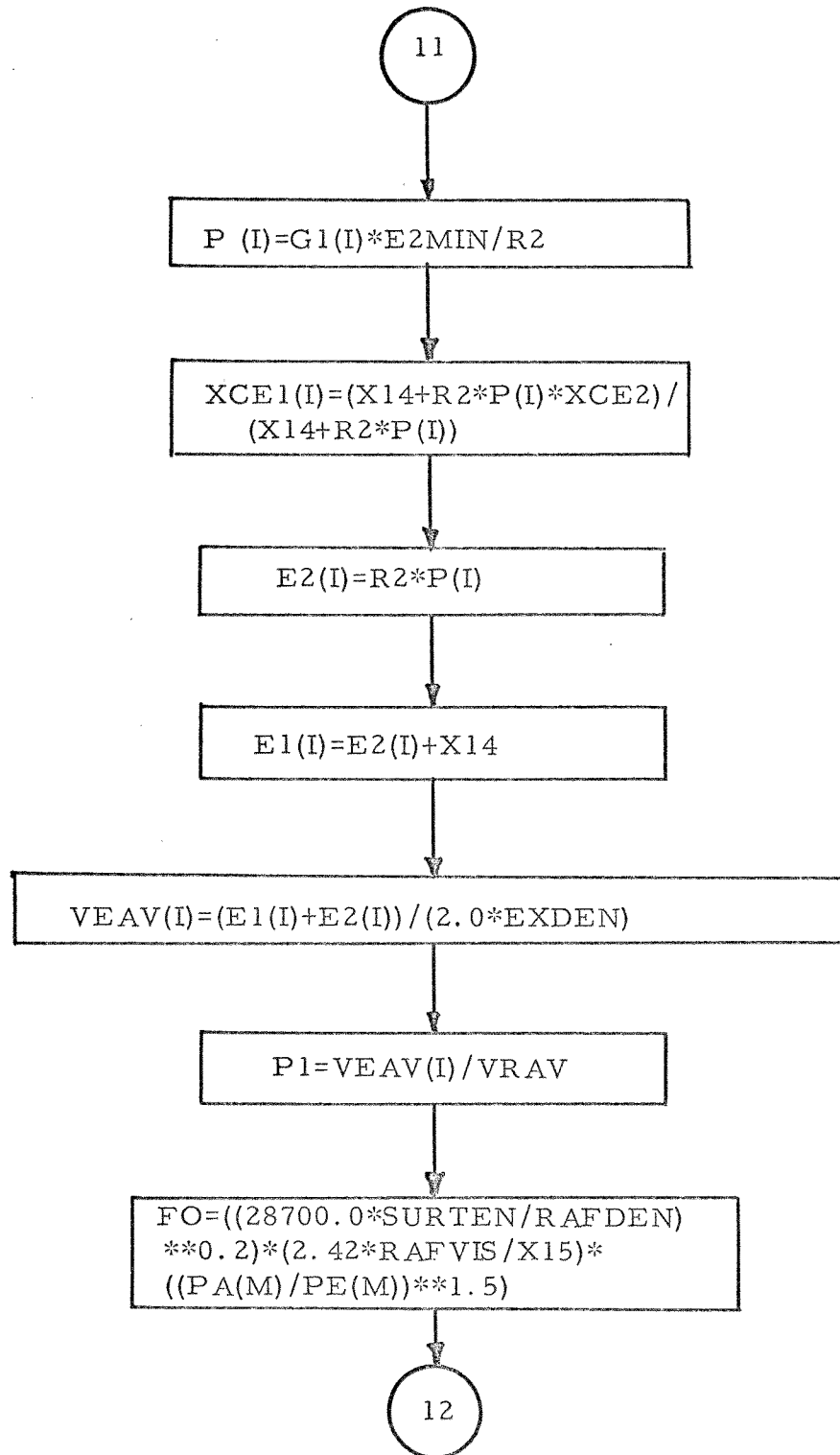


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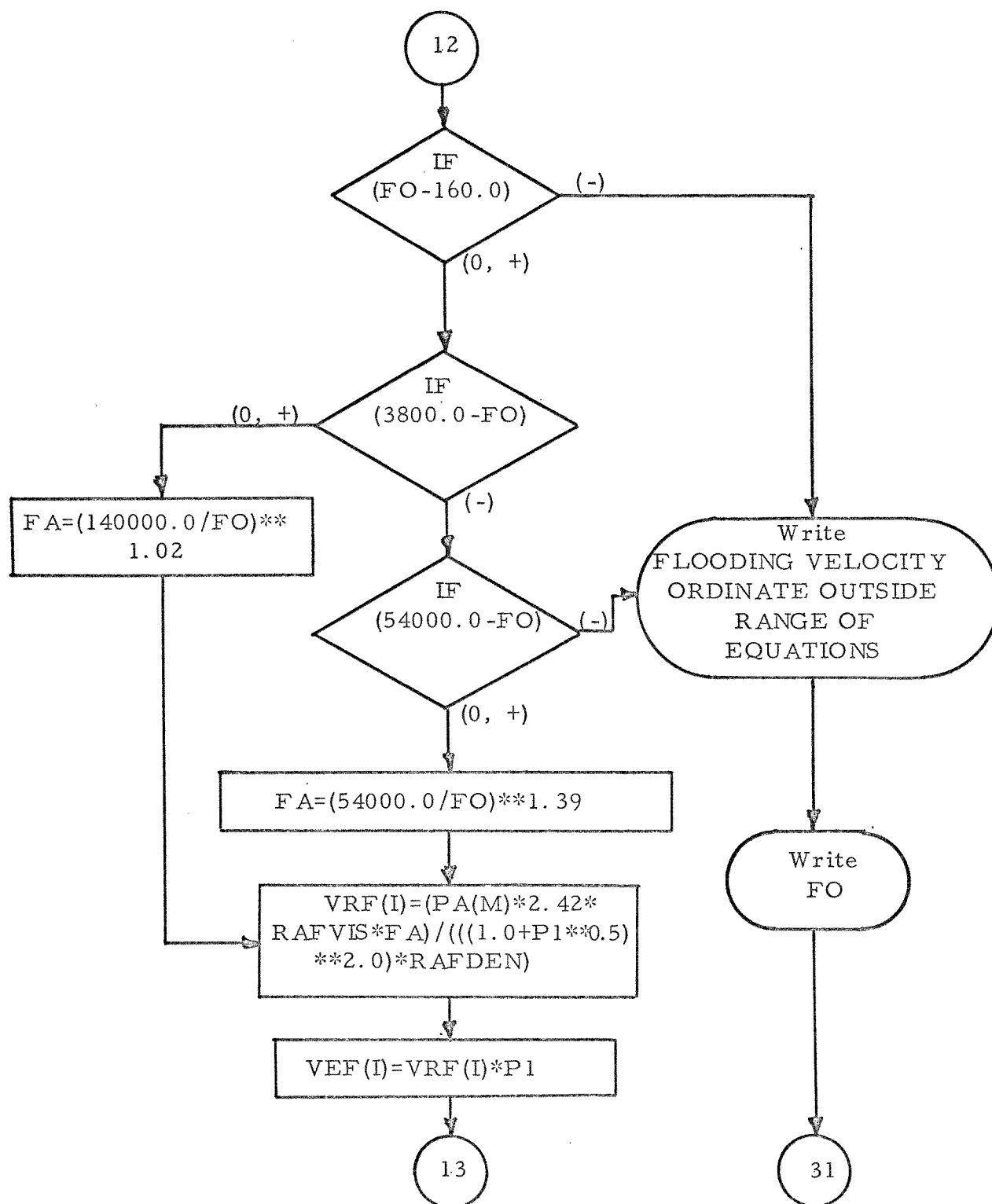


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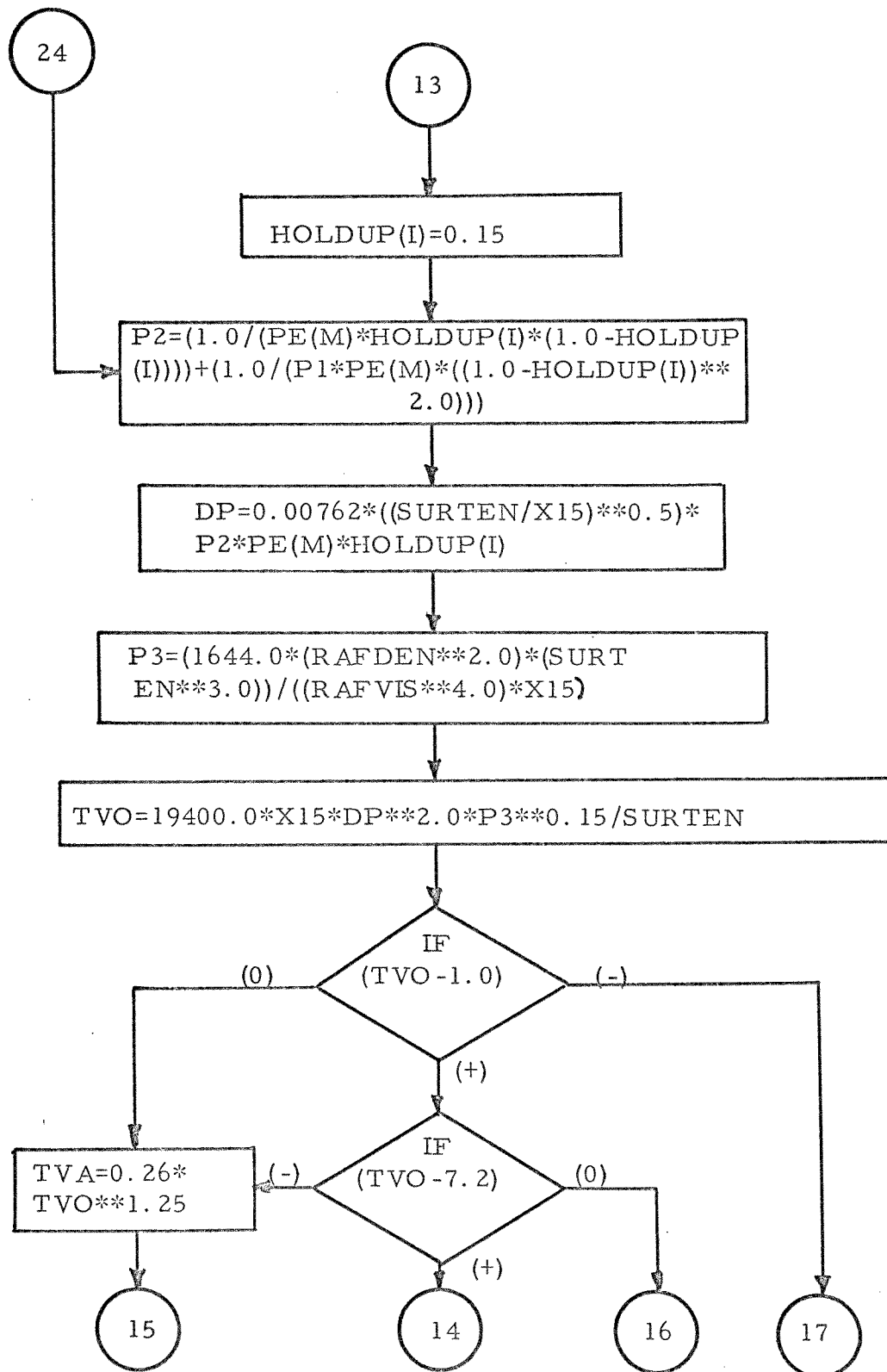
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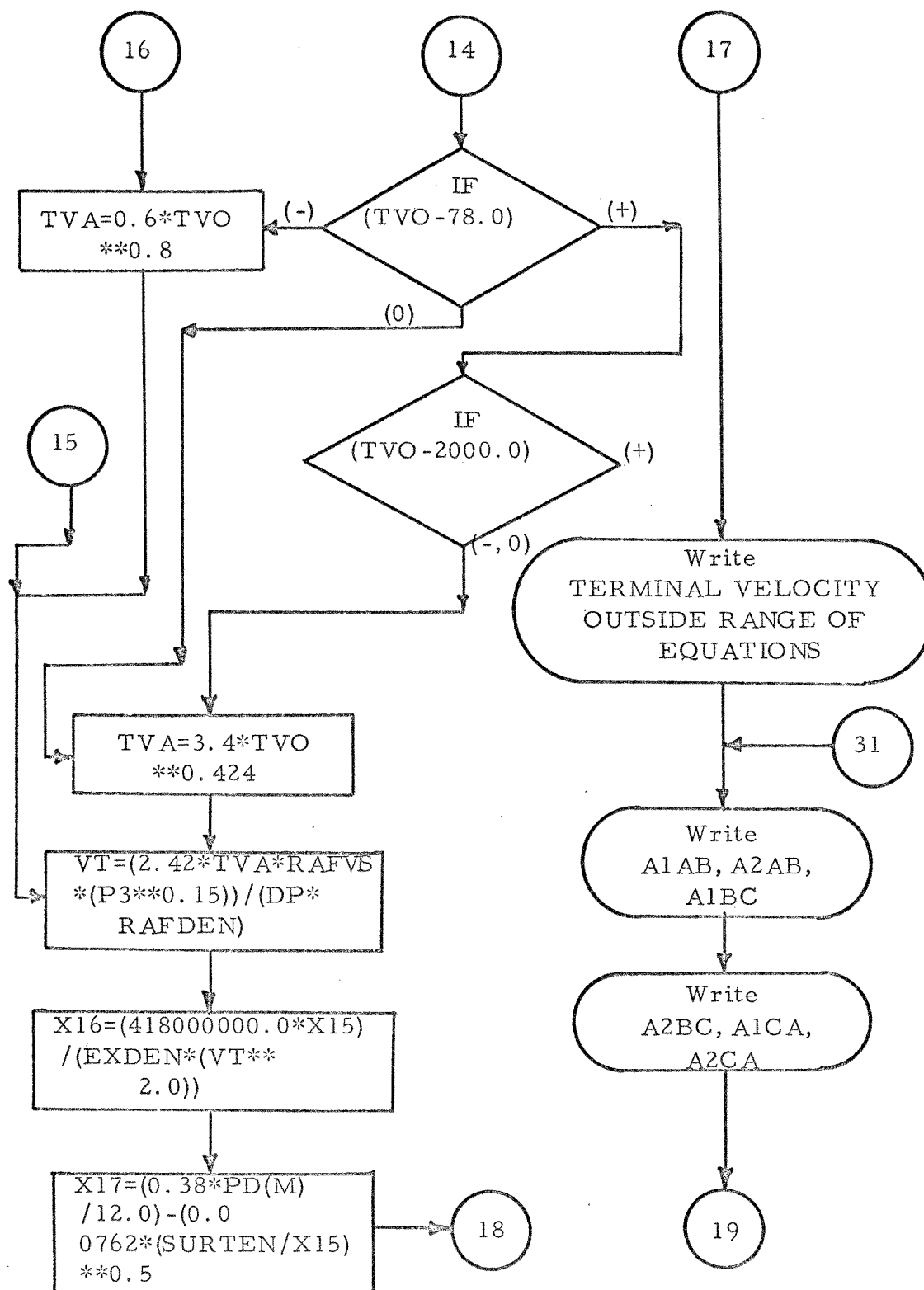
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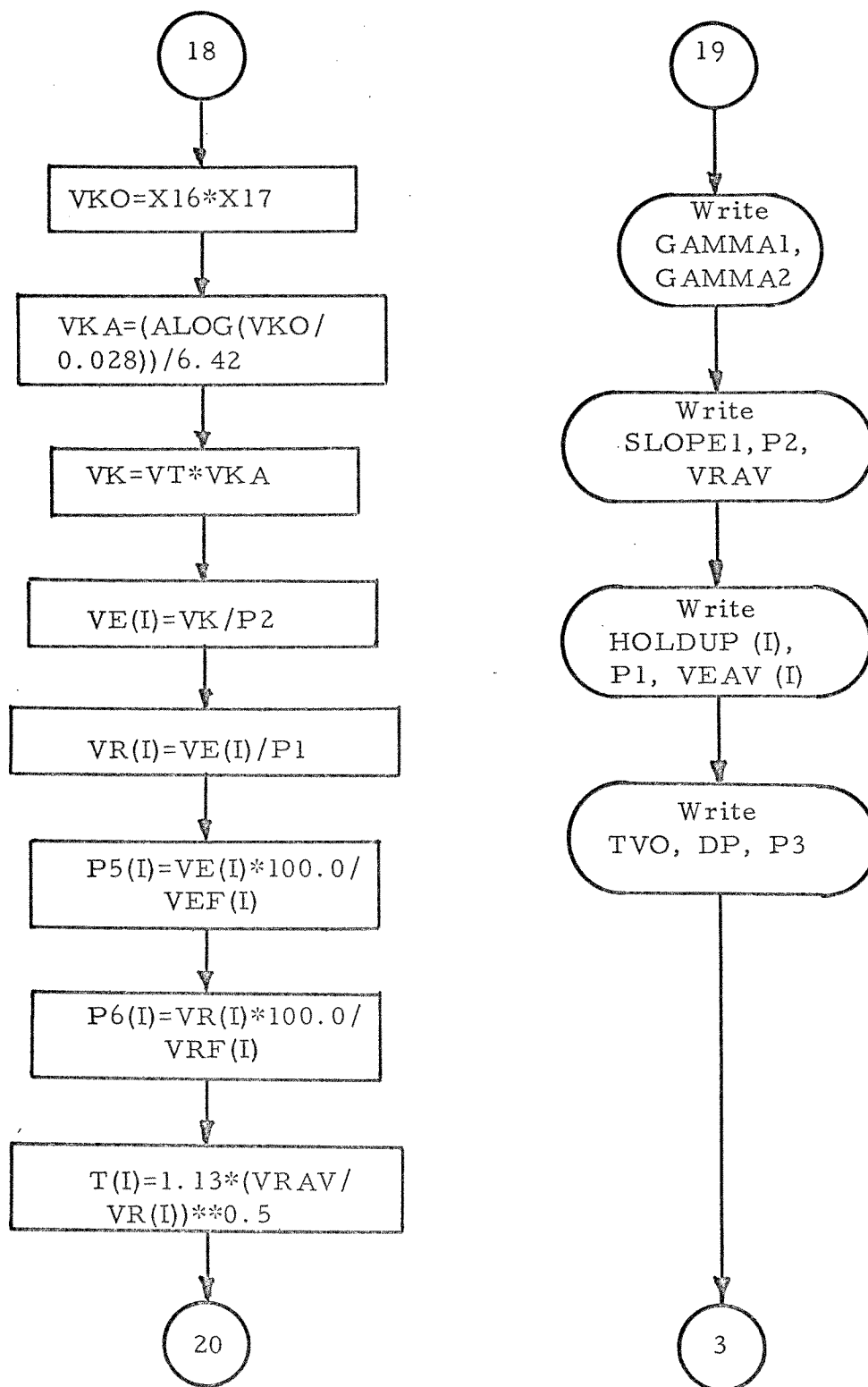


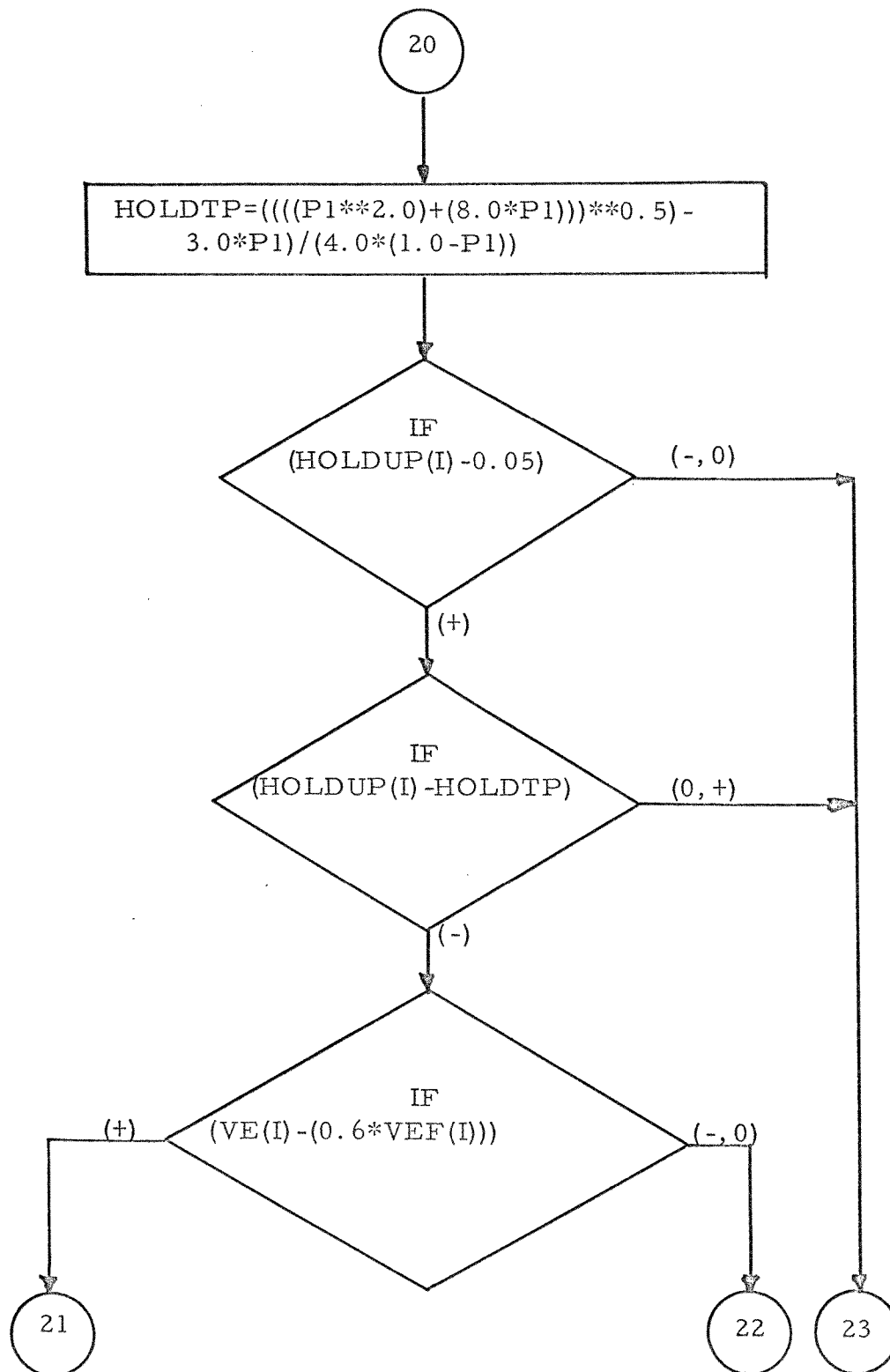
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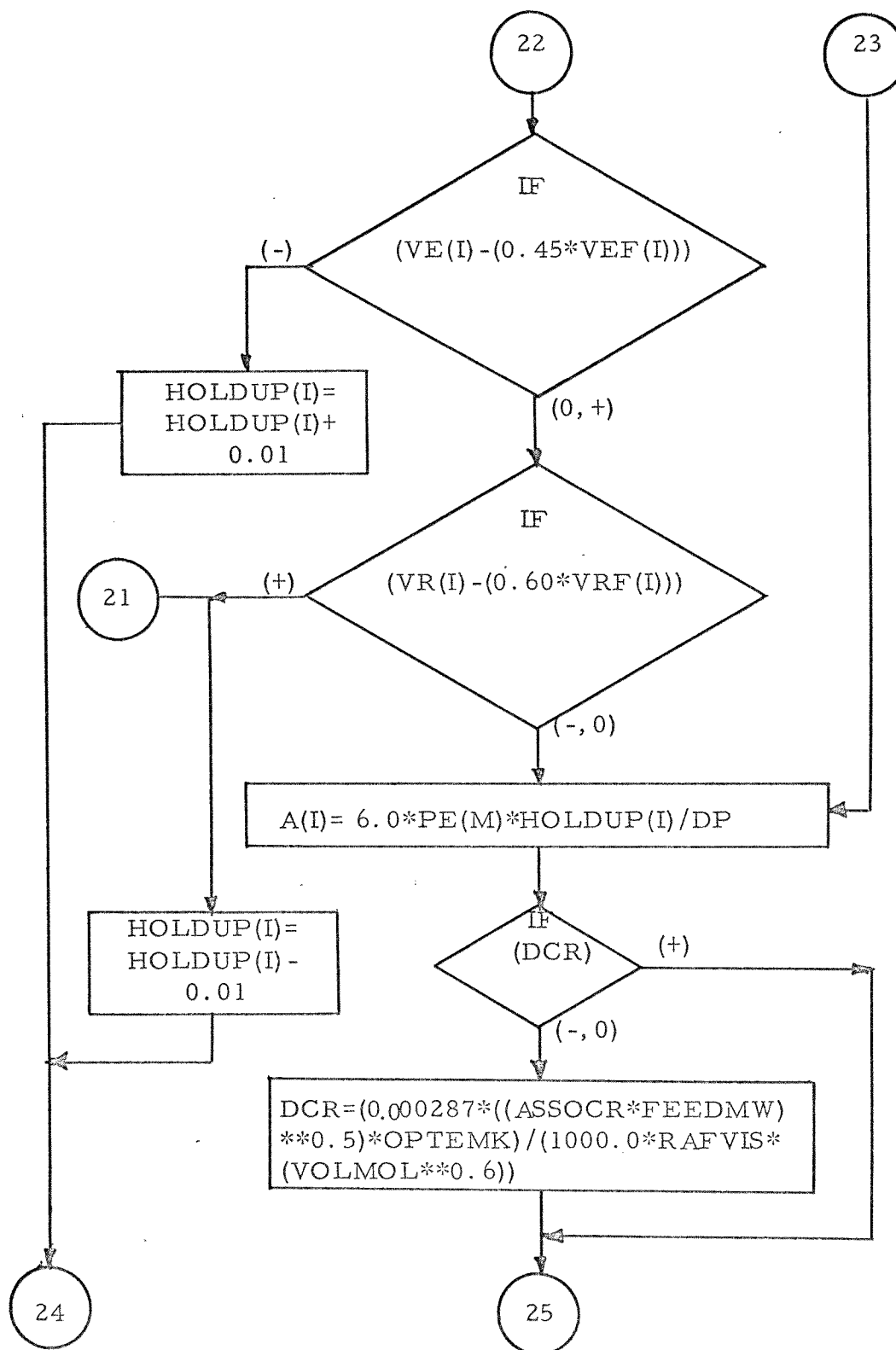
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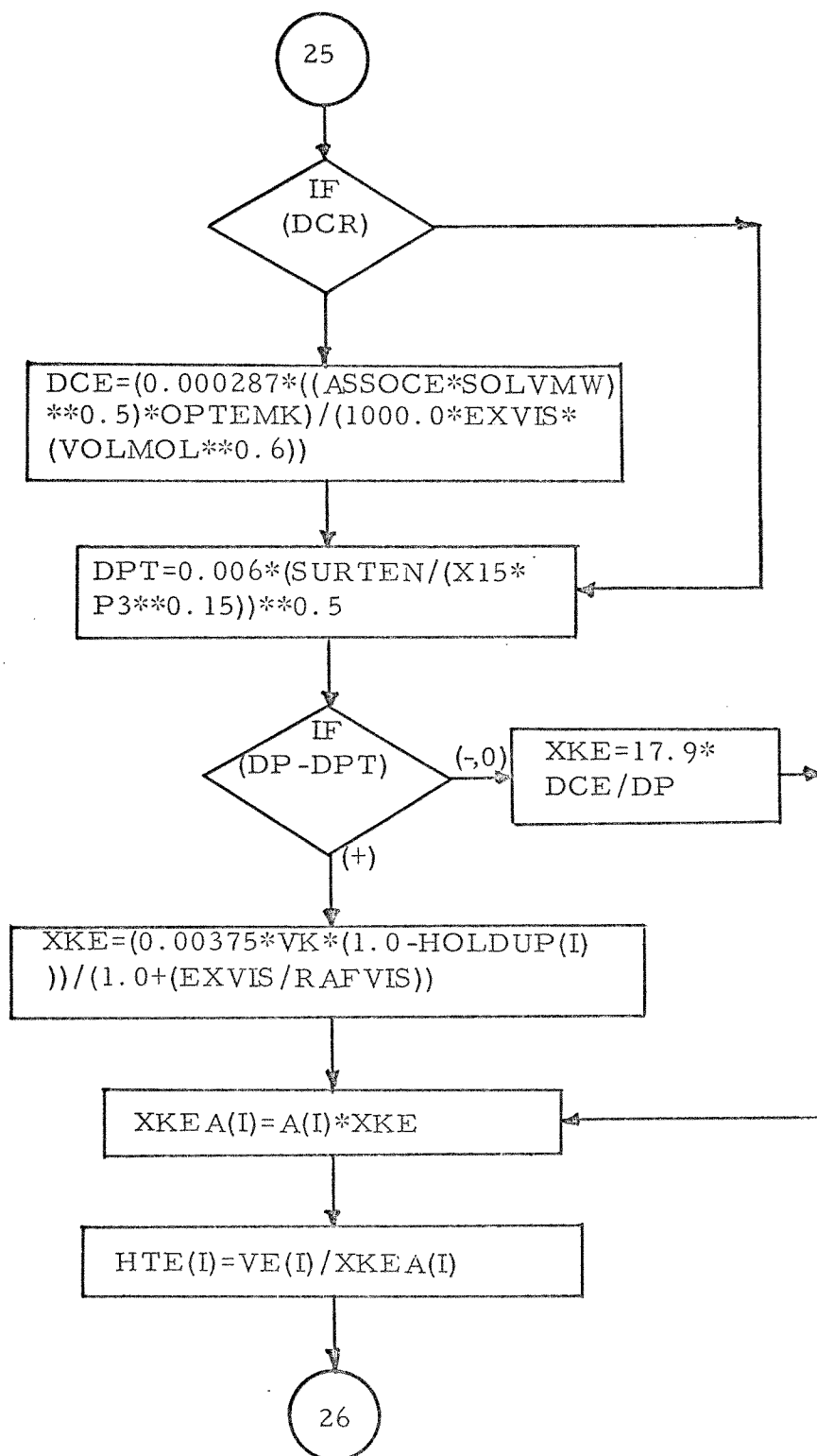
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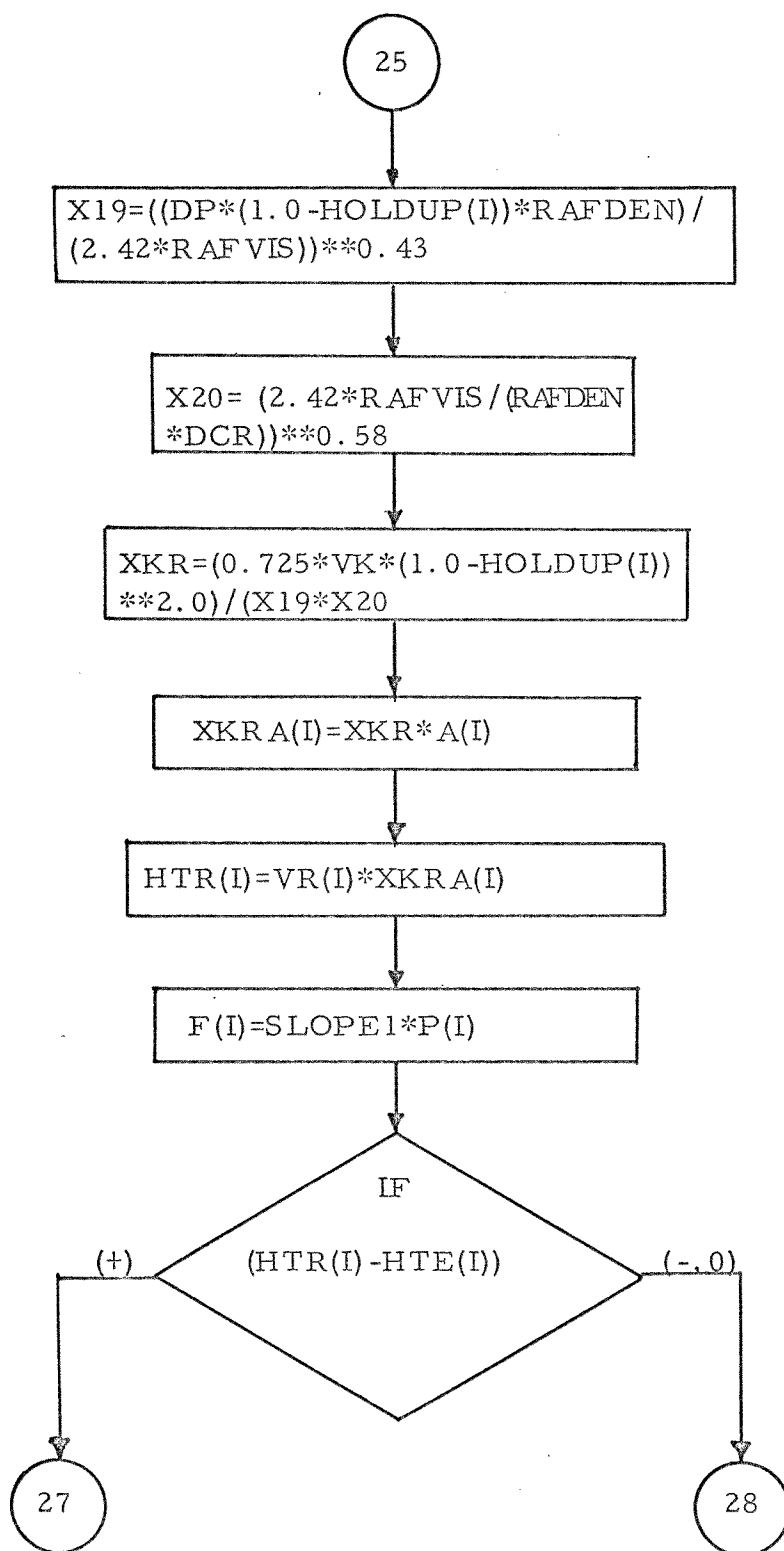
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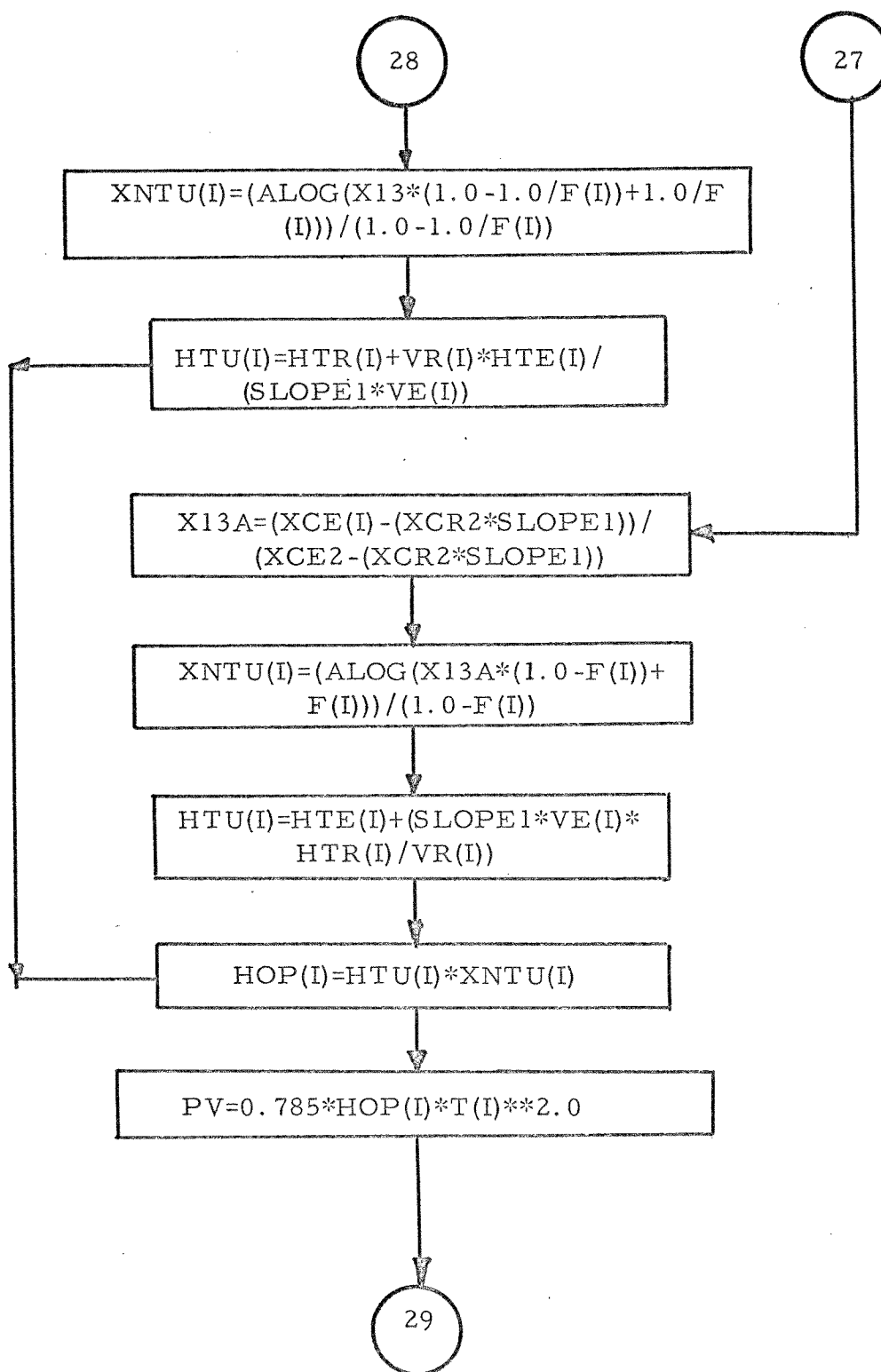
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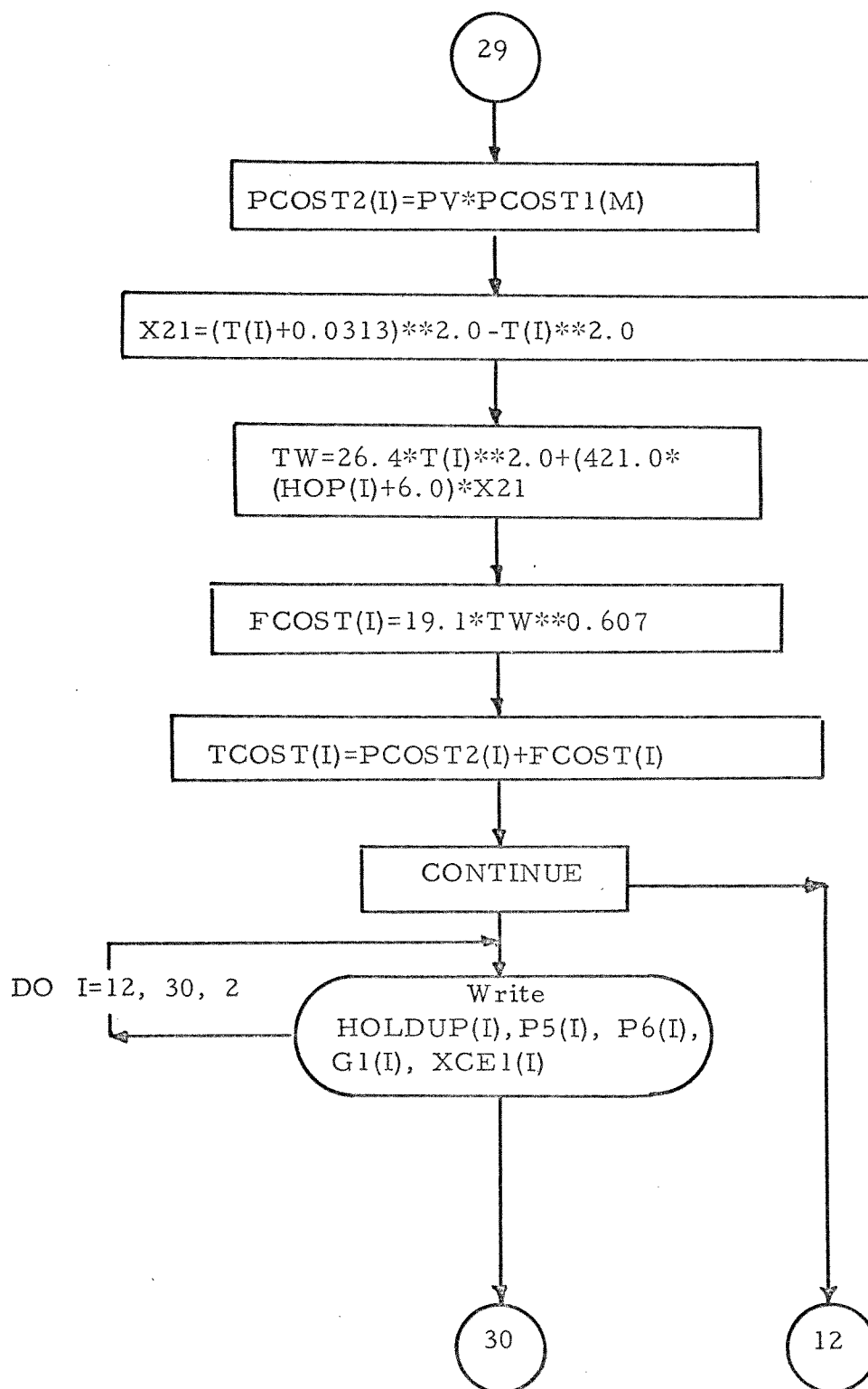


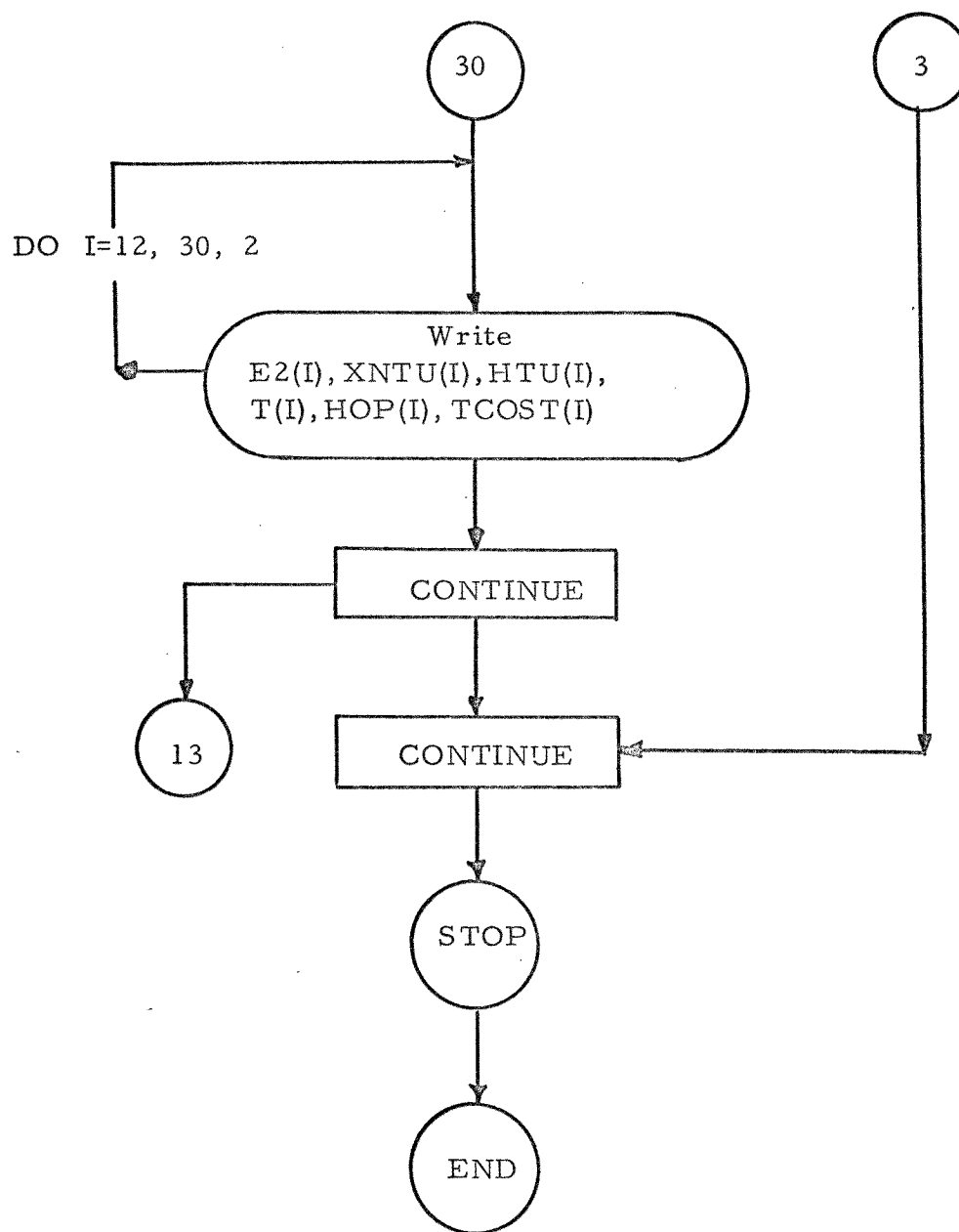
Block Diagram 18



Block Diagram 19



Block Diagram 20

Block Diagram 21

PROGRAM LISTING

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1      PROGRAM COLDES
2 C    DATA INPUT
3      READ (97,1) EXVIS,RAFVIS,FXDEN,RAFDEN,SOLVNW,SOLTIME,VOLMEC
4      1 FORMAT (7F10.0)
5      READ (97,2) SURTEN,SLOPE,R1,DPTMF,CR1,CR2,CE2
6      2 FORMAT (7F10.0)
7 C    A-B MUTUAL SOLUBILITY DATA
8      READ (97,3) XAA1,XBA,XBB1,XAB
9 C    B-C MUTUAL SOLUBILITY DATA
10     READ (97,3) XBC,XCC1,XCB,XBB2
11 C    C-A MUTUAL SOLUBILITY DATA
12     READ (97,3) XAC,XCC2,XCA,XAA2
13     3 FORMAT (4F10.0)
14 C    DISTRIBUTION COEFFICIENT AND HEIGHT OF TRANSFER UNIT DATA
15     READ (97,85) DCR,DCE,FEELMW,ASSOCR,ASSOCE
16     85 FORMAT (5F10.0)
17 C    INPUT OF RASCHIG RING (OR OTHER) PACKING DATA
18     DIMENSION PD(10),PE(10),PA(10),PDEN(10),PCOST1(10)
19     DO 11 J=1,6,1
20     READ (97,12) PD(J),PE(J),PA(J),PDEN(J),PCOST1(J)
21     12 FORMAT (5F10.0)
22     11 CONTINUE
23     IF (SLOPE) 4,6,7
24     4 WRITE (99,5)
25     5 FORMAT (21H ERROR NEGATIVE SLOPE)
26     GO TO 64
27 C    CALCULATION OF EQUILIBRIUM SLOPE USING TWO SUFFIX VAN LAAR EQUATIONS
28 C    CALCULATION OF VAN LAAR CONSTANTS FOR A-B BINARY
29     6 X1=XAA1/XBA+XAB/XBB1
30     X2=ALOG10(XAB/XAA1)
31     X3=ALOG10(XBA/XBB1)
32     X4=2.0*XAA1*XAB*X2
33     X5=XBA*XBB1*X3
34     A1AB=(X1*X2/X3-2.0)/(X1-(X4/X5))
35     X6=(1.0+(A1AB*XAA1/XBA))**2.0
36     X7=(1.0+(A1AB*XAB/XBB1))**2.0
37     A2AB=X2/(1.0/X6-1.0/X7)
38 C    CALCULATION OF VAN LAAR CONSTANTS FOR B-C BINARY
39     X1=XBB2/XCB+XBC/XCC1
40     X2=ALOG10(XBC/XBB2)
41     X3=ALOG10(XCB/XCC1)
42     X4=2.0*XBB2*XBC*X2
43     X5=XCB*XCC1*X3
44     A1BC=(X1*X2/X3-2.0)/(X1-(X4/X5))
45     X6=(1.0+(A1BC*XBB2/XCB))**2.0
46     X7=(1.0+(A1BC*XBC/XCC1))**2.0
47     A2BC=X2/(1.0/X6-1.0/X7)
48 C    CALCULATION OF VAN LAAR CONSTANTS FOR C-A BINARY
49     X1=XCC2/XAC+XCA/XAA2
50     X2=ALOG10(XCA/XCC2)

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51      X3=ALDG10(XAC/XAA2)
52      X4=2.0*XCC2*XCA*X2
53      X5=XAC*XAA2*X3
54      A1CA=(X1*X2/X3-2.0)/(X1-(X4/X5))
55      X6=(1.0+(A1CA*XCC2/XAC))**2.0
56      X7=(1.0+(A1CA*XCA/XAA2))**2.0
57      A2CA=X2/(1.0/X6-1.0/X7)
58 C    CALCULATE SOLUTE ACTIVITY COEFFICIENT IN A RICH LAYER
59      X8=(XAA1**2.0)*A2CA*(1.0/A1CA)**2.0
60      X9=XBA**2.0*(1.0/A1BC)*A2BC*A1BC**2.0
61      X10=XAA1*XBA*(1.0/A1CA)*A1BC
62      X11=A2CA+(1.0/A1BC)*A2BC-(1.0/A1AB)*A2AB*(1.0/A1BC)
63      X12=(XAA1*(1.0/A1CA)+XBA*A1BC)**2.0
64      GAMMA1=(X8+X9+X10*X11)/X12
65 C    CALCULATE SOLUTE ACTIVITY COEFFICIENT IN B RICH LAYER
66      X8=(XAB**2.0)*A2CA*(1.0/A1CA)**2.0
67      X9=XBB1**2.0*(1.0/A1BC)*A2BC*A1BC**2.0
68      X10=XAB*XBB1*(1.0/A1CA)*A1BC
69      X12=(XAB*(1.0/A1CA)+XBB1*A1BC)**2.0
70      GAMMA2=(X8+X9+X10*X11)/X12
71 C    CALCULATION OF EQUILIBRIUM SLOPE
72      SLOPE=10.0**((GAMMA1-GAMMA2))
73 C    CONVERT MOLE FRACTIONS TO WEIGHT FRACTIONS
74      XCR1=(CR1*SOLVMW)/(CR1*SOLVMW+FEEDMW*(1.0-CR1))
75      XCR2=(CR2*SOLVMW)/(CR2*SOLVMW+FEEDMW*(1.0-CR2))
76      XCE2=(CF2*SOLVMW)/(CE2*SOLVMW+SOLVMW*(1.0-CE2))
77 C    CONVERT EQUILIBRIUM SLOPE TO WEIGHT FRACTION BASIS
78      SLOPE1=FEEDMW*SLOPE/SOLVMW
79 C    CHECK SOLUTE CONCENTRATION IN SOLVENT FEED
80      IF (SLOPE1*XCR2-XCE2)8,8,10
81      8 WRITE (77,9)
82      9 FORMAT (50H ERROR,SOLVENT FEED IN EQUILIBRIUM WITH RAFFINATE)
83      GO TO 64
84 C    CALCULATION OF MINIMUM SOLVENT FEED RATE
85      10 X14=R1*(XCR1-XCR2)
86      R2=R1-X14
87      E2MIN=R2/((SLOPE1*XCR1-XCE2)/(XCP1-XCR2))
88      X13=(XCR1-XCE2/SLOPE1)/(XCR2-XCE2/SLOPE1)
89 C    CALCULATION OF CRITICAL PACKING SIZE
90      X15=ABS(RAFDEN-EXDEN)
91      PDC=0.24*(SURTEN/X15)**0.5
92 C    DETERMINATION OF PACKING SIZE
93      DO 14 J=1,6,1
94      K=J
95      IF (PDC=PD(J))22,14,14
96      14 CONTINUE
97      62 WRITE (99,63) PDC
98      63 FORMAT (43H CRITICAL PACKING DIAMETER TOO LARGE PDC=,F10.4)
99      GO TO 64
100     22 VRAV=(R1+R2)/(2.0*RAFDEN)

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101 C      CONVERT OPERATING TEMPERATURE TO KELVIN SCALE
102      OPTEMP=(0.556*(OPTEMP-32.0))+273.0
103      DIMENSION G1(30),P(30),F(30),XNTU(30),XCE1(30),E1(30),E2(30)
104      DIMENSION VEAV(30),VRF(30),VEF(30),HOLDUP(30),VE(30),VR(30)
105      DIMENSION T(30),A(30),XKRA(30),HTE(30),XKRA(30),HTR(30),HTU(30)
106      DIMENSION HOP(30),PCOST(30),FCOST(30),TCOST(30),P5(30),P6(30)
107      DO 67 M=R,6,1
108      WRITE (99,49) PD(M)
109      49 FORMAT (23H1 PACKING DIAMETER (IN)=,F6.3)
110      DO 61 I=12,30,2
111      G=1
112      G1(I)=G/10.0
113      F(I)=G1(I)*F2MIN/R2
114 C      CALCULATION OF EXIT SOLVENT CONCENTRATION
115      XCE1(I)=(X14+R2*P(I)*XCE2)/(X14+R2*P(I))
116 C      CALCULATION OF SOLVENT FEED RATE
117      E2(I)=R2*P(I)
118 C      CALCULATION OF EXTRACT FLOW RATE
119      13 E1(I)=E2(I)+X14
120      VEAV(I)=(E1(I)+E2(I))/(2.0*EXDEN)
121      P1=VEAV(I)/VRAV
122 C      CALCULATION OF FLOODING VELOCITIES
123      33 FD=((28700.0*SURTEN/RAFDEN)**0.2)*(2.42*RAFVIS/X15)*
124      1 ((PA(M)/PE(M))**1.5)
125      IF (FD-160.0)19,15,15
126      15 IF (3800.0-FD)17,16,16
127      16 FA=(140000.0/FD)**1.02
128      GO TO 21
129      17 IF (54000.0-FD)19,18,18
130      18 FA=(54000.0/FD)**1.39
131      GO TO 21
132      19 WRITE (99,20)
133      20 FORMAT (34H FLOODING VELOCITY ORDINATE OUTSIDE RANGE OF EQUATIONS)
134      WRITE (99,65) FD
135      65 FORMAT (4H FD=,F12.1)
136      GO TO 86
137      21 VRF(I)=(PA(M)*2.42*RAFVIS*FA)/(((1.0+P1**0.5)**2.0)*RAFDEN)
138      VEF(I)=VRF(I)*P1
139 C      CALCULATION OF TOWER DIAMETER AND DISPERSED PHASE HOLDUP
140      HOLDUP(I)=0.15
141      39 P2=((1.07/(PE(M)*HOLDUP(I)*(1.0-HOLDUP(I))))+(1.07/(PI*PE(M)*
142      1 ((1.0-HOLDUP(I))**2.0)))
143 C      CALCULATION OF DROP DIAMETER(DP)
144      DP=0.00762*((SURTEN/X15)**0.5)*P2*PE(M)*HOLDUP(I)
145 C      CALCULATION OF TERMINAL DROP VELOCITY
146      P3=(1644.0*(RAFDEN**2.0)*(SURTEN**3.0))/((RAFVIS**4.0)*X15)
147      IVU=19400.0*X15*DP**2.0*P3**0.15/SURTEN
148      IF (IVU-1.0)26,28,23
149      23 IF (IVU-7.2)28,29,24
150      24 IF (IVU-78.0)29,30,25

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151 25 IF (TV0-2000.0)30,30,26
152 26 WRITE (99,27)
153 27 FORMAT (45H TERMINAL VELOCITY OUTSIDE RANGE OF EQUATIONS)
154 86 WRITE (99,72) A1AB,A2AB,A1BC
155 72 FORMAT (6H0A1AB=,F10.5,6H A2AB=,F10.5,6H A1BC=,F10.5)
156 WRITE (99,73) A2BC,A1CA,A2CA
157 73 FORMAT (6H0A2BC=,F10.5,6H A1CA=,F10.5,6H A2CA=,F10.5)
158 WRITE (99,74) GAMMA1,GAMMA2
159 74 FORMAT (6H0GAMMA1=,F10.5,8H GAMMA2=,F10.5)
160 WRITE (99,71) SLOPE1,P2,VRAV
161 71 FORMAT (9H0SLOPE1 =,F10.3,5H P2 =,F10.4,9H VRAV =,F8.1)
162 WRITE (99,68) HOLDUP(I),F1,VEAV(I)
163 68 FORMAT (11H0HOLDUP(I)=,F6.3,4H P1=,F8.3,9H VEAV(I)=,F8.1)
164 WRITE (99,66) TV0,DP,P3
165 66 FORMAT (5H0TV0=,F12.1,4H DP=,F14.8,4H P3=,E12.6)
166 GO TO 64
167 25 IVA=0.26*TV0**1.25
168 GO TO 31
169 29 IVA=0.6*TV0**0.8
170 GO TO 31
171 30 IVA=3.4*TV0**0.424
172 31 VT=(2.42*IVA**RAFEVIS*(P3**0.15))/(DP*RAFDEN)
173 C CALCULATION OF CHARACTERISTIC DROP VELOCITY(VK)
174 X16=(418000000.0*X15)/(EXDEN*(VT**2.0))
175 X17=(0.35*PD(H)/12.0)-(0.00762*(SURTEN/X15)**0.5)
176 VK0=X16*X17
177 VKA=(ALOG(VK0/0.023))/6.42
178 VK=VT*VKA
179 C CALCULATION OF THE TOWER DIAMETER
180 VE(I)=VK/P2
181 VR(I)=VE(I)/PI
182 P5(I)=VE(I)*100.0/VEF(I)
183 P6(I)=VR(I)*100.0/VRF(I)
184 100 T(I)=1.13*(VKAV/VR(I))**0.5
185 C COMPARE HOLD-UP TO HOLD-UP AT TRANSITION
186 HOLDTP=T((PI**2.0)+(8.0*PI))**0.5+3.0*PI)/(4.0*(1.0+PI))
187 IF (HOLDUP(I)-0.05)40,40,84
188 84 IF (HOLDUP(I)-HOLDTP)34,40,40
189 C COMPARISON OF OPERATING AND FLOODING SUPERFICIAL VELOCITIES
190 34 IF (VE(I)-(0.60*VEF(I)))25,35,38
191 35 IF (VE(I)-(0.45*VEF(I)))37,36,36
192 36 IF (VR(I)-(0.60*VRF(I)))40,40,38
193 37 HOLDUP(I)=HOLDUP(I)+0.01
194 GO TO 39
195 38 HOLDUP(I)=HOLDUP(I)-0.01
196 GO TO 39
197 C CALCULATION OF INTERFACIAL AREA
198 40 A(I)=6.0*PE(H)*HOLDUP(I)/DP
199 C CALCULATION OF DIFFUSION COEFFICIENT FOR SOLUTE IN RAFFINATE
200 IF (OCR) 41,41,42

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201 41 DCR=(0.000287*((ASSOCR*FEEDMW)**0.5)*OPTMK)/(1000.0*RAFVIS*
202 1(VOLHDL**0.6))
203 C CALCULATION OF DIFFUSION COEFFICIENT FOR SOLUTE IN EXTRACT
204 42 IF (DCE) 43,43,44
205 43 DCE=(0.000287*((ASSOCE*SOLVMW)**0.5)*OPTMK)/(1000.0*EXVIS*
206 1(VOLHDL**0.6))
207 C CALCULATION OF HEIGHT OF EXTRACT TRANSFER UNIT
208 44 DPI=0.006*(SURTEN/(X15*P3**0.15))**0.5
209 IF (DP-DPT)45,45,46
210 45 XKE=17.9*DCE/DP
211 GO TO 47
212 46 XKE=(0.00375*VR*(1.0-HOLDUP(I)))/(1.0+(EXVIS/RAFVIS))
213 47 XKEA(I)=A(I)*XKE
214 HTE(I)=VE(I)/XKEA(I)
215 C CALCULATION OF HEIGHT OF RAFFINATE TRANSFER UNIT
216 X19=((DP*(1.0-HOLDUP(I))*RAFDEN)/(2.42*RAFVIS))**0.43
217 X20=(2.42*RAFVIS/(RAFDEN+DCR))**0.58
218 XKR=(0.725*VR*(1.0-HOLDUP(I))**2.0)/(X19*X20)
219 XKRA(I)=XKR*A(I)
220 HTR(I)=VR(I)/XKRA(I)
221 C CALCULATION OF HEIGHT OF OVERALL TRANSFER UNIT AND PACKED HEIGHT
222 C CALCULATION OF THE NUMBER OF TRANSFER UNITS
223 F(I)=SLOPE1*P(I)
224 IF (HTR(I)-HTE(I))90,90,91
225 90 XNTU(I)=(ALOG(X13*(1.0-1.0/F(I))+1.0/F(I)))/(1.0-1.0/F(I))
226 HTU(I)=HTR(I)+VR(I)*HTE(I)/(SLOPE1*VE(I))
227 GO TO 92
228 91 X13A=(XCE1(I)-(XCR2*SLOPE1))/(XCE2-(XCR2*SLOPE1))
229 XNTU(I)=(ALOG(X13A*(1.0-F(I))+F(I)))/(1.0-F(I))
230 HTU(I)=HTE(I)+(SLOPE1*VE(I)*HTR(I)/VR(I))
231 92 HOP(I)=HTU(I)*XNTU(I)
232 C CALCULATION OF THE COST OF THE COLUMN
233 PV=0.785*HOP(I)*T(I)**2.0
234 PCOST2(I)=PV*PCOST1(H)
235 X21=(T(I)+0.0313)**2.0-T(I)**2.0
236 TW=26.4*T(I)**2.0+(421.0*(HOP(I)+6.0)*X21)
237 FCOST(I)=19.1*TW**0.607
238 46 TCDST(I)=PCOST2(I)+FCOST(I)
239 61 CONTINUE
240 WRITE (99,78)
241 78 FORMAT (13H0 HOLDUP ,5X,2HP5,10X,2HP6,10X,2HG1,9X,4H XCE1)
242 DD 79 I=12,30,2
243 79 WRITE (99,80) HOLDUP(I),F5(I),P6(I),G1(I),XCE1(I)
244 80 FORMAT (1H ,3X,F6.2,7X,F5.1,7X,F5.1,7X,F4.1,7X,F9.6)
245 WRITE (99,81)
246 81 FORMAT (13H0 E2 ,4X,4HNTU ,8X,4HHTU ,8X,4HJAM,9X,3H HOP,
247 18X,5HTCDST)
248 DD 83 I=12,30,2
249 83 WRITE (99,82) E2(I),XNTU(I),HTU(I),T(I),HOP(I),TCDST(I)
250 82 FORMAT (1H ,3X,F6.0,6X,F6.2,6X,F6.2,7X,F4.1,7X,F6.1,5X,F6.0)

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251 67 CONTINUE
252 64 CONTINUE
253 STOP
254 END

FIGURES

FIGURE 6

EFFECT OF EXTRACT DENSITY ON COLUMN COST
AND THE HEIGHT OF A TRANSFER UNIT

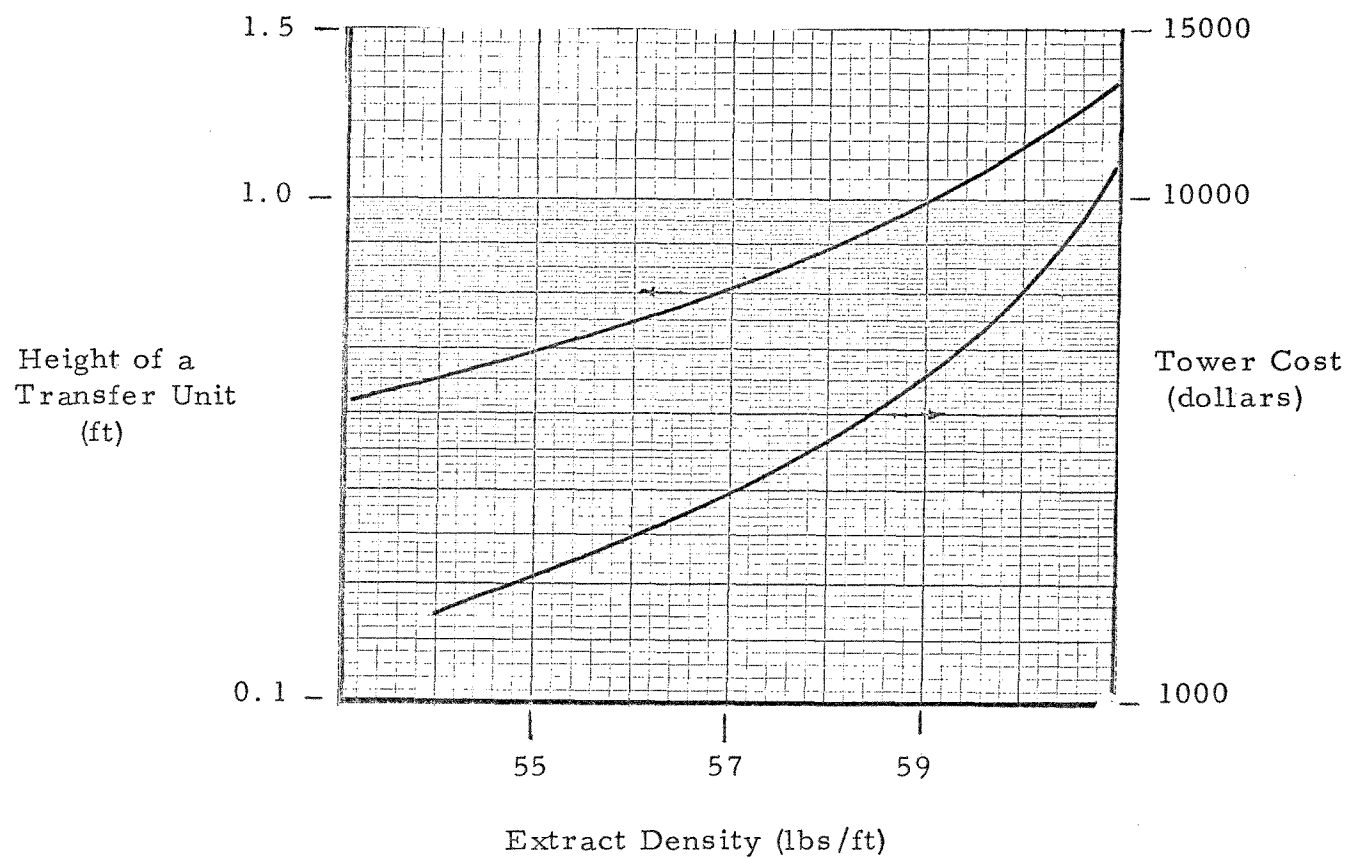


FIGURE 7

EFFECT OF EXTRACT DENSITY ON TOWER DIAMETER

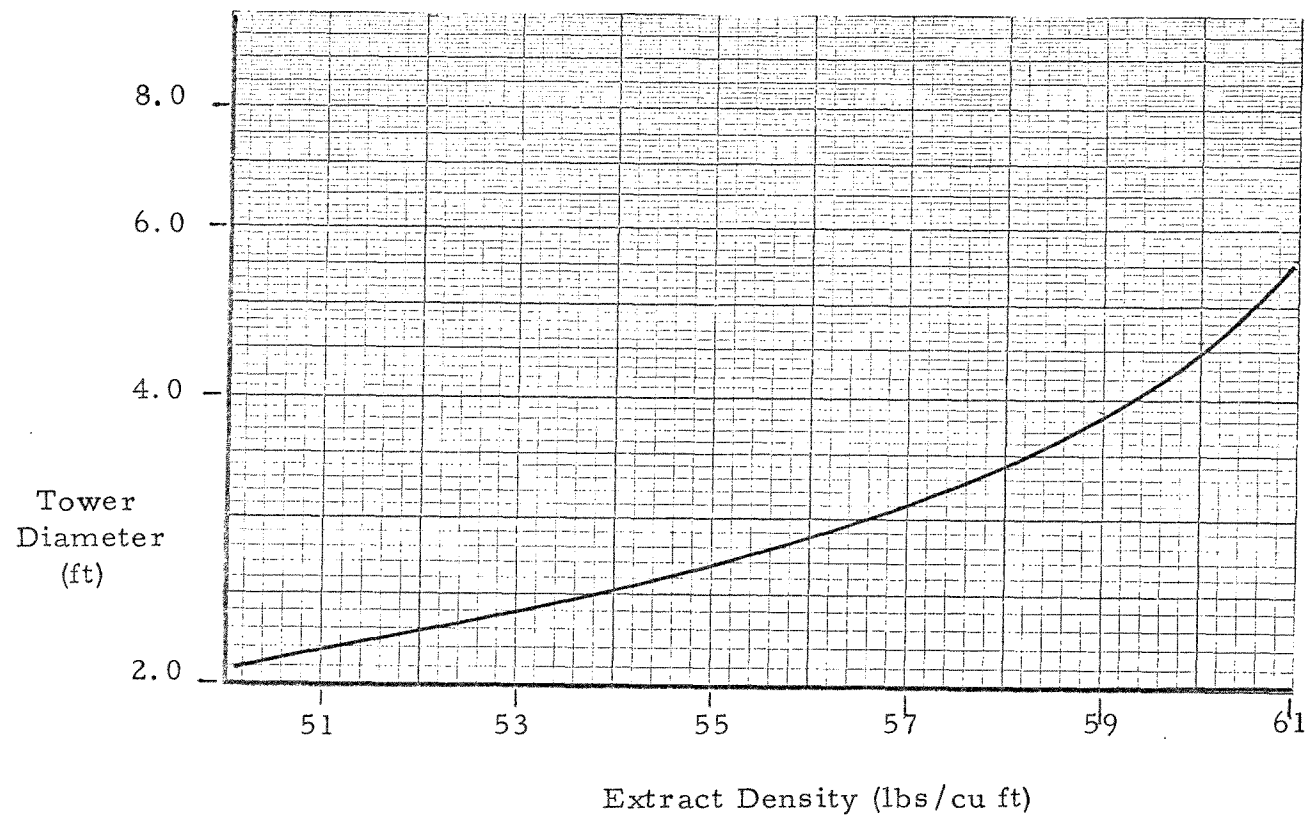


FIGURE 8

EFFECT OF EXTRACT VISCOSITY ON TOWER COST
AND THE HEIGHT OF A TRANSFER UNIT

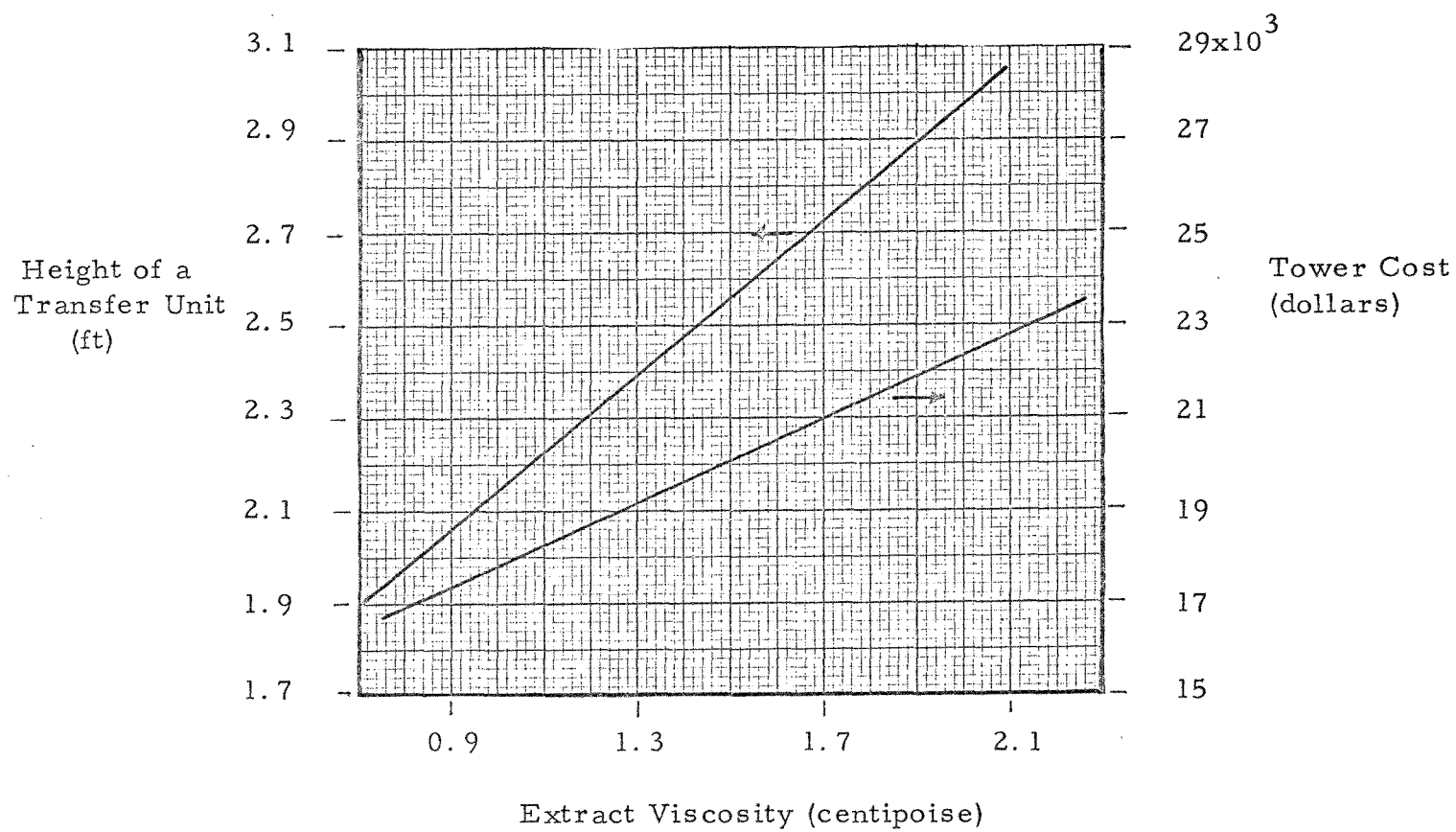


FIGURE 9

EFFECT OF RAFFINATE DENSITY ON TOWER COST
AND THE HEIGHT OF A TRANSFER UNIT

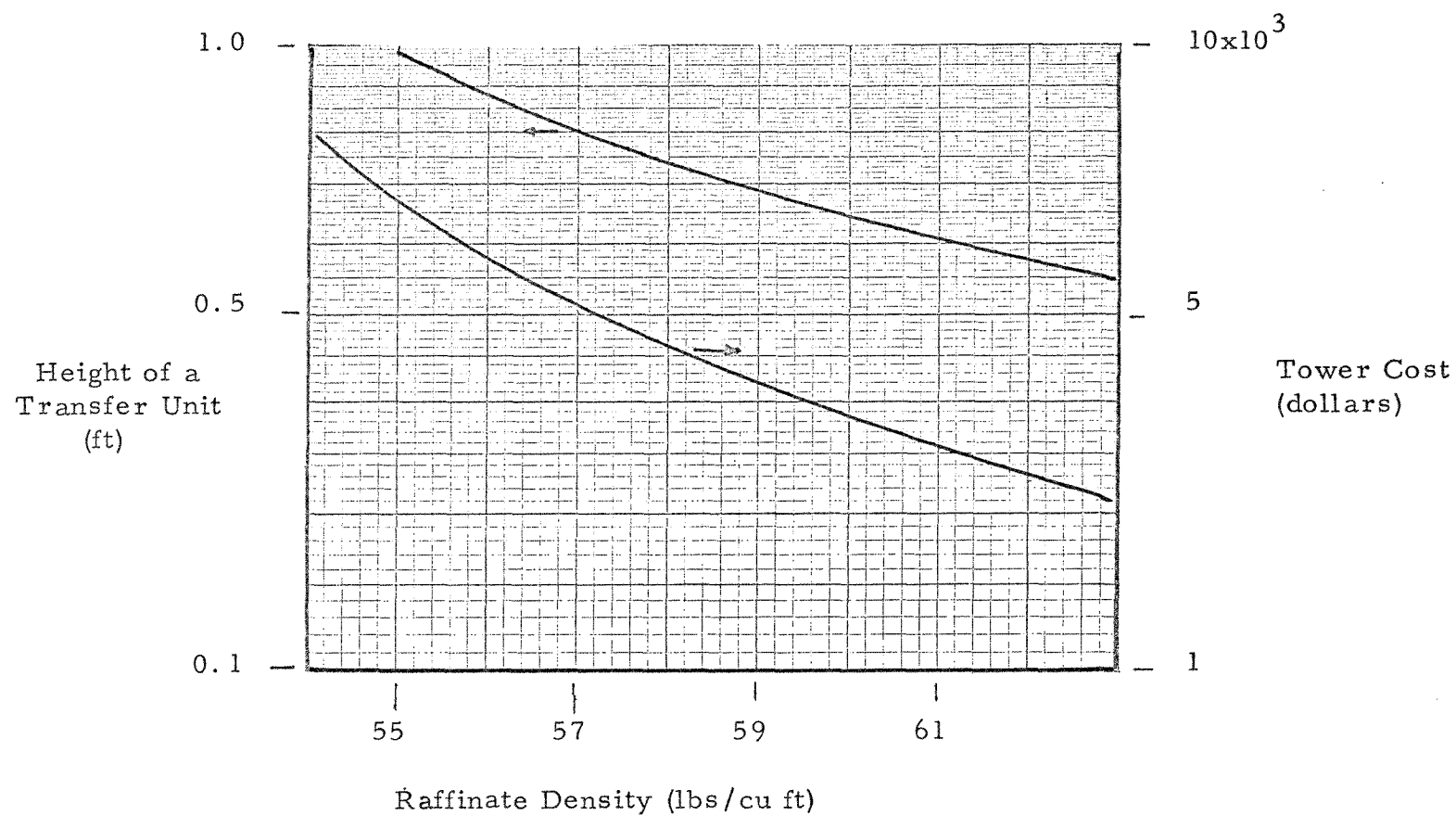


FIGURE 10

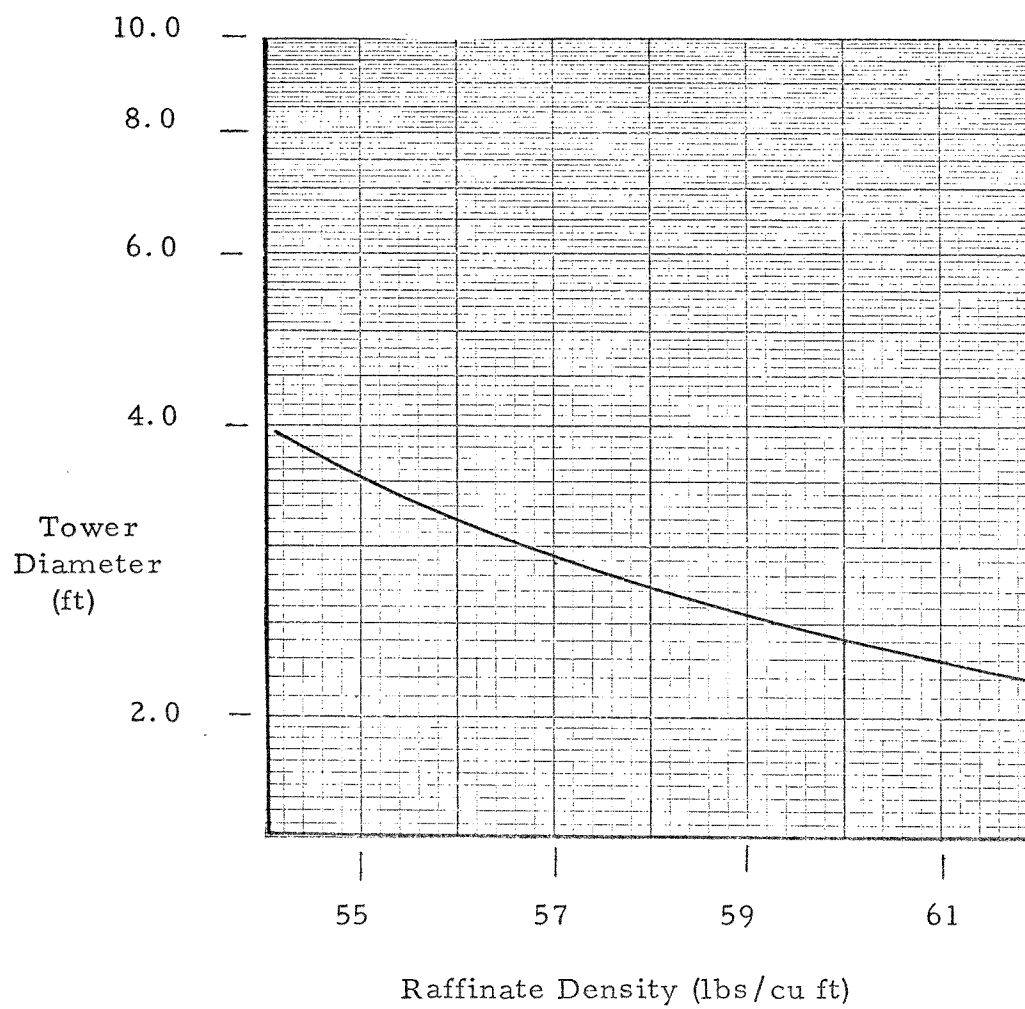
EFFECT OF RAFFINATE DENSITY ON TOWER DIAMETER

FIGURE 11

EFFECT OF INTERFACIAL TENSION ON TOWER COST
AND THE HEIGHT OF A TRANSFER UNIT

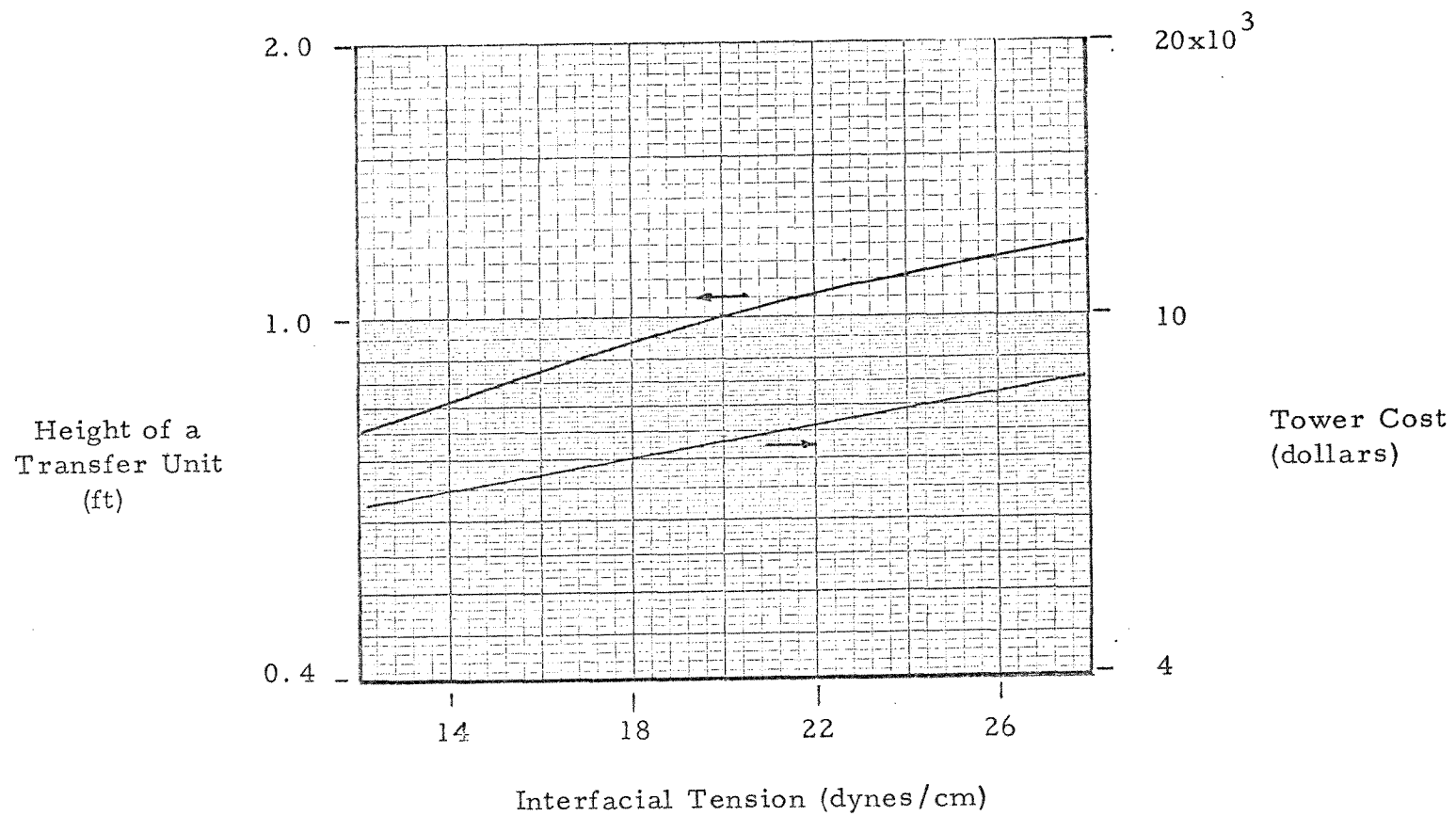


FIGURE 12

EFFECT OF SOLVENT RATE ON THE NUMBER OF TRANSFER UNITS
AND THE HEIGHT OF A TRANSFER UNIT

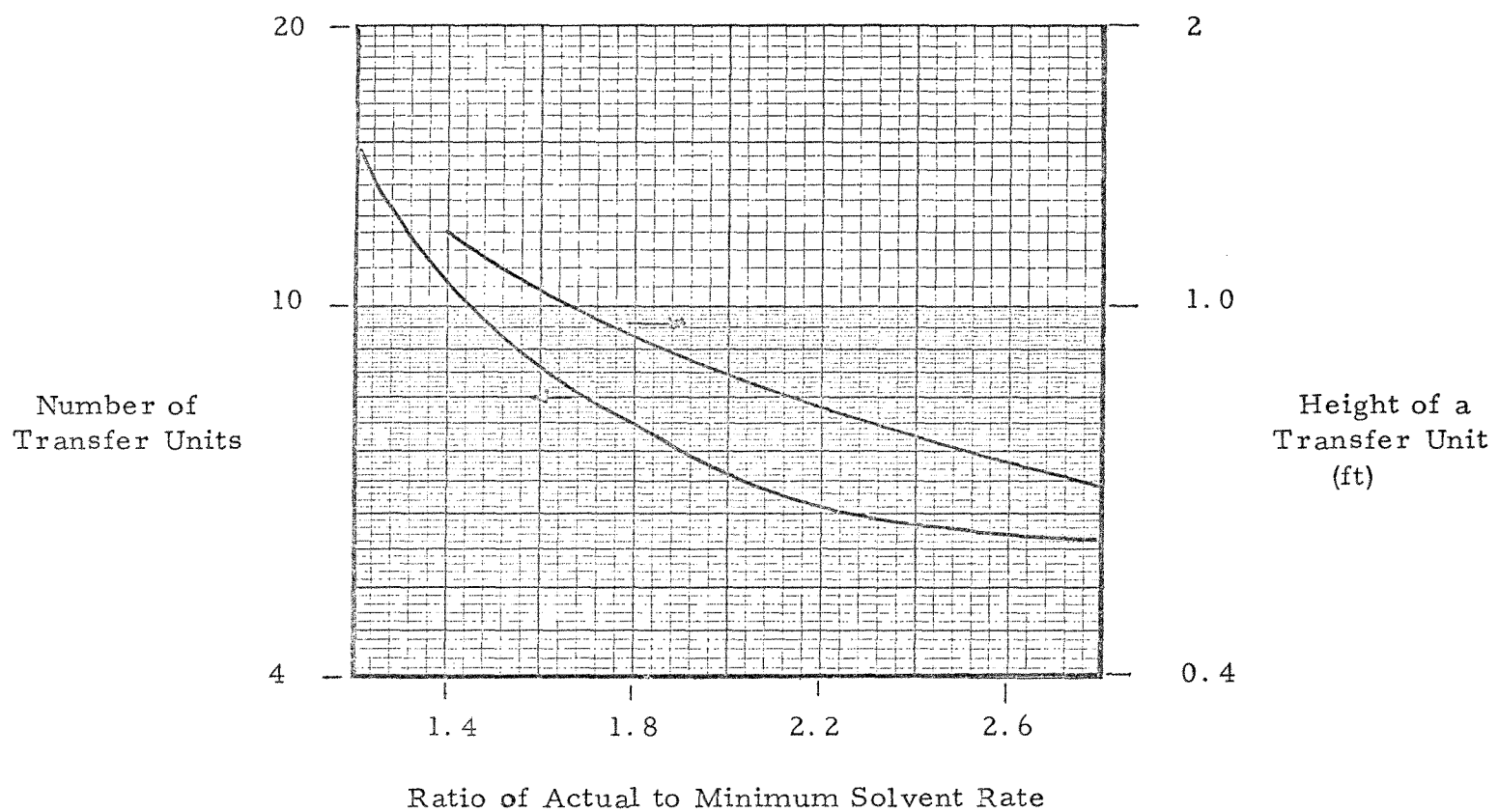


FIGURE 13

EFFECT OF SOLVENT RATE ON TOWER COST AND TOWER DIAMETER

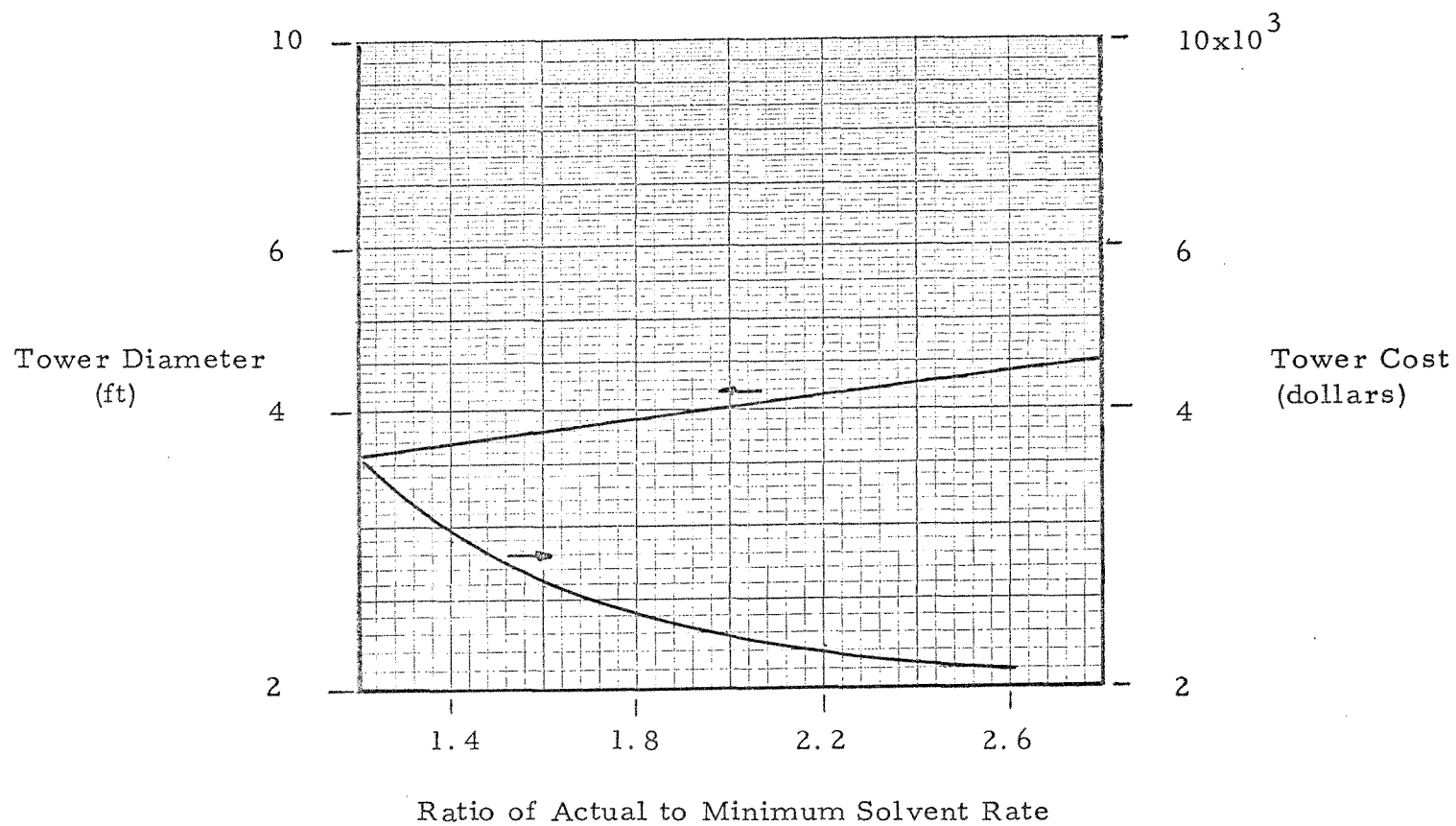
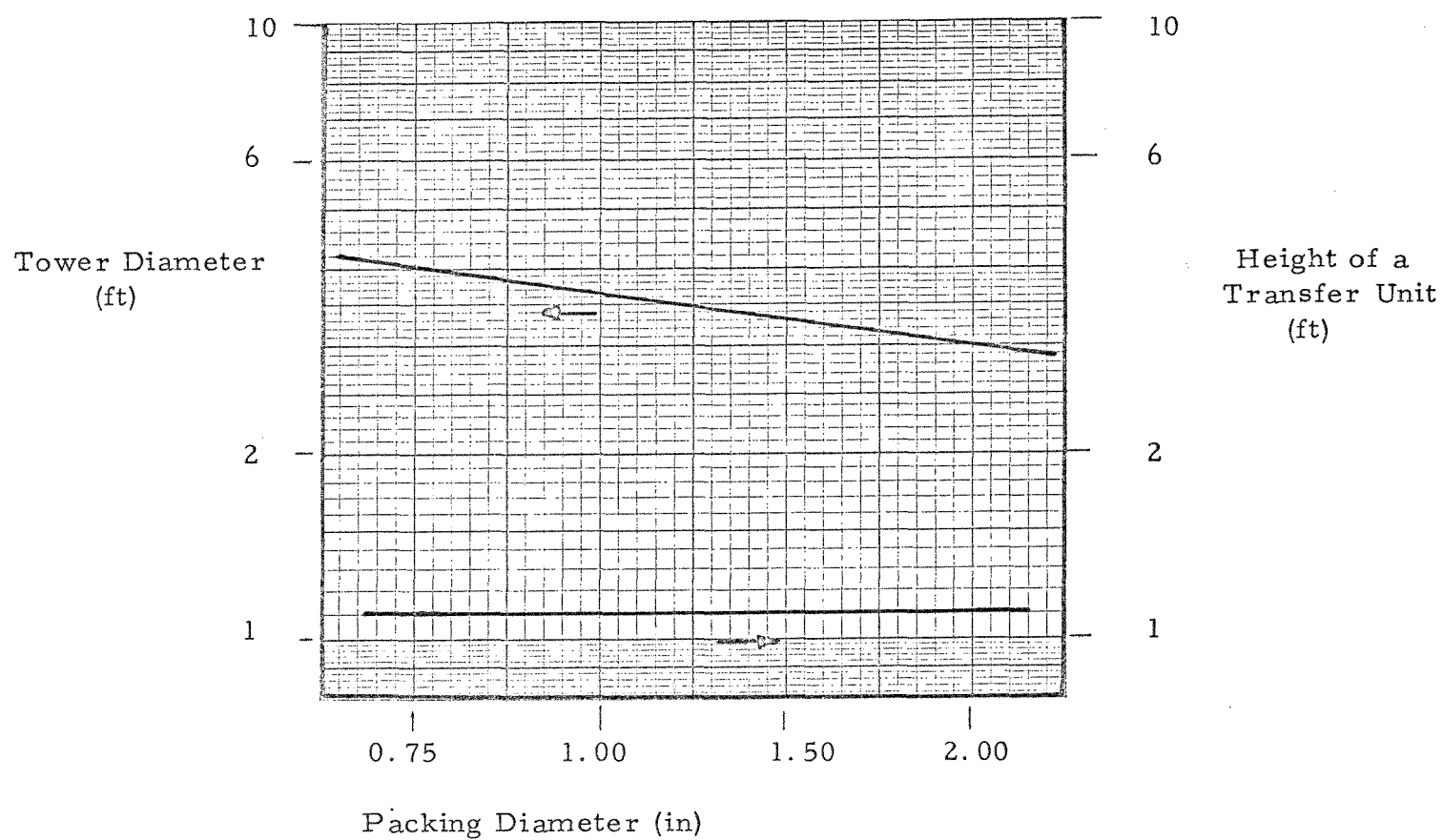


FIGURE 14

EFFECT OF PACKING DIAMETER ON TOWER COST AND THE HEIGHT OF A TRANSFER UNIT



TABLES

TABLE 4
EFFECT OF EXTRACT DENSITY ON COLUMN DESIGN

Packing	=	1.0 inch Raschig Rings
Ratio of Actual to Minimum Solvent Flow Rate	=	1.5
Number of Transfer Units	=	9.23
Raffinate Density	=	64.0 lbs/cu ft

<u>Extract Density (lbs/cu ft)</u>	<u>Dispersed Phase Holdup</u>	<u>Height of Overall Transfer Unit (ft)</u>	<u>Tower Diameter (ft)</u>	<u>Tower Cost (dollars)</u>
50.0	0.13	0.53	2.0	2963
51.0	0.12	0.55	2.1	3134
52.0	0.11	0.58	2.2	3339
53.0	0.10	0.61	2.3	3585
54.0	0.10	0.66	2.4	3751
55.0	0.09	0.70	2.5	4093
57.0	0.07	0.81	2.9	5110
58.0	0.07	0.90	3.0	5565
59.0	0.06	0.99	3.4	6586
60.0	0.05	1.13	4.0	8220
61.0	0.05	1.34	4.4	10248
62.0	0.05	1.74	5.6	15659

TABLE 5

EFFECT OF EXTRACT VISCOSITY ON COLUMN DESIGN

Packing	=	1.0 inch Raschig Rings
Ratio of Actual to Minimum Solvent Flow Rate	=	1.5
Number of Transfer Units	=	9.23
Raffinate Viscosity	=	1.0 centipoise
Extract Density	=	62.0 lbs/cu ft

<u>Extract Viscosity (centipoise)</u>	<u>Dispersed Phase Holdup</u>	<u>Height of Overall Transfer Unit (ft)</u>	<u>Tower Diameter (ft)</u>	<u>Tower Cost (dollars)</u>
0.5	0.06	1.74	5.6	15659
0.7	0.06	1.90	5.6	16583
0.9	0.06	2.07	5.6	17499
1.1	0.06	2.24	5.6	18409
1.3	0.06	2.40	5.6	19312
1.5	0.06	2.57	5.6	20210
1.7	0.06	2.73	5.6	21102
1.9	0.06	2.90	5.6	21989
2.1	0.06	3.06	5.6	22871
2.3	0.06	3.23	5.6	23748
2.5	0.06	3.40	5.6	24620
2.7	0.06	3.56	5.6	25489
2.9	0.06	3.73	5.6	26353

TABLE 6

EFFECT OF RAFFINATE DENSITY ON COLUMN DESIGN

Packing	=	1.0 inch Raschig Rings
Ratio of Actual to Minimum Solvent Flow Rate	=	1.5
Number of Transfer Units	=	9.23
Extract Density	=	50 lbs/cu ft

<u>Raffinate Density (lbs/cu ft)</u>	<u>Dispersed Phase Holdup</u>	<u>Height of Overall Transfer Unit (ft)</u>	<u>Tower Diameter (ft)</u>	<u>Tower Cost (dollars)</u>
54	0.06	1.13	3.8	7993
55	0.06	0.98	3.6	6876
56	0.07	0.88	3.2	5775
57	0.08	0.81	2.9	5018
58	0.08	0.74	2.8	4656
59	0.09	0.69	2.6	4187
60	0.10	0.65	2.4	3820
61	0.11	0.62	2.3	3525
62	0.11	0.58	2.2	3373
63	0.12	0.55	2.1	3154

TABLE 7

EFFECT OF RAFFINATE VISCOSITY ON COLUMN DESIGN

Packing	=	1.0 inch Raschig Rings
Ratio of Actual to Minimum Solvent Flow Rate	=	1.5
Number of Transfer Units	=	9.23
Extract Viscosity	=	0.5 centipoise
Extract Density	=	50.0 lbs/cu ft
Raffinate Density	=	63.0 lbs/cu ft

<u>Raffinate Viscosity (centipoise)</u>	<u>Dispersed Phase Holdup</u>	<u>Height of Overall Transfer Unit (ft)</u>	<u>Tower Diameter (ft)</u>	<u>Tower Cost (dollars)</u>
1.0	0.12	0.55	2.1	3154
1.2	0.12	0.53	2.1	3119
1.4	0.12	0.52	2.1	3096
1.6	0.12	0.51	2.1	3081
1.8	0.12	0.50	2.1	3071
2.0	0.12	0.49	2.2	3063
2.2	0.12	0.49	2.2	3059
2.4	0.12	0.49	2.2	3056

TABLE 8
EFFECT OF INTERFACIAL TENSION ON COLUMN DESIGN

Packing	=	1.0 inch Raschig Rings
Ratio of Actual to Minimum Solvent Flow Rate	=	1.5
Number of Transfer Units	=	9.23

<u>Interfacial Tension (dynes/cm)</u>	<u>Dispersed Phase Holdup</u>	<u>Height of Overall Transfer Unit (ft)</u>	<u>Tower Diameter (ft)</u>	<u>Tower Cost (dollars)</u>
10	0.07	0.69	3.5	5764
12	0.07	0.77	3.5	6001
14	0.06	0.82	3.8	6641
16	0.06	0.89	3.8	6883
18	0.06	0.94	3.8	7125
20	0.06	1.00	3.8	7368
22	0.06	1.06	3.8	7614
24	0.06	1.11	3.8	7865
26	0.06	1.16	3.9	8124
28	0.06	1.21	3.9	8391
30	0.06	1.25	3.9	8669

TABLE 9

EFFECT OF SOLVENT -FEED SOLUBILITY ON COLUMN DESIGN

Packing	=	1.0 inch Raschig Rings
Ratio of Actual to Minimum Solvent Flow Rate	=	1.5
Number of Transfer Units	=	9.23
Extract Density	=	50.0 lbs/cu ft
Raffinate Viscosity	=	3.2 centipoise

Mutual Solubilities
(Mole Fractions)

X_{ba}, X_{ab}	X_{aa}, X_{bb}	Dispersed Phase Holdup	Height of Overall Transfer Unit (ft)	Tower Diameter (ft)	Tower Cost (dollars)
0.001	0.999	0.12	0.48	2.2	3053
0.003	0.997	0.12	0.47	2.2	3067
0.005	0.995	0.12	0.47	2.2	3082
0.007	0.993	0.13	0.48	2.1	3023
0.009	0.991	0.13	0.48	2.2	3036
0.011	0.989	0.13	0.47	2.2	3050
0.013	0.987	0.13	0.47	2.2	3063
0.015	0.985	0.13	0.47	2.2	3076
0.017	0.983	0.13	0.47	2.2	3090

TABLE 10
COMPUTER OUTPUT FOR 0.75 INCH RASCHIG RINGS

PACKING DIAMETER (IN)= 0.750					
HOLDUP	P5	P6	G1	XCE1	
0.07	58.5	58.3	1.2	0.062352	
0.07	55.0	55.0	1.4	0.053925	
0.08	57.7	57.7	1.6	0.047505	
0.08	55.0	55.0	1.8	0.042450	
0.09	57.8	57.8	2.0	0.038368	
0.09	55.7	55.7	2.2	0.035002	
0.10	58.3	58.3	2.4	0.032179	
0.10	56.6	56.6	2.6	0.029778	
0.11	59.1	59.1	2.8	0.027710	
0.11	57.7	57.7	3.0	0.025910	
E2	NTU	HTU	DIAM	HSP	TCOST
7194.	14.95	1.46	4.0	21.8	4543.
8393.	10.30	1.25	4.2	12.9	3544.
9592.	8.48	1.11	4.2	9.4	3006.
10790.	7.49	0.99	4.5	7.4	2826.
11989.	6.87	0.91	4.5	6.2	2611.
13188.	6.44	0.82	4.7	5.3	2556.
14387.	6.13	0.77	4.6	4.7	2432.
15586.	5.89	0.71	4.8	4.2	2417.
16785.	5.70	0.67	4.8	3.8	2334.
17984.	5.54	0.62	4.9	3.5	2330.

TABLE 11

COMPUTER OUTPUT FOR 1.00 INCH RASCHIG RINGS

PACKING DIAMETER (IN)= 1.000

HOLDUP	P5	P6	G1	XCE1
0.05	57.0	57.0	1.2	0.062352
0.05	52.9	52.9	1.4	0.053925
0.06	58.3	58.3	1.6	0.047505
0.06	55.3	55.3	1.8	0.042450
0.06	52.7	52.7	2.0	0.038368
0.07	57.5	57.8	2.2	0.035002
0.07	55.7	55.7	2.4	0.032179
0.07	53.8	53.8	2.6	0.029778
0.08	58.6	58.6	2.8	0.027710
0.08	57.0	57.0	3.0	0.025910

E2	NTU	HTU	DIAM	HDP	TCOST
7194.	14.96	1.41	3.6	21.1	3515.
8393.	10.30	1.21	3.9	12.5	3032.
9592.	8.48	1.08	3.8	9.2	2531.
10790.	7.49	0.96	4.0	7.2	2400.
11989.	6.87	0.87	4.2	6.0	2331.
13188.	6.44	0.80	4.1	5.2	2152.
14387.	6.13	0.73	4.3	4.5	2136.
15586.	5.89	0.68	4.4	4.0	2132.
16785.	5.70	0.64	4.3	3.6	2023.
17984.	5.54	0.60	4.5	3.3	2031.

TABLE 12

COMPUTER OUTPUT FOR 1.50 INCH RASCHIG RINGS

PACKING DIAMETER (IN)= 1.500

HOLDUP	P5	P6	G1	XCE1
0.05	60.3	60.3	1.2	0.062352
0.05	55.9	55.9	1.4	0.053925
0.05	52.4	52.4	1.6	0.047505
0.06	58.4	58.4	1.8	0.042450
0.06	55.6	55.6	2.0	0.038368
0.06	53.3	53.3	2.2	0.035002
0.07	58.9	58.9	2.4	0.032179
0.07	56.9	56.9	2.6	0.029778
0.07	55.1	55.1	2.8	0.027710
0.07	53.5	53.5	3.0	0.025910

E2	NTU	HTU	DIAM	HDP	ICDST
7193.	14.96	1.41	3.2	21.1	3091.
8392.	10.30	1.21	3.4	12.5	2500.
9592.	8.48	1.06	3.6	9.0	2280.
10790.	7.49	0.96	3.8	7.2	2021.
11989.	6.87	0.87	3.7	6.0	1972.
13188.	6.44	0.79	3.9	5.1	1948.
14387.	6.13	0.73	3.8	4.5	1825.
15586.	5.89	0.68	3.9	4.0	1825.
16785.	5.70	0.63	4.1	3.6	1831.
17984.	5.54	0.59	4.2	3.3	1842.

TABLE 13

COMPUTER OUTPUT FOR 2.00 INCH RASCHIG RINGS

PACKING DIAMETER (IN) = 2.000

HOLDUP	P5	P6	G1	XCE1
0.05	56.5	56.5	1.2	0.062352
0.05	52.4	52.4	1.4	0.053925
0.06	57.9	57.9	1.6	0.047505
0.06	54.7	54.7	1.8	0.042450
0.07	59.9	59.9	2.0	0.038368
0.07	57.4	57.4	2.2	0.035002
0.07	55.2	55.2	2.4	0.032179
0.07	53.3	53.3	2.6	0.029778
0.08	58.2	58.2	2.8	0.027710
0.08	56.5	56.5	3.0	0.025910

E2	NTU	HTU	DIAM	HDP	TCOST
7194.	14.96	1.41	2.9	21.1	2819.
8393.	10.30	1.21	3.2	12.5	2290.
9592.	8.48	1.03	3.1	9.2	1949.
10790.	7.49	0.96	3.3	7.2	1861.
11989.	6.87	0.88	3.2	6.0	1714.
13188.	6.44	0.80	3.3	5.2	1693.
14387.	6.13	0.73	3.5	4.5	1685.
15586.	5.89	0.68	3.6	4.0	1686.
16785.	5.70	0.64	3.5	3.6	1608.
17984.	5.54	0.60	3.6	3.3	1617.

TABLE 14

COMPUTER OUTPUT FOR 3.00 INCH RASCHIG RINGS

PACKING DIAMETER (IN) = 3.000

HOLDUP	P5	P6	G1	XCEL
0.05	52.3	52.3	1.2	0.062352
0.06	57.1	57.1	1.4	0.053925
0.06	53.6	53.6	1.6	0.047505
0.07	58.2	58.2	1.8	0.042450
0.07	55.5	55.5	2.0	0.038368
0.08	59.6	59.6	2.2	0.035002
0.08	57.6	57.6	2.4	0.032179
0.08	55.6	55.6	2.6	0.029778
0.09	59.8	59.8	2.8	0.027710
0.09	58.1	58.1	3.0	0.025910

E2	NTU	HTU	DIAM	HDP	TCOST
7194.	14.96	1.41	2.8	21.1	2577.
8393.	10.30	1.23	2.7	12.7	1969.
9592.	8.48	1.08	2.9	9.2	1804.
10790.	7.49	0.98	2.9	7.3	1633.
11989.	6.87	0.88	3.0	6.0	1595.
13188.	6.44	0.81	3.0	5.2	1504.
14387.	6.13	0.75	3.1	4.6	1496.
15586.	5.89	0.69	3.2	4.1	1495.
16785.	5.70	0.65	3.1	3.7	1446.
17984.	5.54	0.61	3.2	3.4	1447.

TABLE 15
CARD FORMAT FOR DATA INPUT

Data Card Number	Card Column Numbers						
	<u>1 - 10</u>	<u>11 - 20</u>	<u>21 - 30</u>	<u>31 - 40</u>	<u>41 - 50</u>	<u>51 - 60</u>	<u>61 - 70</u>
1	EXVIS	RAFVIS	EXDEN	RAFDEN	SOLVMW	SOLUMW	VOLMOL
2	SURTEN	SLOPE	R1	OPTEMF	CR1	CR2	CE2
3	XAA1	XBA	XBB1	XAB			
4	XBC	XCC1	XCB	XBB2			
5	XAC	XCC2	XCA	XAA2			
6	DCR	DCE	FEEDMW	ASSOCR	ASSOCE		
7 - 12	PD(J)	PE(J)	PA(J)	PDEN(J)	PCOST1(J)		

Note: See Equation and Program Nomenclature for definition of program variable names.

TABLE 16
BASIC INPUT DATA FOR COMPUTER RUNS

<u>Data Card Number</u>	<u>Card Column Numbers</u>						
	<u>1 - 10</u>	<u>11 - 20</u>	<u>21 - 30</u>	<u>31 - 40</u>	<u>41 - 50</u>	<u>51 - 60</u>	<u>61 - 70</u>
1	0.5	1.0	60.0	64.0	80.0	100.0	81.0
2	25.0	0	15000.0	70.0	0.006	0.001	0
3	0.9990	0.0010	0.9990	0.0010			
4	0.0003	0.9997	0.1200	0.8800			
5	0.0002	0.9998	0.0100	0.9900			
6	0	0	18.0	2.6	1.0		
7	0.500	0.74	114.0	48.0	13.10		
8	0.750	0.73	80.0	44.0	7.20		
9	1.000	0.73	58.0	40.0	6.50		
10	1.500	0.71	38.0	42.0	5.05		
11	2.000	0.74	28.0	38.0	4.85		
12	3.000	0.74	19.0	40.0	4.30		

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