LBL-15752

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

ENERGY & ENVIRONMENT
DIVISION

VACUUM ETHANOL DISTILLATION TECHNOLOGY

B.L. Maiorella, H.W. Blanch, and C.R. Wilke

March 1983

RECEIVED
FEB 22 2008
By LBNL Library

ENERGY
AND ENVIRONMENT
DIVISION

LBL-15752
c.1

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBL-15752

VACUUM ETHANOL DISTILLATION TECHNOLOGY

B.L. Maiorella

H.W. Blanch

C.R. Wilke

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

March 8, 1983

This work was supported by the Director, Office for Energy Research, Office of Basic Energy Sciences, Division of the Chemical Science Processes and Techniques Branch of the U.S. Department of Energy, and by the Assistant Secretary for Conservation and Solar Energy under Contract No. DE-AC03-76SF00098, and by the Solar Energy Research Institute under Contract No. DR-0-905801.

VACUUM ETHANOL DISTILLATION TECHNOLOGY

1 Introduction

Current distillation technology has been criticized as energy inefficient, requiring as much as the full energy of combustion of the ethanol product separated (5,040 kcal to distill one liter of ethanol) (1,2,3,4,5). While inefficient beverage plants and plants producing ultrapure ethanol utilize nearly this energy, well designed industrial alcohol and alcohol fuel plants employing vapor reuse techniques utilize only about 2.5 kg of steam per liter of 99.9 wt% ethanol product (1,340 kcal) (6,7,8,9).

Many efficient ethanol/water separation methods have been developed or proposed. The purpose of this paper is to illustrate the design principles for one particularly efficient distillation arrangement employing available technology. The newly developed temperature dependent UNIQUAC vapor/liquid equilibrium computation methods are utilized in the design of a minimum cost distillation plant for the production of 100 million liters per year of 95 wt% ethanol product. Vacuum distillation and vapor reuse methods are employed. These methods combine synergystically to reduce the distillation energy requirement in concentrating dilute beer feeds. The vapor reuse methods are then extended to demonstrate how 99.9 wt% ethanol are then produced at virtually no additional energy cost.

2 Ethanol/Water Equilibrium--ETOH Computer Package

The ETOH package of subroutines models ethanol/water vapor/liquid equilibrium behavior for use in separation process design. The UNIQUAC equilibrium model (developed by Abrams and Prausnitz (10))

has been widely adopted by industry and has the advantage of ready expandability to multicomponent system modeling based only upon binary system parameters. For these reasons, the UNIQUAC model was taken as the basis for the ETOH routines. The ethanol/water equilibrium is highly nonideal (varying substantially with temperature) and the simple UNIQUAC model was found inadequate for detailed ethanol distillation design at varying pressures. Instead, a modified temperature dependent model was developed which accurately predicts ethanol/water equilibrium behavior over the temperature range from 298 to 383°K corresponding roughly to the pressure range from 60 to 1070 mmHg.

The overall model for pure ethanol/water vapor/liquid equilibrium is given by the general relation

$$Y_i \, \phi_i \, P^{total} = X_i \, \gamma_i \, f_i^{0,liq} \exp(P^{total} \, V_i^{liq}/RT) \qquad (1)$$

where Y_1 and Y_2 are mole fractions of ethanol and water in the vapor phase respectively, X_1 and X_2 are mole fractions in the liquid and P^{total} and T are the system pressure and temperature.

The ethanol and water liquid pure component specific molar volumes (V_1^{liq} and V_2^{liq}) used in the Poynting correction are given by the modified Rackett equation of Spencer and Danner (75) as:

Modified Rackett Correlation:

$$V_i^{liq} = \frac{R \, T_{c_i} \, Z_i^{\tau}}{P_{c_i}} \qquad (2)$$

where: $\tau = 1 + (1 - T_r)^{0.286}$ for $T_r \leq 0.75$

$$\tau = 1.6 + .00693/(T_r - 0.655) \quad \text{for } T_r \geq 0.75$$

with: $T_r = T/T_c$

and where: T_{c_1} = (ethanol critical temperature) = 516.26°K

T_{c_2} = (water critical temperature) = 647.37°K

P_{c_1} = (ethanol critical pressure) = 63.89 bar

P_{c_2} = (water critical pressure) = 221.20 bar

Z_1 = (ethanol modified Rackett Parameter) = 0.2520

Z_2 = (water modified Rackett parameter) = 0.2380

The zero point reference fugacities for ethanol and water ($f_1^{0,liq}$ and $f_2^{0,liq}$) are given by the expansion of Prausnitz (76):

zero point reference fugacities:

$$f_i^{0,liq} = \exp\,(A_i + B_i/T + C_iT + D_i \ln T + E_iT^2) \qquad (3)$$

with: $A_1 = -0.9091$

$B_1 = -0.3466$

$C_1 = -0.6230$

$D_1 = 0.2049$

$$E_1 = 0.2066$$

and

$$A_2 = 0.5704$$

$$B_2 = 0.7005$$

$$C_2 = 0.3589$$

$$D_2 = 0.6669$$

$$E_2 = 0.8505$$

The ethanol and water vapor phase fugacity coefficients ϕ_1 and ϕ_2 are calculated from second virial coefficients according to:

$$\ln \phi_i = (2 \sum_{j=1}^{n} Y_j B_{ij} - B) \frac{P}{RT} \tag{4}$$

with the mixture coefficient given by:

$$B = \sum_{i=1}^{n} \sum_{j=1}^{n} Y_i Y_j B_{ij}(T) \tag{5}$$

and the ethanol (B_{11}) water (B_{22}) and cross (B_{12}) virial coefficients given by the correlation of Hayden and O'Connell (77) (see "Ethanol/Water Physical and Chemical Properties for Separation Process Design"(73) for a detailed description). For accurate computations, this fugacity correction cannot be ignored as the fugacity coefficient for water deviates by as much as 4% from the ideal gas assumption at 363°K and for $Y_{ethanol} \geq 0.7$.

The activity coefficients for ethanol (γ_1) and water (γ_2) are given by the UNIQUAC model as:

$$\ln \gamma_1 = \ln \frac{\Phi_1}{x_1} + \frac{z}{2} q_2 \ln \frac{\Theta_1}{\Phi_1} + \Phi_2 \left(\ell_1 - \frac{r_1}{r_2} \ell_2\right) + C\, q_1' \left[- \ln(\Theta_1' + \Theta_2' \tau_{21}) + \frac{\Theta_2'\tau_{21}}{\Theta_1' + \Theta_2'\tau_{21}} - \frac{\Theta_2'\tau_{12}}{\Theta_2' + \Theta_1'\tau_{12}} \right] \tag{6}$$

$$\ln \gamma_2 = \ln \frac{\Phi_2}{x_2} + \frac{z}{2} q_2 \ln \frac{\Theta_2}{\Phi_2} + \Phi_1 \left(\ell_2 - \frac{r_2}{r_1} \ell_1\right) + C\, q_2' \left[- \ln(\Theta_2' + \Theta_1'\tau_{12}) + \frac{\Theta_1'\tau_{12}}{\Theta_2' + \Theta_1'\tau_{12}} - \frac{\Theta_1'\tau_{21}}{\Theta_1' + \Theta_2'\tau_{21}} \right] \tag{7}$$

$$\ell_1 = \frac{z}{2}(r_1 - q_1) - (r_1 - 1)$$

$$\ell_2 = \frac{z}{2}(r_2 - q_2) - (r_2 - 1)$$

$$\Phi_1 = \frac{X_1 r_1}{X_1 r_1 + X_2 r_2} \qquad \Phi_2 = \frac{X_2 r_2}{X_1 r_1 + X_2 r_2}$$

$$\Theta_1 = \frac{X_1 q_1}{X_1 q_1 + X_2 q_2} \qquad \Theta_2 = \frac{X_2 q_2}{X_1 q_1 + X_2 q_2}$$

$$\Theta_1' = \frac{X_1 q_1'}{X_1 q_1' + X_2 q_2'} \qquad \Theta_2' = \frac{X_2 q_2'}{X_1 q_1' + X_2 q_2'}$$

where:

z = (coordination number) = 10

r_1 = (ethanol structural size parameter) = 2.11

r_2 = (water structural size parameter) = 0.92

q_1 = (ethanol structural area parameter) = 1.97

q_2 = (water structural area parameter) = 1.40

q_1 = (ethanol modified area parameter) = 0.92

q_2 = (water modified area parameter) = 1.00

are all tabulated physical property parameters (76) calculated from a knowledge of the molecular structures of ethanol and water.

τ_{12} and τ_{21} are the UNIQUAC parameters. The major temperature dependence of these parameters can be removed if they are expressed as:

$$\tau_{12} = \exp\left(\frac{-\Delta U_{12}}{RT}\right)$$
$$\tau_{21} = \exp\left(\frac{-\Delta U_{21}}{RT}\right) \tag{8}$$

$\Delta U_{12}/R$ and $\Delta U_{21}/R$ are then the final parameters which must be found by fitting equilibrium data. To correctly predict the variation of important equilibrium properties (such as azeotrope composition) with pressure, the basic UNIQUAC model must be extended to incorporate a further temperature dependence in these UNIQUAC parameters.

The thermodynamic relationship for the variation of activity coefficient with temperature is:

$$\left(\frac{\partial \sum_{i=1}^{m} X_i \ln \gamma_i}{\partial T}\right)_{P,X} = -\frac{H^E}{RT^2} \tag{9}$$

and

$$\left(\frac{\partial (T \sum_{i=1}^{m} X_i \ln \gamma_i)}{\partial T}\right) = \frac{-S^E}{R} \tag{10}$$

where H^E is the excess heat of mixing and S^E is the excess entropy of mixing. For the ethanol/water system, the heat of mixing is a complex

function of temperature and pressure and neither an athermal solution ($H^E = 0$ so that $\ln \gamma_i$ is independent of T) or a regular solution ($S^E = 0$ so that $\ln \gamma_i \propto \frac{1}{T}$) simplification can be applied.

Prausnitz (76) suggests that where the temperature dependence of activity coefficients cannot be neglected, that the dependence can often be accounted for by representing the characteristic energies in the form:

$$\Delta U_{12} = a_{12} + \frac{b_{12}}{T} \tag{11}$$

Thomsen (78), however, has tested several systems using:

$$\Delta U_{12} = a_{12} + b_{12}/\sqrt{T} \tag{12}$$

$$\Delta U_{12} = a_{12}T \tag{13}$$

$$\Delta U_{12} = a_{12} \exp(b/T) \tag{14}$$

as well as equation 11. All these forms give similar improvement in the overall equilibrium correlation.

To find the temperature dependence of the activity coefficients for the ethanol/water system, rather than a priori assuming a possibly too restrictive form for the UNIQUAC interaction energy parameters, equilibium data measured by Mash and Pemberton (79) was used to fit the UNIQUAC equation at six temperatures (298.15, 303.15, 323.15 343.15, 363.15, 383.15°K) corresponding to the pressure range 60 to 1070 mmHg.

The data was selected, from among 24 sets of data taken from the

literature, based on excellent thermodynamic consistency as measured by the method of Herington (80) as well as other criteria.

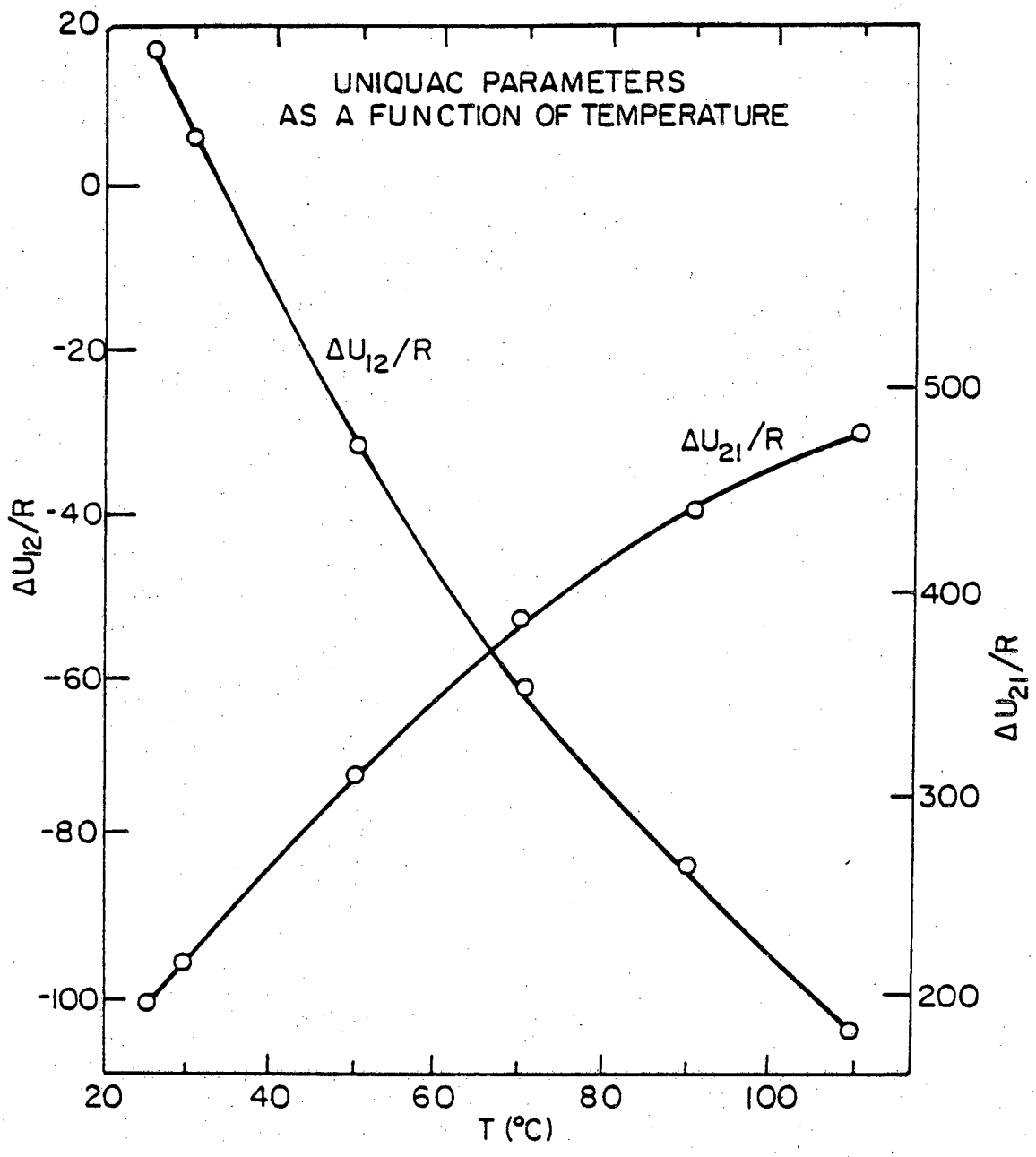
The resulting values of $(\Delta U_{12}/R)$ and $(\Delta U_{21}/R)$ are shown vs temperature in figure 1. Both parameters vary smoothly over the range studied. ΔU_{21} could be fit approximately in the form of equation 11, but ΔU_{12} is better fit in a parabolic form. A five term polynomial expansion was chosen to fit both ΔU_{12} and ΔU_{21} (equations 15 and 16) through the range of interest. This polynominal can fit both interaction energy forms quite accurately.

$$\Delta U_{12}/R = -10845.010853 + 144.454638358\,(T) - 0.692588910466\,(T)^2 + 0.00143459625212\,(T)^3 - 1.096233611 \times 10^{-6}\,(T^4) \quad (15)$$

$$\Delta U_{21}/R = 38765.541772 - 475.052110708\,(T) + 2.1410854923\,(T^2) - 0.004220316593674\,(T)^3 + 3.054583612 \times 10^{-6}\,(T)^4 \quad (16)$$

A telling test of the overall equilibrium model is the prediction of isobaric data -- the model was developed from isothermal data sets while a single isobaric data set covers a range of temperatures.

Figures 2 through 4 compare model predictions as generated by the ETOH package of subroutines with data for the ethanol/water system at 50, 250 and 740 mmHg pressure. Figure 5 shows the predicted equilibrium curve at 50 mmHg expanded near the azeotrope composition. The model closely predicts the slope of the curve in this region (differing with the reported data by less than 0.005 mole fraction).



XBL 812-5289A

Figure 1 Temperature Dependence of the UNIQUAC Parameters for the System Ethanol/Water

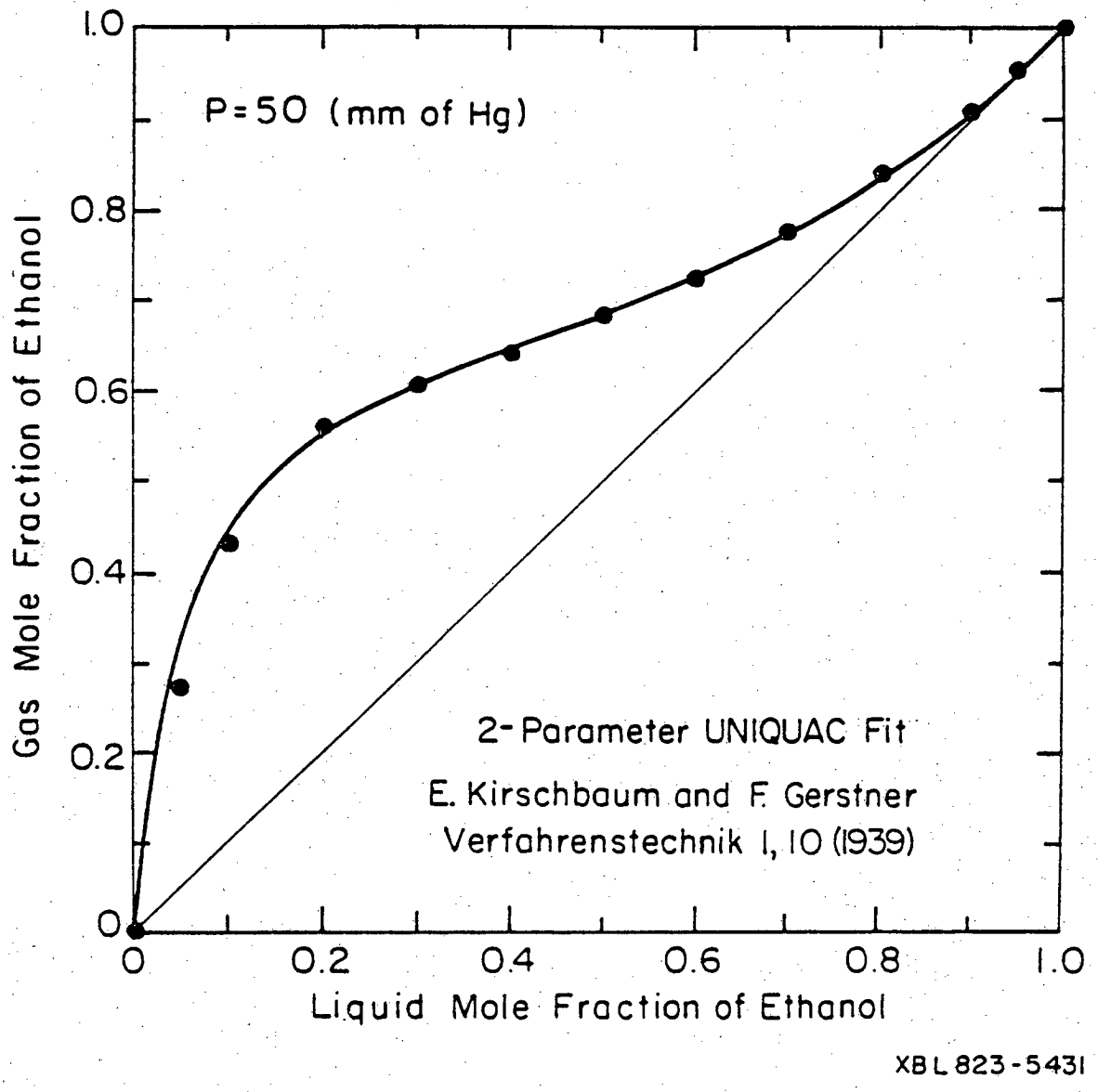


Figure 2 UNIQUAC Model for Ethanol/Water Equilibrium

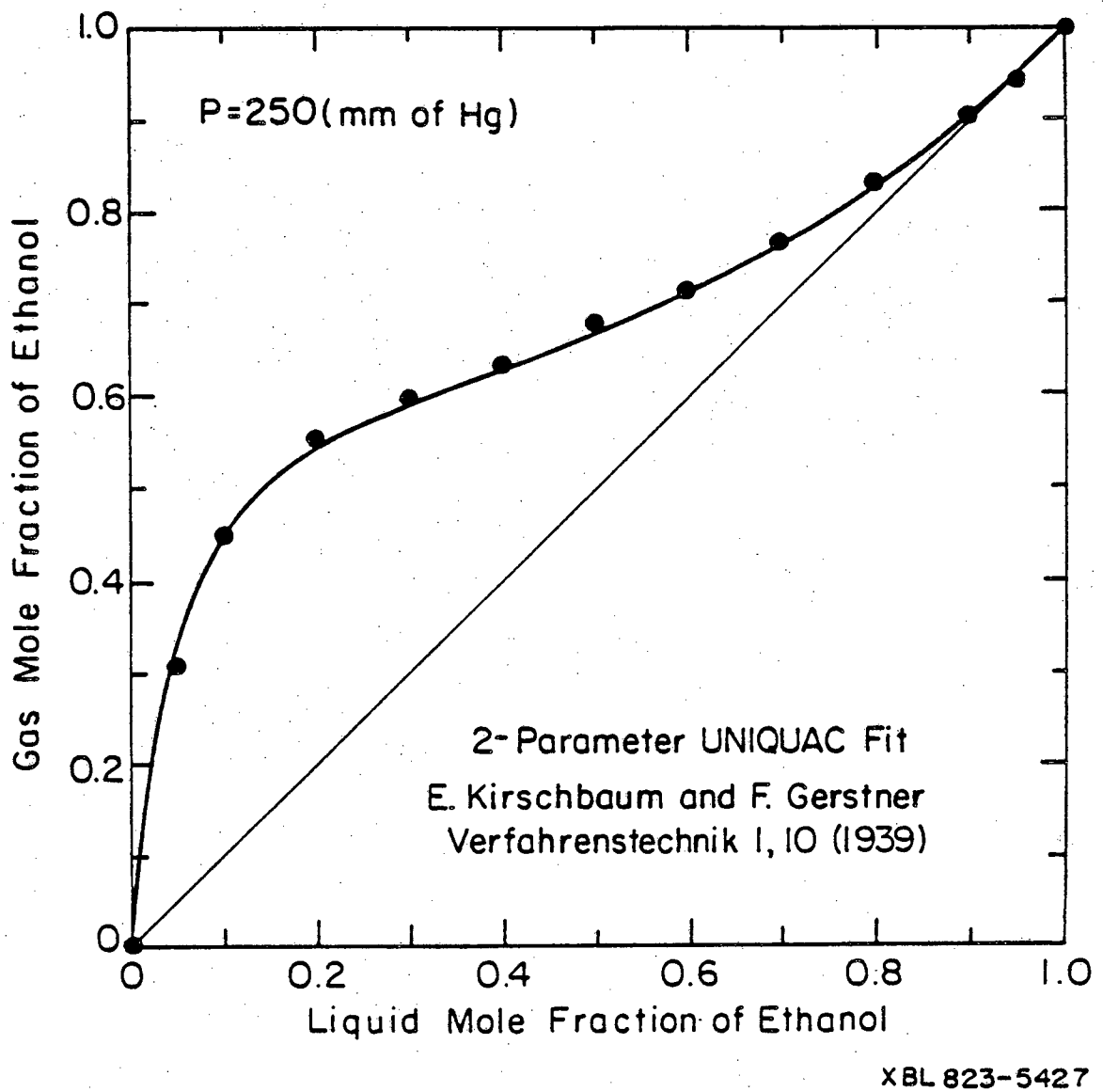

P=250(mm of Hg)
2-Parameter UNIQUAC Fit
E. Kirschbaum and F. Gerstner
Verfahrenstechnik 1, 10 (1939)
Gas Mole Fraction of Ethanol
Liquid Mole Fraction of Ethanol
0
0.2
0.4
0.6
0.8
1.0
XBL 823-5427

Figure 3

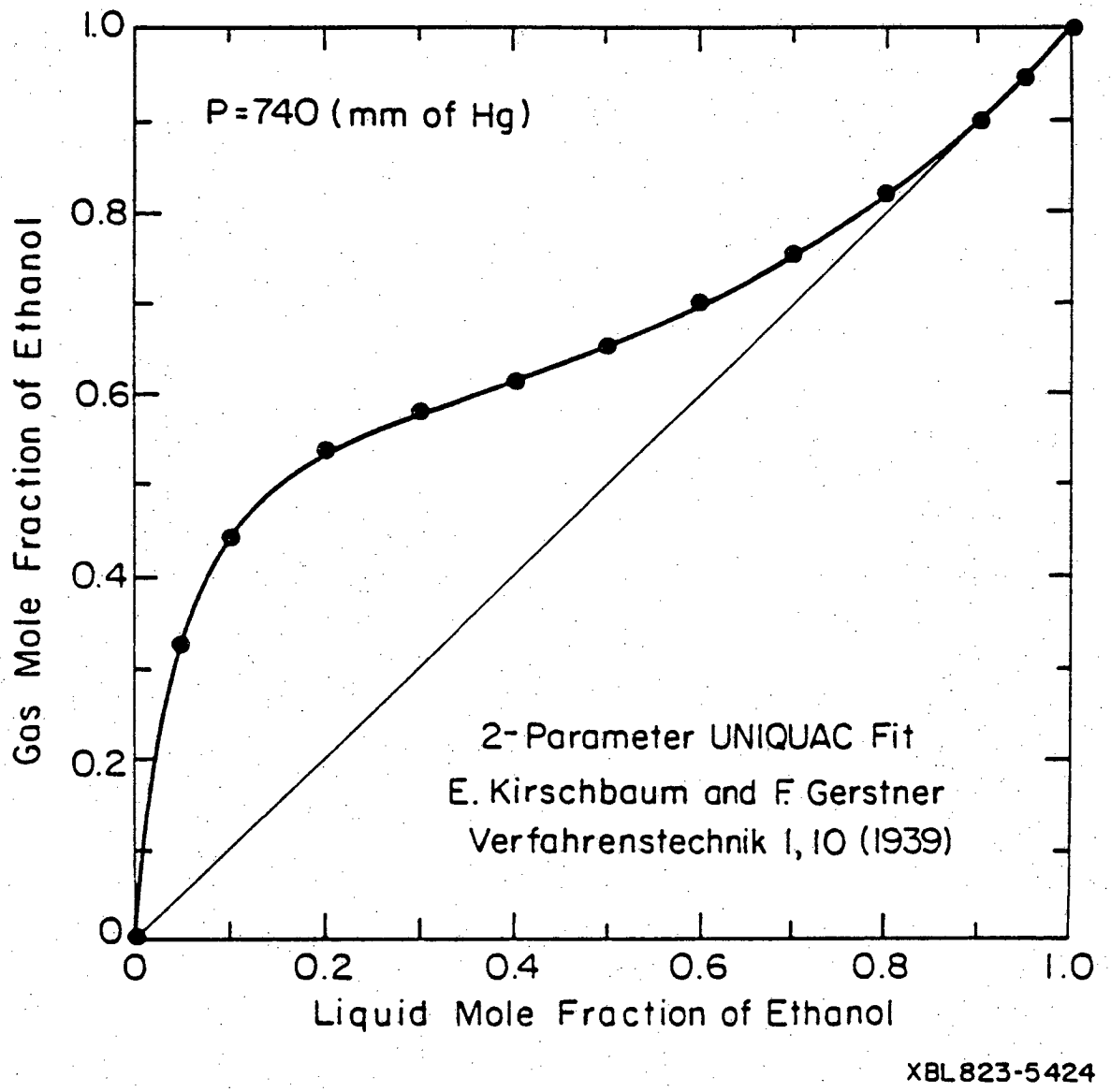

P=740 (mm of Hg)
2-Parameter UNIQUAC Fit
E. Kirschbaum and F. Gerstner
Verfahrenstechnik 1, 10 (1939)
Gas Mole Fraction of Ethanol
Liquid Mole Fraction of Ethanol
0
0.2
0.4
0.6
0.8
1.0
XBL 823-5424

Figure 4

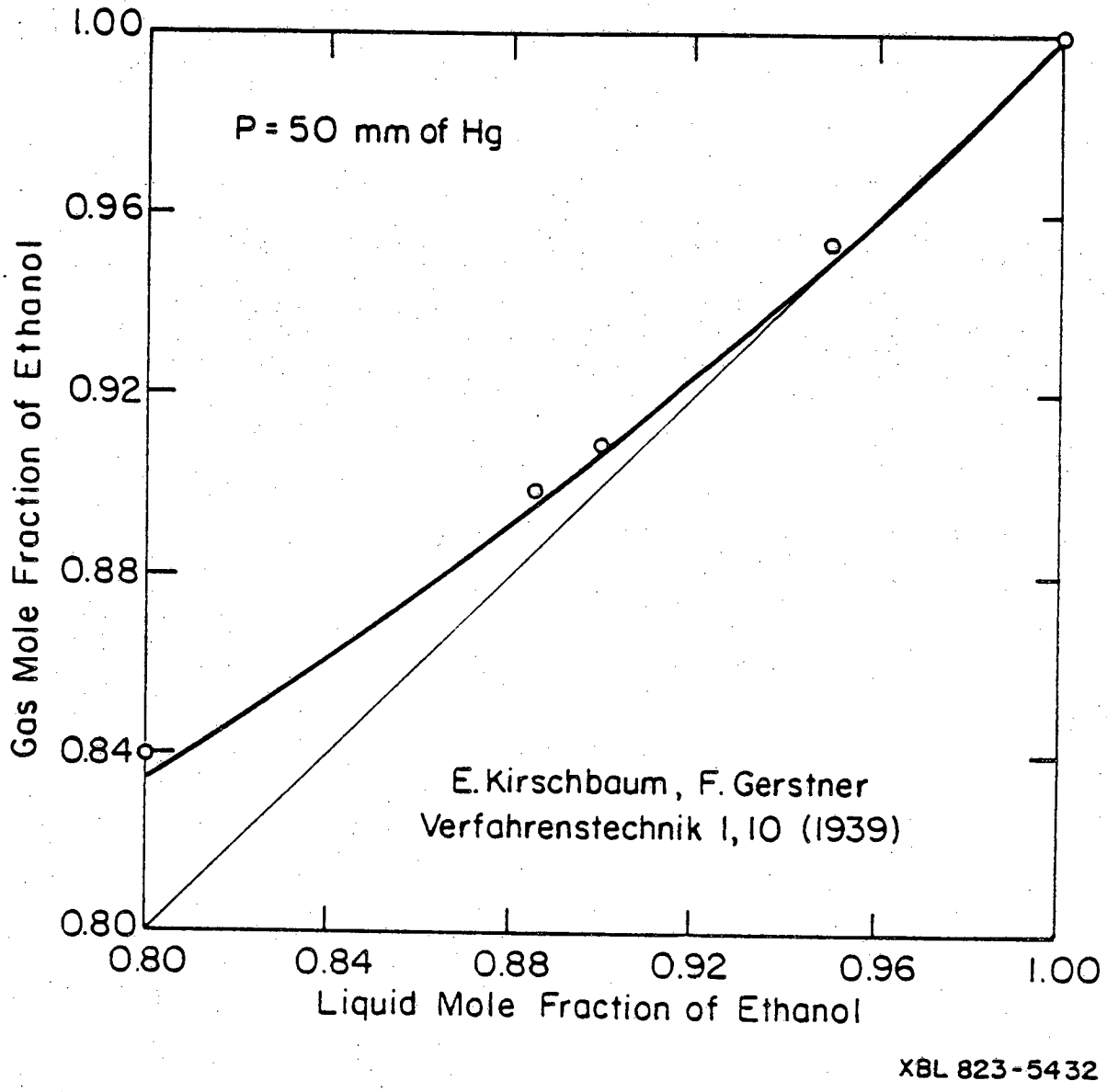


Figure 5 UNIQUAC Model for Ethanol/Water Equilibrium at High Ethanol Concentration

This is critical for prediction of the required reflux ratio in an ethanol/water distillation and for this purpose, as well as for generating plate counts for column design, this model is quite satisfactory.

A detailed description of the development of this model along with a comprehensive bibliography of ethanol/water equilibrium data sources is given in "Ethanol/Water Physical and Chemical Properties for Separation Process Design" (73). This report should be consulted for possible limitations on the use of the model prior to application for separation system design.

3 Vacuum and Vapor Reuse Methods in Ethanol/Water Distillation

The vapor/liquid equilibrium properties of ethanol/water mixtures at one atmosphere are shown in figure 6 (11). The separation of ethanol from water is complicated by azeotrope formation at 95.7 wt% ethanol. To produce pure alcohol, an additional chemical agent must be added (or other method employed) to alter the equilibrium behavior and break the azeotrope (12). In production of 95 wt% industrial ethanol, the "pinch" associated with the azeotrope constrains the distillation design. As the azeotropic composition is approached from below, the relative volatility of ethanol over water decreases. The separation in the pinched region is thus made difficult, requiring many stages and a large reflux. For concentrated feeds, this region becomes controlling in establishing both the column height and distillation energy requirement.

This problem is well illustrated on a McCabe-Thiele diagram (fig. 7) where the equilibrium curve represents the possible equilibrium vapor and liquid compositions achieved on ideal trays, while the operating

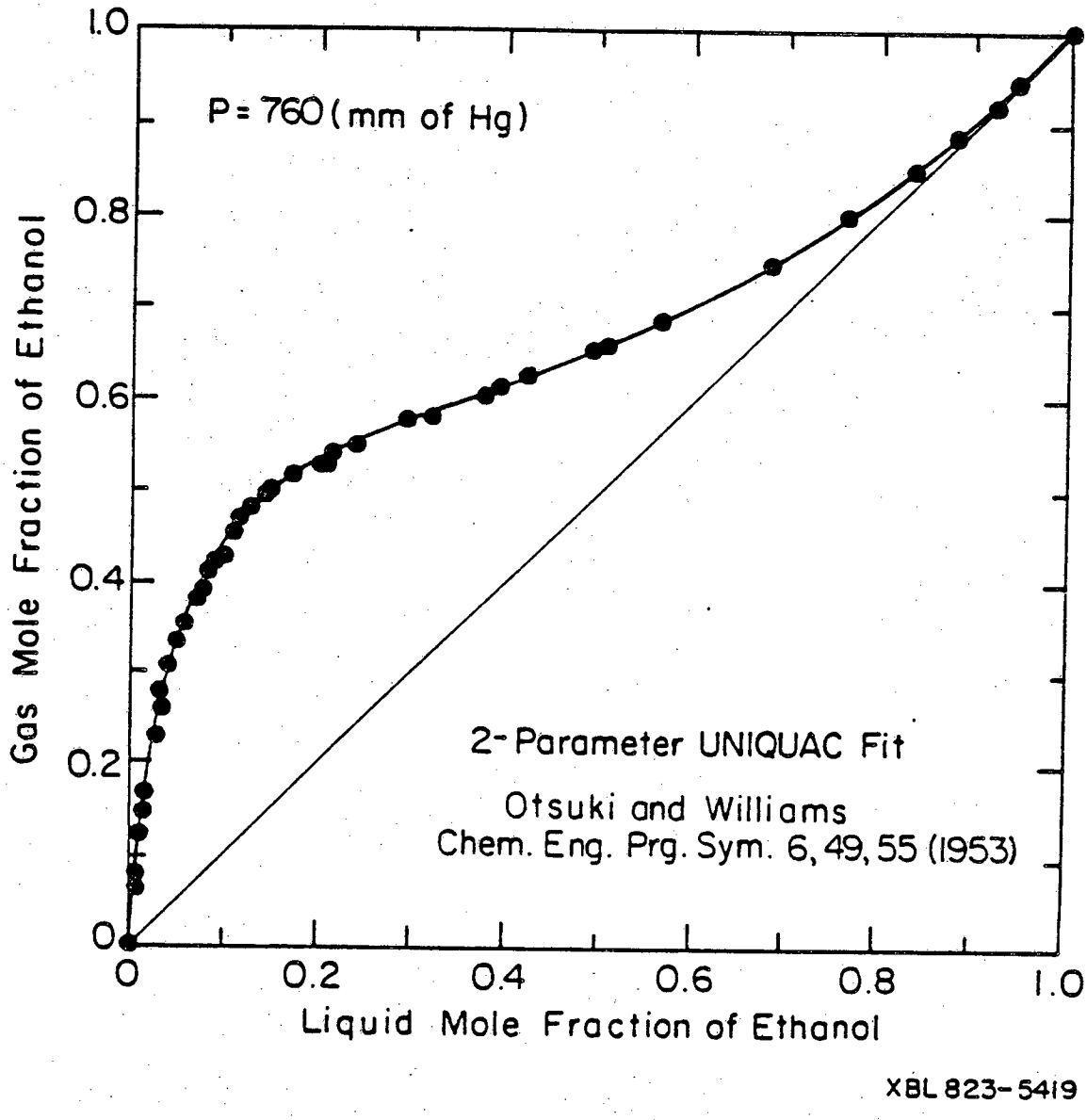


Figure 6 Ethanol/Water - Vapor/Liquid Equilibrium at One Atmosphere

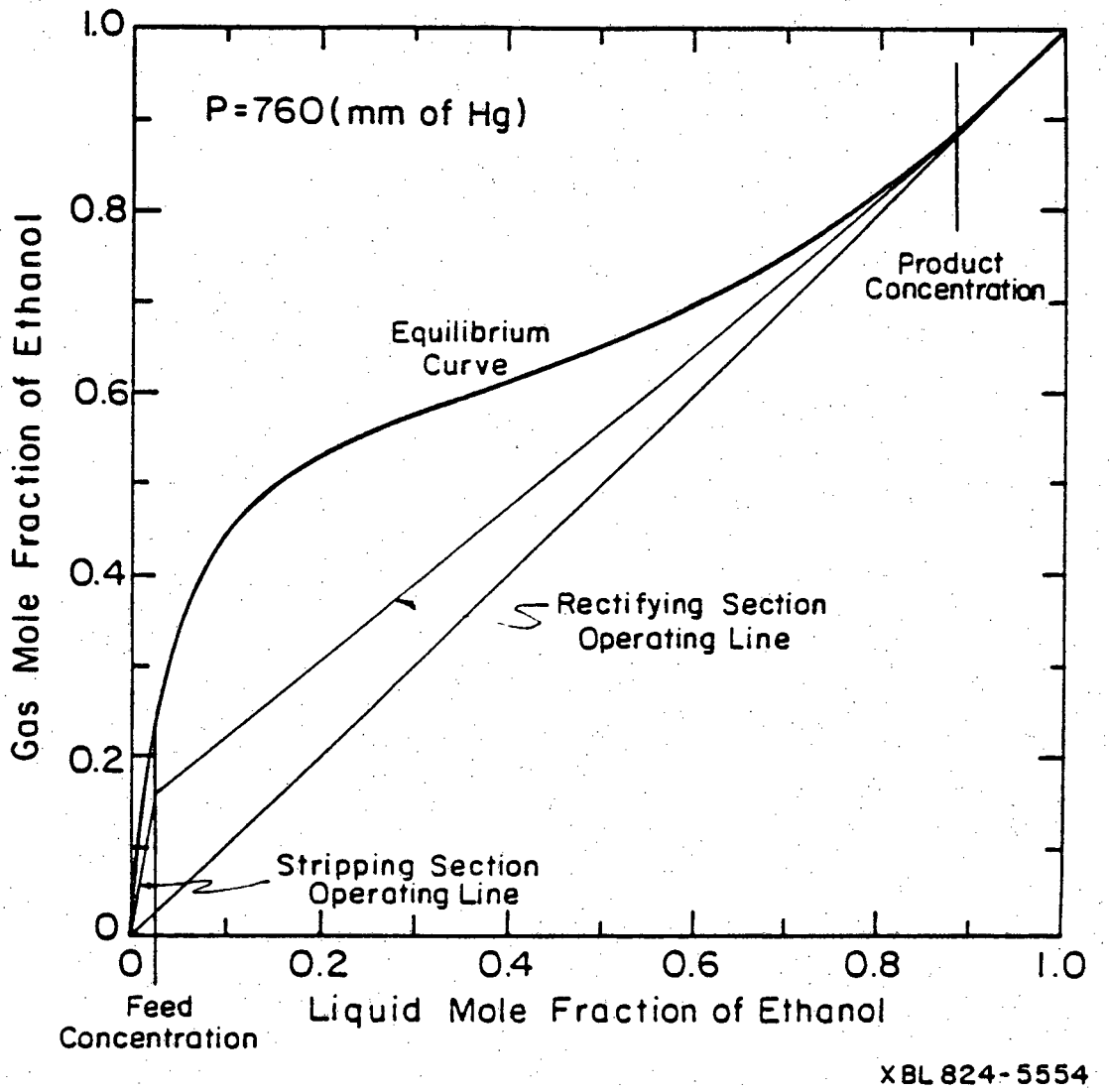


Figure 7 McCabe Thiele Diagram for Ethanol/Water Separation at One Atmosphere

lines are graphical representations of the mass balance equations of the distillation design and represent the possible compositions of vapor and liquid streams passing between plates. The slope of the rectifying operating line gives the required internal reflux ratio (and hence the distillation energy requirement).

The minimum energy input rectifying section operating line is that drawn from the product composition to the feed composition unless otherwise constrained. For the ethanol/water system, the pinch region can offer such a constraint. The operating line crossing the equilibrium curve represents a physically impossible situation. Thus, the operating line may be forced downward (greater slope and required reflux ratio) to avoid crossing the equilibrium curve in the pinched region. At atmospheric pressure and 95 wt% product concentration, the pinch region determines the operating line for all feed compositions above 6.4 wt% ethanol. The extent of this effect is well illustrated in figure 8 which plots minimum possible reflux ratio versus desired product composition for atmospheric pressure distillation of 6 wt% ethanol feed.

The distillation energy increases in a regular manner until a product composition of 94.9 wt% is obtained. Above this composition the pinch limitation takes control and the required reflux increases rapidly. For higher feed concentrations the pinch limitation takes control at lower product concentrations.

The ethanol/water equilibrium is pressure sensitive with the relative volatility of ethanol over water increased at high ethanol concentration as the pressure is reduced. As pressure is reduced from one atmosphere, the ethanol/water azeotropic composition increases

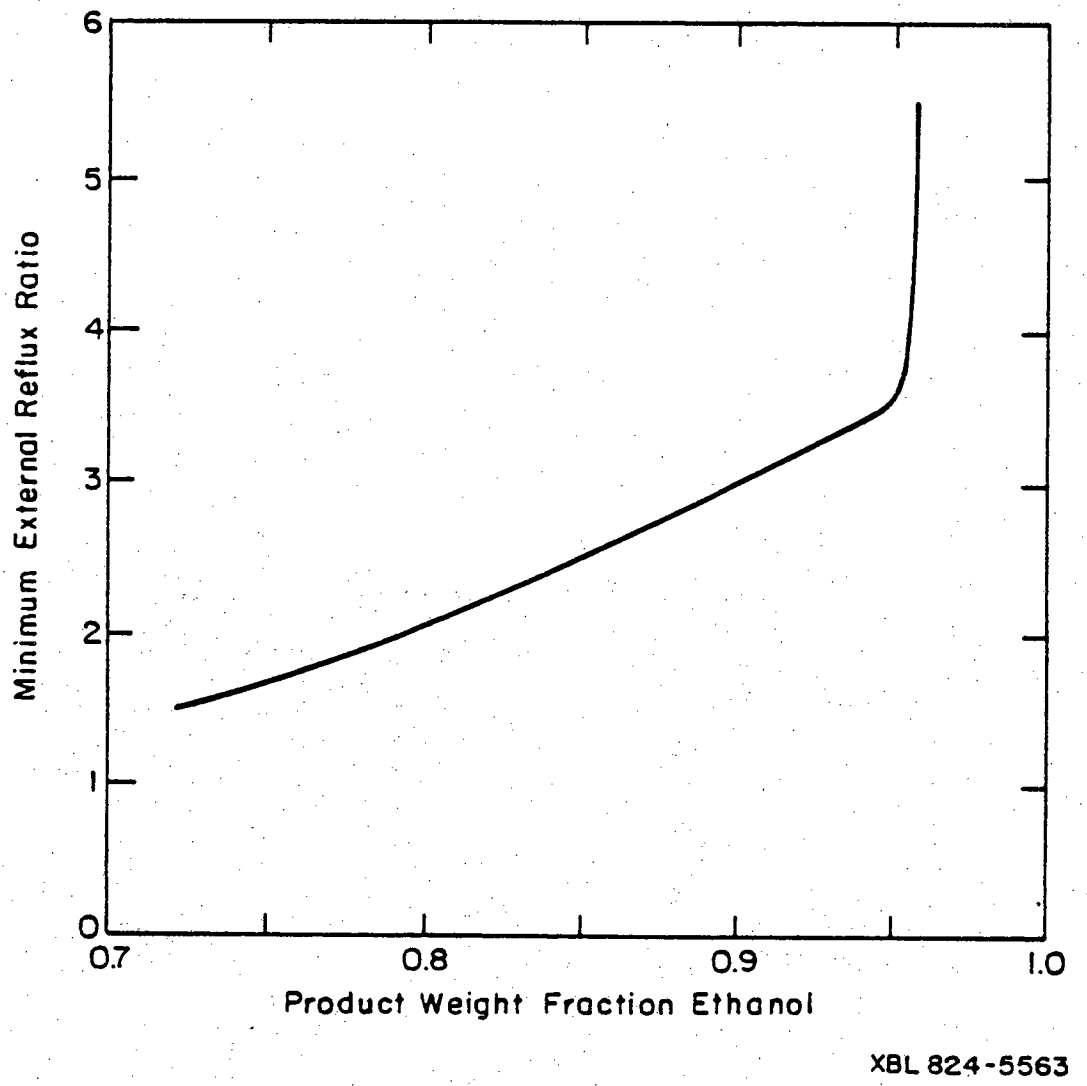


Figure 8 Effect of Product Concentration on Minimum Reflux (6 wt % Feed, One Atmosphere)

until, at about 80 mmHg absolute pressure, the azeotrope disappears. Pure alcohol can thus be distilled from an alcohol/water solution in a single distillation column at reduced pressure. The energy required for this one-step distillation is very high and this process is uneconomical. However, vacuum distillation can be used to reduce the energy requirement for the production of standard 95 wt% industrial ethanol. The shift in the azeotrope is accompanied by a shift in the entire pinched region so that the pinch constraint is made less and less severe as the distillation pressure is reduced. These properties are illustrated in figures 9(a-d) which show a succession of McCabe-Thiele diagrams at decreasing pressures (as generated by the equilibrium computation routine ETOH (73)) along with the corresponding pinch constrained rectifying section operating lines. The operating line slopes decrease at reduced pressures corresponding to a reduction in required reflux ratio.

Vacuum distillation design involves many tradeoffs as illustrated in figures 10, 11, and 12. Assuming a sufficiently concentrated feed so that the pinch limitation is controlling, then the minimum reflux ratio drops off rapidly as pressure is reduced (fig. 10) from 3.3 at one atmosphere to 1.8 at 100 mmHg. Thus at one atmosphere, for every liter of 95 wt% ethanol product, a minimum of 4.3 liters of vapor must be boiled up in the column to effect the separation, while at 100 mmHg only 2.8 L of vapor must be boiled up. These are the minimum possible reflux rates assuming an infinite number of trays in the column to effect the separation. Typically, a reflux of 1.15 to 1.4 times the minimum is used and an economic balance must be made at every pressure, trading off increasing the actual reflux from this theoretical minimum with reducing

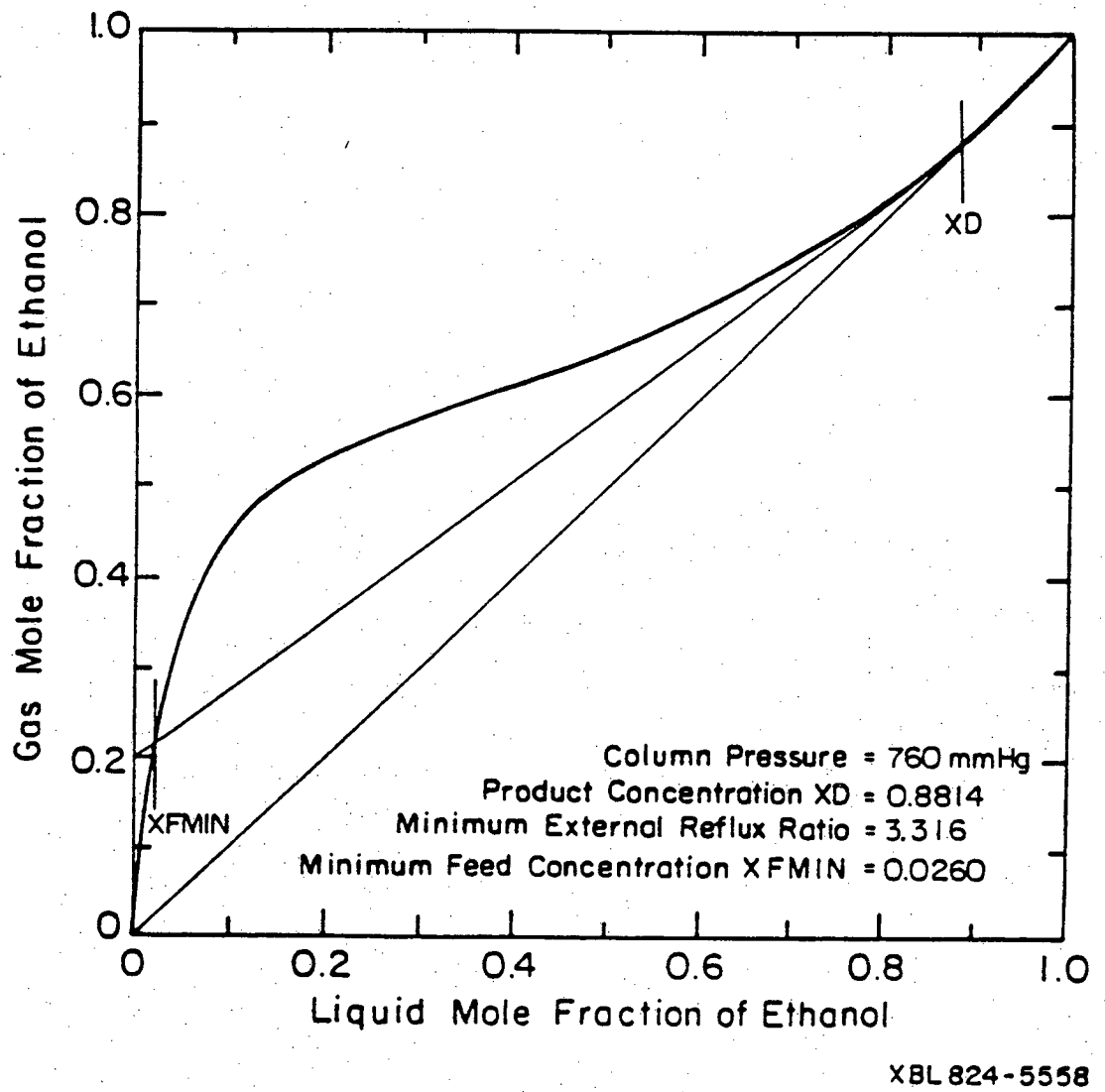
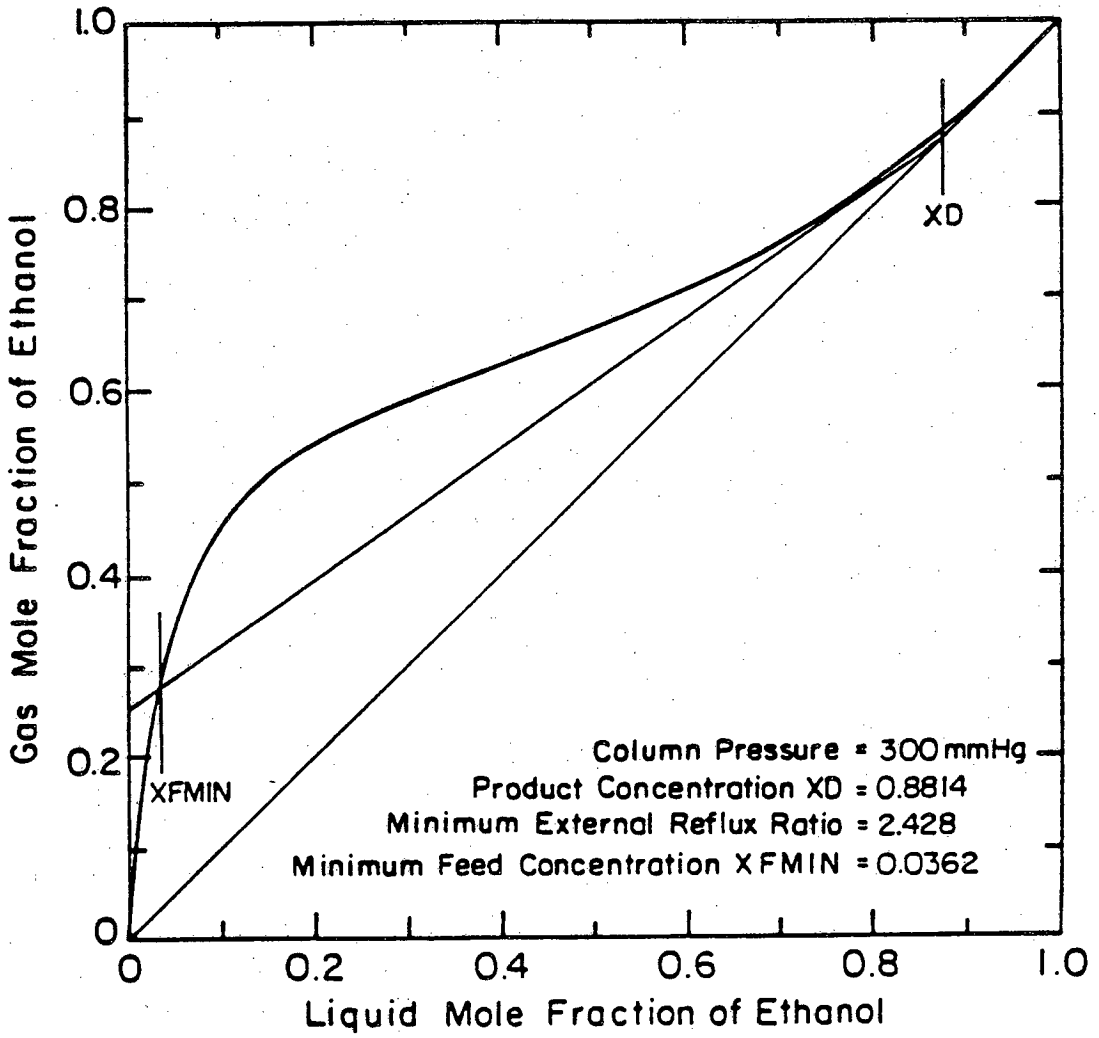


Figure 9a Effect of Pressure on the Azeotropic Pinch for 95 wt % Ethanol Production



XBL 824-5557

Figure 9b

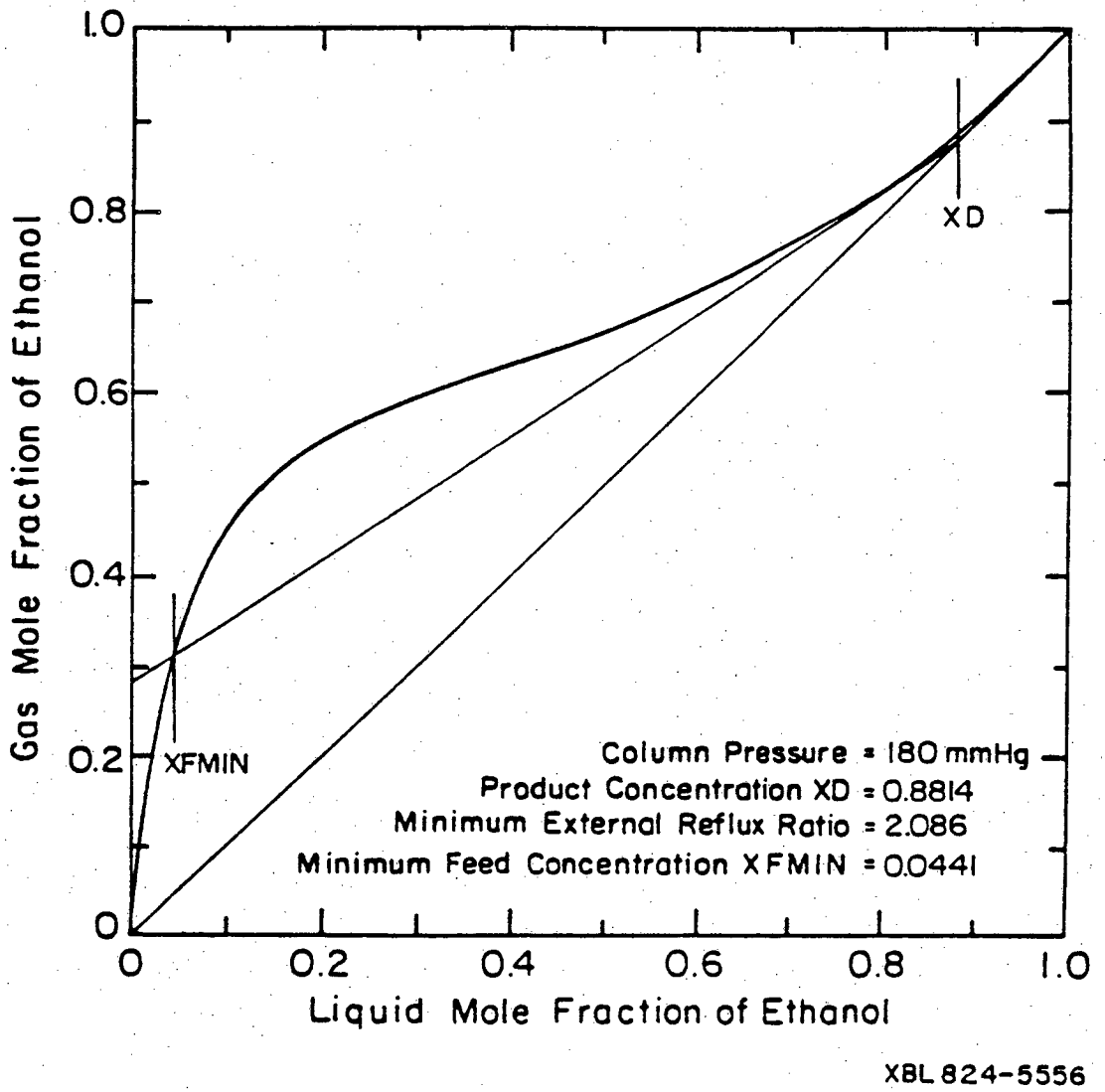
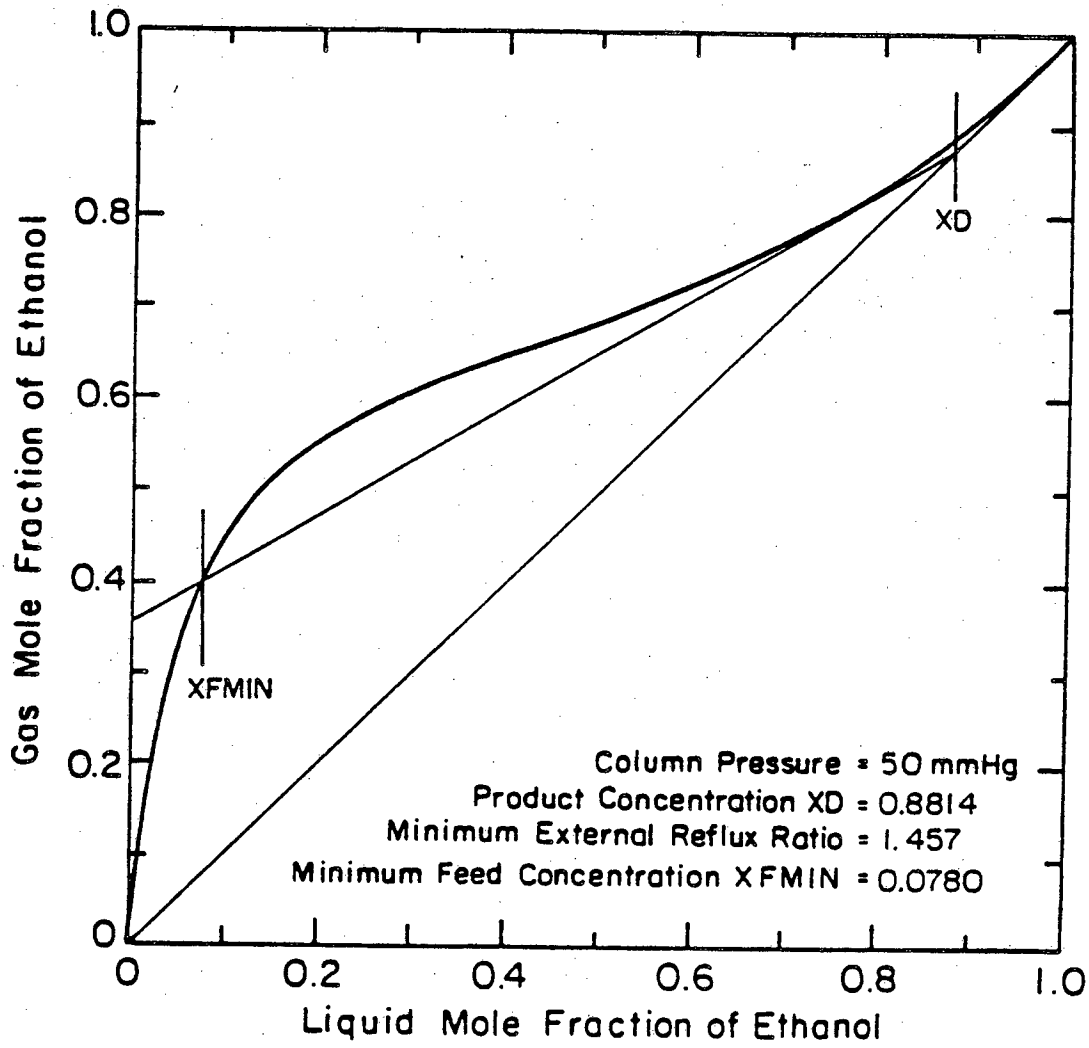
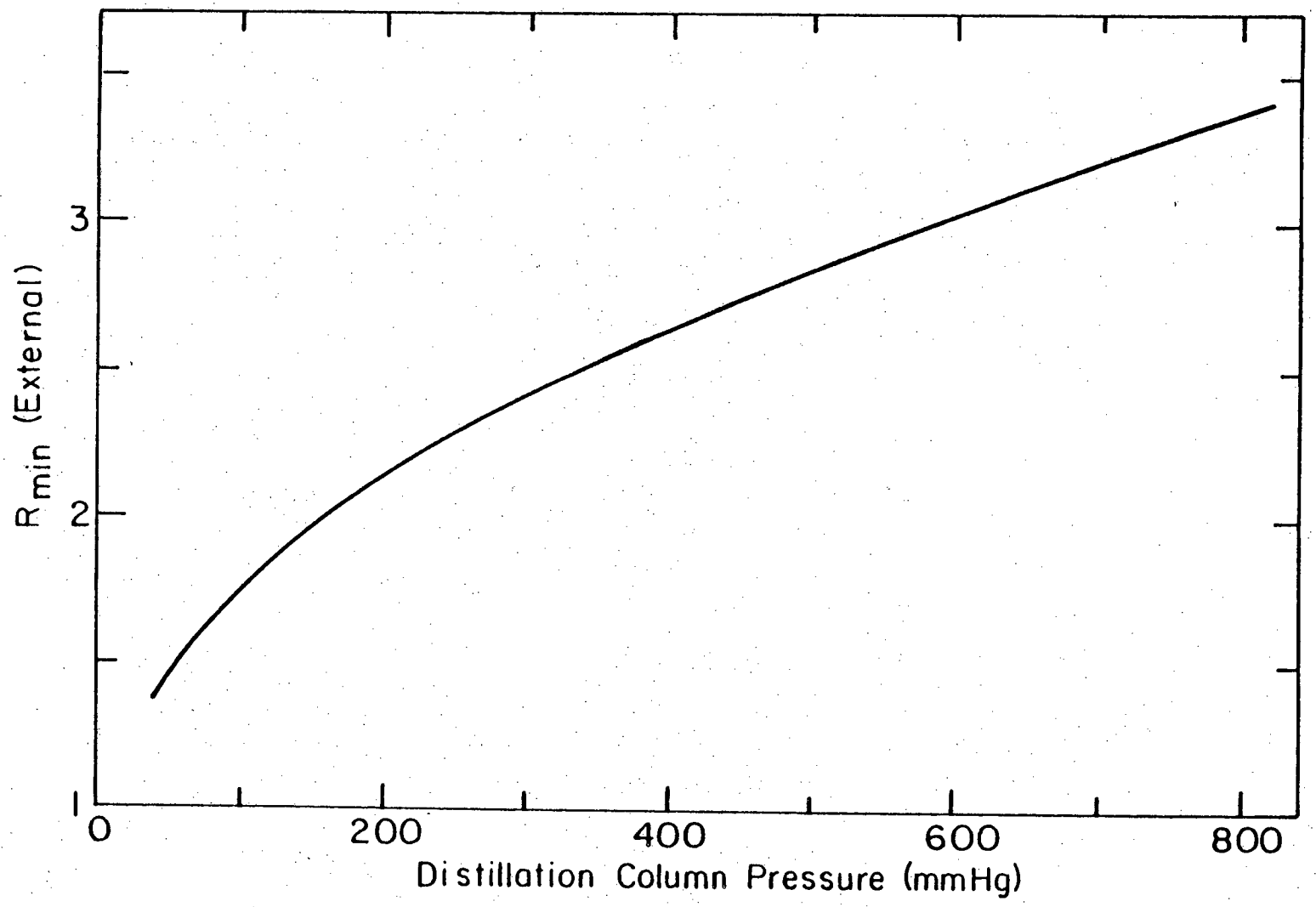

1.0
0.8
0.6
0.4
0.2
0
Gas Mole Fraction of Ethanol
XD
XFMIN
Column Pressure = 180 mmHg
Product Concentration XD = 0.8814
Minimum External Reflux Ratio = 2.086
Minimum Feed Concentration XFMIN = 0.0441
0
0.2
0.4
0.6
0.8
1.0
Liquid Mole Fraction of Ethanol
XBL 824-5556

Figure 9c



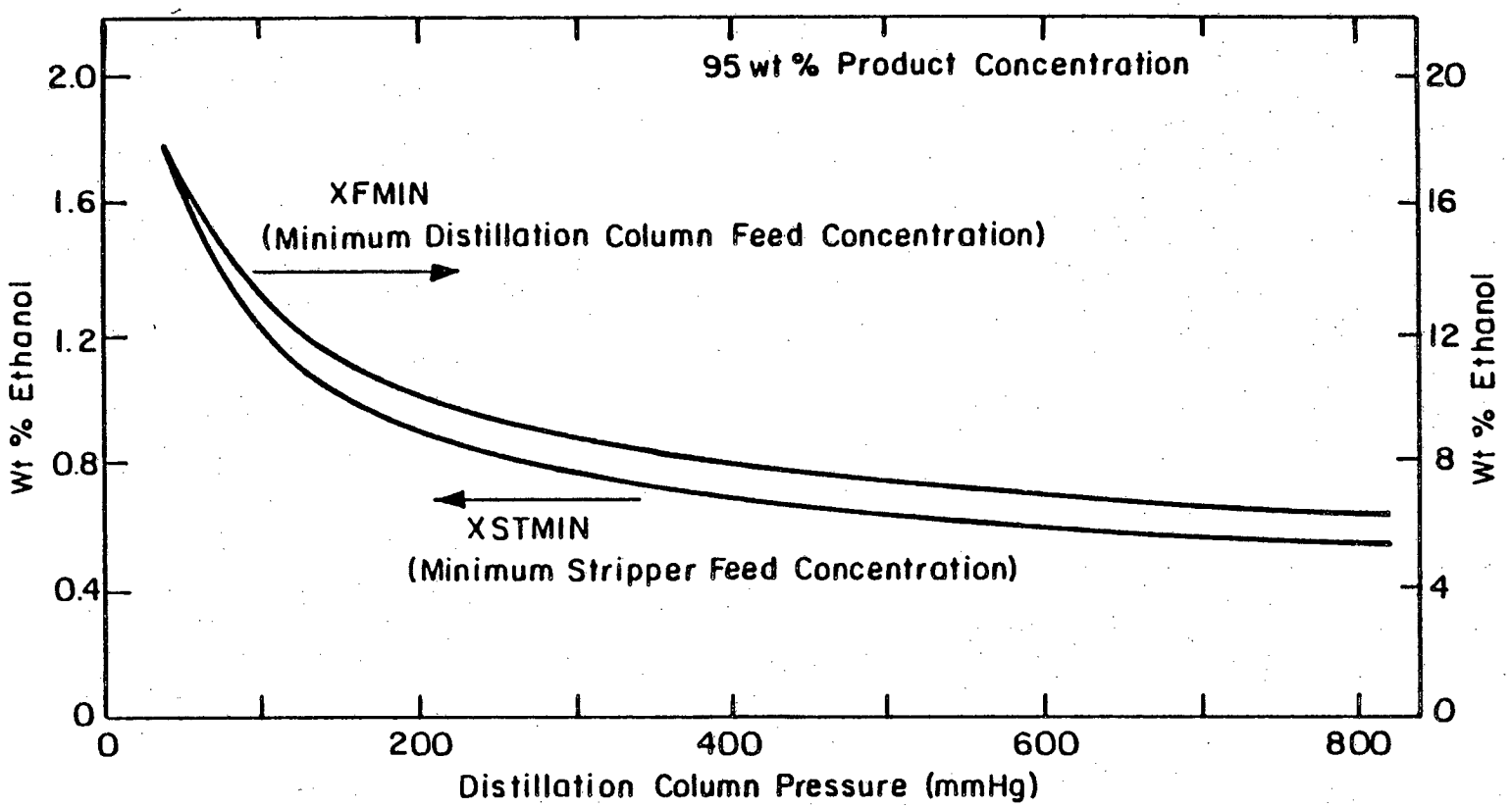
XBL 824-5555

Figure 9d



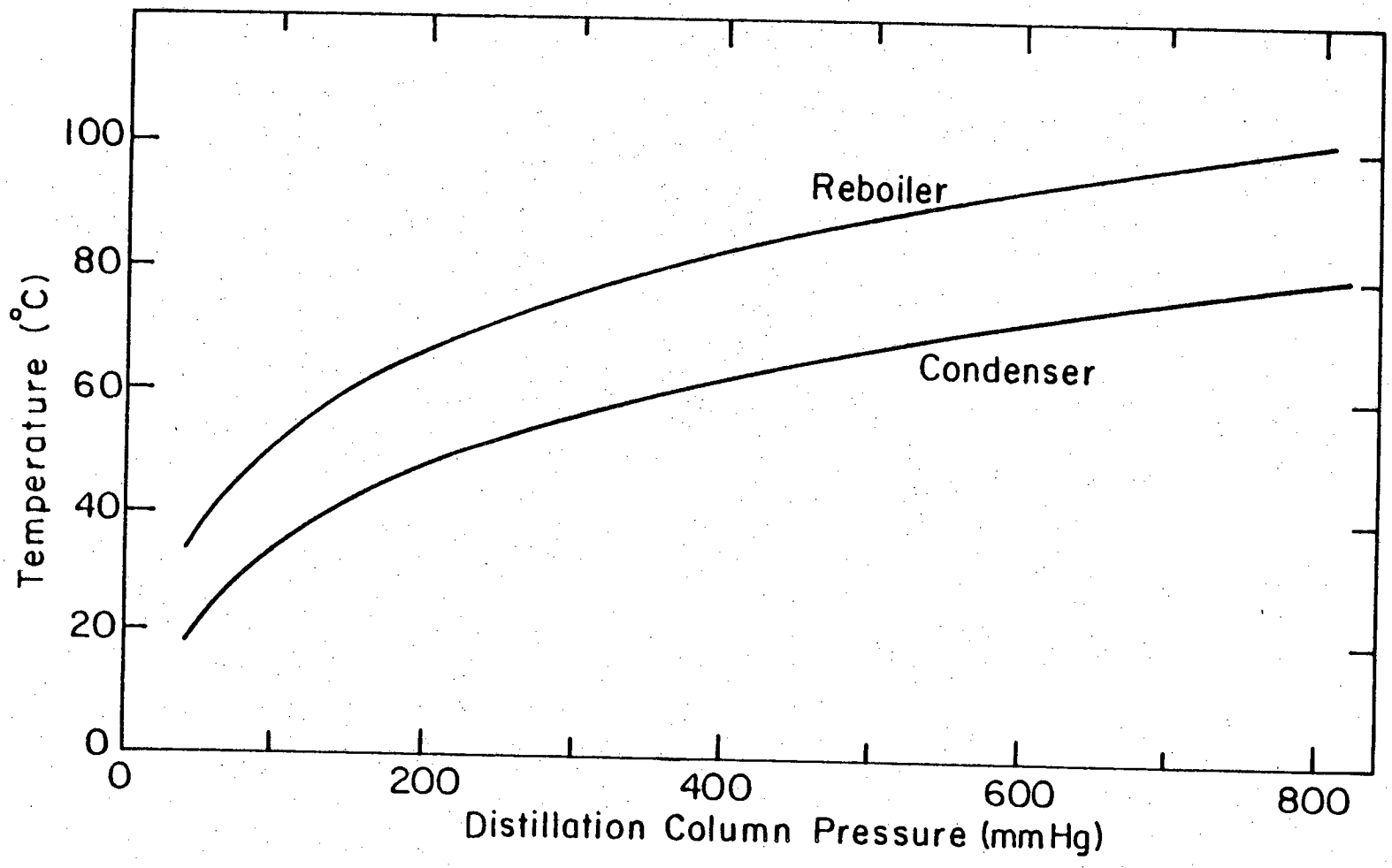
XBL 822-5264

Figure 10 Effect of Pressure on the Minimum Reflux Ratio for 95 wt % Ethanol Production



XBL 824-5562

Figure 11 Minimum Acceptable Feed Concentration for a Single Column System (XFMIN) and a Dual Column System (XSTMIN) to Not Require an Increase in Reflux Over That Set by the Azeotrope Associated Pinch.



XBL 822-5265

Figure 12 Vacuum Distillation Column Condenser and Reboiler Temperatures as a Function of Distillation Pressure

the number of distillation trays to a practical number.

The minimum feed concentration not to induce a constraint more stringent than the pinch limitation (and hence increase required reflux) is given on a McCabe-Thiele diagram as the intersection of the rectifying operating line and the equilibrium curve in the dilute ethanol region (see figs. 9(a-d)). At reduced pressure, not only does the reduced slope of the pinch constrained operating line increase this minimum feed concentration, but the ethanol relative volatility in the dilute region is also reduced, further increasing the minimum feed concentration to not induce a feed constraint. These effects are summarized in figure 11 where the XFMIN curve shows the increase in minimum feed concentration to a vacuum column as a function of pressure not to constrain the reflux ratio beyond the limit set by the pinch. This minimum feed concentration rises from 6.4 wt% ethanol at one atmosphere to 13.2 wt% ethanol at 100 mmHg. High ethanol beer concentrations require the use of specially selected ethanol tolerant microorganisms in the fermentation step with long fermentation times.

This constraint can be lessened somewhat by a special distillation column design in which high pressure drop trays are used. The column head pressure (in the region of the pinch) is maintained low so as to reduce the pinch limitation. Progressing down the column, the pressure increases so that the adverse effect on dilute region ethanol relative volatility is mitigated and the feed constraint is lessened. This method was employed in a design for a column with a head pressure of 77 mmHg and a reboiler pressure of 195 mmHg to overcome the feed limitation for a dual feed system (13).

As the distillation column pressure is reduced, distillation

temperatures also drop (fig. 12). For the reboiler, this is an advantage. The reboiler temperature drops from 100°C at 1 atmosphere to 51°C at 100 mmHg, and low temperature waste heat from elsewhere in the alcohol plant can be recovered to drive the distillation. Unfortunately, the condenser temperature likewise drops from 78°C at 1 atmosphere to 34°C at 100 mmHg. The distillation pressure is thus constrained by the temperature of available cooling water. The cooling water usage and condenser exchanger area are increased at reduced pressure.

A final objection which can be raised regarding the use of vacuum distillation relates to the increased cost of a column to operate under vacuum. This objection is made on two grounds--first, that the column walls must be increased in thickness to compensate the added stresses under vacuum, and second, that owing to the great increase in specific volume of vapors at reduced pressure, the vacuum column must be of a much larger diameter to accommodate the internal vapor flows. Neither of these objections is valid. Applying ASME vessel design code standards (14,15), the wall thickness of a 13 ft diameter vacuum column requires no increase over a conventional column when 4 internal support ring strengtheners are included. For a packed column, two of these are present in any event in the form of reflux distributor tray and packing support plate. While the specific volume of vapors is increased at reduced pressure, the required reflux, and hence the magnitude of internal flows, is reduced, thus compensating for the specific volume effect.

As can be seen from the above analysis, the most severe limitation on the use of vacuum distillation is the requirement of a

relatively concentrated feed not to constrain the required reflux flow and thus negate the possible savings achieved by reducing the pinch effect at low pressures. Here, vapor reuse methods provide a solution. The single vacuum column can be replaced by a two column system. In the first, an atmospheric pressure stripping column operated without reflux, dilute beer is concentated to give a head product of high enough concentration not to limit the vacuum column operation. This head product is then the feed to a full distillation column operated at low pressure. Ordinarily, this two column design would be inefficient as steam would have to be provided to both columns. In the vapor reuse method, however, the vapor product from the atmospheric pressure stripper is condensed in the vacuum column reboiler to provide heat for this column. The concentrated condensed liquid is then fed at a mid-point to the vacuum column. Because the distillation column is operated at reduced pressure and its reboiler temperature is reduced, heat recovery from the hot (1 atmosphere) vapors from the stripper is very efficient--requiring only a standard sized reboiler.

Figure 11 plots XSTMIN, the minimum feed to the stripper of such a dual column system which can be stripped to produce a vapor of high enough concentration to feed a vacuum column without constraining the reflux ratio. This multieffect distillation method is quite efficient--allowing the purification of feed streams of about one tenth the concentration required in the one column method at essentially no increase in distillation energy requirement.

The dual column system also reduces the energy requirements for stillage processing. The stripper bottoms product contains yeast solids and other nonvolatile components from the fermentation. When concentrated, these are valuable as a high protein cattle feed (16). Multieffect evaporation is used for stillage concentration. As only a fraction of the water in the beer leaves as bottoms from the atmospheric pressure stripper (the remainder leaving as bottoms from the vacuum column) this product is more concentrated and less energy must be expended in the subsequent drying processes.

The whole beer, containing organic acids (acetic and lactic) as well as salts, is corrosive (17). Ordinary column materials (carbon steel, copper, aluminum) cannot be used in distillation in contact with the whole beer and costly stainless steel is required (18). The two column design offers a further savings as only the relatively small stripper need be made of stainless steel. The large vacuum column can be constructed of carbon steel and will not be significantly corroded by the purified feed at the reduced vacuum distillation temperatures.

4 Vacuum Distillation Optimization--Program DISTILL

4.1 Program overview

The general vapor reuse vacuum distillation process design is summarized in figure 13. For set feed and product requirements the tradeoffs in design can be summarized by three optimization variables--FRAC, RATIO and P.

For dilute feed concentrations, the beer must first be concentrated in the stripper to provide a concentrated enough feed to the main distillation column to take advantage of the reduction in the

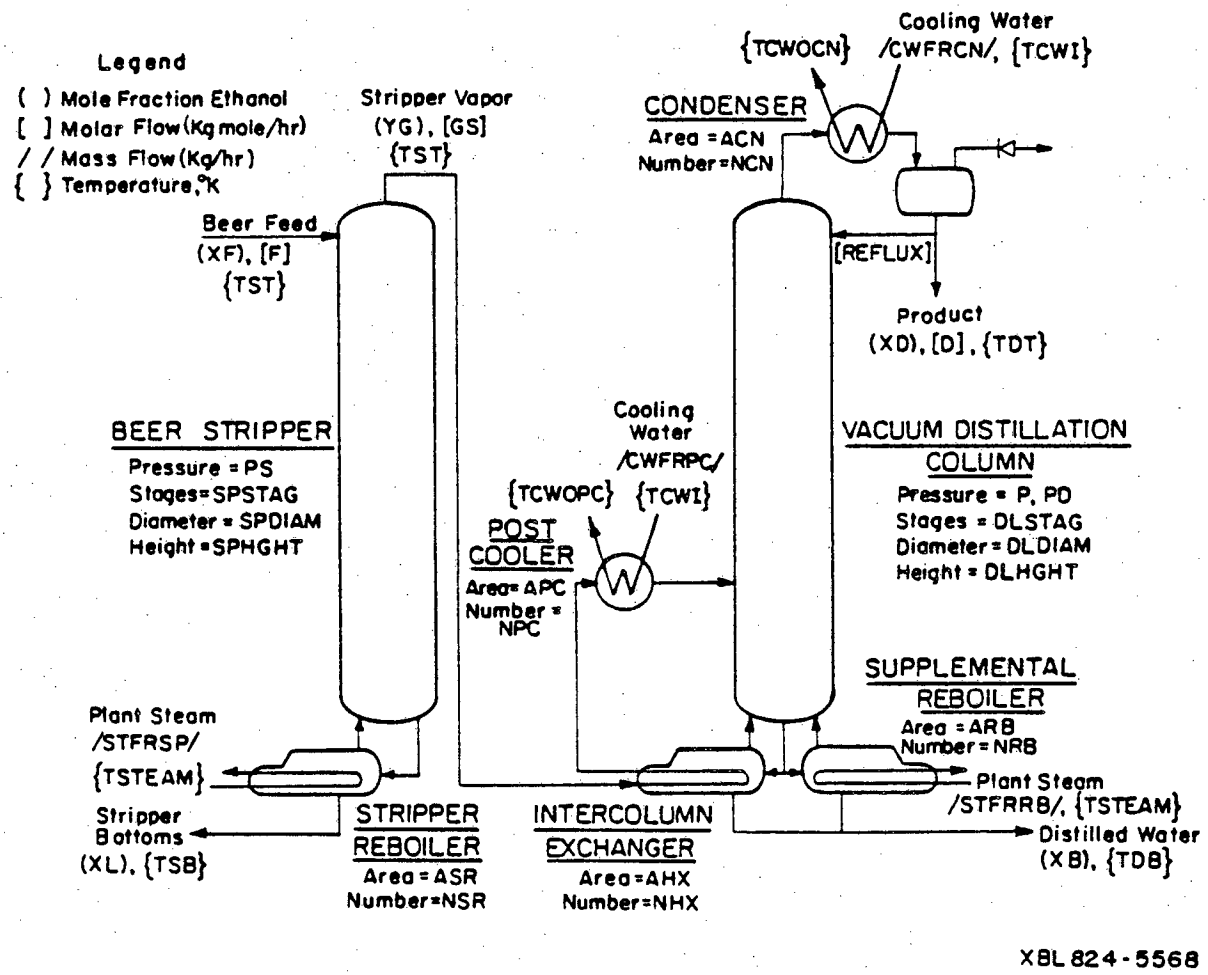


Figure 13 Dual Column Vacuum Ethanol Distillation Design - Variable Names Used in Program DISTILL

pinch at low pressure. FRAC is a scaled variable controlling the extent of concentration by the stripper and representing the fractional approach of the stripper vapor product to its maximum value--equilibrium with the stripper feed.

A close approach to equilibrium with the feed in the stripper requires added plates in the column (increased capital cost) but reduces the vapor flow rate and hence the stripper steam requirement (reduced operating cost). Close equilibrium approach also provides a more concentrated feed to the vacuum distillation column.

With the vacuum distillation column feed concentration established, this column can be designed. As the column operating pressure P (mmHg) is decreased the column head temperature drops increasing the condenser and cooling water costs. However, the lower pressure shifts the ethanol/water equilibrium curve, reducing the effect of the azeotrope associated pinch. The minimum required reflux drops and less steam or fewer stages can be used in the vacuum column to achieve the required separation.

The final design trade off--between reduced steam requirement (operating cost) and reduced vacuum column height (capital cost)--is controlled by the variable RATIO which adjusts the rectifying section operating line slope between its equilibrium pinch constrained minimum value (requiring the minimum possible steam but infinite stages) and one (requiring infinite reflux but minimum stages).

Program DISTILL (Appendix 1) was developed to design combined vapor reuse vacuum distillation systems for minimum cost ethanol/water separation by optimizing the control variables (FRAC, RATIO and P). Design specifications are fixed in common block INPUT. Initial values

for the optimization variables are set in subroutine FUNCT. Given these parameters, subroutine DISTL is called to design the distillation system calling in turn subroutine STRIP for the stripper design and HXCNG for the design of optimized heat exchangers. The distillation cost for the specified design is computed. Subroutine E04JBF (a NAG library optimization routine (19,20)) then specifies new values for the optimization variables to achieve a minimum cost design.

The computational flow of program DISTILL is presented in overview by figure 14.

4.2 Minimum reflux

For the specified vacuum column operating pressure P (mmHg), the minimum distillation reflux is computed by function TPNT. The minimum reflux rectifying section operating line is that line passing through the specified product composition (XD, YD) and just tangent to the equilibrium curve at some lower ethanol concentration. TPNT locates the tangent pinch point and finds the slope of the corresponding minimum reflux rectifying section operating line (TSLOPE). This slope corresponds to the minimum possible molar ratio of vapor upflow to liquid return flow in the rectifying section to allow the separation and thus establishes the minimum distillation energy requirement.

4.3 Minimum acceptable vacuum column feed concentration

The minimum acceptable vacuum column feed concentration (XFMIN) is found using function CROSS. This is the lowest concentration feed which would not impose a greater reflux requirement than that set by the azeotrope associated pinch. The minimum feed composition is found as the intersection of the minimum reflux rectifying operating line (found by TPNT) and the equilibrium curve in the dilute ethanol region.

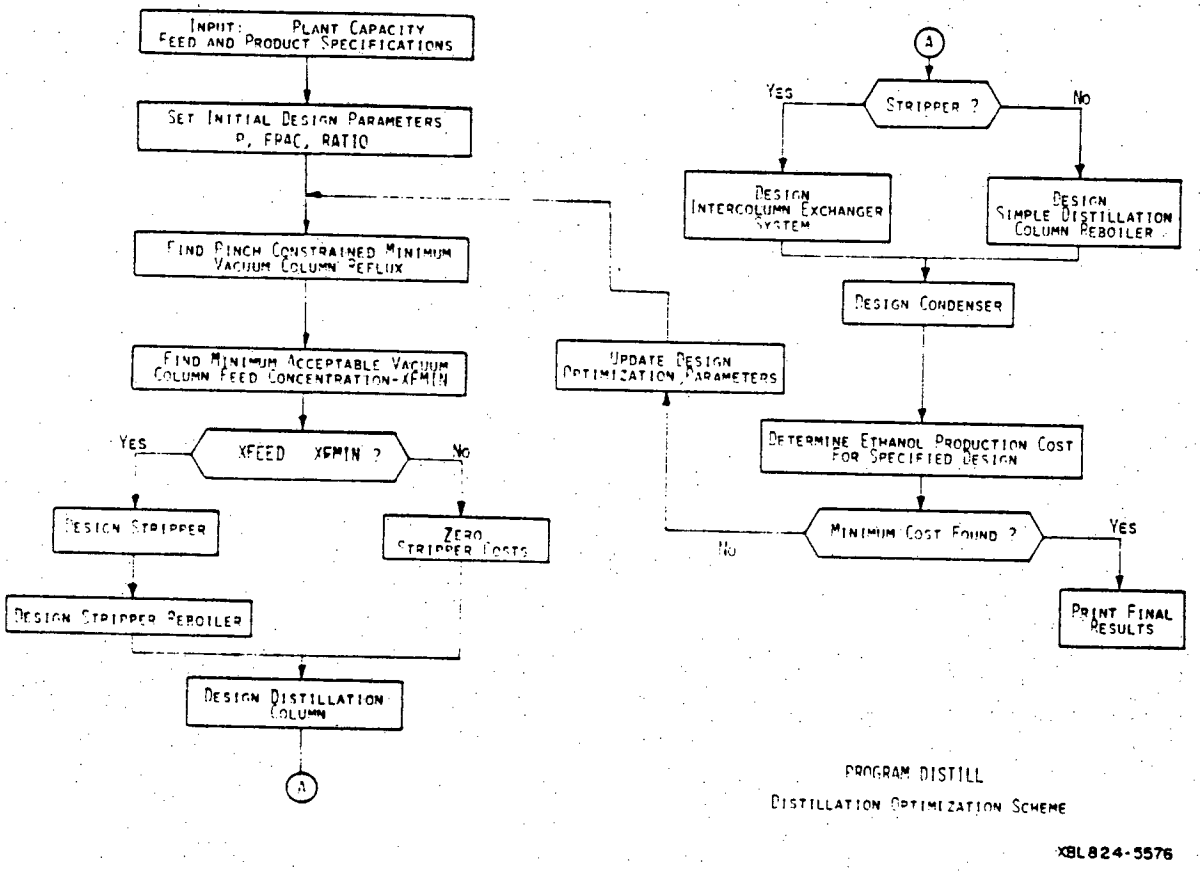


Figure 14 Computational Flow of Program DISTILL

4.4 Atmospheric pressure stripper design

If the specified beer concentration (XF) is less than the minimum acceptable vacuum column feed concentration, then an atmospheric pressure stripper must be designed to concentrate the feed. Even if a stripper is not required by the minimum feed concentration criterion, it may be desirable as high corrosion rates with ordinary materials dictate the use of costly stainless steel construction (table 1 (21)) for all warm beer wetted parts. The cost of a small added stripper can be more than offset by the savings in the use of a carbon steel vacuum column made possible by the removal of most of the corrosive acids and all of the salts in the stripper. Some plants have used distillation columns where only the lower (beer wetted) section is made of stainless steel, but electrolytic corrosion at the stainless steel/carbon steel joint then is problematic (22). The program can be instructed to override the feed concentration criterion and include a stripper in all designs by setting a control flag (MODE(26)).

The stripper (beer column) is designed by function STRIP. Because of the tradeoff between increased number of required trays and reduced steam requirement as the stripper product concentration is increased, the minimum cost design generally does not occur where the stripper product is concentrated to only the minimum required to meet the vacuum column requirement. The optimization variable FRAC then controls the actual stripper vapor composition:

$$YG = YGMIN + FRAC \cdot (YGMAX - YGMIN) \tag{17}$$

where YGMAX is the maximum possible stripper vapor composition

Table 1

Cost Multipliers for Stainless Steel Construction

Equipment	Multiplier
Condenser	1.6
Reboiler	1.6
Columns	2.0

(equilibrium with the feed) and YGMIN is the larger of the stripper feed composition or the minimum acceptable distillation column feed composition.

The stripper bottom composition is determined to give the required ethanol recovery fraction (RFRACT), generally set at 99.8% recovery.

The stripper operating line is set given the head and bottoms compositions and assuming equimolal overflow (constant vapor and liquid flows from stage to stage). This assumption is justified considering the very similar molar heats of vaporization of ethanol and water (differing by only 8.7% at 100°C (23)) and the small temperature increase down the stripper. Sieve plate trays are used. The Murphree vapor efficiency has been measured for ethanol/water separation with values varying from 0.70 to 1.00 (24). The somewhat conservative value of 0.70 was chosen considering that some yeast solids will be present and might adversely affect equilibration. The vapor efficiency is a measure of the approach to equilibrium achieved on each tray. Incorporating this efficiency, a stage by stage calculation is performed to determine the vapor and liquid compositions on each stage. The ETOH ethanol/water equilibrium package (73) is used to find equilibrium compositions and determine the temperatures on each stage. Starting from the column head, trays are added until the specified bottom composition is achieved. A tray spacing of two feet is used to allow for possible foaming caused by proteins in the beer solution.

The stripping column diameter is determined to give a vapor linear velocity at 70% of the flooding limit as determined by Van Winkle (25). A single calculation at typical design conditions established

that this flow was sufficient to prevent weeping (liquid seepage through the sieve tray perforations).

The tower wall thickness is specified at 0.25 inches as determined by a pressure vessel design calculation according to ASME standards (14) and at a typical column diameter of seven feet. Stainless steel construction throughout reduces corrosion rates to negligible levels and no additional corrosion allowance was included for the wall thickness.

The stripper reboiler is designed by subroutine HXCNG. The reboiler could be eliminated by direct steam injection to the stripper but this would add additional water to the stripper bottoms flow, thus increasing the evaporation load on stillage concentrators to produce a dried yeast cattle feed supplement. The reboiler heat load is set by the stripper vapor flow rate, and the hot and cold side temperatures are the plant steam temperature (generally set at 147.15^{o}C for 50 psig steam) and the stripper bottoms product boiling point, respectively. An overall heat transfer coefficient (with a fouling factor already included) of 400 Btu/sq ft$\cdot$hr$\cdot^{o}$F is used (26).

4.5 Vacuum distillation column design

The vacuum distillation column is designed by function DISTL. The feed composition is set as the vapor product composition from the stripper (or the beer feed composition if no stripper is used). The product composition (XD) is that specified in the INPUT data block and the bottom composition is again determined to give the specified ethanol product recovery fraction (generally 99.8% recovery). The distillation pressure P (mmHg) can be fixed but is generally specified as one of the three optimization variables. The vacuum column reflux is then set by

the final optimization variable (RATIO) according to:

$$RATDL = \frac{1}{TSLOPE} + RATIO\ (1.0 - \frac{1}{TSLOPE}) \tag{18}$$

where TSLOPE is the slope of the minimum reflux rectifying section operating line and RATDL is the ratio of the actual operating line slope to the minimum:

$$RSLOPE = RATDL \cdot TSLOPE \tag{19}$$

RATIO can range from 1.0 to 0.0 corresponding to an operating line slope ranging from the minimum (requiring infinite stages) to one (requiring the minimum stages but infinite reflux, and hence, infinite steam to the column reboiler). The stripping section operating line is specified assuming a saturated liquid feed to the vacuum column. At reduced pressure, the difference between ethanol and water heats of vaporization drops (to only 4.9% at 50°C (23)), and constant molar overflow is assumed as in the stripper.

A packed column is specified to reduce pressure drop in the vacuum distillation. If a stripper is not used, then yeast cell solids should be removed prior to distillation to prevent column plugging. This can be achieved by centrifugation.

With the operating lines specified, a stage by stage equilibrium calculation is performed assuming theoretical equilibrium stages. This gives the number of rectifying and stripping equilibrium contacting units required. The height of 2 inch Pall ring packing required to simulate one theoretical equilibrium contacting unit is calculated using

a correlation of Hengstebeck (27), and overdesigned by 15% to allow for uncertainty in the stage height under vacuum conditions. The total column height and the optimum feed location height in the column are thus determined. The packed column diameter is set to give a vapor pressure drop of 50 $(N/m^2)/m$ as recommended by Treybal (28) and with a vapor flow versus pressure drop relation derived from the data of Leva (29).

The column is designed with a wall thickness of 0.375 inches determined according to ASME standards for a vacuum vessel design and calculated for a typical (12 ft diameter column) case assuming four internal support rings (14). The packing support tray and reflux liquid distributor act as two of the support rings. Two "doughnut" vapor flow redistributors in the column provide the remaining support requirement. Carbon steel construction is specified when a stripper is used. At the low vacuum distillation temperatures, corrosion by the clear ethanol/water solution is slight (15). If no stripper is used and organic acids and salts (typical of a fermentor beer) are present, then stainless steel construction is necessary (18).

4.6 Distillation column reboiler design

The distillation column reboiler design is specified by function DISTL.

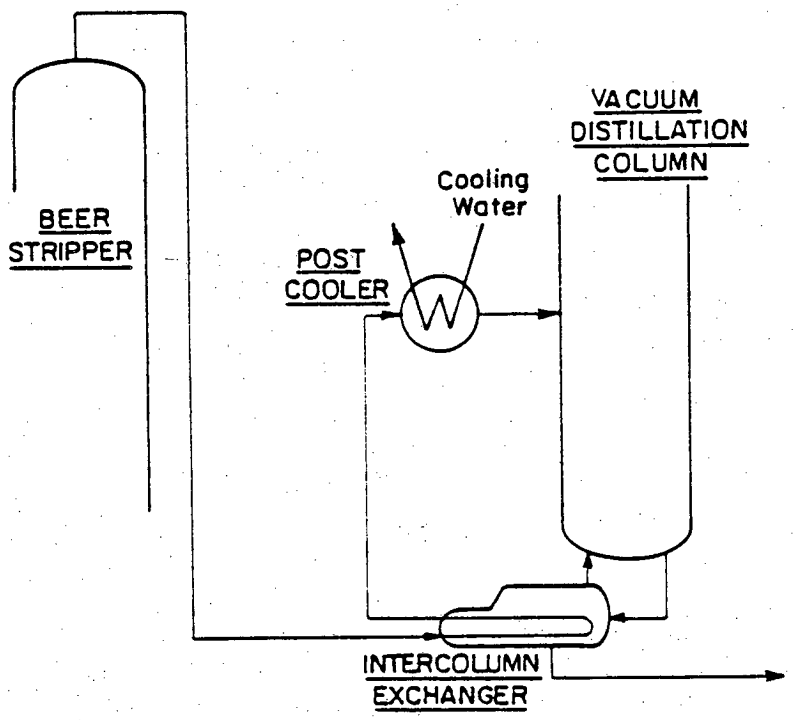
If no stripper is used, then a simple steam heated reboiler is used. The heat load is set to boil up sufficient vapor at the column bottom to provide the specified vapor flow rate. Because the heat of vaporization of the predominantly water bottoms product is slightly higher than that of the predominantly ethanol top product, the vapor flow at the column head (near the pinch) is actually slightly higher

than corresponds to the rectifying slope specification. This results in a conservative design. Hot and cold side temperatures are the plant steam temperature and the column bottom product boiling point (at column pressure), respectively. An overall heat transfer coefficient (with fouling factor included) of 400 Btu/sq ft·^{o}F·hr is used (26). Subroutine HXCNG is called to compute the reboiler size.

If a stripper is used, then vapor reuse methods are employed to recover the stripping heat to drive the vacuum column and a more complex exchanger system is required. The stripper vapor must be totally condensed to provide a saturated liquid feed to the vacuum column. If the heat of condensation of the stripper vapor is greater than the heat requirement of the vacuum column, then an intercolumn exchanger is used as the reboiler for the column and a water cooled post cooler removes the remaining heat to condense the vapor for feed to the column (see fig. 15a). If the heat available from condensing the stripper vapor is insufficient to meet the full requirement for the vacuum column, then an intercolumn exchanger is used to totally condense the stripper vapor and an auxiliary plant steam heated distillation column reboiler is designed to meet the remaining heat requirement (see fig. 15b). A post cooler is generally needed when very dilute feeds are processed as these generate large stripper vapor flows. More concentrated feeds produce smaller more concentrated stripper vapor flows and an auxiliary distillation column reboiler is then required.

Design of the intercolumn exchangers or auxiliary distillation reboiler is simple as all temperatures and heat loads are known. Subroutine HXCNG is called to size these exchangers as in the lone reboiler case.

Figure 15a Intercolumn Heat Exchanger Arrangement For Dilute Beer Feeds



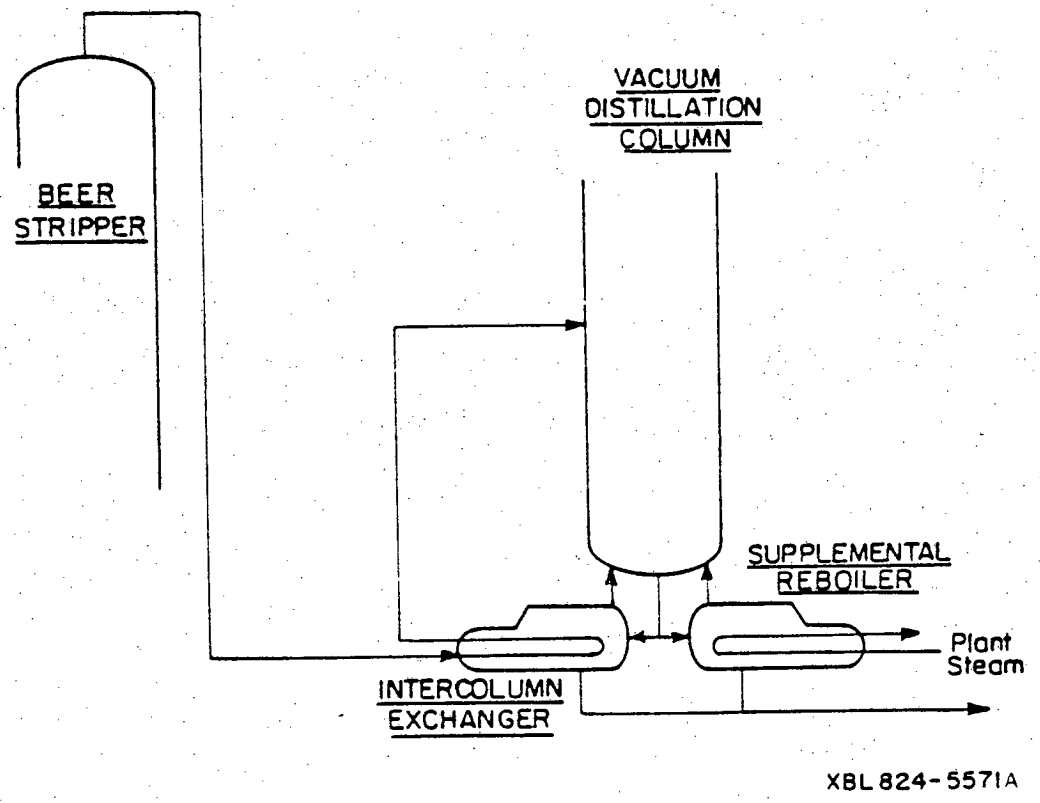


Figure 15b Intercolumn Heat Exchanger Arrangement For Concentrated Beer Feeds

The post cooler design is more complicated, requiring an optimization balancing cooling water costs against post cool exchanger capital cost. Subroutine CNDSR uses function ZERO to minimize function CNCST and provide an optimum post cooler design. The cooling water feed temperature is set at the plant cooling water temperature. The outlet temperature is then varied. As the cooling water outlet temperature is increased, the heat transfer temperature difference driving force decreases necessitating a larger exchanger area (greater capital cost) but, by enthalpy balance, the cooling water usage is decreased (decreasing operating costs).

Standard design four pass exchangers are used. As very close temperature approaches are possible, the effect of imperfect countercurrent flow in the multipass exchangers can result in a further decrease in the effective average temperature driving force. Function FTLM computes a correction to the log mean driving force using correlations derived from figures of Kern (30). With an overall heat transfer coefficient of 350 Btu/hr·sq ft·^{o}F, subroutine HXCNG is used to compute the exchanger area for a given outlet cooling water temperature.

Materials of construction for the distillation column heating system are specified such that all beer wetted surfaces (subject to corrosive organic acids and salts) as made of stainless steel. When no stripper is used, the reboiler is thus constructed of stainless steel. Carbon steel is used for all the intercolumn exchangers when a stripper is used.

4.7 Condenser design

The distillation column condenser is designed by subroutine CNDSR. The cooling load is set by the requirement to condense all the

distillation column overhead vapor (product flow plus reflux). As with the post cooler, an optimization is necessary to find the optimum cooling water flow rate.

The FTLM correction to the log mean temperature driving force is applied using an overall heat transfer coefficient of 350 Btu/sq ft ^{o}F hr. The condenser contacts only purified ethanol/water solutions and carbon steel construction is used.

The effective cost for the exchanger, considering capital and operating associated cost contributions, is then calculated and minimized.

4.8 Distillation system costing

Purchased equipment costs for columns and exchangers are derived from figures presented by Peters and Timmerhaus (21) and corrected to present dollars by the current Marshall Swift Cost Index. The costing equations are summarized in table 2. The total fixed capital cost for the distillation plant is taken as 4.13 times the purchased cost and the total capital investment (including working capital) is 4.89 times purchased equipment cost.

Major operating costs are for cooling water and steam. A base cooling water cost for well water of 18 cents/1000 gallons (Jan. 79) is used and updated by the current Marshall Swift Index. The base steam cost for 50 psig steam of $2.50/1000 lbs is also updated by the Marshall Swift Index. For the assumed design period of mid-1981 with an MSI of 717 (31), the resulting base cooling water and steam costs used are 23 cents/1000 gallons and $3.15/1000 lbs, respectively.

A labor cost is calculated based on the production rate and assuming the distillation plant to be a component in an automated

Table 2

Distillation Equipment
Purchased Cost Equations

Item	Purchased Cost, $	Size Unit	Maximum Size	Construction
Heat Exchanger (Condenser or Reboiler)	$330.69 \times \left(\frac{MSI}{569}\right)(SIZE)^{0.5528}$	Sq. Ft.	7,000	C.S.
Columns:				
Packing	$10.3\left(\frac{MSI}{569}\right)\left(S_h\right)\frac{\pi}{4}\left(S_D\right)^2$	S_h = Height, Ft.	2" Raschig Rings	Porcelain
Trays	$33\left(\frac{MSI}{569}\right)(n)\left(S_D\right)^{1.737}$	n = Number of Trays	16 Ft.	S.S.
Shell Weight	$0.29 \times 144\pi\left(S_h\right)S_D\left(S_t\right)$	S_D = Diameter, Ft. S_t = Wall Thickness, Inches	16 Ft.	C.S.
WTOTAL: Column Total Weight (with heads and skirt)	1.12 x Shell Weight	lbs.		
Column Shell Cost	$\left(\frac{MSI}{569}\right) \times 87.16\ (WTOTAL)^{0.6126}$			
Fittings	$[(85 \times M) + (52 \times N)]\left(\frac{MSI}{369}\right)$	M = Number of Manholes N = Number of Nozzles		C.S.

MSI = Current Marshall Swift cost index.

Purchased cost can be multiplied by factors given in Table 1 to find cost for stainless steel construction.

fermentative ethanol production facility. The labor requirement is given as 0.151 worker hours per ton of product (21). A labor cost (including supervision) of $10/hr (Jan. 1979 dollars) and updated by the Marshall Swift Index is used.

Direct fixed capital related costs are incurred for local taxes, insurance, maintenance and depreciation. These yearly costs are calculated as fractions of the fixed capital investment (summarized in table 3). The depreciation rate corresponds to an 18 year straight line depreciation as specified by the U.S. Internal Revenue code for alcohol plants. This is a reasonable plant lifetime for the equipment as designed.

A further fixed capital related assessment is made as given by (32):

$$\text{Profit} = \frac{\text{INVEST}}{(1.0-\text{TAX})} \tag{20}$$

where INVEST is the desired simple rate of return on fixed capital investment and TAX is the federal income tax rate (assumed 0.50). This assessment corresponds to the profit required to provide the desired return after taxes. For a 15 percent desired return on investment, (INVEST = 0.15) the factor PROFIT equals 0.30 and is the largest capital associated assessment.

Table 3

Standard Capital Related Cost Factors

(Cost per Annum = CFACTR x Fixed Capital)

ITEM	COST FACTOR
Depreciation	0.056
Maintenance	0.060
Insurance	0.010
Local Tax	0.030
Profit Before Income Tax (0.150/0.50)	0.300
CFACTR =	0.456

The total annual price to be charged for distilling a given beer feed is then the sum of yearly operating costs and the fixed capital investment times the capital associated costing factors. It is this charged price which is minimized and the result is the design which will achieve the required purification and provide the required return on investment while producing the product for the minimum sale price.

4.9 Distillation cost minimization

Initial values for the optimization variables FRAC, P (mmHg), and RATIO are set in subroutine FUNCT. A prelminary design is completed at these initial conditions. If only the initial (nonoptimized) design is required, optimization can be overridden by setting a control flag (MODE (27)). Otherwise, new values of the optimization variables are chosen by the NAG library optimization routine E04JBF (19). This routine uses a revised quasi-Newton minimization technique (20,33) to select successive values of the optimization variables and converge on a minimum cost design.

The final distillation system design parameters are stored in design common blocks and details are printed by the main driver program DISTILL.

5 Distillation Optimization Results

5.1 Base case design

Program DISTILL was used to evaluate the economics of vacuum distillation to produce 95 wt% ethanol product.

A typical case is for the purification of a 6 wt% ethanol beer (fig. 16). The complete computer generated design specification for

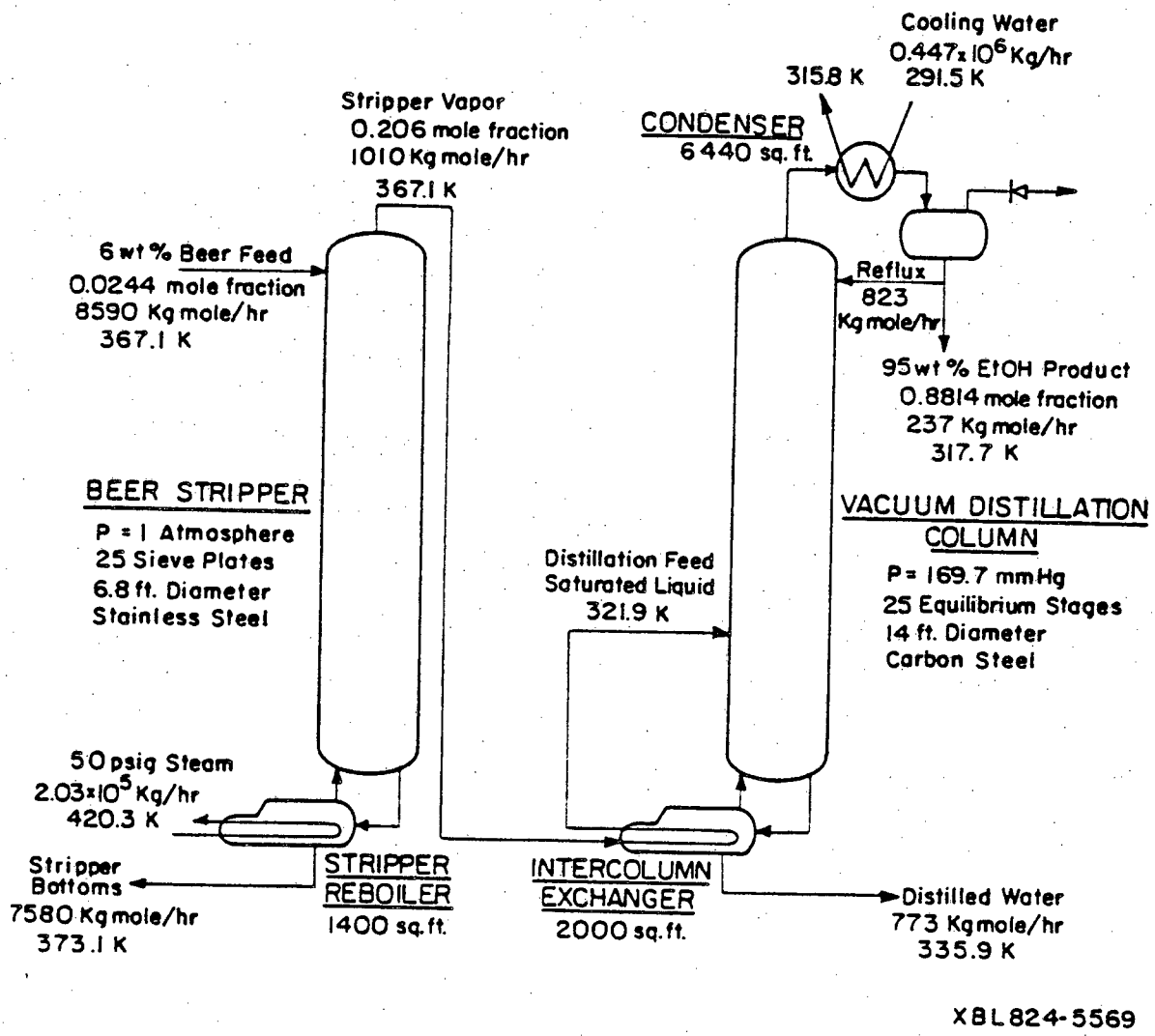


Figure 16 Optimized Base Case Design. Two Column Distillation of 6 wt % Feed to 95 wt % Product

this case (including tray by tray composition changes) is presented as Appendix 2. For the base case, a design capacity of 100 million liters per year of 95 wt% ethanol product and 330 day per year plant operation are assumed. Water at 18.3°C (65°F) is used for cooling (22.6 cents/1000 gallons mid-1981 cost) and plant steam is at 50 psig ($3.15/1000 lbs mid-1981 cost). A labor cost (including a percentage for supervision) of 12.6 dollars per worker hour (mid-1981) is assumed. Depreciation is straight line over eighteen years and a fifteen percent simple return on fixed capital investment is required. No special subsidies or supports are allowed and a fifty percent income tax is assessed.

The 6 wt% beer feed is too dilute to be processed directly in the vacuum distillation without requiring increased reflux above the minimum set by the azeotrope associated pinch (see fig. 11). A preliminary atmospheric pressure stripper is therefore included. At the optimized vacuum column pressure, the minimum acceptable feed concentration is 10.8 wt% ethanol and this sets the minimum allowable vapor product concentration from the stripper. The optimized stripper vapor composition is 39.9 wt% ethanol, far more concentrated than the minimum. This represents the best balance between the number of stripping stages and stripper steam requirement--25 stages and 1.61 kg of steam per liter of ethanol product (13.4 lbs/gal) respectively. The stripper is 54 ft tall and 6.8 ft in diameter.

With a cooling water temperature of 18.3°C, the minimum possible distillation column operating pressure to allow product condensation for reflux is 39.6 mmHg with a corresponding minimum external reflux ratio of 1.38. The optimized pressure is 170 mmHg with a larger corresponding

minimum reflux ratio of 2.06 (62% of the minimum at 1 atmosphere) but allowing a 26.2°C condenser cooling water inlet approach. The optimized reflux ratio is 3.48, 1.69 times the minimum. 25 theoretical equilibrium stages are required at this reflux. At first, the specified reflux may seem excessive--a reflux ratio of 1.15 to 1.35 times minimum is commonly employed in other energy intensive distillation operations. The specified result is however a true optimum and results from the full utilization of recovered stripper heat. 1.61 kg of steam per liter of final product are required to drive the stripper. The optimized intercolumn exchanger design then recovers all of this "free" heat to drive the distillation. Vapor reuse methods thus allow this large reflux and reduced vacuum distillation tower height without the expenditure of additional steam. Using 2-inch Pall ring packing, a 35 foot tall column 14 feet in diameter is required. Because a stripper was used, the distillation column can be constructed of carbon steel.

Purchased costs for the specified plant equipment are summarized in table 4. The total purchased equipment cost is $359,900 with a correspondng total capital investment of $1,759,900. Operating costs are summarized in table 5.

5.2 Effect of feed concentration on distillation design

The effect of feed ethanol concentration on distillation cost and design is summarized in figure 17 and table 6. Figure 17 shows the additive cost contributions for labor, capital associated assessments, steam and cooling water, summed to the total charge for distillation. Costs are all for a dual column system. The distillation cost for a very dilute feed (1 wt% ethanol) is high (7.5 cents/L) but drops off rapidly as feed concentration increases. Above 9 wt% beer feed

Table 4

6 wt% Ethanol Distillation
Purchased Equipment Summary
100 Million Liter Per Year

Equipment	Purchased Cost
Stripping Column 25 sieve trays 6.8 ft. diameter, 54 ft. tall Stainless steel	$105,500
Stripper Reboiler 1400 sq. ft. Stainless steel	$ 36,600
Distillation Column 25.2 stages (Raschig ring packing) 14.0 ft. diameter, 35 ft. tall Carbon steel	$136,700
Intercolumn exchanger 2,000 sq. ft. Carbon steel	$ 27,900
Condenser 6,440 sq. ft. Carbon steel	$ 53,200
Total Purchased Equipment Cost	$359,900
Fixed Capital Investment (4.13 x Purch. Cost)	$1,486,400
Total Capital Investment (4.89 x Purch. Cost)	$1,759,900

Table 5

6 wt% Ethanol Distillation
Operating Cost Summary
100 Million Liter Per Year

	Basis	Charge (¢/L)
DIRECT COSTS		
1. Labor and Supervision	1.81 workers/shift	0.180
2. Utilities		
Steam (50 psig)	1.61 kg/L	1.120
Cooling Water (65°C)	35.4 kg/L	0.212
3. Maintenance	6% Fixed Capital	0.089
		1.601
FIXED COSTS		
1. Depreciation	18 year, Straight Line	0.083
2. Local Taxes	3% Fixed Capital	0.045
3. Insurance	1% Fixed Capital	0.015
		0.143
GROSS PROFIT		
1. Net Profit	15% Simple ROI	0.223
2. Income Tax	50% Rate	0.223
		0.446
	TOTAL CHARGES	2.190

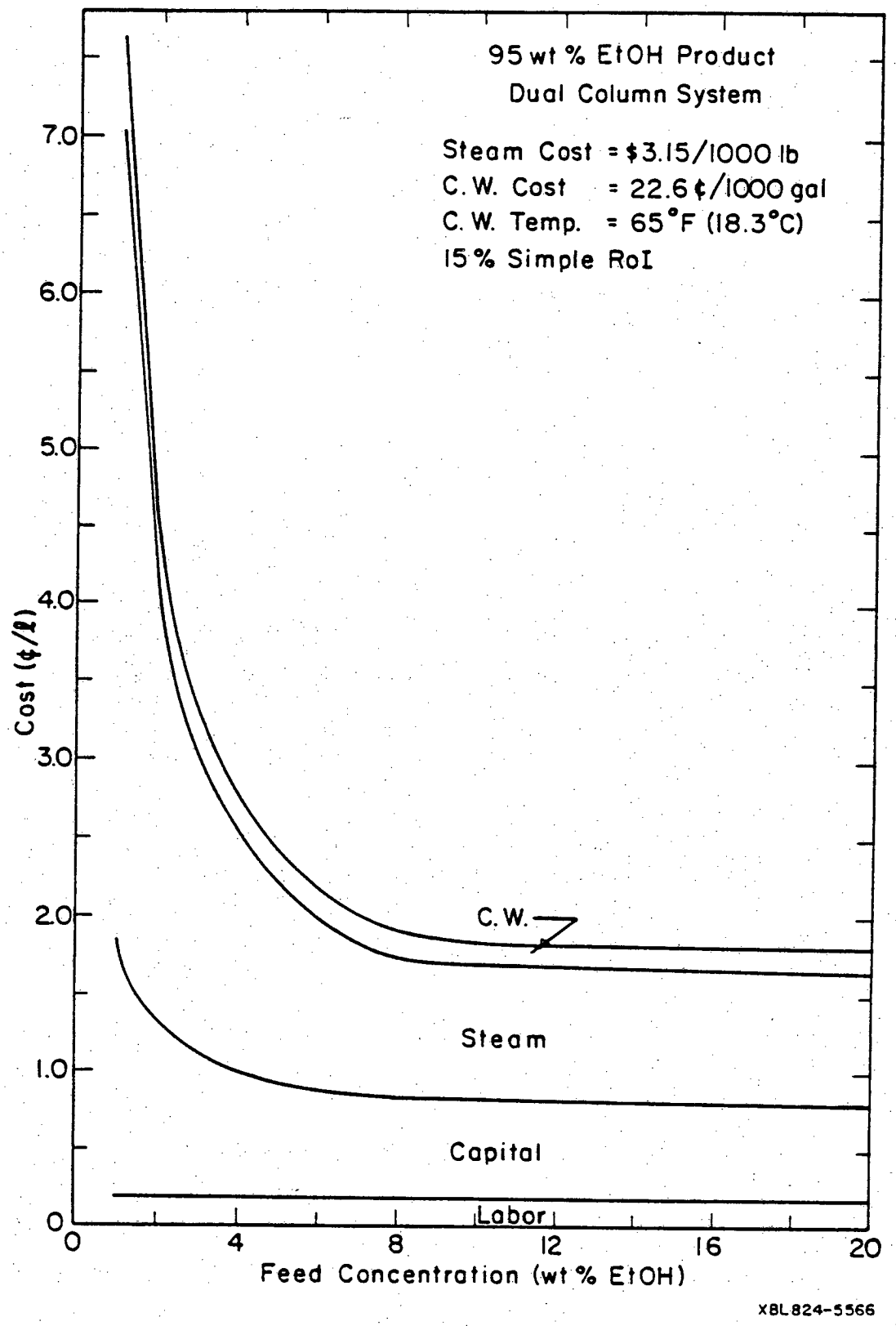


Figure 17 Effect of Feed Ethanol Concentration on Optimized Distillation Design Costs. Base Case Cost Assumptions

Table 6

Effect of Feed Concentration on
Optimized Distillation System Design

Feed wt %	Stripper Trays	Distillation Stages	Exchanger Design	Distillation Pressure	System Capital Cost	Distillation Reflux Ratio	Steam Usage (kg/L)
1	56	35	Post Cooler	289	4,303,000	3.97	7.51
6	25	25	Balanced	170	1,760,000	3.48	1.61
20	11	42	Supplemental Reboiler	162	1,542,000	2.36	1.25

concentration, the design is constrained by the azeotrope associated pinch and the distillation cost becomes constant.

At low feed concentrations, the design is necessarily both capital and energy intensive. To meet the minimum acceptable distillation column feed concentration, a very large stripper is required (56 trays for a 1 wt% beer). The maximum concentration stripper vapor product is still quite dilute and the stripper vapor flow is very large--necessitating a very large steam feed to the stripper reboiler (7.5 kg/L for the optimized 1 wt% feed case). The vacuum column need not be designed for high energy efficiency as excess heat is available through the vapor reuse method in condensing the large vapor stream from the stripper. Relatively high pressures (289 mmHg for the 1 wt% feed case) can be used in the vacuum column. So much heat is available from the stripper vapor that a post cooler is required after the intercolumn exchanger to avoid excessive reflux in the vacuum column which would give rise to an excessive column diameter and increased capital cost.

For typical feed concentrations (5 to 7 wt% ethanol) the heat loads of the stripper and vacuum column can be balanced so that neither a post cooler nor a supplementary distillation column reboiler is required. To maintain the balance while not increasing the vacuum column height, the optimum distillation column pressure is reduced as the feed becomes more concentrated and less heat is available for recovery from the stripper vapor. The height of the stripper can also be decreased as its feed concentration increases.

Very high feed concentrations could result from the development of new end product inhibition resistant fermenting strains. Fermentation processes with selective ethanol product removal could also generate

concentrated feeds for distillation. For feeds above 9 wt% ethanol, only a single column (no stripper) is necessary. However, inclusion of a small stripper is cost effective when processing a corrosive beer. The small stripper can then be made of stainless steel and the large vacuum column can be constructed from carbon steel. Figure 17 presents costs with the dual column system used throughout. Costs for the single column design (using stainless steel construction) are presented for comparison in table 7. If a concentrated feed results from a selective ethanol removal fermentation which gives a clear noncorrosive ethanol/water solution for further distillation (i.e. the vacuferm process (13)) then a single column carbon steel design would be specified at reduced cost.

For a concentrated feed case, the steam usage is set by the azeotrope associated pinch in the vacuum column. This is illustrated for the 20 wt% feed case. The distillation column pressure is reduced to 162 mmHg to reduce the minimum reflux. The number of distillation stages is increased to 42 and the actual reflux reduced to 2.36. For this case then, the actual optimized reflux is just 1.17 times the minimum as is typical in modern distillation design. A small (10 stage) stripper is used. The vacuum column requires more heat than can be recovered from the very concentrated stripper vapors and a supplemental vacuum column reboiler is required.

5.3 Distillation design sensitivity to cost assumptions

5.3.1 Effect of steam cost

The base steam cost of $3.15/1000 lb steam (mid-1981 basis) is based on in-plant coal generated steam. Figure 18 shows the effect of steam cost on the total distillation cost for a typical 6 wt% feed. As

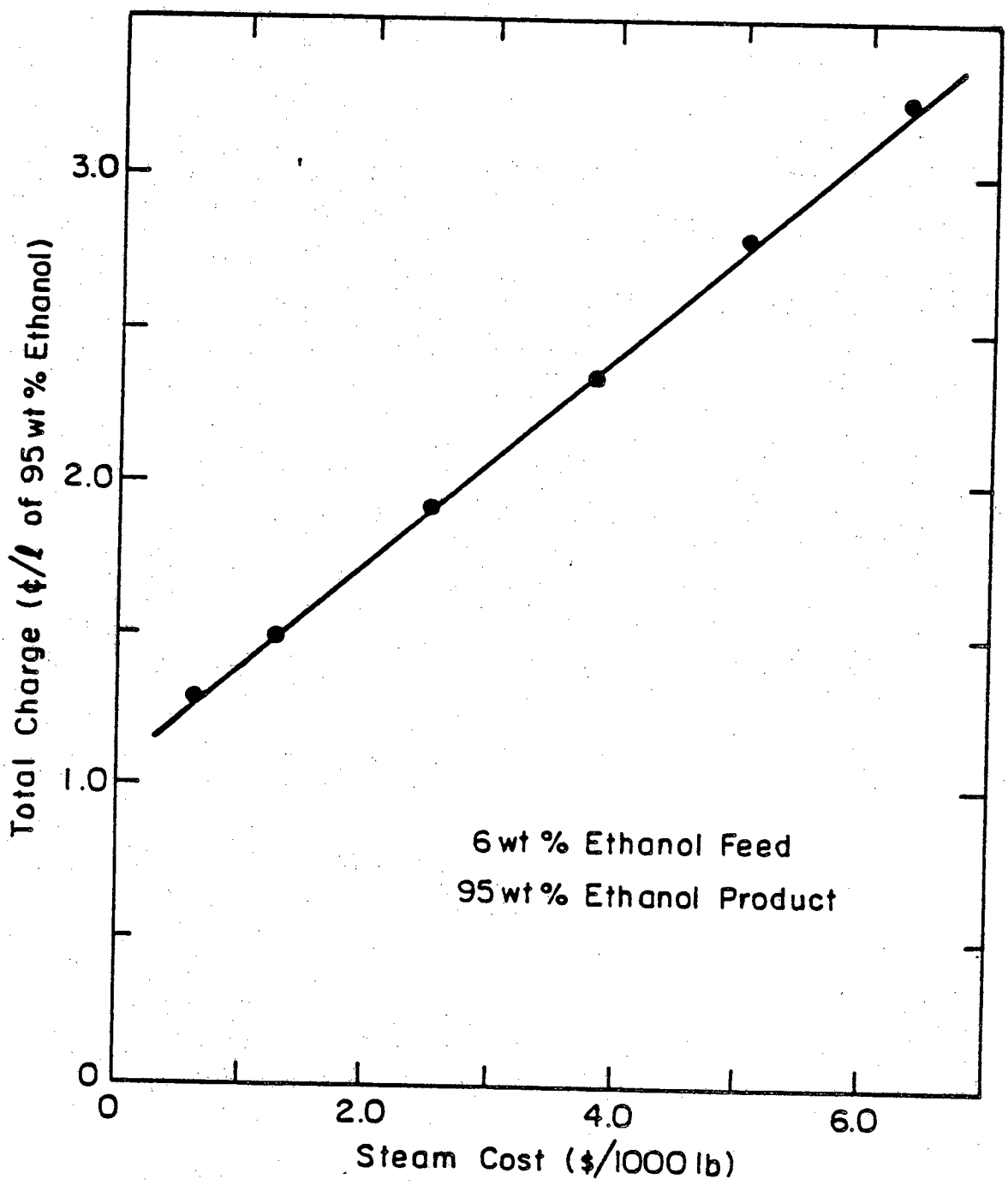
Table 7

Distillation Costs for High Feed Concentrations

Simple versus Dual Column Design

Feed Concentration wt %	Total Charge (¢/L) Single Column Design	Dual Column* Design
11	1.926	1.852
13	1.905	1.840
15	1.901	1.833
17	1.892	1.827
19	1.887	1.819

*Savings result as large vacumn column can be constructed of carbon steel if a stainless steel stripper is used to reduce corrosives.



XBL 824-5559

Figure 18 Effect of Steam Cost on Total Distillation Cost For 6 wt % Ethanol Feed

the steam cost is increased, stages are added to both the stripper and vacuum column and the reflux ratio is reduced. Thus, the increase in steam cost is partially mitigated by a decrease in steam usage, but capital associated costs are increased.

A particularly important case is for steam generated from process wastes. In an integrated ethanol from cellulosic biomass plant, nonhydrolyzable solids will be available as a waste after hydrolysis and sugar recovery. A major waste component material will be lignin, with a fuel value of 29.5×10^6 joules/kg (34). Neglecting the opportunity cost involved is not upgrading and selling these wastes, a steam cost can be computed assuming in-plant burning with no charge for the fuel. Only capital associated costs for the boilers are then assessed and a steam cost (mid-1981 basis) of 75.6 cents/1000 lb results.

Figure 19 summarizes distillation costs for various ethanol feed concentrations using waste generated steam. The use of this "cheap" energy results in very large cost savings for the processing of dilute feeds. Distillation of concentrated feeds is less energy intensive and smaller cost savings are achieved for these. For all concentrations, steam usage is increased, allowing an increase in distillation column pressure and reduction in stripper and distillation column stages for reduced capital costs (table 8).

5.3.2 Effect of cooling water cost

Cooling water cost and temperature depend on the type of cooling water source used (table 9 (21)). In the base case design, low temperature (18.3°C, 65°F) well water is assumed. Ground water usage restrictions in the U.S. Midwest might prevent the use of well water for cooling in corn and grain belt alcohol plants. Recycled cooling tower

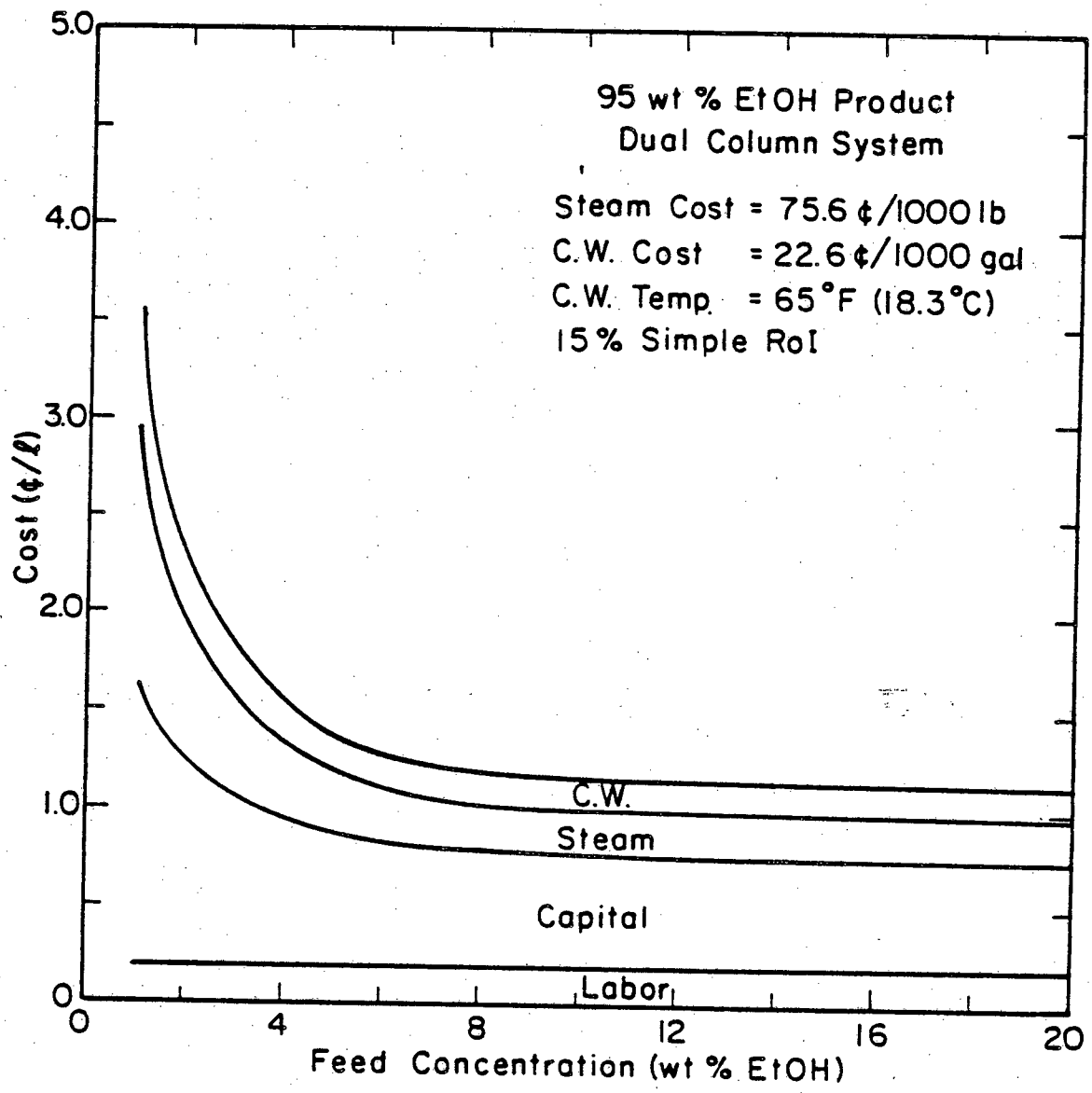


Figure 19 Distillation Cost Using Low Cost (75.6c/1000 lb.) Waste Generated Steam

Table 8

Effect of Steam Cost on Optimized Distillation System Design

Feed wt %	Stripper Trays		Distillation Stages		Distillation Pressure (mmHg)		Distillation Reflux Ratio		Usage (kg/L)	
	Base*	Low	Base	Low	Base	Low	Base	Low	Base	Low
1	56	37	35	34	289	309	3.97	4.40	7.52	7.99
6	25	19	25	27	170	229	3.48	3.79	1.61	1.53
20	11	8	42	39	162	250	2.36	2.85	1.25	1.43

*Base ≡ For base steam cost of $3.15/1000 lb

Low ≡ For low steam cost of 75.6¢/1000 lb (generated from wastes)

Table 9

Typical Cooling Water Costs

Source	Temperature °C (°F)	Cost (¢/1000 gal)
River or Ocean	18-21 (65-70)	10.
Well	18 (65)	23.
Deep Well	13 (55)	32.
Cooling Tower	27-29 (80-85)	13.

water would then be substituted, with a cooling water temperature typically as high as 27.8°C (82°F). Higher cooling water temperature further restricts the minimum pressure in the distillation column to allow product vapor condensation. A larger condenser and larger cooling water flows are required. Balancing these effects, however, is the reduced cost for recycled cooling tower water (12.6 cents/1000 gallons mid-1981 basis) as compared to well water (22.6 cents/1000 gallons).

The distillation cost for various ethanol feed concentrations and using cooling tower water is summarized in figure 20. The overall effect on cost is small (less than 3%) but as shown in table 10, the optimum design specifications are shifted compared to the base case.

5.3.3 Effect of desired ROI

A typical 15% desired simple after tax return on fixed capital investment is assumed in calculating the required price to be charged for distillation in the base case. Capital associated assessments make up roughly one-third of the total distillation price, with the ROI assessment the largest part (66%) of this contribution.

The choice of ROI has a large effect on the calculated distillation price, and the plant design is altered as the specified desired ROI is changed. This is illustrated in figure 21 and table 11 for a typical 6 wt% ethanol feed case assuming various ROI values. A low required ROI results in shifts toward a more capital intensive lower energy consuming plant design while a high required ROI results in a lower capital (smaller columns) more energy intensive plant.

For optimum performance, it is important that a plant be designed based on its true intended desired return on investment. Of course, after a plant is built, market conditions will dictate the actual price

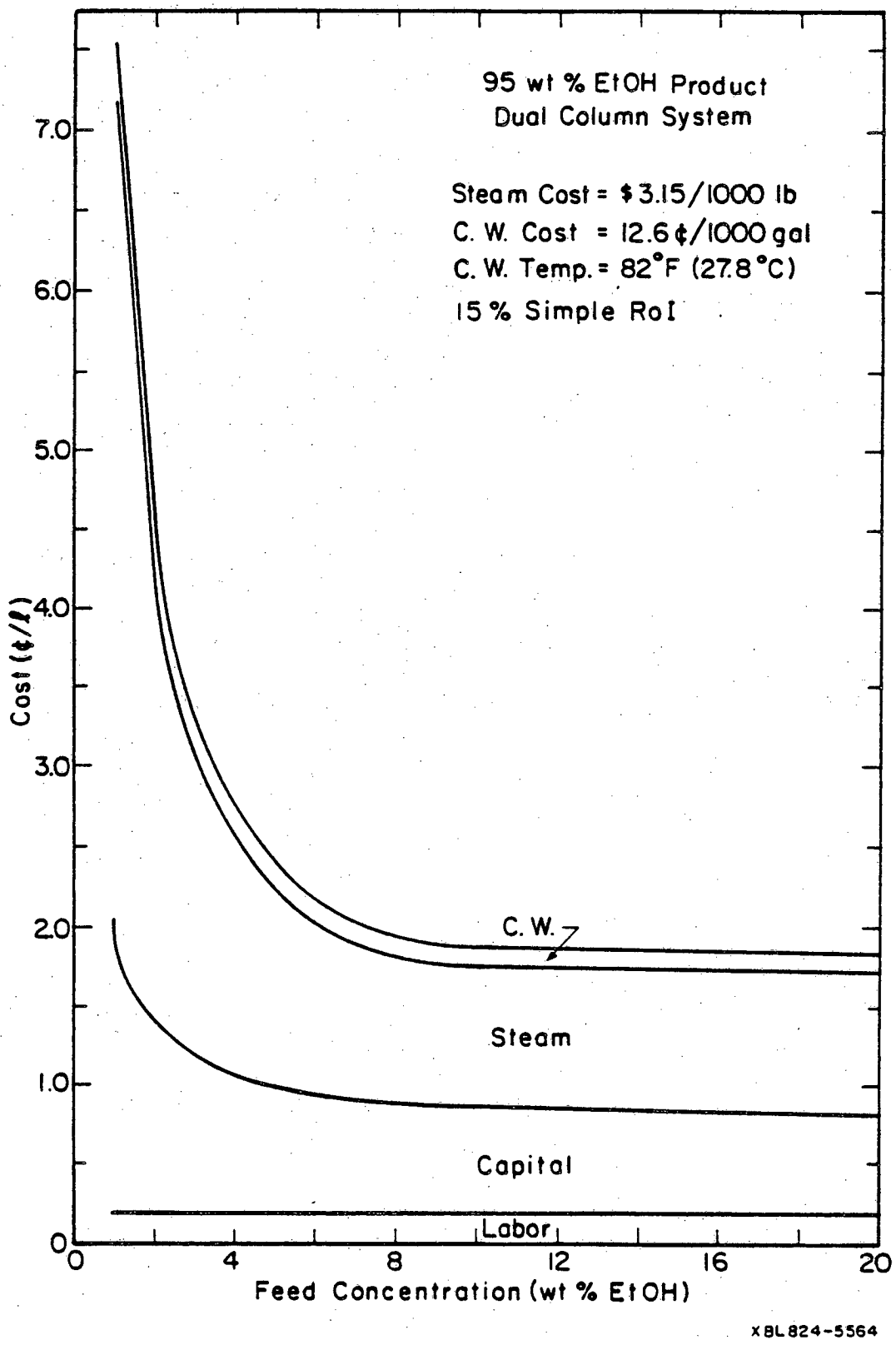


Figure 20 Distillation Cost Using Recycled Cooling Tower Water

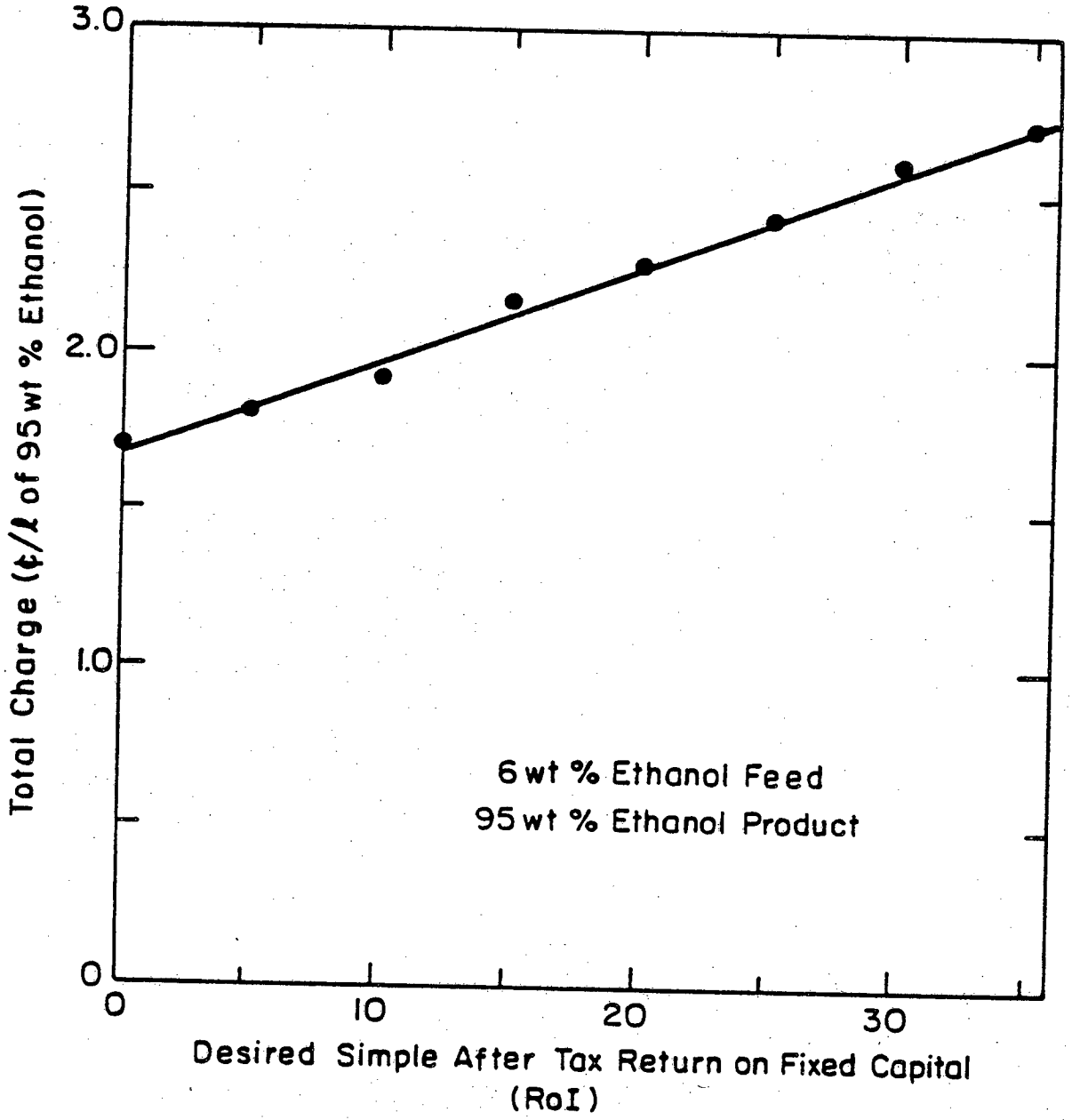
Table 10

Effect of Cooling Water Temperature on Optimized Distillation System Design

Feed wt %	Stripper Trays		Distillation Stages		Distillation Pressure (mmHg)		Cooling Water Usage (kg/L)		Steam Usage (kg/L)	
	Base*	High	Base	High	Base	High	Base	High	Base	High
1	56	66	35	36	289	390	96.6	107.5	7.52	7.38
6	25	30	25	30	170	230	35.4	42.5	1.61	1.57
20	11	10	42	42	162	215	27.8	37.9	1.25	1.35

*Base ≡ For base cooling water temperature (65°F) and cost (22.6¢/1000 gallons)

High ≡ For recycled cooling tower water (82°F, 12.6¢/1000 gallons)



XBL 824-5560

Figure 21 Effect of Required Return on Investment on Distillation Cost

Table 11

Effect of Desired Return on Investment on Distillation Plant Capital Cost

ROI(%)	Capital Cost ($)
30	1,743,900
20	1,821,200
10	1,872,500
0	1,961,000

Capital cost is for optimized plant design distilling 6 wt % ethanol feed to 95 wt % product.

charged for conducting the distillation. If a greater price can be charged than was planned, this will result in an increased return. However, if this actual price had been used in designing the plant, then the resulting design would have been more efficient at the final operating conditions, and an even higher ROI would have been achieved at this actual higher sale price.

5.3.4 Effect of scale

The effect of scale on distillation cost is summarized in figure 22. The maximum capacity for systems using only one distillation train is 100 million lites per year. Above this capacity, the diameter of a single vacuum column would have to be increased beyond 14 feet--the limit for easy rail transportation of column segments. The effective unit cost for distillation rises for plant capacities smaller than the maximum. This increase is due entirely to increases in the capital related costs owing to the loss of economies of scale.

5.4 Simplified costing equations

A particularly important application of these distillation cost results is in the evaluation of alternative fermentation methods. The true extent of advantages in producing more concentrated fermentation beer can be assessed. To facilitate the use of these distillation results in integrated fermentation-distillation plant design, equations have been fit to the final distillation results. Figure 23 and table 12 present these results for the base case costing assumptions giving the purchased equipment cost, cooling water flow, and steam utilization as a function of feed concentration. Table 13 presents equations for the low steam cost (waste fuel) case. These equations can be incorporated into an overall fermentation-distillation design evaluation program to

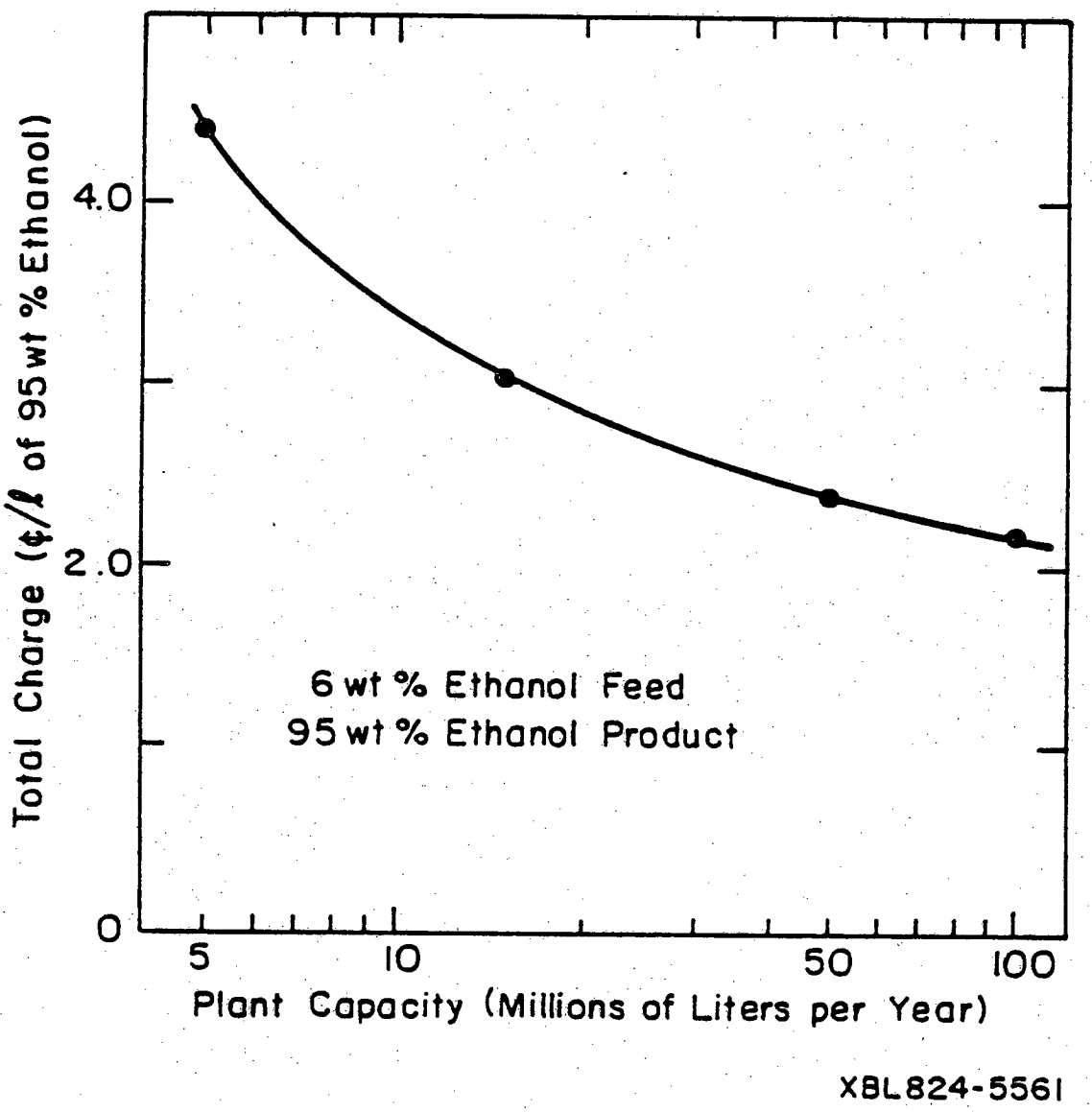


Figure 22 Effect of Plant Scale on Distillation Cost

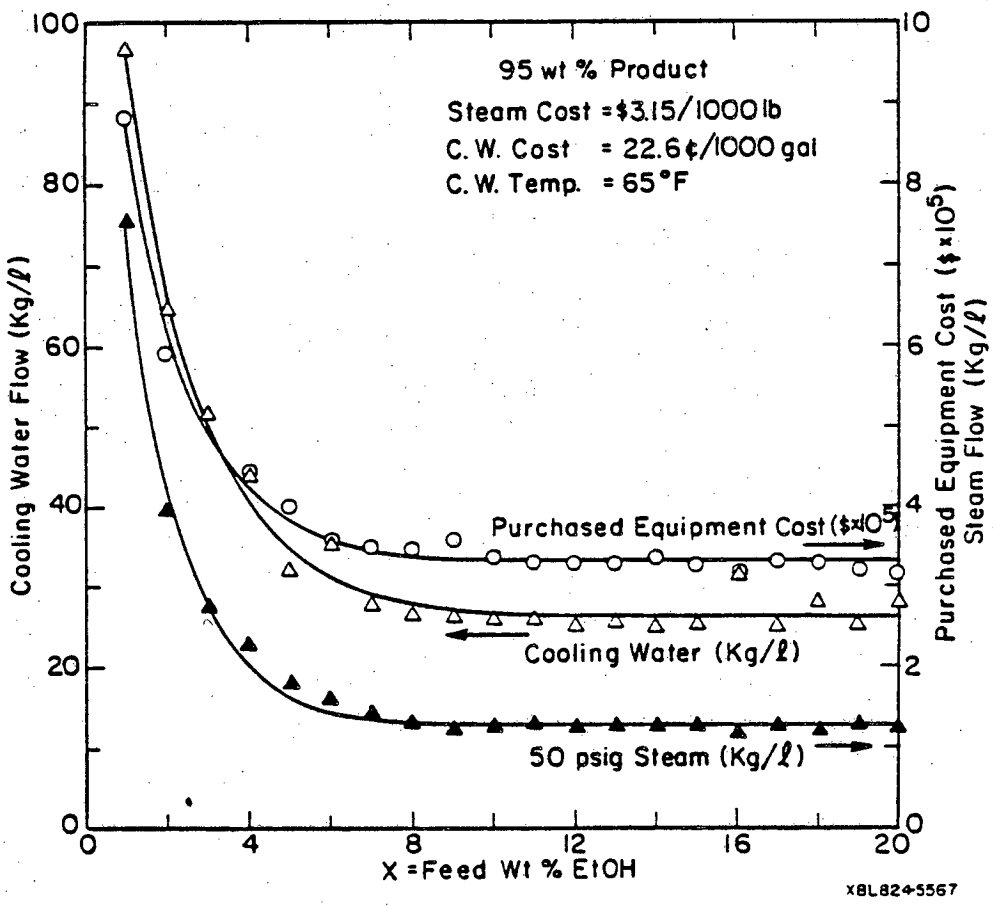


Figure 23 Purchases Equipment Cost, Cooling Water and Steam Flows For the Optimized Distillation Design as a Function of Feed Ethanol Concentration. Base Case Cost Assumptions

Table 12

Simplified Costing Equations
for Base Case Cost Assumptions

Purchased Equipment Cost ($):

$$\text{Cost} = [3.323 + 9.571 \exp(-0.586 \times X)] \times 10^5$$

Steam Usage (kg/L):

$$\text{Steam} = 1.280 + 12.515 \exp(-0.7145 \times X)$$

Cooling Water Usage (kg/L):

$$\text{C.W.} = 26.190 + 116.78 \exp(-0.5203 \times X)$$

X = Feed Ethanol Concentration (wt %).

For distillation to 95 wt % ethanol product with a 100 million liter/year plant capacity.

Table 13

Simplified Costing Equations
Using Waste Generated Steam

Purchased Equipment Cost ($):

$$\text{Cost} = [3.081 + 7.481 \exp(-0.512 \times X)] \times 10^5$$

Steam Usage (kg/L):

$$\text{Steam} = 1.381 + 13.612 \exp(-0.7394 \times X)$$

Cooling Water Usage (kg/L):

$$\text{C.W.} = 26.403 + 132.34 \exp(-0.5941 \times X)$$

X = Feed Ethanol Concentration (wt. %)

For distillation to 95 wt % ethanol product with a 100 million liter/year plant capacity. Base case cost assumptions except for steam cost (75.6¢/1000 lb steam).

determine mass and enthalpy balances as well as the distillation cost.

6 Effect of Secondary Beer Components on Distillation Design

6.1 Secondary components

Secondary components in the feed beer can affect the ethanol/water separation. The fermentation broth contains microbial fermentation by-products as well as nonmetabolized feed components (table 14). Chemical and physical data for essentially all beer trace components have been tabulated by Stage (35,36). The distillation system must be designed to accommodate these secondary components if a pure azeotropic alcohol product is to be produced.

6.2 Dissolved gases

Fermentation beer is saturated with dissolved gases--especially carbon dioxide. Carbon dioxide gas contributes to corrosion at elevated temperatures and interferes with efficient heat transfer in condensers. Dissolved gases are removed from the feed (through an ethanol recovery condenser and demister) after the feed is preheated for addition to the stripper. A small mechanical vacuum pump or steam ejector is also included above the vacuum column reflux drum to assure against the buildup of noncondensables in this column.

6.3 Nonvolatile components

Nonvolatile components--yeast cell debris, salts, nonmetabolized sugars and low volatility components (glycerol, acetic acid)--are removed in the bottom beer stripper product. Stillage typically contains 5 gm/L of salts and 8 gm/L of soluble proteins. If yeast cells are not centrifuged free before stripping, then 10 to 20 gm/L of cells will also be present in the stillage. At these low concentrations, the

Table 14

Secondary Beer Components
Affecting Distillation Design

Carbon Dioxide	
2,3-Butanediol	
Glycerol	
Fusel Oil Components:	Isopropanol
	n-propanol
	Isobutanol
	n-butanol
	Active-amyl alcohol
	Isoamyl alcohol
	n-amyl alcohol
Acetaldehyde	
Organic Acids:	Formic Acid
	Acetic Acid
	Butyric Acid
	Lactic Acid
	Succinic Acid
Dissolved Proteins:	Amino Acids
	Peptides
Whole Yeast Cells	
Non metabolized Salts	

effect of salts, proteins and cells is small. Salts enhance ethanol relative volatility while cells depress it. These effects can be calculated using the methods described by Maiorella (73). The effect of glycerol and the low volatility components has been studied (37,38) and can be calculated using the UNIQUAC method (73). Again, the effect on the equilibrium vapor/liquid distribution of the main components is small due to the low concentrations of the secondary products.

Yeast cell debris and soluble proteins exert an important effect in promoting foaming on the stripper sieve trays. The trays should be widely spaced (2 feet) to allow for the high foaming factor. Mist carryover from tray to tray can adversely affect the separation and a conservative Murphree efficiency should be used in the stripper design.

6.4 Fusel oils

As much as 5 L of fusel oils (see table 15) (39,40,41) are produced for each 1000 L of alcohol produced. Fusel oil is a mixture of amyl and propyl alcohols and their isomers (table 16) (34,42,43,44).

Fusel oils exhibit unusual equilibrium behavior which complicates their separation from the alcohol/water mixture. Dry fusel oils boil in the range from 128-137°C. Dry fusel oils are much less volatile than ethanol and would not be expected as a distillation head product. Fusel oils also are not entirely miscible with water. The volatility of fusel oils is greatly enhanced in the presence of water with only 2.4% amyl alcohol in water exerting the same partial pressure as 90.7% amyl alcohol in 9.3% water (44). The greatly enhanced vapor pressure of dilute amyl alcohol in water forces amyl alcohol into the vapor phase near the bottom of an alcohol purifying column and fusel oils thus cannot be separated as a distillation bottoms product. Fusel oils concentrate in the middle of an alcohol purifying column, building up

Table 15

Fusel Oil Yields

Substrate	Fusel oil; L per 1000 L alcohol	Substrate	Fusel oil; L per 1000 L alcohol
Blackstrap molasses	4-5	Degerminated corn	2.5-3.0
High test molasses	1-3	Wheat	2-3
Corn	4-5	Rye	2-4

Table 16

Composition of Fusel Oil

Constituent	Composition of fusel oil, % constituent from:			
	Corn	Molasses	Potatoes	Rye
Isopropyl alcohol	---	0.6	---	---
n-Propyl alcohol	20.4-11.7	24.3	6.85	---
Isobutyl alcohol	23.9-12.2	7.4	24.35	15.7
n-Butyl alcohol	---	8.1	---	---
active-Amyl alcohol	14.6-23.4	55.3	68.76	79.8
Isoamyl alcohol	36.3-59.7	---	---	---
n-Amyl alcohol	---	4.3	---	---
Undetermined	4.8-3.0	---	0.04	6.5

until they finally "leak" out as contaminants of both the head alcohol and bottoms water streams.

To remove the fusel oils and prevent product contamination, fusel oil laden liquid is bled from the lower plates of the alcohol rectifying section. The liquid is cooled and allowed to separate. A fusel oil layer is removed and washed by contacting with clean water to extract ethanol. The extract is combined with the aqueous layer from the separator and recycled to the distillation column.

Ternary equilibrium data for the ethanol/water system with various fusel oil components has been measured (45,46,47,48). The UNIQUAC method (73) can be used to predict equilibrium behavior for design.

6.5 Acetaldehyde

Typically, one liter of acetaldehyde (and much smaller amounts of the other aldehydes) is produced for every 1000 liters of alcohol product (49,50). This amount can be increased by some selective ethanol removal fermentation systems which also selectively remove acetaldehyde and thus promote its production (i.e. the vacuferm process (13,51)). Acetaldehyde is very volatile, with a normal boiling point of 21°C, and thus, acetaldehyde is easily separated from the ethanol/water mixture as a distillation head product with the primary alcohol product taken as a lower liquid side draw (fig. 24).

Vapor liquid equilibrium for the tenary acetaldehyde/ethanol/water system has been reported by d'Avila (52) and Heitz (53), and the UNIQUAC method can be used for equilibrium calculations (73).

With sufficient trays, a pure acetaldehyde head product can be

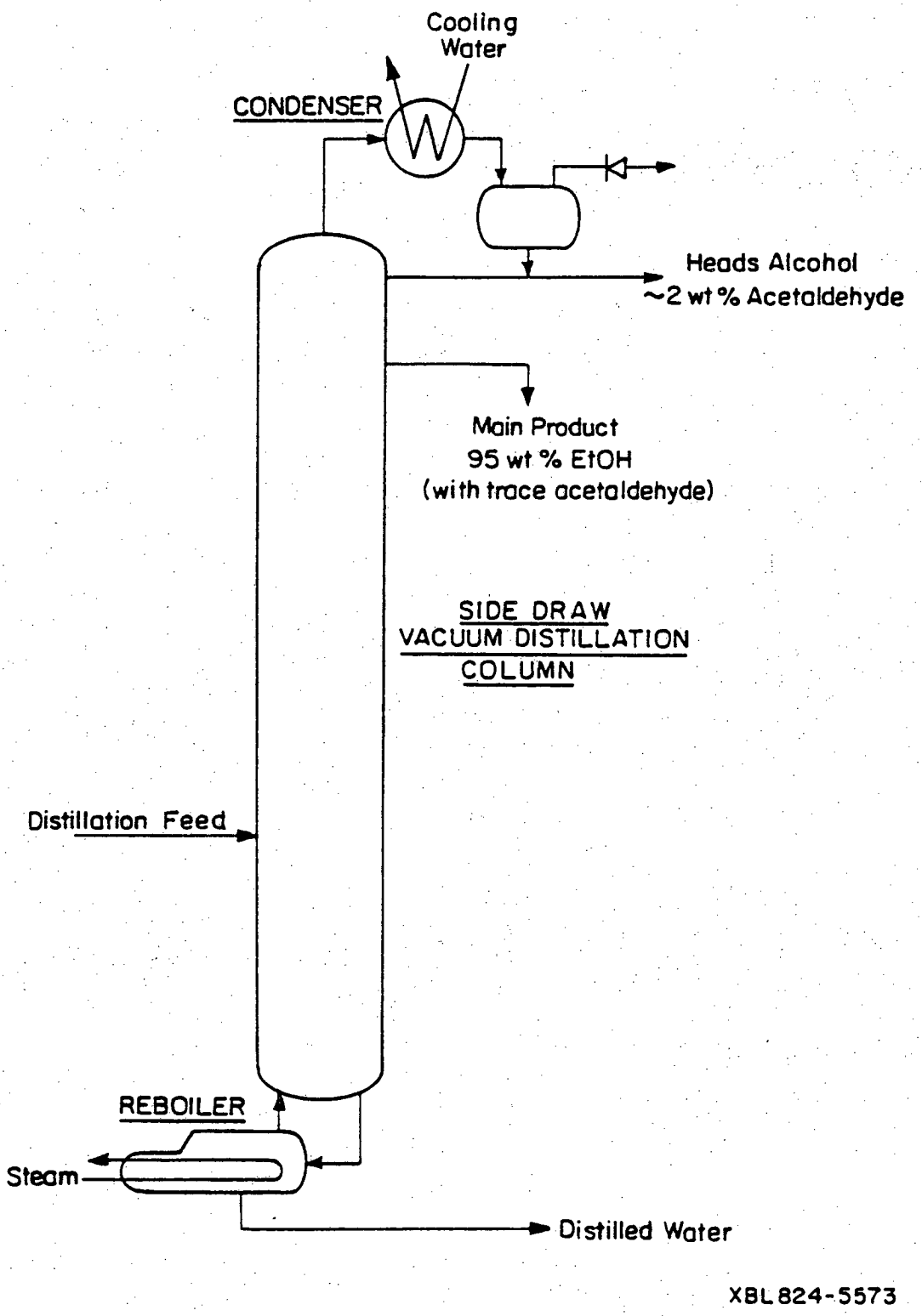


Figure 24 Side Draw Distillation Column With Heads Alcohol Removal For Acetaldehyde Recovery

recovered from the vacuum distillation column. This is impractical though, as a very cold condenser (or higher pressure operation) would be required to condense the volatile acetaldehyde. Instead, approximately five percent of the total ethanol product is withdrawn from the head, thus substantially diluting the acetaldehyde and maintaining a reasonable condenser temperature. This heads product can be sold as a technical grade ethanol containing roughly 2% acetaldehyde. Alternatively, this can be fed to a small auxiliary elevated pressure column for a final separation with pure acetaldehyde as the head product and 95% ethanol as the bottom product. A new possibility is the recycle of the heads product back to the fermentor. Under recycle conditions the acetaldehyde will be largely consumed and converted to additional ethanol (54).

The difference in volatility between acetaldehyde and ethanol is sufficiently large so that very little acetaldehyde will be present in the liquid on the main product draw plate. Nonetheless, the main product, taken as a side draw, is necessarily contaminated by traces of acetaldehyde and other volatiles. Where these trace contaminants cannot be tolerated, a side stripper can be used (fig. 25). The rectifying column side draw is fed directly to the head of the side stripper. An ethanol reboiler provides rising vapors to strip the volatile components from the descending ethanol. Vapors from the side stripper head are returned to the main rectifying column just above the side draw plate to allow acetaldehyde removal from the rectifier head as in the simpler design (fig. 24). With thirty stages, a very high purity 95 wt% ethanol product is recovered from the side stripper bottom.

For dilute feeds, excess heat is available from the beer

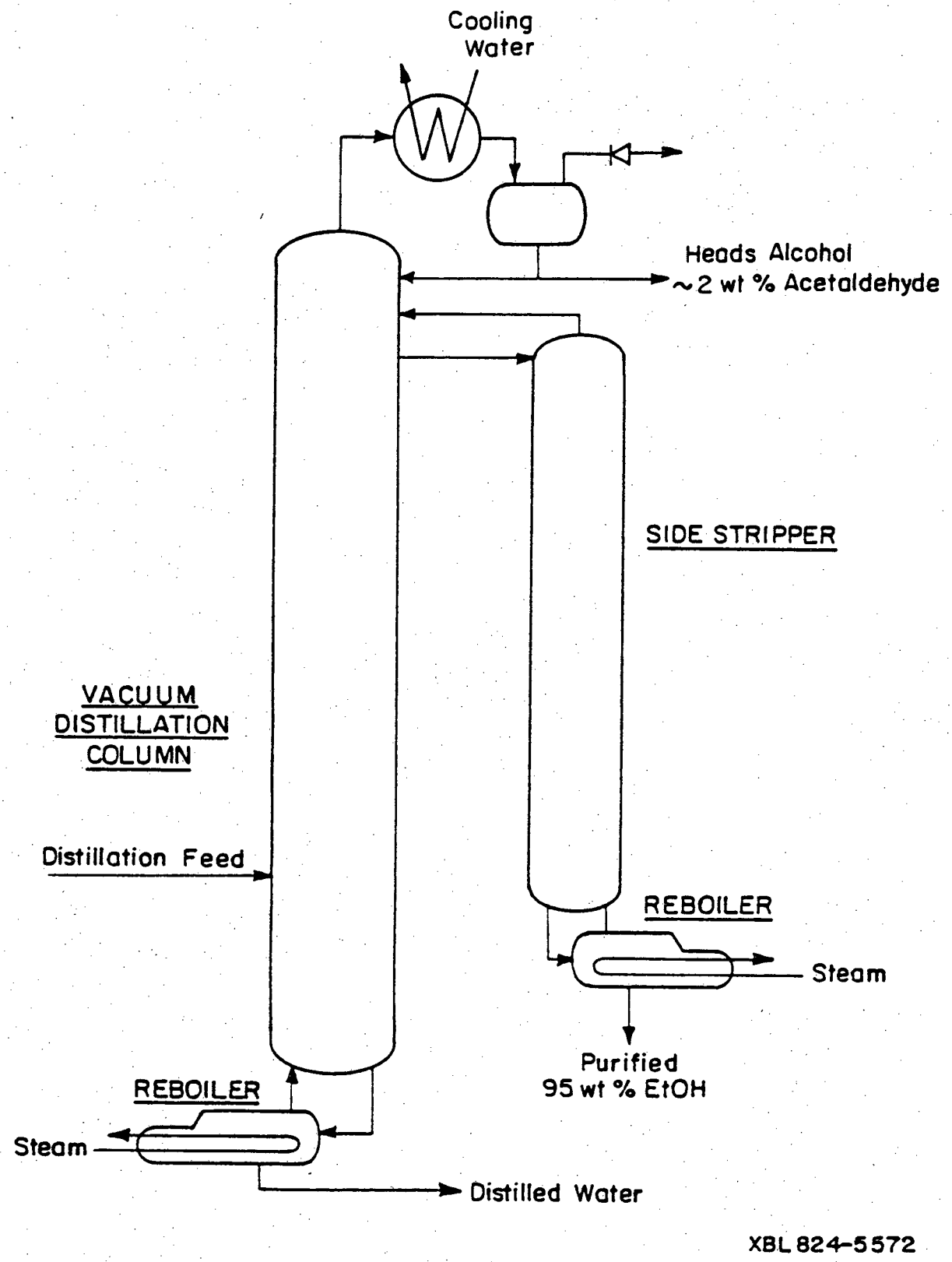


Figure 25 Distillation Column Design With Side Stripper For Acetaldehyde Free Ethanol Production

stripper. Then, the side stripper can be run with no added steam input. The post cooler can be removed and this heat used to drive the ethanol reboiler. For typical feed concentrations (5 to 7 wt% ethanol), again, no added steam input is necessary. For these cases an optimum two column design was found by balancing the heat load of the vacuum column to match the heat available from the stripper. Very large refluxes are used. If a side stripper is added, the main column reflux can be reduced to make sufficient heat available for the ethanol reboiler. Then stages must be added to the main column to maintain product purity, but energy consumption is not raised. For very concentrated feeds (where an auxiliary reboiler is required for the vacuum column) plant steam must be used to drive the ethanol reboiler and overall steam usage is increased.

7. Anhydrous Ethanol Production

7.1 Vapor reuse methods for anhydrous ethanol production

Vapor reuse methods can be extended to allow the production of anhydrous (99.9 wt%) ethanol without added energy input (55). Anhydrous ethanol is generally produced from 94 or higher wt% ethanol by azeotropic distillation with an added entrainer. The entrainer alters the ethanol and water relative volatility forming a constant boiling mixture with water which carries it over as the azeotropic head product. This mixture is then cooled, separated into aqueous and organic layers and is decanted. The organic phase is returned to the column as reflux. Pure ethanol is recovered as the bottom product. Benzene (56,57,58,59,60), n-pentane (61,62,63), trichloroethelene (64,65), diethyl ether (66,67,63,68,69), and even gasoline (63,70) have been used

as entrainers for pure ethanol production. Typical steam requirements for some of these processes, operated independent from the initial distillation system, are given in table 17.

In an integrated distillation plant starting with a beer feed, vapor reuse methods can be used. The condenser temperature for the azeotropic distillation column is generally high and can easily be increased by operating this column at slightly elevated pressure. Then the azeotropic column condenser can be combined with the beer stripper reboiler. The hot azeotropic column vapor condenses and provides heat for boilup to the stripper. No heat is wasted, and the overall process energy requirement need not be increased.

While this approach can be applied to any of the entrainers listed, its use will be illustrated for the diethyl ether case. A 1000 gallon/day capacity pilot plant using diethyl ether azeotropic distillation and employing vapor reuse methods was operated beginning in 1940 by the U.S.D.A. Peoria Laboratories (9). The process description given here is based directly on operating results for this plant (67).

7.2 Diethyl ether azeotropic distillation

A major disadvantage of most entrainers is that they form a ternary constant boiling mixture with ethanol and water. Thus, while pure ethanol can be recovered as the distillation bottom product, the head product contains a mixture of all three species. After decantation, the aqueous phase still contains both ethanol and the added entrainer. This mixture must be fed to an entrainer recovery column (which again produces the ternary azeotrope as head product). The bottom product is not pure water, but an ethanol/water mixture, and a third column is needed to concentrate the ethanol for recycle. This

Table 17

Alternative Azeotropic Distillation Processes
For Anhydrous Ethanol from 95 wt % Feed

Azeotropic Entrainer	Process Description	Energy Consumption
Benzene (1 atmosphere)	50 tray dehydrating Column 30 tray entrainer recovery column Supplementary rectifier	1.0 kg steam per liter
Pentane (50 psig)	18 tray dehydrating column 14 tray entrainer recovery column Supplementary rectifier	0.9 kg steam per liter
Diethylether (130 psig)	30 tray dehydrating column 20 tray entrainer recovery column	2.2 kg steam per liter

complicated arrangement is illustrated for the benzene system in figure 26 (71).

Diethyl ether offers the advantage that it does not form a ternary constant boiling mixture with ethanol and water. Only water is carried overhead by the diethyl ether in the azeotropic column. A second column is needed to strip the ether from the decanted aqueous phase, but now, pure water is taken as this column's bottom product. One column is totally eliminated. The large volatility difference between diethyl ether and water makes for a simple separation and only a small (20 stage) entrainer recovery column is required.

Figure 27 illustrates the diethyl ether azeotropic separation as operated at the Peoria pilot plant. The diethyl ether/water equilibrium is pressure sensitive with the amount of water carried over by the entrainer increasing as the pressure is raised. At the Peoria plant, the azeotropic column was operated at 130 psig with a clean 94 to 95 wt% ethanol feed. At 130 psig the azeotropic column head temperature is 115°C and the head vapors are 4.4 wt% water (the constant boiling mixture composition at this pressure). Using 12.7°C (55°F) deep well cooling water, the overhead vapors are condensed and cooled to 15°C. The organic phase (saturated with 1.15 wt% water) is recycled to the azeotropic column as reflux. The aqueous phase, saturated with traces of diethyl ether, is fed to a small atmospheric pressure packed stripping column with pure water as the bottom product and diethyl ether/water mixture for recycle as the head product.

The difference between water carried over by the diethyl ether and returned as reflux in the saturated diethyl ether from the separator is small as compared to other entrainment systems. 25 to 30 kg of

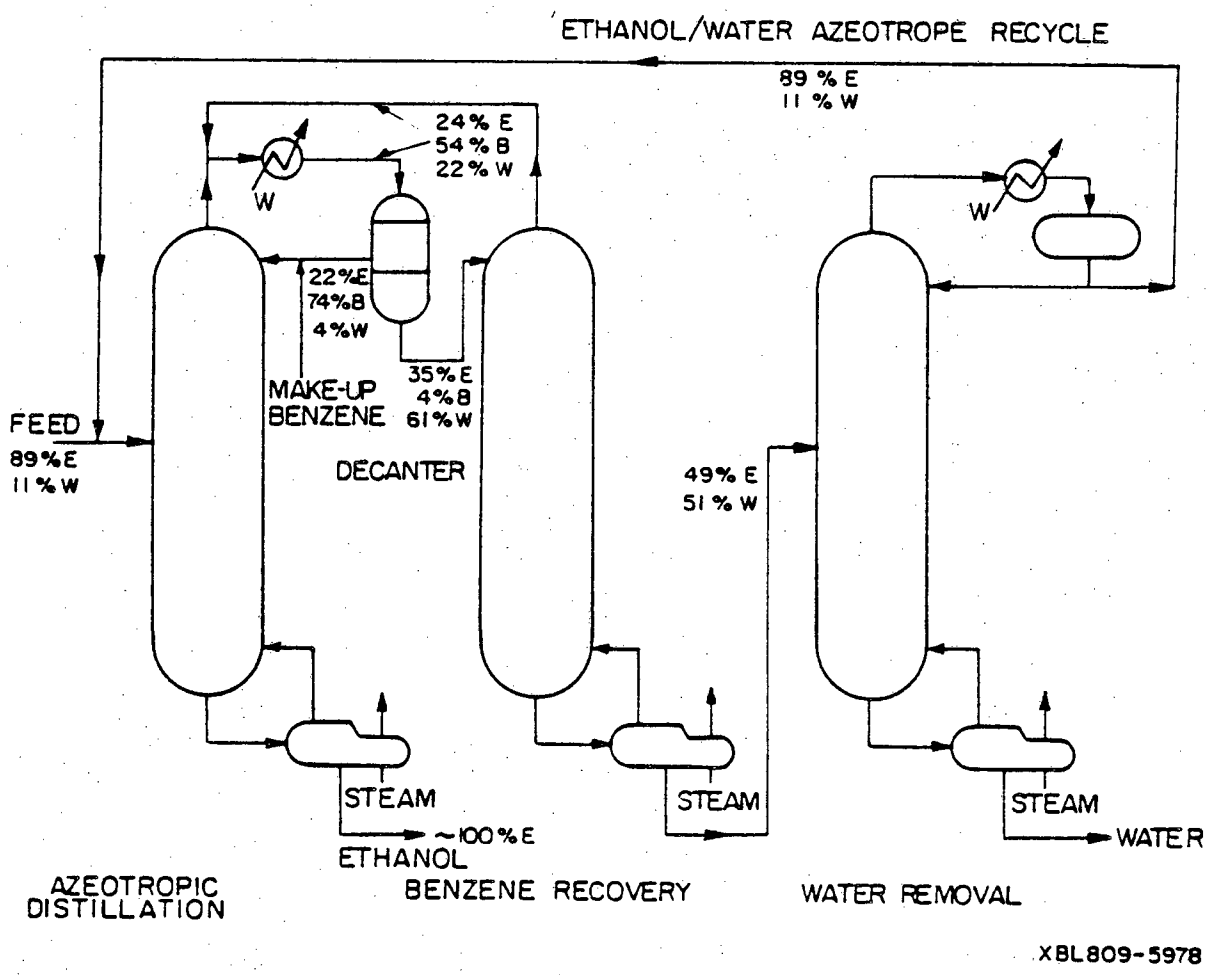


Figure 26 Benzene Azeotropic Distillation For Anhydrous Ethanol Production

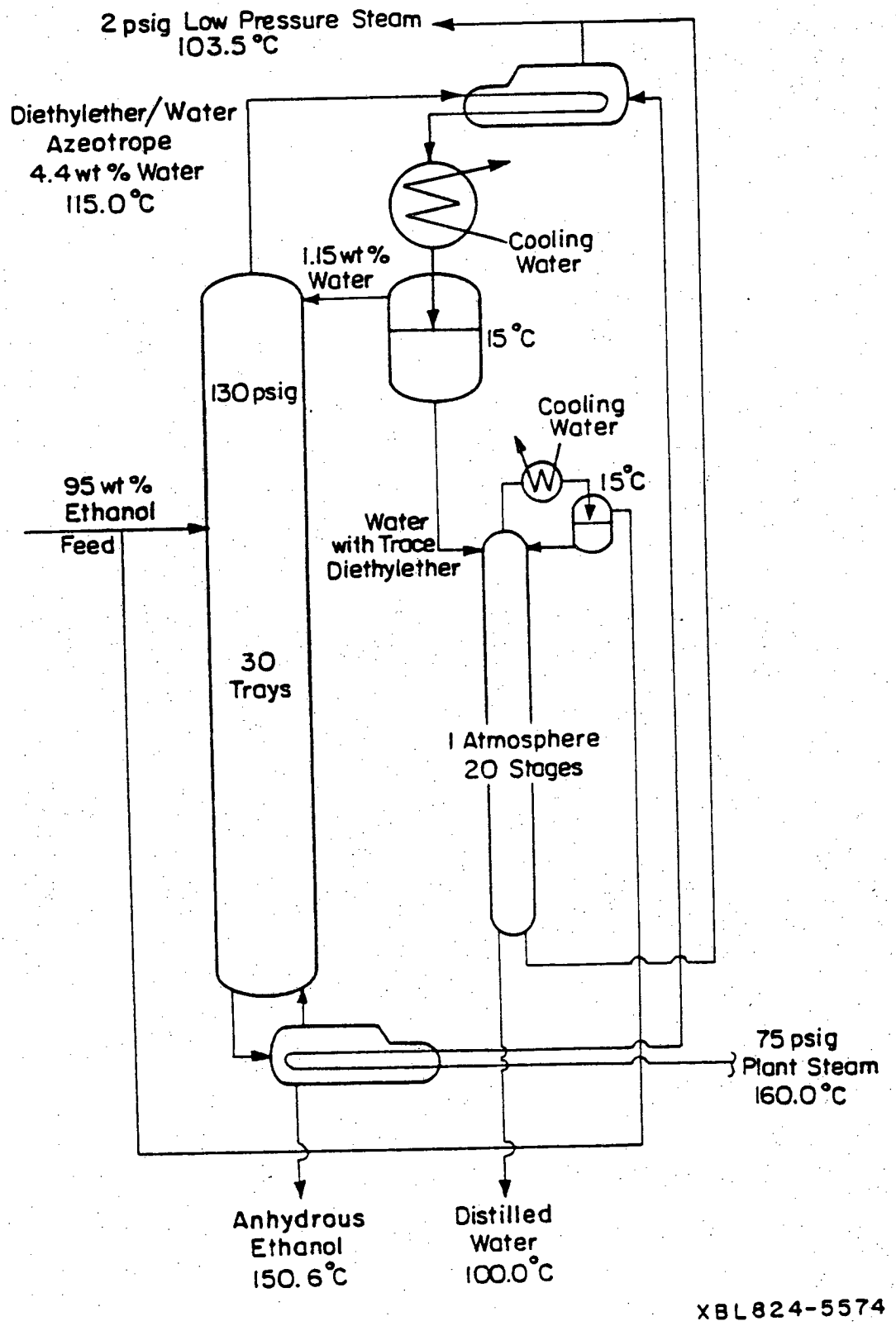


Figure 27 Diethylether Azeotropic Distillation For Anhydrous Ethanol Production

diethyl ether must be distilled to remove one kg of water. Fortunately, the heat of vaporization of diethyl ether is only 89.8 kcal/kg and only 5.7 kg of steam is required to boil up sufficient constant boiling mixture to separate out one kg of water. This results in the minimum steam requirement for the azeotropic column of 0.24 kg of steam per liter of anhydrous ethanol produced starting from a 95 wt% feed. The actual steam consumption in a European distillery is 0.6 kg steam/L (74).

The separation of the constant boiling mixture is difficult and the Peoria plant azeotropic column was operated at 9 to 10 times the minimum reflux rate in a thirty tray column. The steam consumption for this azeotropic column was thus 2.2 to 2.4 kg of steam per liter of anhydrous ethanol product--more than twice the consumption of either the benzene or n-pentane entrainer systems as ordinarily operated.

The UNIQUAC model can be used for azeotropic column design.

7.3 Vapor reuse with the diethyl ether system

The complete integrated processes for anhydrous ethanol production from a fermentor beer is illustrated in figure 28. The diethyl ether azeotropic distillation is combined with the two column vacuum distillation system of section 4 and incorporating fusel oil and acetaldehyde separation. The vapor reuse methods are extended so that the azeotropic column condenser serves as beer stripper reboiler--recoverying heat for reuse. Dilute beer is first degassed and fed to the beer stripper to give a concentrated ethanol vapor for rectification and a bottom stillage product exhausted of ethanol. The stripper vapor is condensed in the reboiler of the main vacuum distillation column and its side stripper. This concentrated liquid is

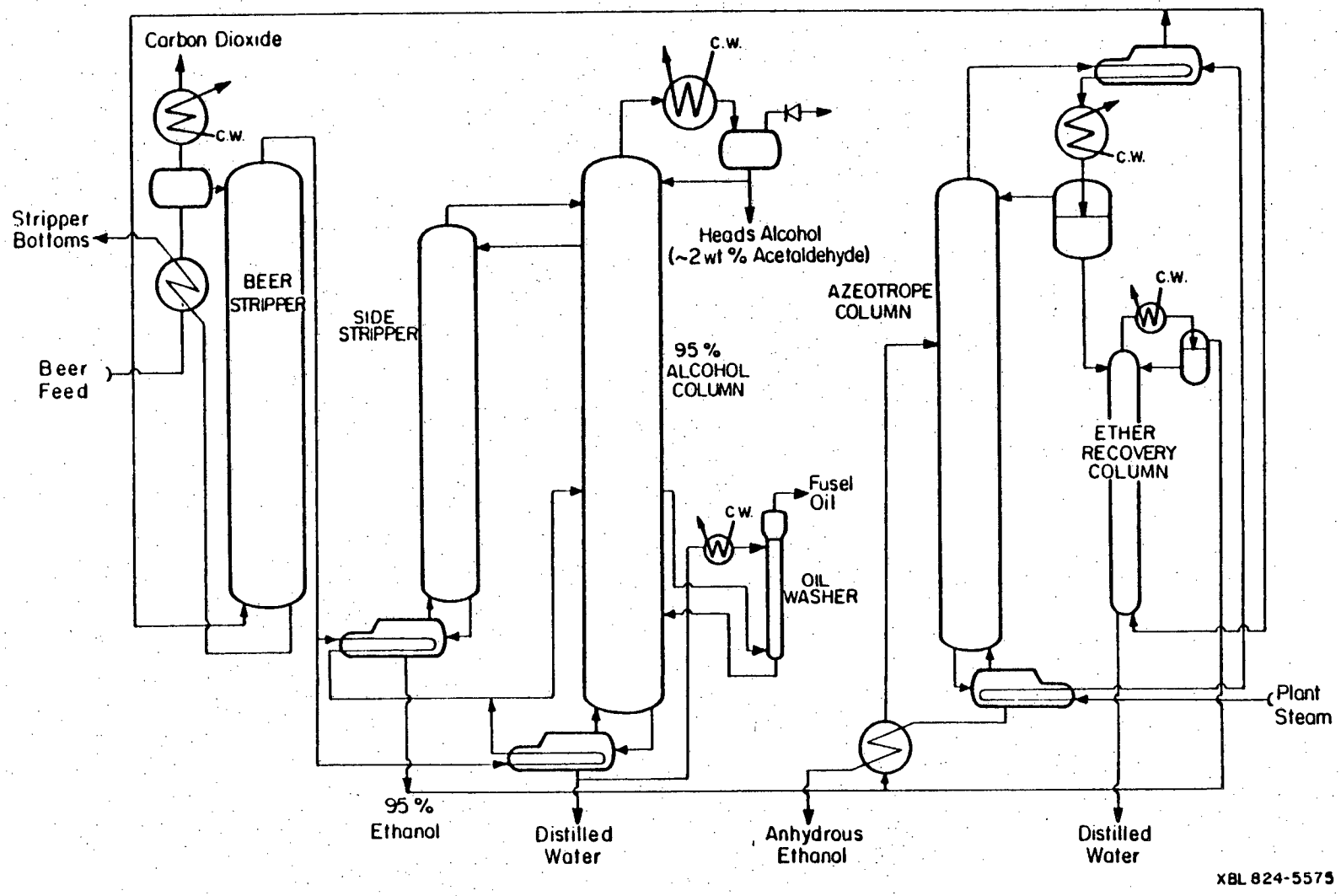


Figure 28 Integrated Distillation Processes For Anhydrous Ethanol Production From Fermentation Beer

then fed to the vacuum column. Pure water is removed as the bottoms. A small side draw from low in the rectifying section is cooled to separate and remove fusel oils. At the column head, a small stream of technical grade alcohol (contaminated with roughly 2 wt% acetaldehyde) is removed. A large side draw, a few plates below the head, feeds the side stripper. Pure 95 wt% ethanol is removed as the side stripper bottom product. This concentrated ethanol is fed to the azeotropic column which produces anhydrous ethanol as the bottom product. A constant boiling mixture of diethyl ether and water is condensed and refluxed at the azeotropic column head. A portion of this is cooled and an aqueous layer separated. The aqueous layer, saturated with traces of diethyl ether, is fed to a small column to strip the ether and produce a pure water bottoms product.

The path of heat flows in this system is as important as the mass flows. Plant steam at 75 psig (160.0°C) is fed to the azeotropic column reboiler and boils up pure ethanol (150.6°C) at 130 psig column pressure. At the head of the azeotropic column, a constant boiling mixture of diethyl ether and water (115.0°C) is condensed, boiling up steam (2 psig, 103.5°) for the main beer stripper and the small diethyl ether recovery column. Vapors from the beer stripper are condensed in the main vacuum column reboiler and its side stripper ethanol reboiler. Finally, the vacuum column vapors (39.8°C) are condensed with cooling water. The original steam heat is thus used in three successive operations.

It is now clear why the large reflux (and hence steam requirement) of the diethyl ether system (as operated at the Peoria pilot plant) compared to other entrainers is not a disadvantage. The

steam flow rate to the azeotropic column was chosen to balance the steam requirements of the successive distillation operations. The number of plates in the azeotropic column, was chosen to give the required separation with the available reflux. In a modern plant with reduced steam requirements for 95 wt% ethanol production, trays should be added to the azeotropic column to reduce its steam consumption and maintain balanced operation.

7.4 Conclusions

The production of anhydrous ethanol as practiced at the U.S.D.A. Peoria alcohol pilot plant has been illustrated. The production of anhydrous ethanol requires additional capital expenditure (for additional columns) as compared to 95 wt% ethanol production. By appropriate application of vapor heat reuse techniques though, essentially no additional energy need be expended for anhydrous ethanol production as compared to 95 wt% ethanol production. The azeotrope associated pinch sets the reflux requirement for 95 wt% ethanol production and thus establishes the overall distillation energy consumption for practical beer feed concentrations.

Many entrainers are available for the final purification of 95 wt% to anhydrous ethanol. By appropriate choice of operating pressures, vapor reuse methods can be applied to any of these. The diethyl ether systems has the advantage of not forming a ternary azeotrope incorporating ethanol and thus using one less column than other systems. Low temperature cooling water is required though for efficient decantation of water from the diethyl ether/water constant boiling mixture, as water solubility in ether rises rapidly with temperature. The n-pentane process uses smaller vapor flow rates and smaller diameter

columns than the others, but foaming problems have been encountered in one trial (72). The benzene distillation is slightly less efficient than n-pentane, but has been tested over many years of in-plant operation.

The UNIQUAC vapor/liquid equilibrium model is a valuable tool and can be used for the design and evaluation of any of these processes. As with the binary ethanol/water equilibrium system, special attention should be paid to nonidealities and the variation of equilibrium properties with temperature. These can be successfully incorporated into the UNIQUAC method as was illustrated for the binary ethanol/water system.

References

1. Scheller, W., B. Mohr, Net Energy Analysis of Ethanol Production, Department of Chemical Engineering, Univ. of Nebraska, Omaha, NE, 1977.

2. Reilly, "Economics and Energy Requirements for Ethanol Production," Department of Chemical Engineering and Nuclear Engineering, Iowa State Univ., Ames, Iowa, January 1978.

3. Chambers, R. S., R. A. Herendeen, J.J. Joyce, and P.S. Penner, Science, 206, 789 (Nov. 16, 1979).

4. Sonnenblick, M., Fusion, p.18 (Sept. 1979).

5. Weisz, P. B., J. F. Marshall, Science, 206, 24 (Oct. 5, 1979).

6. Elias, S., Food Eng. Int., 4(12), 14 (1979).

7. Annon, "Power Alcohol," Process Engineering Co., Mannedorf, Switzerland (1980).

8. Paul, B. P., A. K. Mitra, "Efficient Use of Waste Heat in Rectified Spirit Distillation Plant," in Ethyl Alcohol Production Techniques, Noyes Dev. Corp., Pearl River, New York (1964).

9. Jacobs, P. B., Industrial Alcohol, U.S.D.A., Misc Publ. 695, Washington, D.C. (Feb. 1950).

10. Abrams, D. S., J. M. Prausnitz, AIChE J., 21(1), 116 (1975).

11. Otsuki, H., F. Williams, Chem. Eng. Prog. Symp., 6(49), 55 (1953).

12. Maiorella, B. L., C. R. Wilke, H. W. Blanch, Advances in Biochemical Engineering, 20, 43 (1981).

13. Maiorella, B. L., H. W. Blanch, C. R. Wilke, "Rapid Ethanol Production via Fermentation," LBL-10219, presented at the AIChE Meeting, San Francisco, CA (Nov. 29, 1979).

14. Baumeister, T., Mechanical Engineers' Handbook, McGraw-Hill, N.Y., 1958.

15. Perry, R. H., C. H. Chilton, Chemical Engineers' Handbook, 5th edition, McGraw-Hill, N.Y., 1973.

16. Prescott, S. P., C. G. Dunn, Industrial Microbiology, 2nd edition McGraw-Hill, N.Y., 1949.

17. Tourliere, S., Inds. Agr. et Aliment (Paris), 70, 547 (1953).

18. Plottner, D., Werkstoffe U. Korrosion, 3, 293 (1952).

19. Numerical Algorithms Group "NAGFLIB, 1482/O: Mk6: May 77" Mayfield House, 256 Banbury, Oxford, OX2 7DE, UK.

20. Gill, P. E., W. Murray, Nat'l. Phys. Lab. Rept. No. NAC 72 (1976).

21. Peters, M. S., K. D. Timmerhaus, Plant Design and Economics for Chemical Engineers, McGraw-Hill, N.Y., 1980.

22 Speller, F. N., Corrosion-Causes and Prevention, McGraw-Hill, N.Y., 1951.

23. Polak, J., G. C. Benson, J. Chem. Thermo., 3, 235 (1971).

24. Shilling, G. D., G. H. Beyer, C. C. Watson, Chem. Eng. Prog., 49, 128 (1953).

25. Van Winkle, M., Distillation, McGraw-Hill, N.Y., 1953.

26. Kern, D. Q., Process Heat Transfer, McGraw-Hill, N.Y., 1953.

27. Hengstebeck, R. J., Distillation Principles and Design Procedures, Reinhold, N.Y., 1961.

28. Treybal, R. E., Mass Transfer Operations, 3rd Ed., McGraw-Hill, N.Y., 1980.

29. Leva, M., Chem. Eng. Prog. Symp. Ser., 50(10), 51 (1954).

30. Wales, R. E., Chem. Eng., 88, 77 (1981).

31. Staff, Chemical Engineering, 88(7), 7 (April 1981).

32. Happel, J., D. Jordan, Chemical Process Economics, Marcel Dekker, N.Y., 1975.

33. Gill, P. E., W. Murray, R. A. Pitfield, Nat'l. Phys. Lab. Rept. No. NAC 11, (1972).

34. Falkehag, S., J. Appl. Polymer Sci. (Appl. Polymer Symp. 28), 247 (1975).

35. Stage, H., E. Muller, P. Faldix, Chem. Tech. (Berlin), 6, 31 (1954).

36. Stage, H., P. Faldix, W. Kurth, E. Muller, Chem. Tech (Berlin), 6, 132 (1954).

37. Warren, K. H., U.S. Patent, 2,626,237 (1953).

38. Grolla, K., Branutweinwirtschaft, 75, 453 (1953).

39. Aries, R. S., "Industrial Alcohol," Kirk Othmer Encyclopedia of Chemical Technology, R. Kirk and D. Othmer - eds., p. 252, 1947.

40. Webb, A., J. Ingraham, Adv. Appl. Microbiol., 5, 317 (1963).

41. Suomalainen, H., Suom. Kemistilehti, 41A, 239 (1968).

42. Stevens, R., J. Inst. Brew., 66, 453 (1960).

43. Jansen, W., Paper and Timber (Finland), 32B, 329 (1950).

44. Harrison, J., J. Graham, "Yeast in Distillery Practice," The Yeasts, Vol. 13, Rose and Harrison - eds., Academic Press, N.Y., 1970.

45. Kojima, K., K. Ochi, Y. Nakazawa, Int'l Chem. Eng., 9, 342 (1969).

46. Andiappan, A., A. Y. McClean, Advan. Chem. Ser., 115, 93 (1972).

47. Metyushev, B. D., Fermentnaya i Spirit. Prom., 30(2), 13 (1964).

48. Serebrennaya, I. I., S. S. Byk, Khim Prom (Moscow), 41(9), 669 (1965).

49. Suomalainen, H., P. Ronkainen, Tech. Quart. Master Brewers Assn. Am., 5, 119 (1968).

50. Suomalainen, H., et al., Aspects of Yeast Metabolism--A Guinness Symp., Dublin, Blackwell Scientific Publ., Oxford (1968).

51. Maiorella, B. L., H. W. Blanch, C. R. Wilke, Biotech. Bioeng., 25(1), 103 (1983).

52. d'Avila, S. G., R. S. F. Silva, J. Chem. Eng. Data, 15(3), 421 (1970).

53. Heitz, J. E., An. J. Enol. Viticult., 11, 19 (1960).

54. Maiorella, B. L., H. W. Blanch, C. R. Wilke, "Enhanced Ethanol Yield and Acetaldehyde Disposal in Ethanolic Fermentation," U.C. LBL Invention Case No. IB-425 (1981).

55. Othmer, D. F., Ind. Eng. Chem., 28, 1435 (1936).

56. Norman, W., Trans. Am. Inst. Chem. Eng., 23, 66 (1945).

57. Young, S., Fortey, J. Chem. Soc., 81, 739 (1902).

58. Jumentier, R., Bull. Assoc. Chim. Sucr., 48, 396 (1931).

59. Keyes, D. B., U.S. Patent 1,830,469 (Nov. 3, 1931).

60. Guinot, Clark, Trans. Inst. Chem. Engrs. (London), 16, 189 (1938).

61. Black, C., R. A. Golding, D. E. Ditsler, Adv. Chem., 115, 64 (1972).

62. Black, C., D. E. Ditsler, Adv. Chem., 115, 1 (1972).

63. Black, C., Chem. Eng. Prog., 76(9), 78 (1980).

64. Fritzweiler, R., K. R. Dietrich, Angew. Chem., 45, 605 (1932).

65. Colburn, A. P., J. C. Phillips, Trans. Am. Inst. Chem. Engrs., 40, 333 (1944).

66. Wentworth, T. O., D. F. Othmer, Trans. Am. Inst. Chem. Engrs., 36, 785 (1940).

67. Wentworth, T. O., D. F. Othmer, G. M. Pohler, Trans. Am. Inst. Chem. Engrs., 39, 565 (1943).

68. Othmer, D. F., T. O. Wentworth, Ind. Eng. Chem., 32, 1588 (1940).

69. Wentworth, T. O., U.S. Patent, 2,358,193 (1944).

70. Zieborak, K., and K. Lebecka, Prezemysl. Chem., 31(8), 422 (1940)

71. King., C. J., Separation Processes, McGraw-Hill, N.Y. (1971).

72. Personal communication to H. W. Blanch from R. A. Golding--Shell Development Company (Houston).

73. Maiorella, B. L., H. W. Blanch, C. R. Wilke, Ethanol/Water Physical and Chemical Properties for Separation Process Design, Lawrence Berkeley Laboratory Report, UCLB-14220, May 1982.

74. Chen, C. S., Hawaii Ethanol from Molasses Project--Final Report HNEI-80-03. Hawaii Natural Energy Institute, University of Hawaii at Manoa (1980).

75. Spencer, C. F., R. P. Danner, J. Chem. Eng. Data, 17, 236 (1972).

76. Prausnitz, J., T. Anderson, E. Grens, C. Eckert, R. Hsieh, J. O'Connell, Computer Calculations for Multicomponent Vapor-Liquid and Liquid-Liquid Equilibria, Prentice-Hall, Englewood Cliffs, N.J. (1980).

77. Hayden, J. G., J. P. O'Connell, Ind. Eng. Chem., Proc. Des. Dev., 14(3), 209 (1975).

78. Thomsen, K., M.Sc. Thesis, Instituttet for Kemiteknik, Technical Univ. of Denmark (1977). Reported in A. Fredenslund, J. Gmehling, P. Rasmussen, Vapor-Liquid Equilibria Using UNIFAC, Elsevier, Amsterdam (1977).

79. Pemberton, R.C., C. J. Mash, J. Chem. Thermo., 10, 867 (1978).

80. Herington, E.F., Nature, 160, 610 (1947).

Appendix 1

THE DISTILL COMPUTER PACKAGE

Function DISTL

Purpose: Designs and costs a vacuum distillation column and its associated heat exchanger systems. Resulting parameters are stored in the distillation and heat exchanger common blocks (DLDTA and HXDTA).

Usage: Call DISTL (RATIO, FRAC, P)

Input variables:

(In Call)

Reflux optimization variable	RATIO	
Stripper product fractional equilibrium approach	FRAC	
Distillation column pressure	P	mmHg

(In Common Blocks)

Fraction of capital cost assessed each year	CFACTR	
Distillate product flow rate	D	gmol/hr
Stripper feed flow rate	F	gmol/hr
Distillation column feed flow rate	FD	gmol/hr
Print control flag	LOOK	
Control flags	MODE	
Ethanol recovery fraction	RFRACT	
Cooling water supply temperature	TCWI	deg K
Plant steam temperature	TSTEAM	deg K
Initial guess for distillation column temperature	TD	deg K
Distillate product mole fraction ethanol	XD	
Stripper feed mole fraction ethanol	XF	
Marshall-Stevens Cost Index	XMSI	

Output Variables:

(In Common Blocks)

Condenser area	ACN	sq ft
Number of condensers	NCN	
Intercolumn exchanger area	AHX	
Number of intercolumn exchangers	NHX	
Post cooler area	APC	sq ft
Number of post coolers	NPC	
Distillation column reboiler area	ARB	sq ft
Number of distillation reboilers	NRB	
Distillation column bottom product flow	B	gmol/hr
Distillation column capital cost	CDLCAP	$
Distillation column effective cost	CDLEFF	$
Intercolumn exchanger capital cost	CHXCAP	$
Intercolumn exchanger effective annual cost	CHXFEFF	$
Annual labor cost	CLABR	$

Post cooler capital cost		CPCCAP	$
Post cooler effective annual cost		CPCEFF	$
Post cooler annual operating cost		CPCOP	$
Distillation reboiler capital cost		CRBCAP	$
Distillation reboiler effective cost		CRBEFF	$
Distillation reboiler annual operating cost		CRBOP	$
Total system effective annual cost		CTEFF	$
Total annual operating cost		CTOP	$
Distillation column feed flow rate		FD	gmol/hr
Distillation column vapor flow rate		GD	gmol/hr
Reflux flow rate	REFLUX,	R	gmol/hr
External reflux ratio		RRATIO	
Ratio of rectifying operating line slope to minumum		RATDL	
Y intercept of rectifying operating line		RINT	
Rectifying operating line slope		RSLOPE	
Number of rectifying equilibrium stages		RSTAGE	
Y intercept of stripping section operating line		SINT	
Stripping section operating line slope		SSLOPE	
Number of stripping section equilibrium stages		SSTAGE	
Distillation reboiler steam usage		STFRRB	kg/hr
Cooling water temperature exiting condenser		TCWOCN	deg K
Cooling water temperature exiting post cooler		TCWOPC	deg K
Distillation column reboiler temperature		TDB	deg K
Distillation column head temperature		TDT	deg K
Distillation feed saturation temperature		TDF	deg K
Mole fraction ethanol in distillation bottom product		XB	
Mole fraction ethanol in distillation column feed		XFD	
Vapor composition at intersection of rectifying and stripping lines		YRS	

Other needed subroutines:

CNCST, CNDSR, CROSS, CWCST, DELQ, DIFER, FTLM, HXCNG, STCST, TPNT, ZERO.

Description:

The pressure P (mmHg) is one of the three prime optimization variables specified by the optimization routine (E04 JBF (1)). For the specified pressure, TPNT and CROSS are called to find the minimum reflux rectifying operating line and corresponding minimum distillation column feed composition (XFMIN).

If the system ethanol feed composition (XF) is less than the minimum allowable distillation feed composition (XFMIN) then subroutine STRIP is called to design a stripper with vapor product composition greater than XFMIN. Because of the high added cost of materials for use in contact with the raw beer, a

stripper may be desirable even when the raw beer is sufficiently concentrated without stripping. Thus, by including a small stainless steel stripper, the large distillation column can be made of carbon steel. With MODE(26) = 2, a stripper will always be designed.

The distillation column feed composition (XFD) is specified as the vapor composition from the stripper (or the raw beer composition if no stripper is used). Distillate and bottoms flow rates are calculated by mass balance and knowing the required ethanol recovery fraction (RFRACT).

RATIO is the final prime optimization variable and specifies the rectifying section reflux ratio according to:

$$\text{RATDL} = \frac{1.0}{\text{TSLOPE}} + \text{RATIO}\left(1.0 - \frac{1.0}{\text{TSLOPE}}\right)$$

where TSLOPE is the slope of the minimum reflux operating line and RATDL is the ratio of the actual operating line slope to the minimum:

$$\text{RSLOPE} = \text{RATDL} \times \text{TSLOPE}$$

The distillation column operating lines are thus specified. Theoretical equilibrium stage compositions are then "stairstepped" as with a McCabe-Thiele diagram using equilibrium data generated by BDPTM (the ETOH equilibrium package (2)). The number of rectifying and stripping section stages (RSTAGE, SSTAGE) are thus specified.

The packed column diameter is set to give a vapor pressure drop of $50(N/m^2)/m$ as suggested by Treybal (3). The pressure drop was determined using an equation fit to the data of Leva (4):

$$\alpha = (9.771 \times 10^{-3}) \exp\{-0.6918\ (\beta)\}$$

where:

$$\alpha = \frac{L}{G}\sqrt{\frac{\text{RHOG}}{\text{RHOL} - \text{RHOG}}}$$

and

$$\beta = \frac{(\text{GPRIME})^2\ C_f\ \mu_L\ J}{\text{RHOG}(\text{RHOL} - \text{RHOG})\ g_c}$$

where: $C_f = 20$, for 2 inch Pall ring packing.

These equations are solved for GPRIME (lbs/hr sq ft), which is the allowable mass flow per unit cross section. G is the total column internal vapor mass flow in g/hr, converted to lbs/hr as GLBS. The required column cross-sectional area is then:

$$\text{AREA} = \frac{\text{GLBS}}{\text{GPRIME}}$$

The tower height (DLHGHT) is given by:

$$DLHGHT = (DLSTAG-1) \times (1.15 \times HETP) + 4.0$$

where DLSTAG is the number of required equilibrium stages (includes the reboiler) and HETP is the height of 2" Pall ring packing required per theoretical tray. HETP is given for conditions typical of the vacuum column operation as the larger of HETPR and HETP (5) where:

$$HETP = HETPR \{1.0 + Log_{10} (\frac{DLDIAM}{DIAMR})\}$$

with HETRP = 0.8333 ft and DIAMR = 2.5 ft.

The column is overdesigned by 15% to allow for uncertainty in the stage height under vacuum conditions and four feet of clear space is provided for mist disentrainment.

The tower shell weight is computed using a wall thickness of 0.375 inches as determined by a vacuum vessel design calculation according to ASME standards (6) and assuming four internal support rings (the packing support tray and distributor acting as two support rings).

The column purchased cost (with fittings, supports and packing) is computed according to equations derived from the figures of Peters and Timmerhaus (7). The corresponding total capital investment is given as 4.89 times the purchased cost.

The distillation column reboiler system is then designed to meet the distillation column heat load for boilup (DELQRB). When a stripping column is used, heat from the stripper vapor (DELQFD) is recovered and used through an intercolumn exchanger of heat load DELQRB1. If DELQFD is greater than DELQRB, then an additional post cooler is designed to remove the excess heat (DELQPC) fully condensing the stripper vapor for feed to the vacuum column. If DELQRB is greater than DELQFD, then an auxiliary steam fed distillation column reboiler is designed to meet the remaining required heat load (DELQRB2). Exchanger designs and costs are determined using subroutine HXCNG. The condenser system is then designed using subroutine CNDSR.

Variables in function DISTL

NAME	TYPE	MAIN USE	BLOCKS	DESCRIPTION OF VARIABLES	UNITS
ACN	R	VARIABLE	/HXDTA/	Condenser area	sq ft
AHX	R	VARIABLE	/HXDTA/	Inter column heat exchange	sq ft
ALOG10	R	STANDARD			
AMIN1	R	STANDARD			
APC	R	VARIABLE	/HXDTA/	Post cooler area	sq ft
ARB	R	VARIABLE	/HXDTA/	Distillation column	
AREA	R	VARIABLE		Distillation column cross sectional area	sq ft
B	R	VARIABLE	/DLDTA/	Distillation column bottom	

			product flow	gmol/hr
BDPTM	R EXTERNAL			
CCNCAP	R VARIABLE	/COSTS/	Condenser capital cost	$
CCNEFF	R VARIABLE	/COSTS/	Condenser effective annual cost	$
CCNOP	R VARIABLE	/COSTS/	Condenser annual operating cost	$
CDLCAP	R VARIABLE	/COSTS/	Distillation column capital cost	$
CDLEFF	R VARIABLE	/COSTS/	Distillation column effective annual cost	$
CFACTR	R VARIABLE	/COSTS/	Fraction of capital cost assessed each year	$
CHXCAP	R VARIABLE	/COSTS/	Intercolumn exchanger capital cost	$
CHXEFF	R VARIABLE	/COSTS/	Exchanger effective annual cost	$
CLABR	R VARIABLE	/COSTS/	Annual labor cost	$
CNDSR	R EXTERNAL			
CPCCAP	R VARIABLE	/COSTS/	Post cooler capital cost	$
CPCEFF	R VARIABLE	/COSTS/	Post cooler effective annual cost	$
CPCOP	R VARIABLE	/COSTS/	Post cooler annual operating cost	$
CRBCAP	R VARIABLE	/COSTS/	Distillation reboiler capital cost	$
CRBEFF	R VARIABLE	/COSTS/	Distillation reboiler effective annual cost	$
CRBOP	R VARIABLE	/COSTS/	Distillation reboiler annual operating cost	$
CROSS	R EXTERNAL			
CSPCAP	R VARIABLE	/COSTS/	Stripper capital cost	$
CSPEFF	R VARIABLE	/COSTS/	Stripper effective annual cost	$
CSPOP	R VARIABLE	/COSTS/	Stripper annual operatin cost	$
CSRCAP	R VARIABLE	/COSTS/	Stripper reboiler capital cost	$
CSREFF	R VARIABLE	/COSTS/	Stripper reboiler effective annual cost	$
CTCAP	R VARIABLE	/COSTS/	Total system capital cost	$
CTEFF	R VARIABLE	/COSTS/	Total system effective annual cost	$
CTOP	R VARIABLE	/COSTS/	Total system annual operating cost	$
CWFRCN	R VARIABLE	/HXDTA/	Condenser cooling water usage rate	
CWFRPC	R VARIABLE	/HXDTA/	Post cooler cooling water usage rate	
D	R VARIABLE	/DLDTA/	Distillate flow rate	gmol/hr
DELQ	R EXTERNAL			
DELQCN	R VARIABLE	/HXDTA/	Condenser heat load	kcal/hr
DELQFD	R VARIABLE		Heat load to bring stripper vapor to distillation	

			feed temp	kcal/hr
DELQPC	R VARIABLE	/HXDTA/	Post cooler heat load	kcal/hr
DELQRB	R VARIABLE		Distillation column heat requirement	kcal/hr
DELQRB1	R VARIABLE	/HXDTA/	Intercolumn exchanger heat load if exchanger is used	kcal/hr
DELQRB2	R VARIABLE	/HXDTA/	Distillation column reboiler heat load if reboiler is used	kcal/hr
DIAMO	R VARIABLE		Distillation column outer diameter	ft
DIAMR	R VARIABLE		Packing height correction factor	ft
DISTL	R VARIABLE		Total effective annual distillation cost	$
DLDIAM	R VARIABLE	/DLDTA/	Distillation column inner diameter	ft
DLHGHT	R VARIABLE	/DLDTA/	Distillation column height	ft
DLSTAG	R VARIABLE	/DLDTA/	Number of theoretical stages in distillation column	
EMAT	R VARIABLE		Construction material cost multiplier	
EXP	R STANDARD			
EXTRA	R VARIABLE		Fractional trays required	
F	R VARIABLE	/INPUT/	Stripper feed flow rate	gmol/hr
FD	R VARIABLE	/DLDTA/	Distillation feed flow rate	gmol/hr
FIRST1	L VARIABLE	/INPUT/	Initialization control flag	
FIRST2	L VARIABLE	/INPUT/	Initialization control flag	
FITCST	R VARIABLE		Installed cost of distillation column fittings	$
Frac	R VARIABLE	ARGUMENT	Stripper product fractional equilbirum approach	
GD	R VARIABLE	/SPDTA/	Distillation vapor flow rate	gmol/hr
GLBS	R VARIABLE		Total distillation mass flow rate of vapor	lb/hr
GPRIME	R VARIABLE		Vapor mass flow rate per cross section	lb/sqft/hr
HETP	R VARIABLE		Height of theoretical plate	ft
HETPR	R VARIABLE		Minimum height of theoretical plate	ft
HXCNG	R EXTERNAL			
L	R VARIABLE		stripping section liquid flow rate	gmol/hr
LOOK	I VARIABLE	/DATA3/	print control flag	
MANHLS	I VARIABLE		number of manholes	
MODE	I ARRAY	/DATA3/	control flag	
MWH20	R EQVALENCE	/DATA/	water molecular weight	g/mole
NCN	I VARIABLE	/HXDTA/	number of condensers	
NHX	I VARIABLE	/HXDTA/	number of intercolumn exchangers	
NOZLS	I VARIABLE		number of nozzles	
NPC	I VARIABLE	/HXDTA/	number of post coolers	

NRB	I VARIABLE	/HXDTA/	number of distillation column reboilers	
P	R VARIABLE	ARGUMENT	distillation column pressure	mmHG
PCKCST	R VARIABLE		distillation column packing cost	$
PD	R VARIABLE	/DLDTA/	distillation column packing cost	$
PI04	R VARIABLE		$\pi/4$	
R	R VARIABLE	/DLDTA/	reflux flow rate	gmol/hr
RATDL	R VARIABLE	/DLDTA/	ratio of rectifying operating line slope to minimum	
RATIO	R VARIABLE	ARGUMENT	reflux optimization variable	
REFLUX	R VARIABLE	/DLDTA/	reflux flow rate	gmol/hr
RFRACT	R VARIABLE	/INPUT/	ethanol recovery fraction	
RHOG	R VARIABLE		vapor density	g/cc
RHOL	R VARIABLE		liquid density	g/cc
RINT	R VARIABLE	/DLDTA/	Y intercept of rectifying operating line	
RRATIO	R VARIABLE	/DLDTA/	external reflux ratio	
RSLOPE	R VARIABLE	/DLDTA/	rectifying operating line slope	
RSTAGE	R VARIABLE		Number of theoretical rectifying stages	
SINT	R VARIABLE	/DLDTA/	Y intercept of stripping section operating line	
SQRT	R STANDARD			
SSLOPE	R VARIABLE	/DLDTA/	Slope of stripping section operating line	
SSTAGE	R VARIABLE	/DLDTA/	Number of theoretical stripping stages	
STCST	R ENTERNAL			
STFRB	R VARIABLE	/HXDTA/	Distillation reboiler steam usage	kg/hr
STFRSP	R VARIABLE	/SPDTA/	Stripper reboiler steam usage	kg/hr
STRIP	R EXTERNAL			
SUPCST	R VARIABLE		Vacuum column internal support installed cost	$
TCWI	R VARIABLE	/INPUT/	Cooling water supply temperature	deg K
TCWOCN	R VARIABLE	/HXDTA/	Cooling water temperature exiting condenser	deg K
TCWOPC	R VARIABLE	/HXDTA/	Cooling water temperature exiting post cooler	deg K
TD	R VARIABLE	/DLDTA/	Initial guess for distillation column temp.	deg K
TDB	R VARIABLE	/DLDTA/	Distillation column reboiler temperature	deg K
TDF	R VARIABLE	/DLDTA/	Distillation column saturated feed temp.	deg K
TDT	R VARIABLE	/DLDTA/	Distillation column head temperature	deg K
THICK	R VARIABLE		Distillation column wall	

			thickness	inches
TOWCST	R VARIABLE		Distillation column shell purchased cost	$
TPNT	R EXTERNAL			
TRYCST	R VARIABLE		Packing support and distributor purchased cost	$
TSLOPE	R VARIABLE	/DLDTA/	Minimum reflux rectifying line slope	
TST	R VARIABLE	/SPDTA/	Stripper head temperature	deg K
TSTEAM	R VARIABLE	/HXDTA/	Plant steam temperature	deg K
WORKERS	R VARIABLE	/COSTS/	Operators required for distillation plant	
WTOTAL	R VARIABLE		Distillation column fitted weight	lb
WTSHEL	R VARIABLE		Distillation column empty shell weight	lb
X	R VARIABLE		Liquid composition on current tray	
XB	R VARIABLE	/DLDTA/	Mole fraction ethanol in distillation bottom product	
XD	R VARIABLE	/INPUT/	Mole fraction ethanol in distillation head product	
XF	R VARIABLE	/DLDTA/	Mole fraction ethanol in stripper feed	
XFD	R VARIABLE	/DLDTA/	Mole fraction ethanol in distillation column feed	
XFMIN	R VARIABLE	/DLDTA/	Minimum acceptable distillation feed composition	
XMSI	R VARIABLE	/COSTS/	Marshall-Stevens Index	
XOLD	R VARIABLE		Liquid composition on last tray	
XT	R VARIABLE	/DLDTA/	Minimum reflux pinch point composition	
Y	R VARIABLE		Vapor composition on current tray	
YFD	R VARIABLE	/DLDTA/	Vapor composition in equilibrium with feed composition	
YRS	R VARIABLE	/DLDTA/	Vapor composition at intersection of rectifying and stripping lines	
ZERO	R EXTERNAL			

Function STRIP

Purpose: Designs and costs a stripping column and reboiler system, and stores the resulting parameters in the stripper and heat exchanger common blocks (SPDTA and HXDTA).

Usage: Call STRIP (FRAC)

Input Variables:

(In Call)

Fractional approach of vapor product to equilibrium with feed	FRAC	

(In Common Blocks)

Stripper Murphree vapor efficiency	EMV	
Stripper feed flow rate	F	gmol/hr
Stripper pressure	PS	mmHg
Ethanol recovery fraction	RFRACT	
Initial guess for stripper head temp.	TS	deg K
Steam temperature	TSTEAM	deg K
Stripper feed ethanol mole fraction	XF	
Minimum acceptable distillation column feed composition	XFMIN	
Marshall-Stevens Index	XMSI	
Fraction of capital cost assessed per year	CFACTR	
Print control flag	LOOK	

Output Variables:

(In Common Blocks)

Area of each stripper reboiler	ASR	sq ft
Number of stripper reboilers	NSR	
Capital cost of stripper reboiler system	CSRCAP	$
Steam usage in stripper reboiler	STFRSP	kg/hr
Annual stripper steam cost	CSPOP	$
Effective annual stripper reboiler cost	CSREFF	$
Heat transferred in stripper reboiler system	DELQSTR	kcal/hr
Stripper internal vapor flow rate	GS	gmol/hr
Stripper column diameter	SPDIAM	ft
Stripper column height	SPHGHT	ft
Stripper operating line X intercept	SPINT	
Stripper operating line slope	SPSLOP	
Number of actual stripping stages	SPSTAG	
Stripper reboiler temperature	TSB	deg K
Stripper head temperature	TST	deg K
Distillation column feed ethanol mole fraction	XFD	
Stripper bottom product ethanol		

mole fraction	XL	
Stripper vapor product ethanol mole fraction	YG	
Stripper column capital cost	CSPCAP	$
Stripper column effective yearly cost	CSPEFF	$

Other needed subroutines:

BDPTM, PDEP, TDEP, TXDEP, DELQ, HXCNG, STCST, LHVAP, FTLM, ENTLP.

Description:

The fractional approach of vapor product composition to equilibrium with the feed composition (FRAC) is one of the three prime optimization variables specified by the optimization routine (E04 JBF (1)). The vapor product composition (ethanol mole fracion) is then computed according to:

YG = YGMIN + FRAC x (YGMAX - YMIN)

where YGMAX is the maximum possible stripper vapor composition (equilibrium with the feed) and YGMIN is the larger of the stripper feed composition or the minimum acceptable distillation column feed composition (XFMIN).

The bottom product composition is given by:

XL = XF(1.0-RFRACT)

where XF is the stripper feed concentration and RFRACT is the required ethanol recovery fraction (99.8%).

With feed and product compositions specified, a McCabe-Thiele type analysis is performed, stairstepping stages to get a stage count. Equimolal overflow is assumed. The Murphree vapor efficiency of 0.70 (measured by Shilling (8)) is applied at each stage.

The column diameter is set to give a vapor linear velocity at 70% of flooding with the flooding limit (UFLOOD) determined by a curve fit to the data of Van Winkle (9,10).

The tower weight is computed using a wall thickness of 0.25 inches as determined by a pressure vessel design calculation according to ASME standards (6).

Stainless steel construction is used throughout to reduce corrosion rates in contact with the hot fermentor beer (11).

The column purchased cost (with fittings and trays) is then computed according to equations derived from the figure of Peters and Timmerhaus (7). The corresponding total capital

investment is given as 4.89 times the purchased cost.

A stripper reboiler is designed and costed (using HXCNG) to provide the necessary boilup heat for the stripper vapor flow.

Variables used in subroutine STRIP

NAME	TYPE	MAIN USE	BLOCKS	DESCRIPTION OF VARIABLES	UNITS
AREA	R	VARIABLE		Stripper cross sectional area	sq ft
ASR	R	VARIABLE	/HXDTA/	Stripper reboiler area	sq ft
ATAN2	R	STANDARD			
BDPTM	R	EXTERNAL			
CFACTR	R	VARIABLE	/COSTS/	Fraction of capital cost assessed per year	
CSPCAP	R	VARIABLE	/COSTS/	Stripper capital cost	$
CSPEFF	R	VARIABLE	/COSTS/	Stripper system effective annual cost	$
CSPOP	R	VARIABLE	/COSTS/	Stripper system annual operating cost	$
CSRCAP	R	VARIABLE	/COSTS/	Stripper reboiler cost	$
CSREFF	R	VARIABLE	/COSTS/	Stripper reboiler effective annual cost	$
DELQ	R	EXTERNAL			
DELQST	R	VARIABLE	/HXDTA/	Stripper reboiler heat duty	kcal/hr
EMAT	R	VARIABLE		Stainless steel cost multiplier	
EMV	R	VARIABLE	/INPUT/	Murphree vapor efficiency for stripper	
EXP	R	STANDARD			
F	R	VARIABLE	/INPUT/	Stripper feed flow rate	gmol/hr
FD	R	VARIABLE	/DLDTA/	Distillation column feed flow rate	gmol/hr
FITCST	R	VARIABLE		Cost of stripper manholes and couplings	$
FRAC	R	VARIABLE	ARGMENT	Frational appoach of vapor product to equilibrium with feed	
GS	R	VARIABLE	/SPDTA/	Stripper vapor flow rate	gmol/hr
HXCNG	R	EXTERNAL			
LOOK	I	VARIABLE	/DATA3/	Print control flag	
MANHLS	I	VARIABLE		Number of manholes in stripper	
MODE	I	ARRAY	/DATA3/	Design control flags	
MWH20	R	EQVALENCE	/DATA/	Water molecular weight	g/gmol
NOZLS	I	VARIABLE		Number of nozzles to stripper	
NSR	I	VARIABLE	/HXDTA/	Number of stripper reboilers	
PI04	R	VARIABLE		$\pi/4$	
PS	R	VARIABLE	/SPDTA/	Stripper pressure	mmHg
RFRACT	R	VARIABLE	/INPUT/	Ethanol recovery fraction	
RHOG	R	VARIABLE		Gas density	
RHOL	R	VARIABLE		Liquid density	

SPDIAM	R VARIABLE	/SPDTA/	Stripper column diameter	ft
SPHGHT	R VARIABLE	/SPDTA/	Stripper column height	ft
SPINT	R VARIABLE	/SPDTA/	Stripper operating line intercept	
SPSLOP	R VARIABLE	/SPDTA/	Stripper operating line slope	
SPSTAG	R VARIABLE	/SPDTA/	Number of stripping stages	
SQRT	R STANDARD			
STCST	R EXTERNAL			
STFRSP	R VARIABLE	/SPDTA/	Stripper reboiler steam usage	kg/hr
THICK	R VARIABLE		Stripper wall thickness	inches
TOWCST	R VARIABLE		Purchased cost of stripper tower	$
TRYCST	R VARIABLE		Purchased cost of stripper trays	$
TS	R VARIABLE	/SPDTA/	Initial guess for temperature in stripper	deg K
TSB	R VARIABLE	/SPDTA/	Stripper reboiler temperature	deg K
TST	R VARIABLE	/SPDTA/	Stripper head temperture	deg K
TSTEAM	R VARIABLE	/HXDTA/	Steam temperature	deg K
UACT	R VARIABLE		Vapor flow rate/cross section	lb/hr/sqft
UFLOOD	R VARIABLE		Vapor flow rate flooding limit	lb/hr/sqft
VEL	R VARIABLE		Vapor mass flow rate	lb/hr
WTOTAL	R VARIABLE		Total weight of stripper	lb
WTSHEL	R VARIABLE		Stripper shell weight	lb
X	R VARIABLE		Liquid mole fraction on a stage	
XF	R VARIABLE	/INPUT/	Stripper feed ethanol mole fraction	
XFD	R VARIABLE	/DLDTA/	Distillation column feed ethanol mole fraction	
XFMIN	R VARIABLE	/DLDTA/	Minimum distillation column feed composition	
XL	R VARIABLE	/SPDTA/	Stripper bottom product mole fraction	
XMSI	R VARIABLE	/COSTS/	Marshall-Stevens Index	
Y	R VARIABLE		Vapor mole fraction on a tray	
YG	R VARIABLE	/SPDTA/	Stripper vapor product mole fraction	
YGMAX	R VARIABLE		Equilibrium maximum stripper product concentration	
YGMIN	R VARIABLE		Minimum stripper product concentration	
YOLD	R VARIABLE		Vapor composition at previous plate	

References:

1. Gill, P.E., W. Murray, Nat'l Phys. Lab. Rept. No. NAC 72 (1976).

2. Maiorella, B.L., H.W. Blanch, C.R. Wilke, Ethanol/Water Physical and Chemical Properties for Separation Process Design, Lawrence Berkeley Laboratory Rept., UCLB-14220, May 1982.

3. Treybal, R.E., Mass Transfer Operations, 3rd Ed., McGraw-Hill, N.Y., 1980.

4. Leva, M., Chem. Eng. Pro. Symp. Ser., 50(10),51 (1954).

5. Hengstebeck, R.J., Distillation Principles and Design Procedures, Reinhold, N.Y., 1961.

6. Baumeister, T., Mechanical Engineers' Handbook, McGraw-Hill, N.Y., 1958.

7. Peters, M.S., K.D. Timmerhaus, Plant Design and Economics for Chemical Engineers, McGraw-Hill, N.Y., 1980.

8. Shilling, G.D., G.H. Beyer, C.C. Watson, Chem. Eng. Prog., 49, 128 (1953).

9. Van Winkle, M., Distillation, McGraw-Hill, N.Y., 1967.

10. King, C.J., Separation Processes, McGraw-Hill, N.Y., 1971.

11. Tourliere, S., Inds. Agr. et Aliment (Paris), 70, 547 (1953).

```
DELETE.LGO.OUTPUT.
MNF4.T.
FETCHPS,NAG,NAG,NAG.
LINK.X.P=NAG.RF.
EXIT.
DUMP.O.
GRUMP.
      PROGRAM DISTILL(TAPE5=16,TAPE6=16,OUTPUT=TAPE6)
      LOGICAL FIRST1,FIRST2
      COMMON/ COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $CDLCAP,CDLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
      COMMON/DATA3/ LOOK,MODE(30)
      COMMON/MATCH/NOPAR(3),NAMEPA(3),ORVAL(3),
     $ABOUND(3),BBOUND(3),IMFL,ITAG
      COMMON /CNDTA/DELQ,UCND,THOT,ACND,NUM,CWRATE,CAPITL,OPER8,EFFCST
      COMMON /DLDTA/PD,TD,TDF,TDB,TDT,
     $B,D,FD,R,
     $XT,YT,TSLOPE,TINT,
     $RSLOPE,RINT,
     $SSLOPE,SINT,
     $XB,XFMIN,YFMIN,XFD,YFD,YRS,
     $DLSTAG,SSTAGE,DLDIAM,DLHGHT,
     $RATDL,ANVOL,RMIN,RRATIO,REFLUX
      COMMON /HXDTA/TSTEAM,AHX,NHX,DELQRB1,
     $APC,NPC,TCWOPC,CWFRPC,DELQPC,
     $ARB,NRB,STFRRB,DELQRB2,
     $ASR,NSR,DELQSTR,
     $ACN,NCN,TCWOCN,CWFRCN,DELQCN
      COMMON /INPUT/EMV,F,RFRACT,TCWI,XF,XD,FIRST1,FIRST2
      COMMON /PARMS/PAR(3)
      COMMON /SPDTA/PS,TS,TSB,TST,
     $GS,GD,STFRSP,
     $SPSLOP,SPINT,
     $XL,YG,
     $SPSTAG,SPDIAM,SPHGHT,
     $RATSP
      COMMON/DATA/MW(2),MIDWAY,CPG(5),CPL(2)
      REAL MAINT,INVEST,MW,MST
C     CONNECT FOR INTERACTIVE USE.
      CALL CONNECT(5)
      CALL CONNECT(6)
C
C     PROGRAM DISTILL DESIGNS EFFICIENT ETHANOL/WATER DISTILLATION
C     SYSTEMS EMPLOYING VACUUM DISTILLATION AND DUAL COLUMN VAPOR
C     REUSE METHODS.  OPERATIONAL PARAMETERS ARE INPUT THROUGH THE
C     MAIN PROGRAM.  DESIGN IS DEVELOPED BY SUBROUTINE DISTL AND
C     OPTIMIZED BY E04JBF (A NAG LIBRARY OPTIMIZATION ROUTINE).
C     THIS PROGRAM MUST BE LINKED WITH THE NAG LIBRARY OPTIMIZATION
C     PACKAGE TO RUN.
C
C     FOR FURTHER DETAILS. SEE ≥ETHANOL DISTILLATION TECHNOLOGY≥
C     IN THE ETHANOL SEPARATION HANDBOOK (AVAILABLE FROM THE
C     SOLAR ENERGY RESEARCH INSTITUTE).
C
 5555 CONTINUE
      N=1
```

```
      IMFL=1
      WRITE(6,1000)
 1000 FORMAT(//,* ENTER THE ANNUAL PRODUCTION RATE (MILLIONS OF L)*)
      READ(5,1010) PVOL
      PVOL=PVOL*1000000.
      WRITE(6,4) PVOL
    4 FORMAT(* PVOL=*,F16.3,* LITERS PER YEAR*)
 1010 FORMAT(F15.7)
      WRITE(6,1020)
 1020 FORMAT(* ENTER THE FEED ETHANOL WEIGHT FRACTION*)
      READ(5,1010) WTFRAC
      WRITE(6,1022) WTFRAC
 1022 FORMAT(* FEED WEIGHT FRACTION=*,F5.4)
      FETOH=PVOL*0.8*0.95*1000./(330.*24.)
      F=FETOH/WTFRAC
      FWTR=F-FETOH
      WRITE(6,1024) FETOH,FWTR
 1024 FORMAT(* FEED ETHANOL (G/HR)=*,F12.2,* WATER=*,F12.2)
 1030 FORMAT(* *,F15.7)
      WRITE(6,1040)
 1040 FORMAT(* ENTER THE MARSHALL STEVENS COST INDEX*)
      READ(5,1010) MSI
 1050 FORMAT(* *,F15.7)
      WRITE(6,1050) MSI
      WRITE(6,1060)
 1060 FORMAT(* ENTER THE TEMPERATURE OF PROCESS COOLING WATER (K)*)
      READ(5,1010) T7
      WRITE(6,1070)
 1070 FORMAT(* *,F15.7)
      WRITE(6,1080)
 1080 FORMAT(* EXTENT OF DETAIL NEEDED? (1-9)*)
      READ(5,1005) LOCK
 1005 FORMAT(I1)
 1090 FORMAT(* *,I1)
C
C     DESIGN CONTROL FLAGS:
C       ALLOW 1 COLUMN DESIGN (MODE26=0), FORCE 2 COL (MODE26=1).
C       OPTIMIZE (MODE27=1). DESIGN FOR SPECIFIED INITIAL
C       PARAMETERS (MODE27=0).
C
      MODE(26)=0
      MODE(27)=1
C
C     ETHANOL AND WATER PROPERTY DATA.
C
      MW(1)=46.07
      MW(2)=18.02
      CPL(1)=0.62
      CPL(2)=1.00
      CPG(1)=0.406
      CPG(2)=0.48
      CPG(3)=0.28
      CPG(4)=0.22
      CPG(5)=0.25
      CPCCAP=0.0
      APC=0.0
      NPC=0
      DELQPC=0.0
      CRBCAP=0.0
      CCNCAP=0.0
      CHXCAP=0.0
      CSPCAP=0.0
```

```
      COLCAP=0.0
      HEATB=0.0
      HEATB1=0.0
      HEATO1=0.0
      HEATO2=0.0
      HEATF1=0.0
      HEATARB=0.0
      BETOH=0.0
      BWTR=0.0
      O1ETOH=0.0
      O2ETOH=0.0
      B1ETOH=0.0
      O1WTR=0.0
      O2WTR=0.0
      B1WTR=0.0
      XMSI=MSI
      F=(FETOH/MW(1))+(FWTR/MW(2))
      XF=(FETOH/MW(1))/F
      TCWI=T7
C
C     DEVELOP OPTIMIZED DESIGN.
C
      CALL DESGN
      IF(CSPEFF.GT.0.0.AND.COLEFF.GT.0.0.AND.N.EQ.3) GO TO 5
      IF(COLEFF.GT.0.0.AND.CSPEFF.EQ.0.0) GO TO 10
      GO TO 15
C
C     COMPUTE ENTHALPY BALANCE FOR COMPLETED DESIGN.
C
C     CASE 1. STEAM STRIPPER DESIGN ONLY (NO DIST COLUMN)
C
    5 BETOH=XL*F*MW(1)
      BWTR=(1.-XL)*F*MW(2)
      O1ETOH=YG*GS*MW(1)
      O1WTR=(1.-YG)*GS*MW(1)
      CALL ENTHPY(0.,0.,0.,0.,0.,FETOH,FWTR,TST,1,QB,QV,HEATARB)
      CALL ENTHPY(O1ETOH,O1WTR,0.,0.,0.,0.,0.,TST,3,QB,QV,HEATO1)
      CALL ENTHPY(0.,0.,0.,0.,0.,BETOH,BWTR,TSB,1,QB,QV,HEATB)
      MODE(1)=1
      GOTO 25
   10 IF(CSPCAP.GT.0.0) GOTO 15
C
C     CASE 2. ONE DISTILLATION COLUMN NEEDED.
C
      B1ETOH=XB*B*MW(1)
      B1WTR=(1.0-XB)*B*MW(2)
      O2ETOH=XD*D*MW(1)
      O2WTR=(1.0-XD)*D*MW(2)
      CALL ENTHPY(0.,0.,0.,0.,0.,FETOH,FWTR,TDF,1,QB,QV,HEATARB)
      CALL ENTHPY(0.,0.,0.,0.,0.,O2ETOH,O2WTR,TDT,1,QB,QV,HEATO2)
      CALL ENTHPY(0.,0.,0.,0.,0.,B1ETOH,B1WTR,TDB,1,QB,QV,HEATB1)
      MODE(1)=2
      GOTO 25
C
C     CASE 3. DISTILLATION COLUMN AND STEAM STRIPPER REQUIRED
C
   15 BETOH=XL*(F-GS)*MW(1)
      BWTR=(1.-XL)*(F-GS)*MW(2)
      O1ETOH=YG*GS*MW(1)
      O1WTR=(1.-YG)*GS*MW(2)
      B1ETOH=XB*B*MW(1)
      B1WTR=(1.-XB)*B*MW(2)
```

```
      O2ETOH=XD*D*MW(1)
      O2WTR=(1.-XD)*D*MW(2)
      CALL ENTHPY (0.,0.,0.,0.,0.,FETOH,FWTR,TST,1,QB,QV,HEATARB)
      CALL ENTHPY(O1ETOH,O1WTR,0.,0.,0.,0.,0.,TST,3,QB,QV,HEATO1)
      CALL ENTHPY(0.,0.,0.,0.,0.,BETOH,BWTR,TSB,1,QB,QV,HEATB)
      CALL ENTHPY(0.,0.,0.,0.,0.,O1ETOH,O1WTR,TDF,1,QB,QV,HEATF1)
      CALL ENTHPY(0.,0.,0.,0.,0.,O2ETOH,O2WTR,TDT,1,QB,QV,HEATO2)
      CALL ENTHPY(0.,0.,0.,0.,0.,B1ETOH,B1WTR,TDB,1,QB,QV,HEATB1)
      MODE(1)=3
   25 CONTINUE
C
C     PRINT THE RESULTS.
C
      TITLE=6H  MAIN
      IF(N.EQ.2) TITLE=6H   2ND
      WRITE(6,90) TITLE,ANVOL
      IF(CSPCAP.EQ.0.0) GO TO 95
      WRITE(6,100) SPSTAG
      WRITE(6,110) SPDIAM,SPHGHT
      WRITE(6,120) SPSLOP
      FKGM=F/1000.
      WRITE(6,130) FKGM
      WRITE(6,140) TST
      WRITE(6,150) XF
      GSKGM=GS/1000.
      DBKGM=FKGM-GSKGM
      WRITE(6,170) DBKGM
      WRITE(6,180) TSB
      WRITE(6,190) XL
      WRITE(6,200) GSKGM
      WRITE(6,210) TST
      WRITE(6,220) YG
      WRITE(6,230) CSPCAP
      WRITE(6,250) CSPEFF
      WRITE(6,260)
   95 IF(MODE(1).EQ.1) GOTO 96
      WRITE(6,270) DLSTAG+SSTAGE
      WRITE(6,280) DLDIAM,DLHGHT
      WRITE(6,290) PD
      WRITE(6,300) RATDL
      WRITE(6,305) REFLUX/1000.
      WRITE(6,307) RRATIO,RMIN
      FDKGM=FD/1000.
      WRITE(6,310) FDKGM
      WRITE(6,320) TDF
      WRITE(6,330) XFD
      BKGM=B/1000.
      WRITE(6,340) BKGM
      WRITE(6,350) TDB
      WRITE(6,360) XB
      DKGM=D/1000.
      WRITE(6,370) DKGM
      WRITE(6,380) TDT
      WRITE(6,390) XD
      WRITE(6,400) CDLCAP
      WRITE(6,410) CDLEFF
      WRITE(6,260)
   96 GOTO(911,97,93), MODE(1)
   93 WRITE(6,420) AHX,NHX
      WRITE(6,425) DELQRB1
      WRITE(6,430) CHXCAP
      WRITE(6,440) CHXEFF
```

```
      WRITE(6,260)
      WRITE(6,450) APC,NPC
      WRITE(6,460) CWFRPC
      WRITE(6,470) TCWOPC-TCWI
      WRITE(6,475) DELQPC
      WRITE(6,480) CPCCAP
      WRITE(6,490) CPCOP
      WRITE(6,500) CPCEFF
      WRITE(6,260)
  911 WRITE(6,750) ASR,NSR
      WRITE(6,752) DELQSTR
      WRITE(6,755) STFRSP
      WRITE(6,760) CSRCAP
      WRITE(6,770) CSPOP
      WRITE(6,780) CSREFF
      WRITE(6,260)
      IF(MODE(1).EQ.1) GOTO 900
      IF(CRBEFF.LE.0.0) GOTO 98
   97 WRITE(6,510) ARB,NRB
      WRITE(6,520) STFRRB
      WRITE(6,525) DELQRB2
      WRITE(6,530) CRBCAP
      WRITE(6,540) CRBOP
      WRITE(6,550) CRBEFF
      WRITE(6,260)
   98 WRITE(6,560) ACN,NCN
      WRITE(6,570) CWFRCN
      WRITE(6,580) TCWOCN-TCWI
      WRITE(6,585) DELQCN
      WRITE(6,590) CCNCAP
      WRITE(6,600) CCNOP
      WRITE(6,610) CCNEFF
      WRITE(6,260)
  900 GOTO(910,920,930), MODE(1)
  910 TCWFR=0.0
      TSTFR=STFRSP
      TCTCAP=CSRCAP+CSPCAP
      TCTOP=CLABR+CSPOP
      TCTEFF=CLABR+CSREFF+CSPEFF
      GOTO 950
  920 TCWFR=CWFRCN
      TSTFR=STFRRB
      TCTCAP=COLCAP+CRBCAP+CCNCAP
      TCTOP=CLABR+CRBOP+CCNOP
      TCTEFF=CLABR+COLEFF+CCNEFF+CRBEFF
      GOTO 950
  930 TCWFR=CWFRCN+CWFRPC
      TSTFR=STFRRB+STFRSP
      TCTCAP=CTCAP
      TCTOP=CTOP
      TCTEFF=CLABR+CTEFF
  950 WRITE(6,620) TCWFR
      TSCWCST=CPCOP+CCNOP
      TSCWPL=TSCWCST/ANVOL
      WRITE(6,625) TSCWCST,TSCWPL
      WRITE(6,630) TSTFR
      TSSTCST=CSPOP+CRBOP
      TSSTPL=TSSTCST/ANVOL
      WRITE(6,632) TSSTCST,TSSTPL
      WRITE(6,633) WORKERS
      CLABRPL=CLABR/ANVOL
      WRITE(6,635) CLABR,CLABRPL
```

```
      TCTPL=TCTCAP/ANVOL
      WRITE(6,640) TCTCAP,TCTPL
      TOPPL=TCTOP/ANVOL
      WRITE(6,650) TCTOP,TOPPL
      TEFFPL=TCTEFF/ANVOL
      WRITE(6,660) TCTEFF,TEFFPL
      WRITE(6,960)
  960 FORMAT(////,*DO YOU WANT TO RUN ANOTHER CASE (0=NO. 1=YES)*)
      READ(5,965) IDO
  965 FORMAT(I1)
      FIRST1=.TRUE.
      FIRST2=.TRUE.
      IF(IDO.GT.0) GOTO 5555
   90 FORMAT(///,11X,A6,* DISTILLATION TRAIN*,5X,F10.1,* L/YR CAPACITY*,
     $//)
  100 FORMAT(* STRIPPING COLUMN.  STAGES=*,F10.5)
  110 FORMAT(18X,*DIAMETER=*,E15.5,*FT.  HEIGHT=*,E15.5,*FT.*)
  120 FORMAT(18X,*SLOPE RATIO=*,E15.5)
  130 FORMAT(18X,*FEED FLOW RATE=*,E15.5,* KG-MOLE/HR*)
  140 FORMAT(18X,*FEED TEMPERATURE=*,F10.5,*DEG-K*)
  150 FORMAT(18X,*XF=*,E15.5)
  170 FORMAT(18X,*BOTTOM FLOW RATE=*,E15.5,* KG-MOLE/HR*)
  180 FORMAT(18X,*BOTTOM TEMPERATURE=*,F10.5,* DEG-K*)
  190 FORMAT(18X,*XL=*,E15.5)
  200 FORMAT(18X,*PRODUCT FLOW RATE=*,E15.5,* KG-MOLE/HR*)
  210 FORMAT(18X,*PRODUCT TEMPERATURE=*,F10.5,* DEG-K*)
  220 FORMAT(18X,*YG=*,E15.5)
  230 FORMAT(18X,*CAPITAL COST=$*,E15.7)
  250 FORMAT(18X,*EFFECTIVE COST=$*,E15.5,* PER YR.*)
  260 FORMAT(////)
  270 FORMAT(* DISTILATION COLUMN.  THEORETICAL STAGES=*,F10.5)
  280 FORMAT(21X,*DIAMETER=*,E15.5,*FT.  HEIGHT=*,E15.5,*FT.*)
  290 FORMAT(21X,*PRESSURE=*,F10.5,*MM HG.*)
  300 FORMAT(21X,*SLOPE RATIO=*,E15.5)
  305 FORMAT(21X,*REFLUX FLOW RATE=*,E15.5,* KG-MOLE/HR*)
  307 FORMAT(21X,*REFLUX RATIO=*,F8.5,* RMIN=*,F8.5)
  310 FORMAT(21X,*FEED FLOW RATE=*,E15.5,* KG-MOLE/HR*)
  320 FORMAT(21X,*FEED TEMPERATURE=*,F10.5,* DEG-K*)
  330 FORMAT(21X,*XFD=*,E15.7)
  340 FORMAT(21X,*BOTTOM FLOW RATE=*,E15.5,* KG-MOLE/HR.*)
  350 FORMAT(21X,*BOTTOM TEMPERATURE=*,F10.5,* DEG-K*)
  360 FORMAT(21X,*XB=*,E15.7)
  370 FORMAT(21X,*PRODUCT FLOW RATE=*,E15.5,*KG-MOLE/HR.*)
  380 FORMAT(21X,*PRODUCT TEMPERATURE=*,F10.5,* DEG-K*)
  390 FORMAT(21X,*XD=*,E15.7)
  400 FORMAT(21X,*CAPITAL COST=$*,E15.5)
  410 FORMAT(21X,*EFFECTIVE COST=$*,E15.5,*PER YR*)
  420 FORMAT(* HEAT EXCHANGER, AREA=*,E15.5,*SQ.FT.  NUMBER=*,I4)
  425 FORMAT(16X,*DELTA Q (KCAL/HR)=*,E15.5)
  430 FORMAT(16X,*CAPITAL COST=$*,E15.5)
  440 FORMAT(16X,*EFFECTIVE COST=$*,E15.5,* PER YR.*)
  450 FORMAT(* POST-COOL. AREA=*,E15.5,*SQ.FT.  NUMBER=*,I4)
  460 FORMAT(11X,*COOLING WATER FLOW RATE=*,E15.5,*KG/HR*)
  470 FORMAT(11X,*COOLING WATER TEMPERATURE RISE=*,F10.5,*DEG-K*)
  475 FORMAT(11X,*DELTA Q (KCAL/HR)=*,E15.5)
  480 FORMAT(11X,*CAPITAL COST=$*,E15.5)
  490 FORMAT(11X,*COOLING WATER COST=$*,E15.5,*PER YR.*)
  500 FORMAT(11X,*EFFECTIVE COST=$*,E15.5,* PER YR.*)
  510 FORMAT(* REBOILER,  AREA=*,E15.5,*SQ.FT.  NUMBER=*,I4)
  520 FORMAT(10X,*STEAM FLOW RATE=*,E15.5,*KG/HR*)
  525 FORMAT(10X,*DELTA Q (KCAL/HR)=*,E15.5)
  530 FORMAT(10X,*CAPITAL COST=$*,E15.7)
```

```
540 FORMAT(10X,*STEAM COST=$*,E15.5,* PER YR.*)
550 FORMAT(10X,*EFFECTIVE COST=$*,E15.5,* PER YR.*)
560 FORMAT(* CONDENSER.  AREA=*,E15.5,*SQ.FT.  NUMBER=*,I4)
570 FORMAT(11X,*COOLING WATER FLOW RATE=*,E15.5,*KG/HR*)
580 FORMAT(11X,*COOLING WATER TEMPERATURE RISE=*,F10.5,*DEG-K*)
585 FORMAT(11X,*DELTA Q (KCAL/HR)=*,E15.5)
590 FORMAT(11X,*CAPITAL COST=$*,E15.5)
600 FORMAT(11X,*COOLING WATER COST=$*,E15.5,* PER YR.*)
610 FORMAT(11X,*EFFECTIVE COST=$*,E15.5,* PER YR.*)
620 FORMAT(* SYSTEM. TOTAL COOLING WATER FLOW =*,T38,F10.1,*KG/HR*)
625 FORMAT(8X,*TOTAL COOLING WATER COST=$*,T38,F9.1,* /YR*,
   $T55,F9.6,* /L*)
630 FORMAT(8X,*TOTAL STEAM FLOW RATE=$*,T38,F9.1,*KG.HR.*)
632 FORMAT(8X,*TOTAL STEAM COST=$*,T38,F9.1,* /YR*,
   $T55,F9.7,* /L*)
633 FORMAT(8X,*LABOR REQUIREMENT (WORKERS/SHIFT)=*,F6.2)
635 FORMAT(8X,*LABOR COST=$*,T38,F9.1,* /YR*,T55,
   $F9.7,* /L*)
640 FORMAT(8X,*TOTAL CAPITAL COST=$*,T38,F9.1,
   $T55,F9.7,* /L*)
650 FORMAT(8X,*TOTAL OPERATING COST=$*,T38,F9.1,* /YR*,
   $T55,F9.7,* /L*)
660 FORMAT(8X,*TOTAL EFFECTIVE COST=$*,T38,F9.1,* /YR*,
   $T55,F9.7,* /L*)
750 FORMAT(* STRIPPER REBOILER.  AREA=*,E15.5,*SQ.FT.  NUMBER=*,I4)
752 FORMAT(20X,*DELTA Q (KCAL/HR)=*,E15.5)
755 FORMAT(20X,*STEAM FLOW RATE=*,E15.5,*KG/HR*)
760 FORMAT(20X,*CAPITAL COST=$*,E15.7)
770 FORMAT(20X,*STEAM COST=$*,E15.5,*PER YR.*)
780 FORMAT(20X,*EFFECTIVE COST=$*,E15.5,*PER YR.*)
    RETURN
    END
C
C
C
C
    SUBROUTINE ENTHPY(MASS1,MASS2,MASS3,MASS4,MASS5,
   $MASS11,MASS22,T,IPHASE,QB,QV,Q)
    COMMON/DATA/MW(2),MIDWAY,CPG(5),CPL(2)
    COMMON/DATA3/ LOOK,MODE(30)
    REAL MW,MIDWAY,MASS1,MASS2,MASS3,MASS4,MASS5
    REAL MASS11,MASS22,LHEAT1,LHEAT2,HSOLN1
C
C   SUBROUTINE ENTHPY COMPUTES THE ENTHALPY OF A STREAM
C   GIVEN LIQUID AND VAPOR FLOW RATES AND TEMPERATURE.
C
    QB=0.0
    QV=0.0
    IF(IPHASE.GT.2) GOTO 25
    HEAT11=MASS11*CPL(1)*(T-273.15)
    HEAT22=MASS22*CPL(2)*(T-273.15)
    QB=HEAT11+HEAT22
    IF(IPHASE.EQ.1)GOTO 50
25  CALL LHVAP(273.15,LHEAT1,LHEAT2,HSOLN1)
    HEAT1=(LHEAT1+(CPG(1)*(T-273.15)))*MASS1
    HEAT2=(LHEAT2+(CPG(2)*(T-273.15)))*MASS2
    HEAT3=(HSOLN1+(CPG(3)*(T-273.15)))*MASS3
    HEAT4=CPG(4)*(T-273.15)*MASS4
    HEAT5=CPG(5)*(T-273.15)*MASS5
    QV=HEAT1+HEAT2+HEAT3+HEAT4+HEAT5
50  Q=QB+QV
    RETURN
```

```
540 FORMAT(10X,*STEAM COST=$*,E15.5,* PER YR.*)
550 FORMAT(10X,*EFFECTIVE COST=$*,E15.5,* PER YR.*)
560 FORMAT(* CONDENSER.  AREA=*,E15.5,*SQ.FT.  NUMBER=*,I4)
570 FORMAT(11X,*COOLING WATER FLOW RATE=*,E15.5,*KG/HR*)
580 FORMAT(11X,*COOLING WATER TEMPERATURE RISE=*,F10.5,*DEG-K*)
585 FORMAT(11X,*DELTA Q (KCAL/HR)=*,E15.5)
590 FORMAT(11X,*CAPITAL COST=$*,E15.5)
600 FORMAT(11X,*COOLING WATER COST=$*,E15.5,* PER YR.*)
610 FORMAT(11X,*EFFECTIVE COST=$*,E15.5,* PER YR.*)
620 FORMAT(* SYSTEM. TOTAL COOLING WATER FLOW =*,T38,F10.1,*KG/HR*)
625 FORMAT(8X,*TOTAL COOLING WATER COST=$*,T39,F9.1,* /YR*,
   $T55,F9.6,* /L*)
630 FORMAT(8X,*TOTAL STEAM FLOW RATE=$*,T38,F9.1,*KG.HR.*)
632 FORMAT(8X,*TOTAL STEAM COST=$*,T38,F9.1,* /YR*,
   $T55,F9.7,* /L*)
633 FORMAT(8X,*LABOR REQUIREMENT (WORKERS/SHIFT)=*,F6.2)
635 FORMAT(8X,*LABOR COST=$*,T38,F9.1,* /YR*,T55,
   $F9.7,* /L*)
640 FORMAT(8X,*TOTAL CAPITAL COST=$*,T38,F9.1,
   $T55,F9.7,* /L*)
650 FORMAT(8X,*TOTAL OPERATING COST=$*,T38,F9.1,* /YR*,
   $T55,F9.7,* /L*)
660 FORMAT(8X,*TOTAL EFFECTIVE COST=$*,T38,F9.1,* /YR*,
   $T55,F9.7,* /L*)
750 FORMAT(* STRIPPER REBOILER.  AREA=*,E15.5,*SQ.FT.  NUMBER=*,I4)
752 FORMAT(20X,*DELTA Q (KCAL/HR)=*,E15.5)
755 FORMAT(20X,*STEAM FLOW RATE=*,E15.5,*KG/HR*)
760 FORMAT(20X,*CAPITAL COST=$*,E15.7)
770 FORMAT(20X,*STEAM COST=$*,E15.5,*PER YR.*)
780 FORMAT(20X,*EFFECTIVE COST=$*,E15.5,*PER YR.*)
    RETURN
    END
C
C
C
C
    SUBROUTINE ENTHPY(MASS1,MASS2,MASS3,MASS4,MASS5,
   $MASS11,MASS22,T,IPHASE,QB,QV,Q)
    COMMON/DATA/MW(2),MIDWAY,CPG(5),CPL(2)
    COMMON/DATA3/ LOOK,MODE(30)
    REAL MW,MIDWAY,MASS1,MASS2,MASS3,MASS4,MASS5
    REAL MASS11,MASS22,LHEAT1,LHEAT2,HSOLN1
C
C   SUBROUTINE ENTHPY COMPUTES THE ENTHALPY OF A STREAM
C   GIVEN LIQUID AND VAPOR FLOW RATES AND TEMPERATURE.
C
    QB=0.0
    QV=0.0
    IF(IPHASE.GT.2) GOTO 25
    HEAT11=MASS11*CPL(1)*(T-273.15)
    HEAT22=MASS22*CPL(2)*(T-273.15)
    QB=HEAT11+HEAT22
    IF(IPHASE.EQ.1)GOTO 50
25  CALL LHVAP(273.15,LHEAT1,LHEAT2,HSOLN1)
    HEAT1=(LHEAT1+(CPG(1)*(T-273.15)))*MASS1
    HEAT2=(LHEAT2+(CPG(2)*(T-273.15)))*MASS2
    HEAT3=(HSOLN1+(CPG(3)*(T-273.15)))*MASS3
    HEAT4=CPG(4)*(T-273.15)*MASS4
    HEAT5=CPG(5)*(T-273.15)*MASS5
    QV=HEAT1+HEAT2+HEAT3+HEAT4+HEAT5
50  Q=QB+QV
    RETURN
```

```
      END
C
C
C
C
      SUBROUTINE LHVAP(T,LHEAT1,LHEAT2,HSOLN1)
      COMMON/DATA/MW(2),MIDWAY,CPG(5),CPL(2)
      COMMON/DATA3/ LOCK,MODE(30)
      REAL MW,MIDWAY,LHEAT1,LHEAT2,HSOLN1
C
C     LHVAP COMPUTES THE HEAT OF VAPORIZATION (OR SOLUTION)
C     OF ETHANOL, WATER, AND CO2, AT THE SPECIFIED TEMPERATURE.
C
      LHEAT1=1.987*516.2*(7.08*((1.0-(T/516.2))**0.354)+
     +(10.95*0.635*((1.0-(T/516.2))**0.456)))
      LHEAT1=LHEAT1/MW(1)
      LHEAT2=1.987*647.1*(7.08*((1.0-(T/647.1))**0.354)+
     +(10.95*0.348*((1.0-(T/647.1))**0.456)))
      LHEAT2=LHEAT2/MW(2)
      HSOLN1=(4900/44.01)-CPG(3)*(298.1-273.15)
      RETURN
      END
C
C
C
C
      FUNCTION ENTLP (MFREV,MFRWV,MFREL,MFRWL,T,IPHASE,QL,QV)
      COMMON /DATA/MW(2),MIDWAY,CPG(5),CPL(2)
      COMMON/DATA3/ LOCK,MODE(30)
      REAL MW,MWETH,MWH2O
      EQUIVALENCE (MWETH,MW(1)),
     $(MWH2O,MW(2))
      REAL MFREL,MFRWL,MFREV,MFRWV,LHEATE,LHEATW
      QV =0.0
      QL =0.0
      IF(.NOT.(IPHASE.LE.2))GOTO 30000
      HEATEL =MFREL*CPL(1)*(T-273.15)
      HEATWL =MFRWL*CPL(2)*(T-273.15)
      QL =HEATEL+HEATWL
30000 CONTINUE
      IF(.NOT.(IPHASE.GE.2))GOTO 30002
      CALL LHVAP (273.15,LHEATE,LHEATW,HSOLN)
      HEATEV =(LHEATE+(CPG(1)*(T-273.15)))*MFREV
      HEATWV =(LHEATW+(CPG(2)*(T-273.15)))*MFRWV
      QV =HEATEV+HEATWV
30002 CONTINUE
      ENTLP =QV+QL
      RETURN
      END
C
C
C
C
      FUNCTION FTLM(THOTI,THOTO,TCLDI,TCLDO,N)
C
C     THE LMTD CORRECTION FACTOR.
C          BECAUSE TRUE COUNTER-CURRENT HEAT EXCHANGE IS DIFFICULT
C     TO OBTAIN, THE LOG-MEAN TEMPERATURE MUST BE CORRECTED.
C     THIS ROUTINE COMPUTES THE CORRECTION FACTOR FROM THE INLET-
C     OUTLET TEMPERATURE AND THE NUMBER OF SHELL PASSES.  FOR
C     MORE DETAILS, SEE KERN, PROCESS HEAT TRANSFER, P 155.
C
```

```
      COMMON/DATA3/ LOOK,MODE(30)
      DELHOT =THOTI-THOTO
      DELCLD =TCLDO-TCLDI
      IF(.NOT.(DELHOT.EQ.0.0.OR.DELCLD.EQ.0.0)) GOTO 30000
      IF(.NOT.(DELHOT.EQ.DELCLD)) GOTO 3000
      FTLM =1.0
30002 GOTO 30001
 3000 P=DELCLD/(THOTI-TCLDI)
      R=DELHOT/DELCLD
      X=P/(N-N*P+P)
      F1=(X*SQRT(R*R+1.))/(1.-X)
      F2=ALOG(((2./X)-1.-R+SQRT(R*R+1.))/((2./X)-1.-R-SQRT(R*R+1.)))
      GOTO 30001
30000 CONTINUE
      P =DELCLD/(THOTI-TCLDI)
      R =DELHOT/DELCLD
      G =((1.0-R*P)/(1.0-P))**(1.0/N)
      X =(1.0-G)/(R-G)
      TERM =SQRT(R*R+1.0)
      F1 =TERM*ALOG((1.0-X)/(1.0-R*X))
      F2 =(2.0-X*(R+1.0-TERM))/(2.0-X*(R+1.0+TERM))
      IF(.NOT.(F2.LE.1.0))GOTO 30003
      FTLM =0.001
30005 GOTO 30004
30003 CONTINUE
      F3 =(R-1.0)*ALOG(F2)
      FTLM =F1/F3
30004 CONTINUE
30001 CONTINUE
      RETURN
      END
C
C
C
C
      FUNCTION CNCST(TCWO)
C
C     COMPUTES EFFECTIVE YEARLY COST OF A CONDENSER
C     AS A FUNCTION OF COOLING WATER OUTFLOW TEMPERATURE
C
      COMMON /CNDTA/DELQ,UCND,THOT,ACND,NUM,CWRATE,CAPITL,OPER8,EFFCST
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $CDLCAP,CDLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
      COMMON/DATA3/ LOOK,MODE(30)
      REAL MAINT,INVEST
      COMMON /INPUT/EMV,F,REFACT,TCWI,XF,XD,FIRST1,FIRST2
C
C     DESIGN CONDENSER
C
      CALL HXCNG (DELQ,400.,THOT,THOT,TCWI,TCWO,ACND,NUM,CAPITL)
C
C     CALCULATE COOLING WATER FLOW RATE AND COST
C
      CALL CWCST (DELQ,TCWO-TCWI,CWRATE,OPER8)
C
C     CALCULATE EFFECTIVE YEARLY COST FOR USE IN MINIMIZATION
```

```
C
      EFFCST =OPERB+CFACTR*CAPITL
C     SCALE COST FOR OPTIMIZATION ROUTINE
      CNCST =EFFCST/10000.
      RETURN
      END
C
C
C
C
      SUBROUTINE CNDSR (Q,U,T,TCWO,AREA,NUMBER,RATE,CAPCST,OPCOST,CSTEFF
     $)
      COMMON /CNDTA/DELQ,UCND,THOT,ACND,NUM,CWRATE,CAPITL,OPERB,EFFCST
      COMMON /INPUT/EMV,F,REFACT,TCWI,XF,XD,FIRST1,FIRST2
      COMMON/DATA3/ LOCK,MODE(30)
      EXTERNAL CNCST
C
C     CNDSR FINDS THE MINIMUM COST CONDENSER DESIGN USING CNCST AS
C     MINIMIZED BY ZERO.
C
      IF(.NOT.(Q.LE.0.0))GOTO 30000
      WRITE(6,10)
   10 FORMAT (/21H CNDSR? Q LESS THAN 0)
30000 CONTINUE
      IF(.NOT.(T.LE.TCWI))GOTO 30002
      WRITE(6,20)
   20 FORMAT (/24H CNDSR? T LESS THAN TCWI)
30002 CONTINUE
      IF(.NOT.(Q.LE.0.0.OR.T.LE.TCWI))GOTO 30004
      STOP
30004 CONTINUE
      DELQ =Q
      UCND =U
      THOT =T
C     INITIAL GUESS FOR COOLING WATER EXIT TEMP
      TCWO=TCWI+0.91*(T-TCWI)
      TCWO =ZERO(CNCST,TCWO,2,1.0E-3,TCWI,T,6HCNCST )
      AREA =ACND
      NUMBER =NUM
      RATE =CWRATE
      CAPCST =CAPITL
      OPCOST =OPERB
      CSTEFF =EFFCST
      RETURN
      END
C
C
C
C
      BLOCK DATA CNDTA
C
C     DATA FOR CONDENSER OPTIMIZATION ROUTINES
C
      COMMON /CNDTA/DELQ,UCND,THOT,ACND,NUM,CWRATE,CAPITL,OPERB,EFFCST
      DATA CWRATE /0.0E0/
      END
C
C
C
C
      BLOCK DATA COSTS
C
```

```
C     CAPITAL AND OPERATING COST FACTORS
C
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $COLCAP,COLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
      REAL MAINT,INVEST,LTAX,INSUR
C     LOCAL TAX RATE
      DATA LTAX /0.03/
C     INSURANCE RATE
      DATA INSUR /0.01/
C     EQUIP MAINT COST (FRACTION OF PURCH. COST/YEAR)
      DATA MAINT /0.06E0/
C     DEPRECIATION FACTOR (18 YEAR PLANT LIFE)
      DATA DEPR /0.0556E0/
C     MINIMUM ANNUAL RETURN ON INCREMENTAL INVESTMENT
      DATA INVEST /0.15E0/
C     TAX RATE
      DATA TAX /0.5E0/
C     MARSHALL-STEVENS COST INDEX
      DATA XMSI /717.0E0/
      END
C
C
C
C
      FUNCTION CROSS(X)
C
C     FIND INTERSECTION OF PINCH TANGENT LINE AND EQUILIB CURVE
C
      COMMON /DLOTA/PO,TO,TOF,TOB,TOT,
     $B,D,FD,R,
     $XT,YT,TSLOPE,TINT,
     $RSLOPE,RINT,
     $SSLOPE,SINT,
     $XB,XFMIN,YFMIN,XFD,YFD,YRS,
     $OLSTAG,SSTAGE,DLOTAM,DLHGHT,
     $RATOL,ANVOL,RMIN,RRATIO,REFLUX
      COMMON/DATA3/ LOOK,MODE(30)
      YTAN =TSLOPE*X+TINT
      RMIN=1.0/((1.0/TSLOPE)-1.0)
      YFMIN =YTAN
      CALL BOPTM (PO,TO,X,YFMIN,1)
      CROSS =(YFMIN-YTAN)*100.
      RETURN
      END
C
C
C
C
      SUBROUTINE CWCST (DELQ,DELT,RATE,COST)
C
C     CALCULATE COOLING WATER FLOW RATE AND YEARLY COST
C     FOR A HEAT EXCHANGER
C
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
```

```
      $CDLCAP,COLEFF,CSRCAP,CSREFF,
      $CRBCAP,CRBOP,CRBEFF,
      $CCNCAP,CCNOP,CCNEFF,
      $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
      $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
       COMMON/DATA3/ LOOK,MODE(30)
       REAL MAINT,INVEST
       COMMON /DATA/MW(2),MIDWAY,CPG(5),CPL(2)
       REAL MW,MWETH,MWH2O
       EQUIVALENCE (MWETH,MW(1)),
      $(MWH2O,MW(2))
       RATE =DELQ/(CPL(2)*DELT)
C      COOLING WATER COST ($/1000 GAL)
       WATCOST=.18
       COST =(XMSI/569.0)*RATE*24.0*330.0*WATCOST/3785.0
       RETURN
       END
C
C
C
C
       FUNCTION DELQ (RATE,XFRACT,TVAP,TLIQ)
C
C      CALCULATE THE DIFFERENCE IN ENTHALPY BETWEEN VAPOR AND
C      LIQUID STREAMS OF IDENTICAL FLOW RATE (RATE IN MOLES/HR)
C      AND COMPOSITION (XFRACT=MOLE FRACTION ETHANOL)
C
       COMMON /DATA/MW(2),MIDWAY,CPG(5),CPL(2)
       COMMON/DATA3/ LOOK,MODE(30)
       REAL MW,MWETH,MWH2O
       EQUIVALENCE (MWETH,MW(1)),
      $(MWH2O,MW(2))
       REAL MFRE,MFRW
       MFRE =RATE*XFRACT*MWETH/1000.0
       MFRW =RATE*(1.0-XFRACT)*MWH2O/1000.0
       QVAP =ENTLP(MFRE,MFRW,0.0E0,0.0E0,TVAP,3,QL,QV)
       QLIQ =ENTLP(0.0E0,0.0E0,MFRE,MFRW,TLIQ,1,QL,QV)
       DELQ =ABS(QVAP-QLIQ)
       RETURN
       END
C
C
C
C
       SUBROUTINE DESGN
C
C      DESIGN OF AN ETHANOL/WATER DISTILLATION SYSTEM
C
       COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
      $CHXCAP,CHXEFF,
      $CPCCAP,CPCOP,CPCEFF,
      $CDLCAP,COLEFF,CSRCAP,CSREFF,
      $CRBCAP,CRBOP,CRBEFF,
      $CCNCAP,CCNOP,CCNEFF,
      $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
      $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
       COMMON/DATA3/ LOOK,MODE(30)
       COMMON/MATCH/NOPAR(3),NAMEPA(3),ORVAL(3),
      $ABOUND(3),BBOUND(3),IMFL,ITAG
       REAL LTAX,INSUR,MAINT,INVEST,BL(5),BU(5),W(70),X(5)
      $,DELTA(5),HESL(10),HESD(10),ISTATE(5),G(5)
       INTEGER IW(7),LIW,LW
```

```
      COMMON /DLDTA/PD,TD,TDF,TDB,TDT,
     $B,D,FD,R,
     $XT,YT,TSLOPE,TINT,
     $RSLOPE,RINT,
     $SSLOPE,SINT,
     $XR,XFMIN,YFMIN,XFD,YFD,YRS,
     $DLSTAG,SSTAGE,DLDIAM,DLHGHT,
     $RATDL,ANVOL,RMIN,RRATIO,REFLUX
      COMMON /HXDTA/TSTEAM,AHX,NHX,DELQRB1,
     $APC,NPC,TCWOPC,CWFRPC,DELQPC,
     $ARB,NRB,STFRRB,DELQRB2,
     $ASR,NSR,DELQSTR,
     $ACN,NCN,TCWOCN,CWFRCN,DELQCN
      COMMON /INPUT/EMV,F,RFRACT,TCWI,XF,XD,FIRST1,FIRST2
      COMMON /SPDTA/PS,TS,TSB,TST,
     $GS,GD,STFRSP,
     $SPSLOP,SPINT,
     $XL,YG,
     $SPSTAG,SPDIAM,SPHGHT,
     $RATSP
      EXTERNAL DISTL,MONIT,E04JBQ
      LOGICAL LOCSCH
C
C     COMPUTE CAPITAL COST FACTOR
C
      CFACTR =(4.13/4.89)*(LTAX+INSUR+MAINT+DEPR+INVEST/(1.0-TAX))
C     INITIALIZE FOR OPTIMIZATION
      ITAG=1
      CALL FUNCT(IFLAG,NPAR,X,COST,GC,IW,LIW,W,LW)
C     FIND MINIMUM COST DESIGN
      DO 37 I=1,NPAR
      BL(I)=ABOUND(I)
      BU(I)=BBOUND(I)
      X(I)=ORVAL(I)
   37 CONTINUE
C     TEST DISTL AT STARTING CONDITIONS
      ITAG=3
      CALL FUNCT(IFLAG,NPAR,X,COST,GC,IW,LIW,W,LW)
      WRITE(6,2200)
 2200 FORMAT(* TEST AT INITIAL CONDITIONS COMPLETE.*)
      WRITE(6,2210)
 2210 FORMAT(* GO ON TO OPTIMIZATION? (1=YES,0=NO).*,/)
      READ(5,2220) MODE(27)
 2220 FORMAT(I1)
      IF(MODE(27).EQ.0) RETURN
  111 CONTINUE
      LOCK=10
C
C     SET OPTIMIZATION CONTROL PARAMETERS.
C
      IFAIL=1
      IPRINT=1
      LOCSCH=.TRUE.
      INTYPE=0
      MAXCAL=2000
      ETA=0.1
      XTOL=0.02
      STEPMX=50000.
      FEST=3.5
      DELTA(1)=.00001
      DELTA(2)=.00001
      DELTA(3)=.00001
```

```
      LH=10
      LIW=7
      LW=70
      ITAG=2
      WRITE(6,5010)
 5010 FORMAT(* CALLING E04JBF*)
      WRITE(6,5020)NPAR,IFAIL
 5020 FORMAT(* NPAR=*,I2,*IFAIL=*,I2)
      CALL E04JBF(NPAR,FUNCT,MONIT,IPRINT,LOCSCH,INTYPE,E04JBQ,
     $MAXCAL,ETA,XTOL,STEPMX,FEST,DELTA,0.8L,BU,X,HESL,LH,HESD,
     $ISTATE,VALUE,G,IW,LIW,W,LW,IFAIL)
      IF(IFAIL.EQ.0) GOTO 42
      WRITE(6,96) IFAIL
   96 FORMAT(//,* DIST. OPTIMIZATION FAILURE. IFAIL=*,I2)
   42 ITAG=3
      CALL FUNCT(IFLAG,NPAR,X,COST,GC,IW,LIW,W,LW)
      RETURN
      END
C
C
C
C
      FUNCTION DIFER(F,XO,NUMDIF,DIF1,DIF2,DELTA,XMIN,XMAX,NAME)
      EXTERNAL F
C
C     COMPUTES VALUE AND FIRST (AND SECOND) DERIVATIVE OF F(X) AT XO
C
C     F(XO) IS RETURNED AS THE FUNCTION VALUE (DIFER)
C     THE VALUE(S) OF THE DERIVATIVES ARE RETURNED IN DIF1 (AND DIF2)
C
C     NUMDIF IS THE NUMBER OF DERIVATIVES TO BE COMPUTED (1 OR 2)
C     DELTA IS THE PERTURBATION USED IN COMPUTING THE DERIVATIVES
C
C     CENTRAL DIFFERENCES ARE USED FOR THE DERIVATIVES IF THE POINTS
C     NEEDED TO COMPUTE THEM LIE WITHIN THE OPEN INTERVAL (XMIN,XMAX)
C     OTHERWISE, FORWARD OR BACKWARD DIFFERENCES ARE USED
C
C     NAME IS THE NAME OF THE FUNCTION F (IN HOLERITH)
C
      COMMON/DATA3/ LOCK,MODE(30)
      IF(.NOT.(XMAX-XMIN.LE.DELTA+DELTA))GOTO 30000
      WRITE(6,10)NAME
   10 FORMAT (/53H DIFER? XMAX-XMIN LESS THAN 2*DELTA (DIFFERENTIATING ,
     $A6,1H))
      STOP
30000 CONTINUE
      X1 =XO-DELTA
      X2 =XO+DELTA
      IF(.NOT.(X1.LE.XMIN))GOTO 30002
      X1 =XO
30004 GOTO 30003
30002 CONTINUE
      IF(.NOT.(X2.GE.XMAX))GOTO 30005
      X2 =XO
30005 CONTINUE
30003 CONTINUE
      DELX =X2-X1
      F1 =F(X1)
      F2 =F(X2)
      DIFER =F(XO)
      DIF1 =(F2-F1)/DELX
      IF(.NOT.(NUMDIF.EQ.2))GOTO 30007
```

```
      DIF2 =(F2-DIFER-DIFER+F1)/(DELTA*DELTA)
30007 CONTINUE
      RETURN
      END
C
C
C
C
      SUBROUTINE FUNCT(IFLAG,NPAR,PARAM,COST,GC,IW,LIW,W,LW)
C
C     SUBROUTINE FUNCT SERVES AS A BRIDGE BETWEEN THE DISTILLATION
C     DESIGN ROUTINES AND THE NAG MATHLIB OPTIMIZATION ROUTINE
C     E04JAF.
C
      COMMON/MATCH/NOPAR(3),NAMEPA(3),ORVAL(3),
     $ABOUND(3),BBOUND(3),IMFL,ITAG
      REAL PARAM(3),GC(3),W(70)
      INTEGER IW(7)
      COMMON /DLDTA/PO,TD,TDF,TDB,TDT,
     $B,D,FD,R,
     $XT,YT,TSLOPE,TINT,
     $FSLOPE,RINT,
     $SSLOPE,SINT,
     $XB,XFMIN,YFMIN,XFD,YFD,YPS,
     $DLSTAG,SSTAGE,DLDIAM,DLHGHT,
     $RATDL,ANVOL,RMIN,RRATIO,REFLUX
      COMMON/INPUT/EMV,F,REFACT,TCWI,XF,XD,FIRST1,FIRST2
      COMMON/DATA3/LOOK,MODE(30)
      IF(LOOK.GT.3) GOTO 47
      WRITE(6,149) ITAG
  149 FORMAT(/,* ENTERING FUNCT. ITAG=*,I2)
      WRITE(6,153) NPAR,PARAM(1),PARAM(2),PARAM(3)
  153 FORMAT(/,* NPAR=*,I2,*PARAM1=*,F12.7,*PARAM2=*,F12.7,*PARAM3=*,
     $F12.7)
   47 CONTINUE
      IF(ITAG.GT.1) GOTO 400
C     ITAG=1, READ IN PARAMETERS FOR OPTIMIZATION
      LOOKX=LOOK
      LOOK=10
      WRITE(6,200)
  200 FORMAT(* 2 OR 3 PARAMETER OPTIMIZATION?*)
      WRITE(6,205)
  205 FORMAT(* 2 PARAM OPTIMIZATION HOLDS DIST PRESSURE FIXED*)
      READ(5,215) NPAR
  215 FORMAT(I1)
  210 FORMAT(* *,I1)
      WRITE(6,210) NPAR
C     SET INITIAL GUESSES AND BOUNDS FOR PARAMETERS
C
      NOPAR(1)=1
      NAMEPA(1)=10HSLOPERATIO
      ORVAL(1)=.88
      ABOUND(1)=0.3
      BBOUND(1)=.99
C
      NOPAR(2)=2
      NAMEPA(2)=10HEQUAPROACH
      ORVAL(2)=0.9
      ABOUND(2)=0.0
      BBOUND(2)=0.99
C
C     FIND MINIMUM DISTILLATION PRESSURE FOR CONDENSATION
```

```
C
      PMIN=80.
      TCW=TCWI
      XDIST=XD
      WRITE(6,764) TCW
      WRITE(6,765) XDIST
  764 FORMAT(/* COOLING WATER TEMP. (DEG K)*,F7.2)
  765 FORMAT(* DISTILLATE MOLE FRACTION=*,F6.5)
      CALL BCPTM(PMIN,TCW,XDIST,XDIST,3)
      WRITE(6,220) PMIN
  220 FORMAT(* MINIMUM COLUMN PRESSURE TO CONDENSE PRODUCT =*,F5.2)
      IF(NPAR.NE.3) GOTO 300
      NOPAR(3)=3
      ORVAL(3)=(PMIN+150.)/100.
      ABOUND(3)=(PMIN+3.0)/100.
      BBOUND(3)=700./100.
      GOTO 310
  300 WRITE(6,230)
  230 FORMAT(* DISTILLATION COLUMN PRESSURE (MMHG)?*)
      READ(5,235) P
  235 FORMAT(F10.3)
  240 FORMAT(* *,F10.3)
  310 RETURN
  400 CONTINUE
C     FIND COST FOR GIVEN PARAMETERS
      IF(NPAR.NE.3) GOTO 410
      P=PARAM(3)*100.
  410 IF(ITAG.NE.3) GOTO 500
      LOOK=LCOKX
  500 TCOST=DISTL(PARAM(1),PARAM(2),P)
      ANVOL=330.*24.*D*(XD*46.+(1-XD)*18.)/(0.8*1000.)
      COST=100.*TCOST/ANVOL
      RETURN
      END
C
C
C
C
      SUBROUTINE MONIT(NPAR,X,COST,GC,ISTATE,GPJNRM,COND,
     $POSDEF,NITER,NF,IW,LIW,W,LW)
C
C     MONIT REPORTS ON THE PROGRESS OF THE OPTIMIZATION.
C     NO COMPUTATION TAKES PLACE IN MONIT.
C
      INTEGER ISTATE(3),IW(70),LIW,IW
      REAL X(3),GC(3),W(70)
      COMMON/DATA3/ LOOK,MODE(30)
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $CDLCAP,CDLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
      DATA N /0/
      IF(LOOK.GT.11) GOTO 500
      N=N+1
      WRITE(6,120) NPAR,NF,NITER
  120 FORMAT(/,* NPAR=*,I2,* NF=*,I4,*NITER=*,I4)
      WRITE(6,140) X(1),X(2),X(3)
  140 FORMAT(* PARAM1=*,F15.11,* PARAM2=*,F15.11,* PARAM3=*,F15.11)
```

```
      IF(N.LE.5) GOTO 400
      N=0
  200 WRITE(6,220) CSPCAP,CSPEFF
  220 FORMAT(* STRIPPER COSTS. CAPITAL=*,F10.2,
     $* ANNUAL=*,F10.2)
  230 WRITE(6,235) CSRCAP,CSPOP,CSREFF
  235 FORMAT(* STRIPPER REBOILER COSTS. CAPITAL=*,F10.2,* OPER=*,
     $F10.2,* ANNUAL=*,F10.2)
      WRITE(6,240) CHXCAP,CHXEFF
  240 FORMAT(* EXCHANGER COSTS. CAPITAL=*,F10.2,* ANNUAL=*,F10.2)
      WRITE(6,260) CPCCAP,CPCOP,CPCEFF
  260 FORMAT(* POST COOLER COSTS. CAPITAL=*,F10.2,* OP=*,F10.2,
     $* ANNUAL=*,F10.2)
      WRITE(6,280) CRBCAP,CRBOP,CRBEFF
  280 FORMAT(* REBOILER COSTS. CAPITAL=*,F10.2,* OP=*,F10.2,
     $* ANNUAL=*,F10.2)
      WRITE(6,300) CCNCAP,CCNOP,CCNEFF
  300 FORMAT(* CONDENSER COSTS. CAPITAL=*,F10.2,* OP=*,F10.2,
     $* ANNUAL=*,F10.2)
      WRITE(6,320) CDLCAP,CDLEFF
  320 FORMAT(* DIST COL COSTS. CAPITAL=*,F10.2,* ANNUAL=*,F10.2)
      WRITE(6,330) CLABR
  330 FORMAT(* LABOR COST=*,F10.2)
      WRITE(6,340) CTCAP,CTOP,CTEFF
  340 FORMAT(* TOTAL COSTS. CAPITAL=*,F12.2,* OP=*,F12.2,
     $* ANNUAL=*,F12.2)
  400 CONTINUE
      WRITE(6,160) COST
  160 FORMAT(* COST=*,F18.12,* CENTS/LITER*)
  500 CONTINUE
      RETURN
      END
C
C
C
C
      FUNCTION DISTL(RATIO,FRAC,P)
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $CDLCAP,CDLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
      COMMON/DATA3/ LOOK,MODE(30)
      REAL MAINT,INVEST
      COMMON /DLDTA/PO,TD,TDF,TDB,TDT,
     $B,D,FD,R,
     $XT,YT,TSLOPE,TINT,
     $RSLOPE,RINT,
     $SSLOPE,SINT,
     $XB,XFMIN,YFMIN,XFD,YFD,YRS,
     $DLSTAG,SSTAGE,DLDIAM,DLHGHT,
     $RATDL,ANVOL,RMIN,RRATIO,REFLUX
      COMMON /HXDTA/TSTEAM,AHX,NHX,DELQRB1,
     $APC,NPC,TCWOPC,CWFRPC,DELQPC,
     $ARB,NRB,STFRRB,DELQRB2,
     $ASR,NSR,DELQSTR,
     $ACN,NCN,TCWOCN,CWFRCN,DELQCN
      COMMON /INPUT/EMV,F,REFRACT,TCWI,XF,XD,FIRST1,FIRST2
      COMMON /DATA/MW(2),MIDWAY,CPG(5),CPL(2)
```

```
      REAL MW,MWETH,MWH2O
      EQUIVALENCE (MWETH,MW(1)),
     $(MWH2O,MW(2))
      COMMON /SPDTA/PS,TS,TSB,TST,
     $GS,GD,STFRSP,
     $SPSLOP,SPINT,
     $XL,YG,
     $SPSTAG,SPDIAM,SPHGHT,
     $PATSP
      EXTERNAL CROSS,STRIP,TPNT
      REAL L
      LOGICAL FIRST1,FIRST2
C
C     DISTL PERFORMS THE STAGE BY STAGE VACUUM DISTILLATION
C     COLUMN DESIGN.
C
      DATA MANHLS /2/
      DATA NOZLS /8/
      DATA THICK /0.375E0/
      DATA RHOL /1.0E0/
      DATA HETPR,DIAMR /0.833333E0,2.5E0/
      DATA FIRST1 /.TRUE./
      DATA FIRST2 /.TRUE./
      MODE(1)=2
C
      IF(LOOK.GT.2) GOTO 210

      WRITE(6,205)
  205 FORMAT(//,*   ENTERING FUNCTION DISTL*,/)
  210 CONTINUE
C
C     INITIAL PRESSURE AND OPERATING LINE RATIO
C
      PO =P
      IF(LOOK.GT.2) GOTO 220
      WRITE(6,215) PO,RATOL
  215 FORMAT(* DIST COLUMN PRES = *,F6.2,*(MMHG). OP RATIO =*,F6.4)
  220 CONTINUE
C
C     FIND THE TANGENT TO THE EQUILIB CURVE PASSING THRU (XD,YD)
C
      XT =ZERO(TPNT,XT,1,1.0E-5,0.50,XD,6HTPNT  )
C
C     FIND THE MINIMUM ALLOWABLE FEED COMPOSITION
C
      XFMIN =ZERO(CROSS,XFMIN,1,1.0E-5,0.0,XD,6HCROSS )
      IF(LOOK.GT.2) GOTO 230
      WRITE(6,225) XFMIN,XF
  225 FORMAT(* XFMIN=*,F6.5,* XFEED=*,F6.5)
  230 CONTINUE
C
C     CHECK THAT MOLE FRACTION OF ETHANOL IN FEED IS ABOVE MINIMUM
C     IF NOT: ADD A STRIPPING COLUMN
C
      WRITE(6,1917)
 1917 FORMAT(* ALLOW SINGLE COLUMN DESIGN? (0=YES, 1=NO).*)
      READ(5,1919) MODE(26)
 1919 FORMAT(I2)
C
C     IF MODE26=1. OVERRIDE PROGRAM DECISION AND USE TWO COLUMN
C     DESIGN.
C
```

```
      IF(MODE(26).EQ.1) GOTO 240
      IF(.NOT.(XF.LE.XFMIN))GOTO 30000
      IF(LOOK.GT.2) GOTO 240
      WRITE(6,235)
  235 FORMAT(* XFEED<XFMIN. STRIPPER REQUIRED*)
  240 CONTINUE
      IF(XF.GT.XFMIN) XFMIN=XF
      CALL STRIP(FRAC)
30002 GOTO 30001
30000 CONTINUE
      FD=F
      XFD=XF
      CSPCAP =0.0
      CSPOP =0.0
      CSPEFF =0.0
      STFRSP =0.0
      CHXCAP=0.0
      CHXEFF=0.0
      CPCCAP=0.0
      CPCOP=0.0
      CPCEFF=0.0
      CWFRPC=0.0
      CSREFF=0.0
      CSRCAP=0.0
30001 CONTINUE
C
C     CALCULATE DISTILLATE AND BOTTOM FLOW RATES
C
      D =RFRACT*FD*XFD/XD
      RATDL=(1.0/TSLOPE)+RATIO*(1.0-(1.0/TSLOPE))
      B =FD-D
      XB =(FD*XFD-D*XD)/B
C
C     FIND THE OPERATING LINES
C
      RSLOPE =RATDL*TSLOPE
      RRATIO=1.0/((1.0/RSLOPE)-1.0)
      RINT =XD*(1.0-RSLOPE)
      YRS =RSLOPE*XFD+RINT
      SSLOPE =(YRS-XB)/(XFD-XB)
      SINT =XB*(1.0-SSLOPE)
      IF(LOOK.GT.2) GOTO 260
      WRITE(6,242)
  242 FORMAT(///,*     DISTILLATION COLUMN DETAIL*,/)
      WRITE(6,245) RSLOPE,RINT
  245 FORMAT(* RECTIFYING SLOPE=*,F6.4,* INTERCEPT=*,F6.4)
      WRITE(6,255) SSLOPE,SINT
  255 FORMAT(* STRIPPING SLOPE=*,F6.4,* INTERCEPT=*,F6.4,/)
  260 CONTINUE
C
C     FIND TEMPERATURE OF SATURATED FEED, AND EQUILIBRIUM
C     ETHANOL VAPOR MOLE FRACTION
C
      YFD =YRS
      TDF =TD
      CALL BDPTM (PD,TDF,XFD,YFD,1)
C
C     CALCULATE REFLUX FLOW RATE
C
      R =D*RSLOPE/(1.0-RSLOPE)
      REFLUX=R
      IF(LOOK.GT.2.) GOTO 270
```

```
      WRITE(6,265) R
  265 FORMAT(* REFLUX FLOW (GMOL/HR)=*,E11.3)
  270 CONTINUE
C
C     SUCCESIVELY CALCULATE STAGES
C
      X =XD
      Y =XD
      DLSTAG =0.0
      RSTAGE =0.0
30003 IF(.NOT.(X.GT.XB))GOTO 30004
      DLSTAG =DLSTAG+1.0
      IF(.NOT.(DLSTAG.GT.1.0))GOTO 30005
C
C     DOWN TO OP LINE
C
      IF(.NOT.(X.GT.XFD))GOTO 30007
      Y =RSLOPE*X+RINT
      IF(LOOK.GT.2) GOTO 272
      WRITE(6,271) X,Y
  271 FORMAT(* RECTIFYING OPERATING LINE.  X=*,F6.5,*  Y=*,F6.5)
  272 CONTINUE
30009 GOTO 30008
30007 CONTINUE
      Y =SSLOPE*X+SINT
      IF(LOOK.GT.2) GOTO 280
      WRITE(6,275) X,Y
  275 FORMAT(* STRIPPING OPERATING LINE.  X=*,F6.5,*  Y=*,F6.5)
  280 CONTINUE
30008 CONTINUE
30005 CONTINUE
C
C     BACK TO EQUILIBRIUM CURVE
C
      XOLD =X
      CALL BOPTM (PO,TO,X,Y,2)
      IF(LOOK.GT.2) GOTO 290
      WRITE(6,285) X,Y
  285 FORMAT(* EQUILIBRIUM CURVE.  X=*F6.5,*  Y=*,F6.5)
  290 CONTINUE
      IF(.NOT.(DLSTAG.EQ.1.0))GOTO 30010
      TDT =TO
30010 CONTINUE
      IF(.NOT.(X.GT.XFD))GOTO 30012
      RSTAGE =RSTAGE+1.0
30014 GOTO 30013
30012 CONTINUE
      IF(.NOT.(XOLD.GT.XFD))GOTO 30015
      RSTAGE =RSTAGE+(XOLD-XFD)/(XOLD-X)
      SSTAGE =(XFD-X)/(XOLD-X)
30017 GOTO 30016
30015 CONTINUE
      SSTAGE =SSTAGE+1.0
30016 CONTINUE
30013 CONTINUE
      IF(.NOT.(X.LT.XB))GOTO 30018
      EXTRA =(XB-X)/(XOLD-X)
      DLSTAG =DLSTAG-EXTRA
      SSTAGE =SSTAGE-EXTRA
      X =XB
30018 CONTINUE
30020 GOTO 30003
```

```
30004 CONTINUE
      IF(LOOK.GT.2) GOTO 300
      WRITE(6,295) DLSTAG,SSTAGE
  295 FORMAT(/,* THEORETICAL RECT. STAGES=*,F3.0,* STRIP. STAGES=*,F3.0)
  300 CONTINUE
      TDB =TD
C
C     CALCULATE DISTILLATION COLUMN DIAMETER
C
      GD =R+C
      L =R+FD
      RHOG =MWH2O*PD/(62.36E3*TDB)
      GPRIME =SQRT(5.206E8*RHOG*(RHOL-RHOG)
     $*EXP(-0.6918*L*SQRT(RHOG/(RHOL-RHOG))/GD))
      GLBS =GD*MWH2O/454.0
      AREA =GLBS/GPRIME
      PI04=3.14159/4.0
      DLDIAM =SQRT(AREA/PI04)
C
C     CALCULATE DISTILLATION COLUMN HEIGHT
C
      HETP =HETPR*(1.0+0.7*ALOG10(DLDIAM/DIAMR))
      DLHGHT =(DLSTAG-1)*1.15*HETP+4.0
      IF(LOOK.GT.2) GOTO 310
      WRITE(6,305) DLDIAM,DLHGHT
  305 FORMAT(* DIST COLUMN DIAM (FT)=*,F4.2,*  HT=*,F4.2)
  310 CONTINUE
C
C     ESTIMATE CAPITAL COST OF DISTILLATION COLUMN
C
      DIAMO =DLDIAM+THICK/12.0
      WTSHEL=DLHGHT*3.14159*DIAMO*THICK*0.29*144.0
      WTOTAL=1.12*WTSHEL
C     STAINLESS STEEL CONSTRUCTION IF BEER IS HANDLED DIRECTLY
C     CARBON STEEL IF A CLEAN FEED FROM STRIPPER IS HANDLED
      EMAT=1.0
      IF(MODE(1).EQ.2) EMAT=2.0
      TOWCST=EMAT*(XMSI/569.)*87.16*(WTOTAL**0.6126)
      FITCST=EMAT*(XMSI/569.)*((MANHLS*95.)+(NOZLS*52.))
      TRYCST=2.0*(XMSI/569.)*33.*(DIAMO**1.737)
      SUPCST=EMAT*2.0*(XMSI/569.)*5.0*(DIAMO**1.737)
      PCKCST =(XMSI/569.)*PI04*DLDIAM*DLDIAM*DLHGHT*10.3
      COLCAP =4.89*(TOWCST+PCKCST+FITCST+SUPCST+TRYCST)
      COLEFF =CFACTR*COLCAP
C
C     CALCULATE REBOILER ENTHALPY CHANGE
C
      DELQRB =DELQ(R+C,XB,TDB,TDB)
      IF(.NOT.(CSPEFF.NE.0.0))GOTO 30021
C
C     CALCULATE CHANGE IN ENTHALPY TO PREPARE STRIPPER VAPOR
C     FOR FEED TO DISTILLATION COLUMN
C
      DELQFD =DELQ(FD,XFD,TST,TDF)
C
C     DESIGN HEAT EXCHANGER BTWN DIST COL FEED AND BOTTOMS
C     (REPLACES REBOILER WHEN STRIPPER IS USED)
C
C     IS ADDITIONAL HEATING REQUIRED FOR DIST COLUMN?
      DELQRB1=DELQRB
      IF(DELQRB.GT.DELQFD) DELQRB1=DELQFD
      CALL HXCNG (DELQRB1,400.0E0,TST,TST,TDB,TDB,AHX,NHX,CHXCAP)
```

```
      IF(LOOK.GT.2) GOTO 900
      WRITE(6,800)
  800 FORMAT(//,* INTER COLUMN EXCHANGER*)
      WRITE(6,810)TST,TDB
  810 FORMAT(* THOT (DEG K)=*,F6.2,* TCOLD=*,F6.2)
      WRITE(6,820) DELQRB1
  820 FORMAT(* DELQ (KCAL/HR)=*,E15.6)
      WRITE(6,830) AHX,NHX
  830 FORMAT(* EXCH AREAS (FT2)=*,F8.1,* NO. OF UNITS=*,I3)
  900 CONTINUE
      CHXEFF=CFACTR*CHXCAP
      IF(DELQRB.GT.DELQFD) GOTO 1700
C
C     DESIGN ADDITIONAL FEED PRECOOLER (TO SAT. LIQ. FEED TEMP.)
C
      IF(.NOT.(FIRST1))GOTO 30023
      TCWOPC =(TCWI+TDF)/2.0
      FIRST1=.FALSE.
30025 GOTO 30024
30023 CONTINUE
      TCWOPC =AMIN1(TCWOPC,TDF-1.0)
30024 CONTINUE
      DELQPC=DELQFD-DELQRB
      CALL CNDSR (DELQPC,4.0E2,TDF,TCWOPC,
     $APC,NPC,CWFRPC,CPCCAP,CPCOP,CPCEFF)
      IF(LOOK.GT.2) GOTO 1100
      WRITE(6,1000)
 1000 FORMAT(//,* POST COOLER*)
      WRITE(6,1010) TDF,TCWI,TCWOPC
 1010 FORMAT(* THOT (DEG K)=*,F6.2,* TCOLDIN=*,F6.2,* TCOLDOUT=*,F6.2)
      WRITE(6,1020)DELQPC
 1020 FORMAT(* DELTA Q (KCAL/HR)=*,E15.6)
      WRITE(6,1030)APC,NPC
 1030 FORMAT(* EXCH AREAS (FT2)=*,F8.1,* NO. OF UNITS=*,I3)
 1100 CONTINUE
C
C      ZERO REBOILER COSTS
C
      CRBCAP =0.0
      CRBOP =0.0
      CRBEFF =0.0
      STFRRB =0.0
30026 GOTO 30022
 1700 CONTINUE
C
C     SUPPLEMENTAL REBOILER REQUIRED
C
      DELQRB2=DELQRB-DELQFD
      GOTO 1710
C
C     NO STRIPPER: DESIGN STEAM FED REBOILER
C
30021 CONTINUE
      DELQRB2=DELQRB
C
C     SET INTER-COLUMN HEAT EXCHANGER COST TO ZERO
C      (NO STRIPPER USED)
C
      CHXCAP =0.0
      CHXEFF =0.0
 1710 CONTINUE
C
```

```
C     ZERO POST COOLER COSTS
C
      CPCCAP =0.0
      CPCOP =0.0
      CPCEFF =0.0
      CWFRPC =0.0
      CALL HXCNG (DELQRB2,3.5E2,TSTEAM,TSTEAM,TDB,TDB,ARB,NRB,CRBCAP)
C
C     S.S. REBOILER IF NO STRIPPER TO PURIFY FEED
C
      IF(MODE(1).NE.2) GOTO 1301
      CRBCAP=1.6*CRBCAP
 1301 CONTINUE
      IF(LOOK.GT.2)GOTO 1300
      WRITE(6,1200)
 1200 FORMAT(//,* DISTILLATION COLUMN REBOILER*)
      WRITE(6,1210) TSTEAM,TDB
 1210 FORMAT(* THOT (DEG K)=*,F6.2,* TCOLD=*,F6.2)
      WRITE(6,1220) DELQRB2
 1220 FORMAT(* DELTA Q (KCAL/HR)=*,E15.6)
      WRITE(6,1230)ARB,NRB
 1230 FORMAT(* EXCH AREAS (FT2)=*,F8.1,* NO. OF UNITS=*,I3)
 1300 CONTINUE
      CRBOP =STCST(STFRRB,DELQRB2,2)
      CRBEFF =CRBOP+CFACTR*CRBCAP
C
30022 CONTINUE
C
C     CAN*T CONDENSE PRODUCT - USE HIGHER COLUMN PRESSURE
C
      IF(.NOT.(TDT.LE.TCWI))GOTO 30027
      WRITE(6,10)
   10 FORMAT (/23H CAN*T CONDENSE PRODUCT/19H TDT LESS THAN TCWI/
     $20H USE HIGHER PRESSURE)
      STOP
30027 CONTINUE
C
C     CALCULATE REQUIRED CONDENSER ENTHALPY CHANGE
C
      DELQCN =DELQ(R+C,XD,TDT,TDT)
C
C     DESIGN FINAL PRODUCT CONDENSER
C
      IF(.NOT.(FIRST2))GOTO 30029
      TCWOCN =(TCWI+TDT)/2.0
      FIRST2=.FALSE.
30031 GOTO 30030
30029 CONTINUE
      TCWOCN =AMIN1(TCWOCN,TDT-1.0)
30030 CONTINUE
      CALL CNDSR (DELQCN,4.0E2,TDT,TCWOCN,ACN,NCN,CWFRCN,CCNCAP,CCNOP,CC
     $NEFF)
      IF(LOOK.GT.2) GOTO 1500
      WRITE(6,1400)
 1400 FORMAT(//,* PRODUCT CONDENSER*)
      WRITE(6,1410) TDT,TCWI,TCWOCN
 1410 FORMAT(* THOT (DEG K)=*,F6.2,* TCOLDIN=*,F6.2,* TCOLDOUT=*,F6.2)
      WRITE(6,1420) DELQCN
 1420 FORMAT(* DELTA Q (KCAL/HR)=*,E15.6)
      WRITE(6,1430)ACN,NCN
 1430 FORMAT(* EXCH AREAS (FT2)=*,F8.1,* NO. OF UNITS=*,I3)
 1500 CONTINUE
```

```
C
C     CALCULATE TOTAL DISTILLATION SYSTEM COST
C
C     .151 EMPLOYEE HR PER TON PRODUCT
C     P+T, FIG 5-8
      WORKERS=0.151*(D*46.*2.2/(2000.*1000.))
      CLABR=(XMSI/569.)*24.*330.*10.*WORKERS
      CTCAP =CSRCAP+CSPCAP+CHXCAP+CPCCAP+CDLCAP+CRBCAP+CCNCAP
      CTOP =CLABR+CSPOP+CPCOP+CRBOP+CCNOP
      CTEFF =CSREFF+CSPEFF+CHXEFF+CPCEFF+CDLEFF+CRBEFF+CCNEFF
      DISTL =CTEFF
      RETURN
      END
C
C
C
C
      BLOCK DATA DLDTA
      COMMON /DLDTA/PD,TD,TDF,TDB,TDT,
     $B,D,FD,R,
     $XT,YT,TSLOPE,TINT,
     $RSLOPE,RINT,
     $SSLOPE,SINT,
     $XB,XFMIN,YFMIN,XFD,YFD,YRS,
     $DLSTAG,SSTAGE,DLDIAM,DLHGHT,
     $RATDL,ANVOL,RMIN,RRATIO,REFLUX
C
C     INITIAL GUESS FOR PRESSURE IN DISTILLATION COLUMN (MMHG)
      DATA PD /170.0E0/
C     INITIAL GUESS FOR TEMPERATURE
      DATA TD /300.0E0/
C     INITIAL GUESS FOR SLOPE INCREASE RATIO IN DIST COLUMN
      DATA RATDL /1.1E0/
C     INITIAL GUESS FOR TANGENT POINT
      DATA XT /0.8E0/
      DATA YT /0.8E0/
      DATA XFMIN /0.05E0/
      END
C
C
C
C
      SUBROUTINE HXCNG (Q,U,THOTI,THOTO,TCLDI,TCLDO,AREA,NUMBER,COST)
C
C     DESIGN A HEAT EXCHANGER AND ESTIMATE ITS CAPITAL COST
C
C     Q IS THE HEAT TO BE TRANSFERED
C     U IS THE HEAT TRANSFER COEFICIENT IN BTU/(FT**2 HR DEG F)
C     THOTI, THOTO, ARE THE IN AND OUTGOING HOT STREAM TEMPS (DEG K)
C     TCLDI, TCLDO, ARE THE COLD STREAM TEMPS
C     AREA IS EXCHANGE ARE PER EXCHANGER (FT**2)
C     NUMBER IS THE NUMBER OF EXCHANGERS NEEDED
C     COST IS THE ESTIMATED CAPITAL COST
C
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $CDLCAP,CDLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
```

```
      COMMON/DATA3/ LOOK,MODE(30)
      REAL MAINT,INVEST
      DATA AMAX /5.0E3/
C
C     CALCULATE LOG MEAN DELTA T
C
      DELT1 =THOTI-TCLDO
      DELT2 =THOTO-TCLDI
      IF(.NOT.(DELT1.EQ.DELT2))GOTO 30000
      DTLM =DELT1
30002 GOTO 30001
30000 CONTINUE
      DTLM =(DELT1-DELT2)/ALOG(DELT1/DELT2)
30001 CONTINUE
C
C     CALCULATE AREA
C
      AREA =Q/(0.454*U*DTLM*FTLM(THOTI,THOTO,TCLDI,TCLDO,1))
C
C     CALCULATE NUMBER OF EXCHANGERS
C
      RATIO=AREA/AMAX
      NUMBER=RATIO
      IF (RATIO.GT.NUMBER) NUMBER=NUMBER+1
      AREA =AREA/NUMBER
C
C     ESTIMATE COST
C
      COST=4.89*NUMBER*(XMSI/569.)*331.*(AREA**0.5528)
      RETURN
      END
C
C
C
C
      BLOCK DATA HXDTA
      COMMON /HXDTA/TSTEAM,AHX,NHX,DELQRB1,
     $APC,NPC,TCWOPC,CWFRPC,DELQPC,
     $ARB,NRB,STFRRB,DELQRB2,
     $ASR,NSR,DELQSTR,
     $ACN,NCN,TCWOCN,CWFRCN,DELQCN
      DATA STFRRB /0.0E0/
      DATA TCWOPC /298.0/
      DATA CWFRPC /0.0E0/
      DATA CWFRCN /0.0E0/
      END
C
C
C
C
      BLOCK DATA INPUT
      COMMON /INPUT/EMV,F,RFRACT,TCWI,XF,XD,FIRST1,FIRST2
C
C     MURPHREE VAPOR EFFICIENCY
      DATA EMV /0.7E0/
C     FEED TO DISTILLATION SYSTEM (MOLES/HR, MOLE FRACTION)
      DATA F /1.0E6/
      DATA XF /0.01E0/
C     REQUIRED ETHANOL PRODUCT COMPOSITION (MOLE FRACTION)
      DATA XD /0.8814E0/
C     RECOVERY FRACTION
      DATA RFRACT /0.998/
```

```
C       COOLING WATER TEMPERATURE
        DATA TCWI /298.0E0/
        END
C
C
C
C
        BLOCK DATA MAINT
        COMMON /MAINT/IFLAG1
        DATA IFLAG1 /0/
        END
C
C
C
C
        BLOCK DATA MAINTX
        COMMON /MAINTX/IFLAG2,NOP
        DATA IFLAG2 /0/
        DATA NOP /1/
        END
C
C
C
C
        SUBROUTINE OPTIM (F,X,Y,DELTAX,DELTAY,XMIN,XMAX,YMIN,YMAX,NAME)
C
C       FINDS LOCAL MINIMUM OR MAXIMUM OF F(X,Y)
C       USING NEWTON-RAPHSON ALGORITHM
C
C       (X,Y) AS PASSED ON CALL IS THE INITIAL GUESS
C       DELTAX, DELTAY ARE USED FOR COMPUTING DERIVATIVES OF F WRT X,Y
C       XMIN, XMAX ARE MINIMUM AND MAXIMUM ALLOWABLE X VALUES
C       NAME IS THE NAME OF FUNCTION F (IN HOLERITH)
C
        EXTERNAL F
        COMMON/DATA3/ LOCK,MODE(30)
        DATA ABSTOL,RELTOL /1.0E-7,1.0E-4/
        DATA ITRMAX /200/
        IF(.NOT.(XMAX.LE.XMIN))GOTO 30000
        WRITE(6,10)NAME
   10   FORMAT (/37H OPTIM? XMAX LESS THAN XMIN (SOLVING ,A6,1H))
30000   CONTINUE
        IF(.NOT.(YMAX.LE.YMIN))GOTO 30002
        WRITE(6,20)NAME
   20   FORMAT (/37H OPTIM? YMAX LESS THAN YMIN (SOLVING ,A6,1H))
30002   CONTINUE
        IF(.NOT.(XMAX.LE.XMIN.OR.YMAX.LE.YMIN))GOTO 30004
        STOP
30004   CONTINUE
        OLDX =X
        OLDY =Y
        DO 30006 ITER=1,ITRMAX
        VALUE =PARTL(F,X,Y,DFDX,DFDY,D2FDX,D2FDY,D2FDXY,DELTAX,DELTAY,
       $XMIN,XMAX,YMIN,YMAX,NAME)
        DENOM =D2FDX*D2FDY-D2FDXY*D2FDXY/4.0
        DELX =(D2FDXY*DFDY-D2FDY*DFDX)/DENOM
        DELY =(D2FDXY*DFDX-D2FDX*DFDY)/DENOM
        X =X+DELX
        Y =Y+DELY
        IF(.NOT.(ABS(DELX).LT.RELTOL*AMIN1(ABS(X),ABS(OLDX))+ABSTOL.AND.AB
       $S(DELY).LT.RELTOL*AMIN1(ABS(Y),ABS(OLDY))+ABSTOL))GOTO 30008
        X=AMAX1(X,XMIN+DELTAX)
```

```
      X=AMIN1(X,XMAX-DELTAX)
      Y=AMAX1(Y,YMIN+DELTAY)
      Y=AMIN1(Y,YMAX-DELTAY)
      VALUE =F(X,Y)
      RETURN
30008 CONTINUE
      IF(.NOT.(X.LE.XMIN))GOTO 30010
      X =(XMIN+OLDX)/2.0
30012 GOTO 30011
30010 CONTINUE
      IF(.NOT.(X.GE.XMAX))GOTO 30013
      X =(XMAX+OLDX)/2.0
30013 CONTINUE
30011 CONTINUE
      IF(.NOT.(Y.LE.YMIN))GOTO 30015
      Y =(YMIN+OLDY)/2.0
30017 GOTO 30016
30015 CONTINUE
      IF(.NOT.(Y.GE.YMAX))GOTO 30018
      Y =(YMAX+OLDY)/2.0
30018 CONTINUE
30016 CONTINUE
      OLDX =X
      OLDY =Y
30006 CONTINUE
30007 CONTINUE
      WRITE(6,30)NAME,ITRMAX,X,Y,VALUE,DELX,DELY
   30 FORMAT (/31H OPTIM? NO CONVERGENCE SOLVING ,A6,7H AFTER ,I3,
     $11H ITERATIONS/
     $10H          X=,1PE10.3,4H, Y=,E10.3,4H, F=,E10.3,
     $7H, DELX=,E10.3,7H, DELY=,E10.3)
      RETURN
      END
C
C
C
C
      BLOCK DATA PARMS
      COMMON /PARMS/PAR(3)
      END
C
C
C
C
      FUNCTION PARTL(F,XO,YO,DFDX,DFDY,D2FDX,D2FDY,D2FDXY,DELTAX,DELTAY,
     $XMIN,XMAX,YMIN,YMAX,NAME)
C
C     CALCULATES PARTIAL DERIVATIVES.  SEE FUNCTION DIFFER FOR
C     EXPLANATION OF CALCULATIONAL METHOD.
C
      EXTERNAL F
      COMMON/DATA3/ LOOK,MODE(30)
      IF(.NOT.(XMAX-XMIN.LE.DELTAX+DELTAX))GOTO 30000
      WRITE(6,10)NAME
   10 FORMAT (/54H PARTL? XMAX-XMIN LESS THAN 2*DELTAX (DIFFERENTIATING
     $,
     $A6,1H))
30000 CONTINUE
      IF(.NOT.(YMAX-YMIN.LE.DELTAY+DELTAY))GOTO 30002
      WRITE(6,20)NAME
   20 FORMAT (/54H PARTL? YMAX-YMIN LESS THAN 2*DELTAY (DIFFERENTIATING
     $,
```

```
     $A6,1H))
30002 CONTINUE
      IF(.NOT.(XMAX-XMIN.LE.DELTAX+DELTAX.OR.YMAX-YMIN.LE.DELTAY+DELTAY)
     $)GOTO 30004
      STOP
30004 CONTINUE
      XM =XO-DELTAX
      XP =XO+DELTAX
      IF(.NOT.(XM.LE.XMIN))GOTO 30006
      XM =XO
30008 GOTO 30007
30006 CONTINUE
      IF(.NOT.(XP.GE.XMAX))GOTO 30009
      XP =XO
30009 CONTINUE
30007 CONTINUE
      DELX =XP-XM
      YM =YO-DELTAY
      YP =YO+DELTAY
      IF(.NOT.(YM.LE.YMIN))GOTO 30011
      YM =YO
30013 GOTO 30012
30011 CONTINUE
      IF(.NOT.(YP.GE.YMAX))GOTO 30014
      YP =YO
30014 CONTINUE
30012 CONTINUE
      DELY =YP-YM
      FMM =F(XM,YM)
      FOM =F(XO,YM)
      FPM =F(XP,YM)
      FMO =F(XM,YO)
      FPO =F(XP,YO)
      FMP =F(XM,YP)
      FOP =F(XO,YP)
      FPP =F(XP,YP)
      PARTL =F(XO,YO)
      DFDX =(FPO-FMO)/DELX
      DFDY =(FOP-FOM)/DELY
      D2FDX =(FPO-PARTL-PARTL+FMO)/(DELTAX*DELTAX)
      D2FDY =(FOP-PARTL-PARTL+FOM)/(DELTAY*DELTAY)
      D2FDXY =(FPP-FMP-FPM+FMM)/((DELTAX+DELTAX)*(DELTAY+DELTAY))
      RETURN
      END
C
C
C
C
      BLOCK DATA SPOTA
C
C     STRIPPING COLUMN DATA
C
      COMMON /SPOTA/PS,TS,TSB,TST,
     $GS,GO,STFRSP,
     $SPSLOP,SPINT,
     $XL,YG,
     $SPSTAG,SPDIAM,SPHGHT,
     $RATSP
C     PRESSURE
      DATA PS /760.0EC/
C     INITIAL GUESS FOR TEMPERATURE
      DATA TS /300.0EC/
```

```
      DATA RATSP /0.0/
      END
C
C
C
C
      FUNCTION STCST(RATE,Q,KIND)
C
C     COMPUTES REQUIRED STEAM FLOW RATE AND COST FOR A GIVEN
C     HEAT DUTY.
C
      COMMON /HXDTA/TSTEAM,AHX,NHX,DELQRB1,
     $APC,NPC,TCWOPC,CWFRPC,DELQPC,
     $ARB,NRB,STFRRB,DELQRB2,
     $ASR,NSR,DELQSTR,
     $ACN,NCN,TCWOCN,CWFRCN,DELQCN
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $CDLCAP,CDLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
      COMMON/DATA3/ LOOK,MODE(30)
      REAL MAINT,INVEST
      REAL LHEATW
C     50 PSIG SAT. STEAM
      DATA TSTEAM /420.3E0/
      IF(.NOT.(KIND.EQ.2))GOTO 30000
      CALL LHVAP (TSTEAM,DUMMY,LHEATW,HSOLN)
      RATE =Q/LHEATW
30000 CONTINUE
C     COST OF STEAM ($/1000 LB)
      STMCST=2.50
      STCST =(XMSI/569.0)*RATE*24.0*330.0*STMCST/454.0
      RETURN
      END
C
C
C
C
      SUBROUTINE STRIP(FRAC)
C
C     DESIGN A STRIPPING COLUMN ASSUMING CONST MOLAR FLOWS
C
      COMMON /HXDTA/TSTEAM,AHX,NHX,DELQRB1,
     $APC,NPC,TCWOPC,CWFRPC,DELQPC,
     $ARB,NRB,STFRRB,DELQRB2,
     $ASR,NSR,DELQSTR,
     $ACN,NCN,TCWOCN,CWFRCN,DELQCN
      COMMON /COSTS/CSPCAP,CSPOP,CSPEFF,
     $CHXCAP,CHXEFF,
     $CPCCAP,CPCOP,CPCEFF,
     $CDLCAP,CDLEFF,CSRCAP,CSREFF,
     $CRBCAP,CRBOP,CRBEFF,
     $CCNCAP,CCNOP,CCNEFF,
     $CTCAP,CTOP,CTEFF,CLABR,WORKERS,
     $XMSI,MAINT,DEPR,INVEST,LTAX,INSUR,TAX,CFACTR
      COMMON/DATA3/ LOOK,MODE(30)
      REAL MAINT,INVEST
      COMMON /DLDTA/PD,TD,TDF,TDB,TDT,
```

```
      $B,D,FD,R,
      $XT,YT,TSLOPE,TINT,
      $RSLOPE,RINT,
      $SSLOPE,SINT,
      $XB,XFMIN,YFMIN,XFD,YFD,YRS,
      $DLSTAG,SSTAGE,DLDIAM,DLHGHT,
      $RATDL,ANVOL,RMIN,RRATIO,REFLUX
       COMMON /INPUT/EMV,F,RFRACT,TCWI,XF,XD,FIRST1,FIRST2
       COMMON /DATA/MW(2),MIDWAY,CPG(5),CPL(2)
       REAL MW,MWETH,MWH2O
       EQUIVALENCE (MWETH,MW(1)),
      $(MWH2O,MW(2))
       COMMON /SPDTA/PS,TS,TSB,TST,
      $GS,GD,STFRSP,
      $SPSLOP,SPINT,
      $XL,YG,
      $SPSTAG,SPDIAM,SPHGHT,
      $RATSP
       DATA RHOL /1.0E0/
       DATA THICK /0.25/
       DATA EMAT /1.6E0/
       DATA MANHLS /2/
       DATA NOZLS /9/
       MODE(1)=3
       MODE(19)=0
C
       IF(LOOK.GT.3)GOTO 87
       WRITE(6,83)
   83  FORMAT(//,* ENTERING SUBROUTINE STRIP*)
   87  CONTINUE
C
C      CALCULATE BOTTOM LIQUID PRODUCT COMPOSITION (XL)
C
       XL =XF*(1.0-RFRACT)
C
C      CALCULATE VAPOR PRODUCT FLOW (GS), COMPOSITION (YG)
C
C      CAN A PRODUCT OF REQUIRED Y=XFMIN BE PRODUCED (1=NO)
       YGMAX=XF
       CALL BDPTM(PS,TS,XF,YGMAX,1)
       YGMIN=XFMIN*1.03
       IF(YGMAX.LT.YGMIN) MODE(19)=1
C      TOP PRODUCT COMPOSITION FOR THIS ITERATION
       YG=YGMIN+FRAC*(YGMAX-YGMIN)
C      VAPOR PRODUCT FLOW RATE
       GS=F*XF*RFRACT/YG
C
C      FIND OPERATING LINE
C
       SPSLOP=F/GS
       SPINT =-SPSLOP*XL
       IF(LOOK.GT.3)GOTO 12
       WRITE(6,4)
    4  FORMAT(//,*  STRIPPING COLUMN DETAIL*,/)
       WRITE(6,8)GS,YG
    8  FORMAT(* STRIPPER PROD FLOW (GMOLE/HR)=*,F12.3,* MOLE FRAC =*,
      $F5.4)
       WRITE(6,6) SPSLOP,SPINT
    6  FORMAT(* STRIPPER OP LINE SLOPE=*,F7.5,* INTERCEPT=*,F7.5,/)
   12  CONTINUE
       IF(MODE(19).LT.1) GOTO 105
       IF(LOCK.GT.6) GOTO 105
```

```
      WRITE(6,104)
  104 FORMAT(* WARNING, DISTILLATION FEED IS TOO DILUTE*)
      WRITE(6,134) XF,YG
  134 FORMAT(* XF=*,F6.5,*  YG=*,F6.5)
  105 CONTINUE
C
C     STEP OFF STAGES
C
      X =XL
      Y =0.0
      SPSTAG =0.0
30000 IF(.NOT.(Y.LT.YG))GOTO 30001
      SPSTAG =SPSTAG+1.0
      IF(.NOT.(SPSTAG.GT.1.0))GOTO 30002
C
C     ACROSS TO OPERATING LINE
C
      X =(Y-SPINT)/SPSLOP
      IF (LOCK.GT.2) GOTO 248
      WRITE(6,247) X,Y
  247 FORMAT(* OPERATING LINE, X=*,F6.5,* Y=*,F6.5)
  248 CONTINUE
30002 CONTINUE
C
C     UP TO EQUILIBRILM CURVE
C
      YOLD =Y
      CALL BOPTM (PS,TS,X,Y,1)
      IF (LOCK.GT.2) GOTO 258
      WRITE(6,256) X,Y
  256 FORMAT(* EQUILIB LINE, X=*,F6.5,* Y=*,F6.5)
  258 CONTINUE
      IF(.NOT.(SPSTAG.EQ.1.0))GOTO 30004
      TSB =TS
30004 CONTINUE
      Y =YOLD+EMV*(Y-YOLD)
      IF (LOCK.GT.2) GOTO 188
      WRITE(6,186) X,Y
  186 FORMAT(* WITH EMV, X=*,F6.5,* Y=*,F6.5)
  188 CONTINUE
      IF(.NOT.(Y.GT.YG))GOTO 30006
      SPSTAG =SPSTAG-(Y-YG)/(Y-YOLD)
      Y =YG
30006 CONTINUE
30008 GOTO 30000
30001 CONTINUE
C
C     SET OUTLET VAPOR FLOW TEMPERATURE
      TST=TS
C
C     SET FEED SPECIFICATIONS FOR DISTILLATION COLUMN
C
      FD =GS
      XFD =YG
C
C     ESTIMATE STRIPPER COLUMN DIAMETER
C
      RHOG =MWH2O*PS/(62.36E3*TST)
      UFLOOD=.347*EXP(-0.932*F*SQRT(RHOG/RHOL)/GS)/SQRT(RHOG/(RHOL-RHOG
     $))
      UACT =0.7*UFLOOD
      VEL =GS*MWH2O*9.811E-9/RHOG
```

```
      AREA =VEL/UACT
      PI04 =ATAN2(1.0E0,1.0E0)
      SPDIAM =SQRT(AREA/PI04)
      IF(LOOK.GT.3) GOTO 115
      WRITE(6,111) SPDIAM
  111 FORMAT(/,* STRIPPER DIAMETER=*,F7.3)
  115 CONTINUE
C
C     ESTIMATE CAPITAL COST
C
      SPHGHT =SPSTAG+SPSTAG+4.0
      WTSHEL=SPHGHT*3.14159*SPDIAM*THICK*0.29*144.
      WTOTAL=1.12*WTSHEL
C     S.S. STRIPPER
      TOWCST=2.0*(XMSI/569.)*87.16*(WTOTAL**0.6126)
      TRYCST=SPSTAG*(XMSI/569.)*33.*(SPDIAM**1.737)
      FITCST=2.0*(XMSI/569.)*((MANHLS*85.)+(NOZLS*52.))
      CSPCAP =4.89*(TOWCST+TRYCST+FITCST)
C
C     ESTIMATE OPERATING (STEAM) COST
C
      DELQSTR=DELQ(GS,XL,TSB,TSB)
      CALL HXCNG(DELQSTR,350.,TSTEAM,TSTEAM,TSB,TSB,ASR,NSR,
     $CSRCAP)
C     STAINLESS STEEL REBOILER
      CSRCAP=1.6*CSRCAP
      CSPOP=STCST(STERSP,DELQSTR,2)
      CSREFF=CSPOP+CFACTR*CSRCAP
      IF(LOOK.GT.2) GOTO 2200
      WRITE(6,2110)
 2110 FORMAT(//,* STRIPPER REBOILER*)
      WRITE(6,2120) TSTEAM,TSB
 2120 FORMAT(* THOT (DEG K)=*,F6.2,* TCOLD=*,F6.2)
      WRITE(6,2130) DELQSTR
 2130 FORMAT(* DELTA Q (KCAL/HR)=*,E15.5)
      WRITE(6,2140) ASR,NSR
 2140 FORMAT(* REBOILER AREAS (FT2)=*,F8.1,* NO. OF UNITS=*,I3)
 2200 CONTINUE
      IF(LOOK.GT.3) GOTO 125
      WRITE(6,121) STERSP
  121 FORMAT(* STRIPPER REBOILER STEAM FEED (KG/HR)=*,F6.2)
      WRITE(6,123) CSPOP
  123 FORMAT(* YEARLY STEAM COST=*,F11.2)
  125 CONTINUE
C
C     CALCULATE EFFECTIVE YEARLY COST
C
      CSPEFF =CFACTR*CSPCAP
      IF(LOOK.GT.3)GOTO 177
      WRITE(6,8) GS,YG
  177 CONTINUE
      RETURN
      END
C
C
C
C
      FUNCTION TPNT(X)
C
C     WHEN TPNT=0, X IS THE ETHANOL MOLE FRACTION AT THE OPERATING
C     LINE AND EQUILIBRIUM CURVE TANGENT POINT.
C
```

```
      COMMON /DLDTA/PC,TD,TDF,TDB,TDT,
     $B,D,FD,R,
     $XT,YT,TSLOPE,TINT,
     $RSLOPE,RINT,
     $SSLOPE,SINT,
     $XB,XFMIN,YFMIN,XFD,YFD,YRS,
     $DLSTAG,SSTAGE,DLDIAM,DLHGHT,
     $RATDL,ANVOL,RMIN,RRATIO,REFLUX
      COMMON/DATA3/ LCCK,MODE(30)
      COMMON /INPUT/EMV,F,RFRACT,TCWI,XF,XD,FIRST1,FIRST2
      DATA DELTA /5.0E-6/
      CALL BDPTM (PD,TD,X,YT,1)
      Y1 =YT
      CALL BDPTM (PD,TD,X-DELTA,Y1,1)
      Y2 =YT
      CALL BDPTM (PD,TD,X+DELTA,Y2,1)
      TSLOPE =(Y2-Y1)/(DELTA+DELTA)
      TINT =YT-TSLOPE*X
      DINT =XD*(1.0-TSLOPE)
      TPNT =(TINT-DINT)*100.
      RETURN
      END
C
C
C
C
      FUNCTION ZERO(F,XO,KIND,DELTA,XMIN,XMAX,NAME)
C
C     KIND=1:   FIND ROOT (0) OF F(X)
C         =2:   FIND LOCAL MINIMUM OR MAXIMUM
C
C     USES NEWTON-RAPHSON ALGORITHM
C
C     XO PASSED IN CALL IS USED AS INITIAL GUESS
C     DELTA IS USED IN COMPUTING THE DERIVATIVE OF F WRT X
C     XMIN, XMAX ARE MINIMUM AND MAXIMUM ALLOWABLE X VALUES
C     NAME IS THE NAME OF FUNCTION F (IN HOLERITH)
C
      EXTERNAL F
      COMMON/DATA3/ LCCK,MODE(30)
      DATA ABSTOL,RELTOL /5.0E-7,5.0E-4/
      DATA ITRMAX /40C/
      IF(.NOT.(XMAX.LE.XMIN))GOTO 30000
      WRITE(6,10)NAME
   10 FORMAT (/36H ZERO? XMAX LESS THAN XMIN (SOLVING ,A6,1H))
      STOP
30000 CONTINUE
      X =XO
      OLDX =X
      DO 30002 ITER=1,ITRMAX
      VALUE =DIFER(F,X,KIND,DIF1,DIF2,DELTA,XMIN,XMAX,NAME)
      IF(.NOT.(KIND.EQ.2))GOTO 30004
      DELX =-DIF1/DIF2
30006 GOTO 30005
30004 CONTINUE
      DELX =-VALUE/DIF1
30005 CONTINUE
      X =X+DELX
      IF(.NOT.(ABS(DELX).LT.RELTOL*AMIN1(ABS(X),ABS(OLDX))+ABSTOL))GOTO
     $30007
      IF(KIND.EQ.1.AND.ABS(VALUE).GT.(10.*ABSTOL)) GOTO 30007
 1000 X=AMAX1(X,XMIN+DELTA)
```

```
      X=AMIN1(X,XMAX-DELTA)
      VALUE =F(X)
      ZERO =X
      RETURN
30007 CONTINUE
      IF(.NOT.(X.LE.XMIN))GOTO 30009
      X =(XMIN+OLDX)/2.0
30011 GOTO 30010
30009 CONTINUE
      IF(.NOT.(X.GE.XMAX))GOTO 30012
      X =(XMAX+OLDX)/2.0
30012 CONTINUE
30010 CONTINUE
      OLDX =X
30002 CONTINUE
30003 CONTINUE
      WRITE(6,20)NAME,ITRMAX,X,VALUE,DELX
  20  FORMAT (/30H ZERO? NO CONVERGENCE SOLVING ,A6,7H AFTER ,I3,
     $11H ITERATIONS/
     $9H        X=,1PE10.3,4H, F=,E10.3,7H, DELX=,E10.3)
      GOTO 1000
      STOP
      END
C
C
C
C
      SUBROUTINE BOPTM (P,T,XETH,YETH,ITYPE)
C
C THIS SUBROUTINE PERFORMS ONE OF THE FOLLOWING CALCULATIONS...
C
C ITYPE=  1-BUBBLE POINT TEMPERATURE (GIVEN P,X-FIND T,Y)
C ITYPE=  2-DEW POINT TEMPERATURE    (GIVEN P,Y-FIND T,X)
C ITYPE=  3-BUBBLE POINT PRESSURE    (GIVEN T,X-FIND P,Y)
C ITYPE=  4-DEW POINT PRESSURE       (GIVEN T,Y-FIND P,X)
C
C FOR ITYPE=1 OR 2...
C THIS SUBROUTINE CALCULATES THE BUBBLE OR DEW TEMPERATURE (DEG K) FOR
C A GIVEN PRESSURE (MMHG) AND FEED COMPOSITION X(ITYPE=1) OR Y(ITYPE=2),
C IT RETURNS T (K) AND Y (ITYPE=1) OR X (ITYPE=2). A GUESSED T MUST BE
C SUPPLIED, BUT IF IT IS .LT. 200.0 OR .GT. 600.0, A GUESS OF 325.0
C WILL BE SUPPLIED.
C
C FOR ITYPE=3 OR 4...
C THIS SUBROUTINE CALCULATES THE BUBBLE OR DEW PRESSURE (MMHG) FOR A
C GIVEN TEMPERATURE (K) AND FEED COMPOSITION X(ITYPE=3) OR Y(ITYPE=4).
C IT RETURNS P (MMHG) AND Y(ITYPE=3) OR X(ITYPE=4). A GUESSED P MUST BE
C SUPPLIED, BUT IF IT IS .LT. 1.0E-4 .OR .GT. 76000.0, A GUESS OF 350.0
C WILL BE SUPPLIED.
C
C USES PASSED X AND Y AS INITIAL GUESS.
C
C SUBROUTINES TDEP, TXDEP, AND PDEP ARE CALLED.
C
C BOPTM IS BASED IN PART ON SUBROUTINES BUDET AND BUDEP,
C FOUND IN #COMPUTER CALCULATIONS FOR MULTICOMPONENT VAPOR-LIQUID AND
C LIQUID-LIQUID EQUILIBRIA# BY PRAUSNITZ,ANDERSON,GRENS,ECKERT,HSIEH,AND
C O,CONNELL,   PRENTICE-HALL, 1980.
C
      DIMENSION X(2),Y(2),DUMMY(2),E2(2),F6(3)
      COMMON/DATA3/ LOOK,MODE(30)
      REAL K(2)
```

```
      DATA ITMAX /40/
C
C CHECK VALIDITY OF INPUT PARAMETERS.
C
      IF (ITYPE .LT. 1 .OR. ITYPE .GT. 4) GO TO 510
      IF (ITYPE .GT. 2) GO TO 10
C
C CHECK FOR VALIDITY OF GUESSED T.
C
      IF (T .LT. 200.0 .OR. T .GT. 600.0) T=325.0
C
C CHECK FOR VALIDITY OF INPUT P.
C
      IF (P .GT. 1.0E-4 .AND. P .LT. 76000.0) GO TO 20
      IERROR=1
      GO TO 300
C
C CHECK FOR VALIDITY OF GUESSED P.
C
   10 IF (P .LT. 1.0E-4 .OR. P .GT. 76000.0) P=350.0
C
C CHECK FOR VALIDITY OF INPUT T.
C
      IF (T .GT. 200.0 .AND. T .LT. 600.0) GO TO 20
      IERROR=2
      GO TO 300
   20 IT=0
C
C  INITIALIZE X
C
      X(1)=XETH
      X(2)=1.0-X(1)
C
C INITIALIZE Y
C
      Y(1)=YETH
      Y(2)=1.0-Y(1)
C
C TOP OF ITERATION LOOP
C
   40 IT=IT+1
      IF (IT .LT. ITMAX) GO TO 50
      IERROR=3
      GO TO 300
C
C GET K VALUES FOR P,T,X,Y
C
   50 IF (ITYPE .EQ. 4 .AND. IT .GT. 1) GO TO 55
      IF (ITYPE .EQ. 3 .AND. IT .GT. 1) GO TO 56
      CALL TDEP (T)
   55 CALL TXDEP (T,X)
   56 CALL PDEP (P,T,Y,K)
C
C CALCULATE SUM OF KX (BP) OR Y/K (DP).
C
      S=0.0
      DO 80 I=1,2
         IF (ITYPE .EQ. 2 .OR. ITYPE .EQ. 4) GO TO 60
         DUMMY(I)=K(I)*X(I)
         GO TO 70
   60    DUMMY(I)=Y(I)/K(I)
   70    S=S+DUMMY(I)
```

```
   80  CONTINUE
C
C BRANCH TO TWO METHODS OF CONVERGENCE FOR BUBDEWT AND BUBDEWP.
C
       IF (ITYPE .GT. 2) GO TO 160
       F1=ALOG(S)
C
C CHECK FOR CONVERGENCE.
C
       IF (ABS(F1) .LT. 5.0E-9) GO TO 130
C
C FIND K VALUES AT T+1.0 FOR FINITE DIFFERENCE DERIVITIVE.
C
       CALL TDEP (T+1.0)
       CALL TXDEP (T+1.0,X)
       CALL PCEP (P,T+1.0,Y,K)
       SS=0.0
       IF (ITYPE .EQ. 2) GO TO 100
C
C CALCULATE NEW VAPOR COMPOSITION FOR BP AND SUM OF KX AT T+1.0.
C
       DO 90 I=1,2
          Y(I)=DUMMY(I)/S
          SS=SS+K(I)*X(I)
   90  CONTINUE
       GO TO 120
C
C CALCULATE NEW VAPOR COMPOSITION FOR DP AND SUM OF Y/K AT T+1.0.
C
  100  DO 110 I=1,2
          X(I)=DUMMY(I)/S
          SS=SS+Y(I)/K(I)
  110  CONTINUE
  120  F2=ALOG(SS)
C
C CALCULATE NEW NEWTON-RAPHSON TEMPERATURE
C
       T=(F2-F1)*T/(F2-T*F1/(T+1.0))
C
C BREAK LOOP IF T IS GETTING OUT OF RANGE.
C
       IF (T .GT. 100.0 .AND. T .LT. 1000.0) GO TO 40
       IERROR=4
       GO TO 300
C
C NORMALIZE CONVERGED X OR Y.
C
  130  DO 150 I=1,2
          IF (ITYPE .EQ. 2) GO TO 140
          Y(I)=DUMMY(I)/S
       GO TO 150
  140     X(I)=DUMMY(I)/S
  150  CONTINUE
       GO TO 900
  160  IF (ITYPE .EQ. 4) GO TO 180
       DO 170 I=1,2
          Y(I)=DUMMY(I)/S
  170  CONTINUE
       GO TO 200
  180  DO 190 I=1,2
          X(I)=DUMMY(I)/S
  190  CONTINUE
```

```
 200  IF (S .LT. 5.0 .AND. S .GT. 0.2) GO TO 220
      IF (S .LT. 1.0) GO TO 210
      S=5.0
      GO TO 220
 210  S=0.2
 220  IF (ITYPE .EQ. 4) GO TO 230
      P=P*S
      GO TO 240
 230  P=P/S
 240  IF (P .GT. 1.0E-4 .AND. P .LT. 76000.0) GO TO 250
      IERROR=5
      GO TO 300
 250  IF (ABS(S-1.0) .LT. 5.0E-9) GO TO 900
      GO TO 40
C
C PRINT AN ERROR MESSAGE.
C
 300  IF (ITYPE .GT. 2) GO TO 310
      E1=1HP
      E2(1)=4HMM O
      E2(2)=4HF HG
      E5=4HTEMP
      GO TO 320
 310  E1=1HT
      E2(1)=4HDEG
      E2(2)=1HK
      E5=4HPRES
 320  IF (ITYPE .EQ. 2 .OR. ITYPE .EQ. 4) GO TO 330
      E3=1HX
      E4=3H2BL
      GO TO 340
 330  E3=1HY
      E4=3HDEW
 340  GO TO (350,360,370,380,390), IERROR
 350  E6(1)=4HINPU
      E6(2)=4HT PR
      E6(3)=2HES
      GO TO 400
 360  E6(1)=4HINPU
      E6(2)=4HT TE
      E6(3)=2HMP
      GO TO 400
 370  E6(1)=4HNUMB
      E6(2)=4H. IT
      E6(3)=2HER
      GO TO 400
 380  E6(1)=4HCALC
      E6(2)=4H. TF
      E6(3)=2HMP
      GO TO 400
 390  E6(1)=4HCALC
      E6(2)=4H. PR
      E6(3)=2HES
 400  GO TO (410,420,440,450), ITYPE
 410  WRITE (6,470) E1,P,E2(1),E2(2),E3,X(1),E4,E5,(E6(I),I=1,3)
      GO TO 430
 420  WRITE (6,470) E1,P,E2(1),E2(2),E3,Y(1),E4,E5,(E6(I),I=1,3)
 430  T=0.0
      GO TO 1000
 440  WRITE (6,470) E1,T,E2(1),E2(2),E3,X(1),E4,E5,(E6(I),I=1,3)
      GO TO 460
 450  WRITE (6,470) E1,T,E2(1),E2(2),E3,Y(1),E4,E5,(E6(I),I=1,3)
```

```
 460  P=0.0
      GO TO 1000
 470  FORMAT (/1X,*AT *,A1,*=*,F10.5,* *,2A4,* AND *,A1,*(1)=*,F8.5,*, *,
     2        A3,* POINT *,A4,* HAS NOT BEEN*/1H ,*CALCULATED BECAUSE *,
     2        2A4,A2,* EXCEEDS ITS ALLOWED RANGE IN SUBR. BOPTM.*/)
C
C ITYPE HAS NOT BEEN INPUT PROPERLY.
C
 510  WRITE (6,520)
 520  FORMAT (/1H ,*SUBR. BOPTM ABORTED BECAUSE ITYPE WAS SET WRONG.*/)
      GO TO 1000
C
C  STORE RESULTS IN PASSED ARGUMENTS
C
 900  XETH=X(1)
      YETH=Y(1)
C
C  EXIT
C
 1000 RETURN
      END
C
C
C
C
      SUBROUTINE PDEP (P,T,Y,K)
C
C THIS SUBROUTINE CALCULATES K,S AS FUNCTIONS OF P,T,Y AND TDEP VARIBLES.
C THIS SUBROUTINE SHOULD BE CALLED ANYTIME P,T,X,OR Y ARE CHANGED, SINCE
C THE K VALUES ARE DEPENDENT ON GAMMA(T,X), P, AND T.
C T IS EXPRESSED IN DEGREES KELVIN, AND P IS EXPRESSED IN MMHG.
C PDEP IS BASED IN PART ON SUBROUTINES PHIS2 AND VPLOK,
C FOUND IN -COMPUTER CALCULATIONS FOR MULTICOMPONENT VAPOR-LIQUID AND
C LIQUID-LIQUID EQUILIBRIA- BY PRAUSNITZ,ANDERSON,GRENS,ECKERT,HSIEH,AND
C O.CONNELL.   PRENTICE-HALL. 1980.
C
      DIMENSION PHI(2),Y(2)
      COMMON/DATA3/ LOOK,MODE(30)
      COMMON /SUBT/ VLIQ(2),F(2),B(3)
      COMMON /SUBTX/ GAMMA(2)
      REAL K(2)
C CONVERT P FROM MMHG TO BARS, WHICH IS THE UNIT USED BY TDEP TO FIND
C ZERO PRESSURE REFERENCE FUGACITY.
      P=P*1.01325/760.0
      PRT=P/(T*83.1473)
      BM=Y(1)*Y(1)*B(1)+Y(2)*Y(2)*B(3)+2.0*Y(1)*Y(2)*B(2)
      PHI(1)=EXP((2.0*(Y(1)*B(1)+Y(2)*B(2))-BM)*PRT)
      PHI(2)=EXP((2.0*(Y(2)*B(3)+Y(1)*B(2))-BM)*PRT)
      DO 20 I=1,2
         K(I)=GAMMA(I)*F(I)*EXP(PRT*VLIQ(I))/(PHI(I)*P)
   20 CONTINUE
C CONVERT P BACK TO MMHG FROM BARS.
      P=P*760.0/1.01325
      RETURN
      END
C
C
C
C
      BLOCK DATA SUBT
      COMMON /SUBT/ VLIQ(2),F(2),B(3)
      END
```

```
C
C
C
C
      BLOCK DATA SUBTX
      COMMON /SUBTX/ GAMMA(2)
      END
C
C
C
C
      SUBROUTINE TDEP (T)
C
C THIS SUBROUTINE CALCULATES ALL THE TEMPERATURE DEPENDENT VARIABLES.
C THESE ARE- LIQUID MOLAR VOLUMES,ZERO PRESSURE REFERENCE FUGACITIES,
C AND VIRIAL COEFFICIENTS. TEMPERATURE IS EXPRESSED IN DEGREES KELVIN.
C THIS SUBROUTINE MUST BE CALLED EACH TIME A NEW T IS USED.
C IN ADDITION, SUBROUTINE TXDEP SHOULD ALSO BE CALLED, BECAUSE ACTIVITY
C COEFFICIENTS ARE FUNCTIONS OF T AS WELL AS X.
C IF THIS SUBROUTINE IS USED, IFLAG1 MUST BE COMMONED TO THE MAIN
C PROGRAM. IFLAG1 =0 WHEN THE SUBROUTINE IS USED FOR THE FIRST TIME.
C TDEP IS BASED IN PART ON SUBROUTINES MVOLM,REFUG,AND BIJS2.
C FOUND IN -COMPUTER CALCULATIONS FOR MULTICOMPONENT VAPOR-LIQUID AND
C LIQUID-LIQUID EQUILIBRIA- BY PRAUSNITZ,ANDERSON,GRENS,ECKERT,HSIEH,AND
C O.CONNELL.   PRENTICE-HALL, 1980.
C
      DIMENSION C1(2),C2(2),C3(2),C4(2),C5(2),PC(2),TC(2),ZRA(2),
     2          RD(2),DM(2),ETA(3),W(3),SGM(3),EOK(3),ROP(3),A(3),DH(3),
     3          E(3),EC(3),BD(3)
      COMMON /MAINT/ IFLAG1
      COMMON/DATA3/ LOCK,MODE(30)
      COMMON /SUBT/ VLIQ(2),F(2),B(3)
      IF (IFLAG1 .GT. 0) GO TO 100
C INITIALIZE CONSTANTS FOR ETHANOL (1) AND WATER (2).
C CRITICAL TEMPERATURES (DEG K) AND PRESSURES (BARS).
      TC(1)=516.26
      TC(2)=647.37
      PC(1)=63.80
      PC(2)=221.20
C ZERO PRESS. REF. FUGACITY (BARS) EQUATION CONSTANTS FOR ETHANOL.
      C1(1)=-90.909918893565
      C2(1)=-3465.8734683496
      C3(1)=-0.06230139174076 8
      C4(1)=20.486492956207
      C5(1)=0.0000206642210427 73
C ZERO PRESS. REF. FUGACITY (BARS) EQUATION CONSTANTS FOR WATER.
      C1(2)=57.041597918252
      C2(2)=-7004.8416152596
      C3(2)=0.0035888444369749
      C4(2)=-6.6669397843423
      C5(2)=-0.0000008505428734 4029
C DIPOLE MOMENT (DEBYES).
      DM(1)=1.69
      DM(2)=1.83
C MEAN RADIUS OF GYRATION (ANGSTROMS).
      RD(1)=2.25
      RD(2)=0.615
C RACKETT PARAMETERS FOR SATURATED-LIQUID MOLAR VOLUME CORRELATION.
      ZRA(1)=0.2520
      ZRA(2)=0.2380
C ASSOCIATION PARAMETER FOR ETHANOL.
      ETA(1)=1.40
```

```
C SOLVATION PARAMETER FOR ETHANOL-WATER BINARY.
      ETA(2)=1.55
C ASSOCIATION PARAMETER FOR WATER.
      ETA(3)=1.70
      EX=0.28571429
C CALCULATE TEMP. DEPENDENT PURE-COMPONENT PARAMETERS (SUB. BIJS2).
      DO 10 I=1,2
         J=(I+1)*I/2
         W(J)=RD(I)*(RD(I)*(-0.001366*RD(I)+0.02096)+0.006026)
         EOK(J)=TC(I)*(0.748+0.91*W(J))
         EOK(J)=EOK(J)-TC(I)*0.4*ETA(J)/(2.0+20.0*W(J))
         SGM(J)=(2.4507-W(J))**3*TC(I)/PC(I)
C ANGLE AVERAGING IS USED TO ACCOUNT FOR THE EFFECT OF POLARITY DUE TO
C A LARGE DIPOLE ON THE ENERGY AND SIZE PARAMETERS.
         PN=16.0+400.0*W(J)
         P1=PN/(PN-6.0)
         P2=3.0/(PN-6.0)
         CONT=2.882-1.882*W(J)/(0.03+W(J))
         XI=1.7941E07*DM(I)**4/(CONT*EOK(J)*SGM(J)**2*TC(I))
         EOK(J)=EOK(J)*(1.0-XI*P1+P1*(1.0+P1)*XI*XI/2.0)
         SGM(J)=SGM(J)*(1.0+XI*P2)
         RDP(J)=7243.8*DM(I)**2/(EOK(J)*SGM(J))
   10 CONTINUE
C CALCULATE TEMPERATURE INDEPENDENT CROSS PARAMETERS.
      IJ=2
      I=1
      J=3
      W(IJ)=0.5*(W(I)+W(J))
      EOK(IJ)=0.7*SQRT(EOK(I)*EOK(J))+0.6/(1.0/EOK(I)+1.0/EOK(J))
      SGM(IJ)=SQRT(SGM(I)*SGM(J))
      RDP(IJ)=7243.8*DM(1)*DM(2)/(EOK(IJ)*SGM(IJ))
C CALCULATE REMAINDER OF TEMPERATURE INDEPENDENT PARAMETERS.
      DO 40 I=1,3
         BO(I)=1.2618*SGM(I)
         A(I)=-0.3-0.C5*RDP(I)
         DH(I)=1.99+0.2*RDP(I)**2
C CALCULATE THE MODIFIED REDUCED DIPOLE TO BE USED IN CALCULATING THE
C FREE-POLAR CONTRIBUTION TO THE VIRIAL COEFFICIENT.
         IF (RDP(I) .LT. 0.25) GO TO 20
         RDP(I)=RDP(I)-0.25
         GO TO 30
   20    IF (RDP(I) .LT. 0.04) GO TO 30
         RDP(I)=0.0
C CALCULATE E(IJ) VALUES FOR EACH ETA(IJ).
   30    E(I)=ETA(I)*(650.0/(EOK(I)+300.0)-4.27)
   40 CONTINUE
      IFLAG1=1
  100 CONTINUE
C CALCULATE LIQUID MOLAR VOLUMES (FROM SUB. MVOLM).
      DO 130 I=1,2
         TR=T/TC(I)
         IF (TR .GT. 0.75) GO TO 110
         TAU=1.0+(1.0-TR)**EX
         GO TO 120
  110    TAU=1.6+6.93026E-3/(TR-0.655)
  120    VLIQ(I)=83.1473*TC(I)*ZRA(I)**TAU/PC(I)
  130 CONTINUE
C CALCULATE ZERO PRESSURE REFERENCE FUGACITIES (FROM SUB. REFUG).
      DO 140 I=1,2
         F(I)=EXP(C1(I)+C2(I)/T+C3(I)*T+C4(I)*ALOG(T)+C5(I)*T**2)
  140 CONTINUE
C CALCULATE THE SECOND VIRIAL COEFFICIENTS (FROM SUB. BIJS2).
```

```
      DO 160 I=1,3
         TS=T/EOK(I)
         TSP=1.0/TS-1.6*W(I)
C CALCULATE THE FREE CONTRIBUTION TO THE SECOND VIRIAL COEFFICIENT.
         B(I)=0.94-1.47*TSP-0.85*TSP**2+1.015*TSP**3
         IF (ROP(I) .LT. 1.0E-19) GO TO 150
         B(I)=B(I)-ROP(I)*(0.75-3.0*TSP+2.1*TSP**2+2.1*TSP**3)
 150     B(I)=BO(I)*B(I)
C CALCULATE THE METASTABLE, BOUND, AND CHEMICAL CONTRIBUTIONS.
         BO(I)=A(I)*EXP(DH(I)/TS)
         BO(I)=BO(I)+EXP(E(I))-EXP(1500.0*ETA(I)/T+E(I))
         BO(I)=BO(I)*BO(I)
         B(I)=B(I)+BO(I)
 160  CONTINUE
      RETURN
      END
C
C
C
C
      SUBROUTINE TXDEP (T,X)
C
C THIS SUBROUTINE CALCULATES THE ACTIVITY COEFFICIENTS, WHICH ARE
C FUNCTIONS OF T AND X.  IT SHOULD BE CALLED ANYTIME T OR X ARE CHANGED.
C
C T IS EXPRESSED IN DEGREES KELVIN. TXDEP IS PARTIALLY BASED ON ACTIV2,
C FOUND IN #COMPUTER CALCULATIONS FOR MULTICOMPONENT VAPOR-LIQUID AND
C LIQUID-LIQUID EQUILIBRIA# BY PRAUSNITZ,ANDERSON,GRENS,ECKERT,HSIEH,AND
C O.CONNELL.   PRENTICE-HALL, 1980.
C
C IF THIS SUBROUTINE IS USED, IFLAG2 AND NOP MUST BE COMMONED TO THE
C MAIN PROGRAM. IFLAG2=0 WHEN THE SUBROUTINE IS CALLED FOR THE FIRST
C TIME. NOP=1  FOR THE 2-PARAMETER UNIQUAC
C          =2  FOR THE 3-PARAMETER UNIQUAC
C          =3  FOR THE 3-PARAMETER NRTL
C FIT OF ACTIVITY COEFFICIENTS.
C
      DIMENSION R(2),Q(2),QP(2),X(2)
      COMMON /MAINTX/ IFLAG2,NOP
      COMMON/DATA3/ LOCK,MODE(30)
      COMMON /SUBTX/ GAMMA(2)
      COMMON /PARMS/ PAR(3)
      REAL LG1,LG2
C
C COEFFICIENTS FOR 3-PARAMETER UNIQUAC FIT
C
      DATA CTHO,CTH1 /-16.03058823E0, 0.0470588235 3E0/
      DATA CP10,CP11,CP12,CP13,CP14,CP15
     1     /-89.32844525E0, 24.27541863E0, 68.698815592E0,
     2      14.5937136E0, -10.42198857E0, -4.522048302E0/
      DATA CP20,CP21,CP22,CP23,CP24,CP25,CP26
     1     /327.3816357E0, 198.6002199E0, 152.9937678E0, -8.512191087E0,
     2      -58.2073705E0, 0.7547851961E0, 7.061925131E0/
      DATA CP30,CP31,CP32,CP33,CP34,CP35,CP36
     1     /1.3325301106E0, -0.7627075015E0, -0.3210071756E0,
     2      0.2267275941E0, 0.1384721276E0, -0.0313666795E0,
     3      -0.0170849291E0/
C
      IF (IFLAG2 .GT. 0) GO TO 10
C INITIALIZE CONSTANTS FOR ETHANOL (1) AND WATER (2).
C STRUCTURAL VOLUME PARAMETERS FOR UNIQUAC EQUATION.
      R(1)=2.1
```

```
      R(2)=0.92
C STRUCTURAL AREA PARAMETERS FOR UNIQUAC EQUATION.
      Q(1)=1.97
      Q(2)=1.40
C MODIFIED STRUCTURAL AREA PARAMETERS FOR UNIQUAC EQUATION.
      QP(1)=0.92
      QP(2)=1.00
      IFLAG2=1
   10 CONTINUE
C  CALCULATE PARAMETERS AND ACTIVITY COEFFICIENTS (FROM SUB. ACTIV2).
      IF (NOP .GT. 1) GO TO 20
C EQUATIONS FOR PARAMETERS OF 2-PARAMETER UNIQUAC FIT.
C INSERT FUNCTION FOR PARAMETER 1 HERE
      PAR(1)=-10845.0108153+144.454638358*T-0.692588910446*T**2+
     2        0.00143455625212*T**3-1.096233611E-6*T**4
C INSERT FUNCTION FOR PARAMETER 2 HERE
      PAR(2)=38765.541772-475.052110708*T+2.14108540923*T**2-
     2        0.00420316593674*T**3+3.054583612E-6*T**4
      PAR(3)=1.0
      GO TO 30
   20 IF (NOP .GT. 2) GO TO 40
C EQUATIONS FOR PARAMETERS OF 3-PARAMETER UNIQUAC FIT.
      THETA=CTH0+CTH1*T
C INSERT FUNCTION FOR PARAMETER 1 HERE
      PAR(1)=CP10+THETA*(CP11+THETA*(CP12+THETA*(CP13+THETA*(CP14
     1        +THETA*CP15))))
C INSERT FUNCTION FOR PARAMETER 2 HERE
      PAR(2)=CP20+THETA*(CP21+THETA*(CP22+THETA*(CP23+THETA*(CP24
     1        +THETA*(CP25+THETA*CP26)))))
C INSERT FUNCTION FOR PARAMETER 3 HERE
      PAR(3)=CP30+THETA*(CP31+THETA*(CP32+THETA*(CP33+THETA*(CP34
     1        +THETA*(CP35+THETA*CP36))))
C NOW CALCULATE ACTIVITY COEFFIENTS FOR UNIQUAC FIT.
   30 T12=EXP(-PAR(1)/T)
      T21=EXP(-PAR(2)/T)
      EL1=5.0*(R(1)-Q(1))-(R(1)-1.0)
      EL2=5.0*(R(2)-Q(2))-(R(2)-1.0)
      PHS=X(1)*R(1)+X(2)*R(2)
      PH1=X(1)*R(1)/PHS
      PH2=1.0-PH1
      THS=X(1)*Q(1)+X(2)*Q(2)
      THP1=X(1)*QP(1)/(X(1)*QP(1)+X(2)*QP(2))
      THP2=1.0-THP1
      S1=THP2+THP1*T12
      S2=THP1+THP2*T21
      LG1=ALOG(R(1)/PHS)+5.0*Q(1)*ALOG(Q(1)*PHS/R(1)/THS)+
     2     PH2*(EL1-EL2*R(1)/R(2))
      LG1=LG1+PAR(3)*QP(1)*(-ALOG(S2)+THP2*(T21/S2-T12/S1))
      LG2=ALOG(R(2)/PHS)+5.0*Q(2)*ALOG(Q(2)*PHS/R(2)/THS)+
     2     PH1*(EL2-EL1*R(2)/R(1))
      LG2=LG2+PAR(3)*QP(2)*(-ALOG(S1)+THP1*(T12/S1-T21/S2))
      GO TO 100
C  3-PARAMETER NRTL
   40 CONTINUE
C INSERT FUNCTION FOR PARAMETER 1 HERE
C INSERT FUNCTION FOR PARAMETER 2 HERE
C INSERT FUNCTION FOR PARAMETER 3 HERE
      T12=PAR(1)/(1.987*T)
      T21=PAR(2)/(1.987*T)
      G12=EXP(-PAR(3)*T12)
      G21=EXP(-PAR(3)*T21)
      GS12=(X(2)+X(1)*G12)**2
```

```
      GS21=(X(1)+X(2)*G21)**2
      LG1=X(2)**2*(T21*G21**2/GS21+T12*G12/GS12)
      LG2=X(1)**2*(T12*G12**2/GS12+T21*G21/GS21)
100   GAMMA(1)=EXP(LG1)
      GAMMA(2)=EXP(LG2)
      RETURN
      END
```

Appendix 2

COMPUTER GENERATED DISTILLATION DESIGN

```
 ENTER THE ANNUAL PRODUCTION RATE (MILLIONS OF L)
102.
 PVOL=   102000000.000 LITERS PER YEAR
 ENTER THE FEED ETHANOL WEIGHT FRACTION
0.06
 FEED WEIGHT FRACTION=.0600
 FEED ETHANOL (G/HR)=  9787878.79 WATER=153343434.34
 ENTER THE MARSHALL STEVENS COST INDEX
717.0
     717.0000000
 ENTER THE TEMPERATURE OF PROCESS COOLING WATER (K)
291.48

 EXTENT OF DETAIL NEEDED? (1-9)
2

 ENTERING FUNCT. ITAG= 1

 NPAR=-IPARAM1=-INDEF      PARAM2=-INDEF      PARAM3=-INDEF
 2 OR 3 PARAMETER OPTIMIZATION?
 2 PARAM OPTIMIZATION HOLDS DIST PRESSURE FIXED
3
 3

 COOLING WATER TEMP. (DEG K) 291.48
 DISTILLATE MOLE FRACTION=.88140
 MINIMUM COLUMN PRESSURE TO CONDENSE PRODUCT =39.62


   ENTERING FUNCTION DISTL

 DIST COLUMN PRES = 169.74(MMHG), OP RATIO =1.1000
 XFMIN=.04509 XFHED=.02436
 ALLOW SINGLE COLUMN DESIGN? (0=YES, 1=NO).
0
 XFEED<XFMIN, STRIPPER REQUIRED


 ENTERING SUBROUTINE STRIP


  STRIPPING COLUMN DETAIL

 STRIPPER PROD FLOW (GMOLE/HR)= 1027877.273 MOLE FRAC =.2063
 STRIPPER OP LINE SLOPE=8.48553 INTERCEPT=-.00041

 EQUILIB LINE, X=.00005 Y=.00062
 WITH EMV, X=.00005 Y=.00043
 OPERATING LINE, X=.00010 Y=.00043
 EQUILIB LINE, X=.00010 Y=.00126
 WITH EMV, X=.00010 Y=.00101
 OPERATING LINE, X=.00017 Y=.00101
```

EQUILIB LINE, X=.00017 Y=.00213
WITH EMV, X=.00017 Y=.00180
OPERATING LINE, X=.00026 Y=.00180
EQUILIB LINE, X=.00026 Y=.00329
WITH EMV, X=.00026 Y=.00284
OPERATING LINE, X=.00038 Y=.00284
EQUILIB LINE, X=.00038 Y=.00484
WITH EMV, X=.00038 Y=.00424
OPERATING LINE, X=.00055 Y=.00424
EQUILIB LINE, X=.00055 Y=.00690
WITH EMV, X=.00055 Y=.00610
OPERATING LINE, X=.00077 Y=.00610
EQUILIB LINE, X=.00077 Y=.00962
WITH EMV, X=.00077 Y=.00856
OPERATING LINE, X=.00106 Y=.00856
EQUILIB LINE, X=.00106 Y=.01319
WITH EMV, X=.00106 Y=.01180
OPERATING LINE, X=.00144 Y=.01180
EQUILIB LINE, X=.00144 Y=.01782
WITH EMV, X=.00144 Y=.01601
OPERATING LINE, X=.00194 Y=.01601
EQUILIB LINE, X=.00194 Y=.02377
WITH EMV, X=.00194 Y=.02144
OPERATING LINE, X=.00258 Y=.02144
EQUILIB LINE, X=.00258 Y=.03127
WITH EMV, X=.00258 Y=.02832
OPERATING LINE, X=.00339 Y=.02832
EQUILIB LINE, X=.00339 Y=.04055
WITH EMV, X=.00339 Y=.03688
OPERATING LINE, X=.00439 Y=.03688
EQUILIB LINE, X=.00439 Y=.05174
WITH EMV, X=.00439 Y=.04728
OPERATING LINE, X=.00562 Y=.04728
EQUILIB LINE, X=.00562 Y=.06484
WITH EMV, X=.00562 Y=.05957
OPERATING LINE, X=.00707 Y=.05957
EQUILIB LINE, X=.00707 Y=.07967
WITH EMV, X=.00707 Y=.07364
OPERATING LINE, X=.00873 Y=.07364
EQUILIB LINE, X=.00873 Y=.09579
WITH EMV, X=.00873 Y=.08915
OPERATING LINE, X=.01055 Y=.08915
EQUILIB LINE, X=.01055 Y=.11262
WITH EMV, X=.01055 Y=.10558
OPERATING LINE, X=.01249 Y=.10558
EQUILIB LINE, X=.01249 Y=.12945
WITH EMV, X=.01249 Y=.12229
OPERATING LINE, X=.01446 Y=.12229
EQUILIB LINE, X=.01446 Y=.14558
WITH EMV, X=.01446 Y=.13859
OPERATING LINE, X=.01638 Y=.13859
EQUILIB LINE, X=.01638 Y=.16046

```
WITH EMV, X=.01638 Y=.15390
OPERATING LINE, X=.01819 Y=.15390
EQUILIB LINE, X=.01819 Y=.17369
WITH EMV, X=.01819 Y=.16775
OPERATING LINE, X=.01982 Y=.16775
EQUILIB LINE, X=.01982 Y=.18510
WITH EMV, X=.01982 Y=.17990
OPERATING LINE, X=.02125 Y=.17990
EQUILIB LINE, X=.02125 Y=.19469
WITH EMV, X=.02125 Y=.19025
OPERATING LINE, X=.02247 Y=.19025
EQUILIB LINE, X=.02247 Y=.20258
WITH EMV, X=.02247 Y=.19888
OPERATING LINE, X=.02349 Y=.19888
EQUILIB LINE, X=.02349 Y=.20897
WITH EMV, X=.02349 Y=.20594
OPERATING LINE, X=.02432 Y=.20594
EQUILIB LINE, X=.02432 Y=.21406
WITH EMV, X=.02432 Y=.21163

STRIPPER DIAMETER=  6.875


STRIPPER REBOILER
THOT (DEG K)=420.30 TCOLD=373.14
DELTA Q (KCAL/HR)=      .10665E+08
REBOILER AREAS (FT2)=  1423.1 NO. OF UNITS=  1
STRIPPER REBOILER STEAM FEED (KG/HR)=20624.
YEARLY STEAM COST= 1133417.56
STRIPPER PROD FLOW (GMOLE/HR)= 1027877.273 MOLE FRAC =.2063


   DISTILLATION COLUMN DETAIL

RECTIFYING SLOPE= .7764 INTERCEPT= .1971
STRIPPING SLOPE=1.7337 INTERCEPT=-.0004

REFLUX FLOW (GMOL/HR)=    .834E+06
EQUILIBRIUM CURVE.  X=.87351  Y=.88140
RECTIFYING OPERATING LINE.  X=.87351  Y=.87528
EQUILIBRIUM CURVE.  X=.86584  Y=.87528
RECTIFYING OPERATING LINE.  X=.86584  Y=.86932
EQUILIBRIUM CURVE.  X=.85826  Y=.86932
RECTIFYING OPERATING LINE.  X=.85826  Y=.86344
EQUILIBRIUM CURVE.  X=.85064  Y=.86344
RECTIFYING OPERATING LINE.  X=.85064  Y=.85752
EQUILIBRIUM CURVE.  X=.84285  Y=.85752
RECTIFYING OPERATING LINE.  X=.84285  Y=.85147
EQUILIBRIUM CURVE.  X=.83473  Y=.85147
RECTIFYING OPERATING LINE.  X=.83473  Y=.84517
EQUILIBRIUM CURVE.  X=.82613  Y=.84517
```

```
RECTIFYING OPERATING LINE.  X=.82613  Y=.83849
EQUILIBRIUM CURVE.  X=.81684  Y=.83849
RECTIFYING OPERATING LINE.  X=.81684  Y=.83127
EQUILIBRIUM CURVE.  X=.80658  Y=.83127
RECTIFYING OPERATING LINE.  X=.80658  Y=.82331
EQUILIBRIUM CURVE.  X=.79499  Y=.82331
RECTIFYING OPERATING LINE.  X=.79499  Y=.81431
EQUILIBRIUM CURVE.  X=.78154  Y=.81431
RECTIFYING OPERATING LINE.  X=.78154  Y=.80387
EQUILIBRIUM CURVE.  X=.76546  Y=.80387
RECTIFYING OPERATING LINE.  X=.76546  Y=.79138
EQUILIBRIUM CURVE.  X=.74549  Y=.79138
RECTIFYING OPERATING LINE.  X=.74549  Y=.77588
EQUILIBRIUM CURVE.  X=.71953  Y=.77588
RECTIFYING OPERATING LINE.  X=.71953  Y=.75572
EQUILIBRIUM CURVE.  X=.68363  Y=.75572
RECTIFYING OPERATING LINE.  X=.68363  Y=.72786
EQUILIBRIUM CURVE.  X=.62959  Y=.72786
RECTIFYING OPERATING LINE.  X=.62959  Y=.68589
EQUILIBRIUM CURVE.  X=.53707  Y=.68589
RECTIFYING OPERATING LINE.  X=.53707  Y=.61406
EQUILIBRIUM CURVE.  X=.34946  Y=.61406
RECTIFYING OPERATING LINE.  X=.34946  Y=.46841
EQUILIBRIUM CURVE.  X=.11124  Y=.46841
STRIPPING OPERATING LINE.  X=.11124  Y=.19247
EQUILIBRIUM CURVE.  X=.02026  Y=.19247
STRIPPING OPERATING LINE.  X=.02026  Y=.03473
EQUILIBRIUM CURVE.  X=.00278  Y=.03473
STRIPPING OPERATING LINE.  X=.00278  Y=.00442
EQUILIBRIUM CURVE.  X=.00034  Y=.00442

THEORETICAL RECT. STAGES=22. STRIP. STAGES= 3.
DIST COLUMN DIAM (FT)=14.1  HT=34.6


INTER COLUMN EXCHANGER
THOT (DEG K)=367.06 TCOLD=335.84
DELQ (KCAL/HR)=     .115044E+08
EXCH AREAS (FT2)=  2029.5 NO. OF UNITS=  1


DISTILLATION COLUMN REBOILER
THOT (DEG K)=420.30 TCOLD=335.84
DELTA Q (KCAL/HR)=     .108299E+05
EXCH AREAS (FT2)=       .8 NO. OF UNITS=  1


PRODUCT CONDENSER
THOT (DEG K)=317.72 TCOLDIN=291.48 TCOLDOUT=315.81
DELTA Q (KCAL/HR)=     .110227E+08
EXCH AREAS (FT2)=  6536.7 NO. OF UNITS=  1
```

MAIN DISTILLATION TRAIN 101440147. L/YR CAPACITY

```
STRIPPING COLUMN,  STAGES=  25.05949
                DIAMETER=     .68752E+01FT.  HEIGHT=     .54119E+02FT.
                SLOPE RATIO=     .84855E+01
                FEED FLOW RATE=     .87221E+04 KG-MOLE/HR
                FEED TEMPERATURE= 367.05987DEG-K
                XF=     .24358E-01
                BOTTOM FLOW RATE=     .76942E+04 KG-MOLE/HR
                BOTTOM TEMPERATURE= 373.13587 DEG-K
                XL=     .48717E-04
                PRODUCT FLOW RATE=     .10279E+04 KG-MOLE/HR
                PRODUCT TEMPERATURE= 367.05987 DEG-K
                YG=     .20628E+00
                CAPITAL COST=$   .5192281E+06
                EFFECTIVE COST=$     .19979E+06 PER YR.


DISTILATION COLUMN,  THEORETICAL STAGES=  25.23404
                  DIAMETER=     .14080E+02FT.  HEIGHT=     .34579E+02FT.
                  PRESSURE= 169.73693MM HG.
                  SLOPE RATIO=     .11547E+01
                  REFLUX FLOW RATE=     .83362E+03 KG-MOLE/HR
                  REFLUX RATIO= 3.47223 RMIN= 2.05254
                  FEED FLOW RATE=     .10279E+04 KG-MOLE/HR
                  FEED TEMPERATURE= 321.90729 DEG-K
                  XFD=   .2062812E+00
                  BOTTOM FLOW RATE=     .78750E+03 KG-MOLE/HR.
                  BOTTOM TEMPERATURE= 335.84451 DEG-K
                  XB=   .5322911E-03
                  PRODUCT FLOW RATE=     .24008E+03KG-MOLE/HR.
                  PRODUCT TEMPERATURE= 317.71918 DEG-K
                  XD=   .8814000E+00
                  CAPITAL COST=$     .67558E+06
                  EFFECTIVE COST=$     .25996E+06PER YR


HEAT EXCHANGER, AREA=     .20295E+04SQ.FT.  NUMBER=   1
              DELTA Q (KCAL/HR)=     .11504E+08
              CAPITAL COST=$     .13736E+06
              EFFECTIVE COST=$     .52855E+05 PER YR.
```

```
POST-COOL, AREA=    0.          SQ.FT.  NUMBER=   0
          COOLING WATER FLOW RATE=    0.          KG/HR
          COOLING WATER TEMPERATURE RISE=   6.52000DEG-K
          DELTA Q (KCAL/HR)=    0.
          CAPITAL COST=$    0.
          COOLING WATER COST=$    0.          PER YR.
          EFFECTIVE COST=$    0.          PER YR.


STRIPPER REBOILER,  AREA=     .14231E+04SQ.FT.  NUMBER=   1
                    DELTA Q (KCAL/HR)=     .10665E+08
                    STEAM FLOW RATE=     .20624E+05KG/HR
                    CAPITAL COST=$   .1806205E+06
                    STEAM COST=$     .11334E+07PER YR.
                    EFFECTIVE COST=$     .12029E+07PER YR.


REBOILER,  AREA=     .80700E+00SQ.FT.   NUMBER=   1
         STEAM FLOW RATE=     .20943E+02KG/HR
         DELTA Q (KCAL/HR)=     .10830E+05
         CAPITAL COST=$   .1811601E+04
         STEAM COST=$     .11509E+04 PER YR.
         EFFECTIVE COST=$     .18480E+04 PER YR.


CONDENSER,  AREA=     .65367E+04SQ.FT.  NUMBER=   1
          COOLING WATER FLOW RATE=     .45307E+06KG/HR
          COOLING WATER TEMPERATURE RISE=  24.32897DEG-K
          DELTA Q (KCAL/HR)=     .11023E+08
          CAPITAL COST=$     .26222E+06
          COOLING WATER COST=$     .21503E+06 PER YR.
          EFFECTIVE COST=$     .31593E+06 PER YR.
```

```
SYSTEM, TOTAL COOLING WATER FLOW =     453069.2KG/HR
        TOTAL COOLING WATER COST=$    215032.1 /YR       .002120 /L
        TOTAL STEAM FLOW RATE=$        20645.0KG,HR.
        TOTAL STEAM COST=$           1134568.5 /YR      .0111846 /L
        LABOR REQUIREMENT (WORKERS/SHIFT)=  1.83
        LABOR COST=$                  183070.3 /YR      .0018047 /L
        TOTAL CAPITAL COST=$         1776829.7          .0175160 /L
        TOTAL OPERATING COST=$       1532670.9 /YR      .0151091 /L
        TOTAL EFFECTIVE COST=$       2216378.9 /YR      .0218491 /L
```

NREL
National Renewable Energy Laboratory
02LIB078192