Lehigh University
Lehigh Preserve

Theses and Dissertations

1973

Steady-state consideration of a binary distillation column sidestream composition control

Mehmet Nihat Elbi
Lehigh University

Follow this and additional works at: https://preserve.lehigh.edu/etd

Part of the Chemical Engineering Commons

STEADY-STATE CONSIDERATIONS OF A BINARY DISTILLATION

COLUMN SIDESTREAM COMPOSITION CONTROL

by

Mehmet Nihat Elbi

A Research Report

Presented to the Graduate Faculty

of Lehigh University

in Candidacy for the Degree of

Master of Science

in

Chemical Engineering

Lehigh University

1973

CERTIFICATE OF APPROVAL

This research report is accepted and approved in partial
fulfillment of the requirements for the degree of
Master of Science in Chemical Engineering.

Nov. 28, 1973
(Date)

Dr. W. L. Luyben
Professor in charge

Dr. L. A. Wenzel
Chairman of the Department
of Chemical Engineering

ACKNOWLEDGEMENTS

TABLE OF CONTENTS

LIST OF FIGURES

NOMENCLATURE

B : Bottoms rate (mole. gr./hr.)

D : Distillate rate (mole. gr./hr.)

E_1, E_2, E_3 : Tray efficiencies

F : Feed rate (mole. gr./hr.)

h : Liquid phase enthalpy (cal./mole. gr.)

H : Vapor phase enthalpy (cal./mole. gr.)

i : Component index

k : Index for trays at rectifying section

L : Liquid rate (mole. gr./hr.)

m : Index for trays at stripping section

n : Index for trays between feed and sidestream

P : Total pressure of trays (atm.)

p : Vapor pressure of pure components (atm.)

Q_B : Heat duty of reboiler (cal./hr.)

Q_L : Heat loss (cal./hr.)

R : Reflux rate (mole. gr./hr.)

S : Steam rate (gr./hr.)

SS : Sidestream draw off rate (mole. gr./hr.)

T : Tray temperature ($^{\circ}$C)

T_F : Feed temperature ($^{\circ}$C)

T_R : Reflux temperature ($^{\circ}$C)

V : Vapor rate (mole. gr./hr.)

X : Liquid phase mole fraction of more volatile component

X_B : Bottoms mole fraction

X_D : Distillate mole fraction

X_F : Feed mole fraction

X_S : Sidestream mole fraction

Y : Vapor phase mole fraction of more volatile component

NF : Feed plate number from bottom

NS : Sidestream tray number from bottom

NT : Total number of trays

γ : Activity coefficients

ABSTRACT

Sidestream draw off distillation columns have a wide application in industry. They are very important for multicomponent mixture separations, especially in petroleum industry.

This thesis investigates the steady-state behavior of a nonequal molar overflow binary distillation column with a sidestream. Then the control aspect is considered from steady-state point of view. The system is methanol-water distillation column.

A steady-state model was developed. A digital computer program predicted sidestream composition, flow, temperature, composition profiles and heat duty of the column for specified feed rate, feed temperature, feed composition, end products compositions, sidestream rate, total trays, feed tray, sidestream tray. Then these predictions were checked by experiments.

It is concluded that sidestream draw off rate had a very little effect on its tray composition. The changes that were made on the end products compositions had considerable effect on sidestream composition as expected. However, for specified end compositions, moving the sidestream tray up and down covers wide range of sidestream compositions.

For vapor sidestream at stripping section, the effect of draw off rate on its composition was considerable.

No dynamic studies were made but from steady-state point of view alone we can conclude that to control the sidestream composition

1

by its draw off rate will not be effective. Using multiple sidestreams
and adjusting individual stream rates to control the composition is
a better scheme.

INTRODUCTION

Even though mathematical methods were first applied to distillation in 1890's, Van Winkle (1) points out that sidestream columns that are considered modern unit operations were first suggested as early as 1600's.

Sidestream draw off columns are economical for multi-component distillations. Without any sidestream, we require N-1 columns for N component mixture separation.

For binary mixtures, however, this is not generally true. We can obtain any desired composition by mixing feed with the overhead or feed with the bottoms products. Depending on the difficulty of separation, sidestream draw off may still be more economical. However, Van Winkle (1) points out that economical considerations alone can not be a decisive factor. The control difficulties should also be kept in mind. The dynamics of sidestream draw off columns has received little attention despite the challenging control problems.

Ruszkay (2) developed a dynamic model for a solvent recovery column, where the sidestream was vapor at stripping section. There were two feeds (rich and poor). He made analog simulations of various control schemes for this system.

Luyben (3) made a qualitative discussion of some ten control schemes. Both liquid sidestream at rectifier and vapor sidestream at stripper are considered.

Buckley (4) applied protective control to sidestream draw

3

off columns. His quantitative arguments were for an equal molar over-flow system.

Buckley and Cox (5) studied override and auto-override (non-linear control) techniques for sidestream columns. Their study involved numerous simulations for different control schemes and gains, with different disturbances.

Luyben (6) explains dynamic modeling of both ideal binary and multicomponent distillation columns, the latter having sidestreams.

Franks (7) also gives a dynamic model and computer program for multicomponent distillation column with sidestream.

Dynamic models are essential for a control scheme studies. However, steady-state models give valuable information on deciding the manipulative variable. Even the small changes in this variable must effect the controlled variable. Steady-state model can give us this information very easily within a shorter computation time.

For a binary system with sidestream it is always possible to apply a graphical method at steady-state. Coulson and Richardson (8) explains a Ponchon – Savarit graphical techniques for specified internal reflux ratio and separation. For our purpose where we have a specific column in hand with total number of trays given this method requires some trial and error procedure. Because of this reason it is more efficient to use computer simulations.

For this Ponchon method we need three delta points. D point is found exactly the usual way. Fictitious feed F'=F-S point is used instead of F for ΔB point. ΔS point is the intersection of

4

line $\overline{\Delta BF}$ and $\overline{\Delta DF}$ where S is the sidestream point. Then we proceed in usual manner using appropriate delta points and tie lines.

The maximum rate of sidestream draw off is limited by operation conditions. Component balance dictates the maximum sidestream rate. This value is reached when one of the end product rates vanishes. If the column conditions, including the reflux rate were established before hand, then by increasing the sidestream draw off rate we can have a pinch point in the column (for the system in hand this occurs at feed plate) which corresponds to a maximum sidestream draw off rate. Actually at this point the operation is at "minimum reflux."

A dynamic model of distillation columns with sidestream drawoff does not suffer from additional convergence difficulties since a sidestream is merely an additional term in the differential equations of that tray. For steady-state model, however, only one additional sidestream changes the convergence procedure of the program as explained in Appendix B, that stage of the program becomes the time consuming part in simulations.

SCOPE OF THE WORK

The purpose of this work was to determine the best manipulative variable to control the sidestream composition. This is done by steady-state computations alone.

Following areas are investigated for liquid sidestream at rectifying section:

1. Find the steady-state profile of the column using a mathematical model and compare with experiments.

2. The effect of sidestream drawoff rate on sidestream composition.

3. The effect of sidestream drawoff tray location.

4. The effect of distillate and bottoms composition on sidestream composition.

5. The effect of feed tray location.

These predictions were first made by simulating the model then some verified by experiments.

Also similar effects are studied for vapor sidestream at stripping section. In this case no experimental verification is made.

DESCRIPTION OF THE SYSTEM

A simplified sketch of the system is shown in Figure 1. Methanol-water binary system was studied in pilot plant scale distillation column. Product streams were fed back to the feed tank and recycled.

Distillation column was manufactured by Vulcan Copper and Supply Company. The column has 24 trays. Its diameter is 8" and each tray contains two bubble cups.

The reboiler is vertical thermo syphon type. Also there is a feed preheater. Reflux tank is a vertical cylinder. Table 1 shows the equipment.

There are two cascade loops to control distillate and bottom compositions. In each case master controller is a temperature controller which controls a tray temperature, its output is used as a set point in slave loop, at top this controls the reflux flow; at bottom it controls the steam flow rate.

The sidestream was taken out from trays 15, 17 or 19 as liquid at rectifying section of the column. These lines are 3/8" OD copper refrigeration tubing and sufficient amount can be taken out by syphon action. The procedure of mounting these sidestreams are explained in detail at "Experimental Work" section.

A Leeds and Northrup Speedomax multipoint recorder was available to record 7 tray temperatures and 4 stream temperatures continuously during experiments. Sidestream composition was
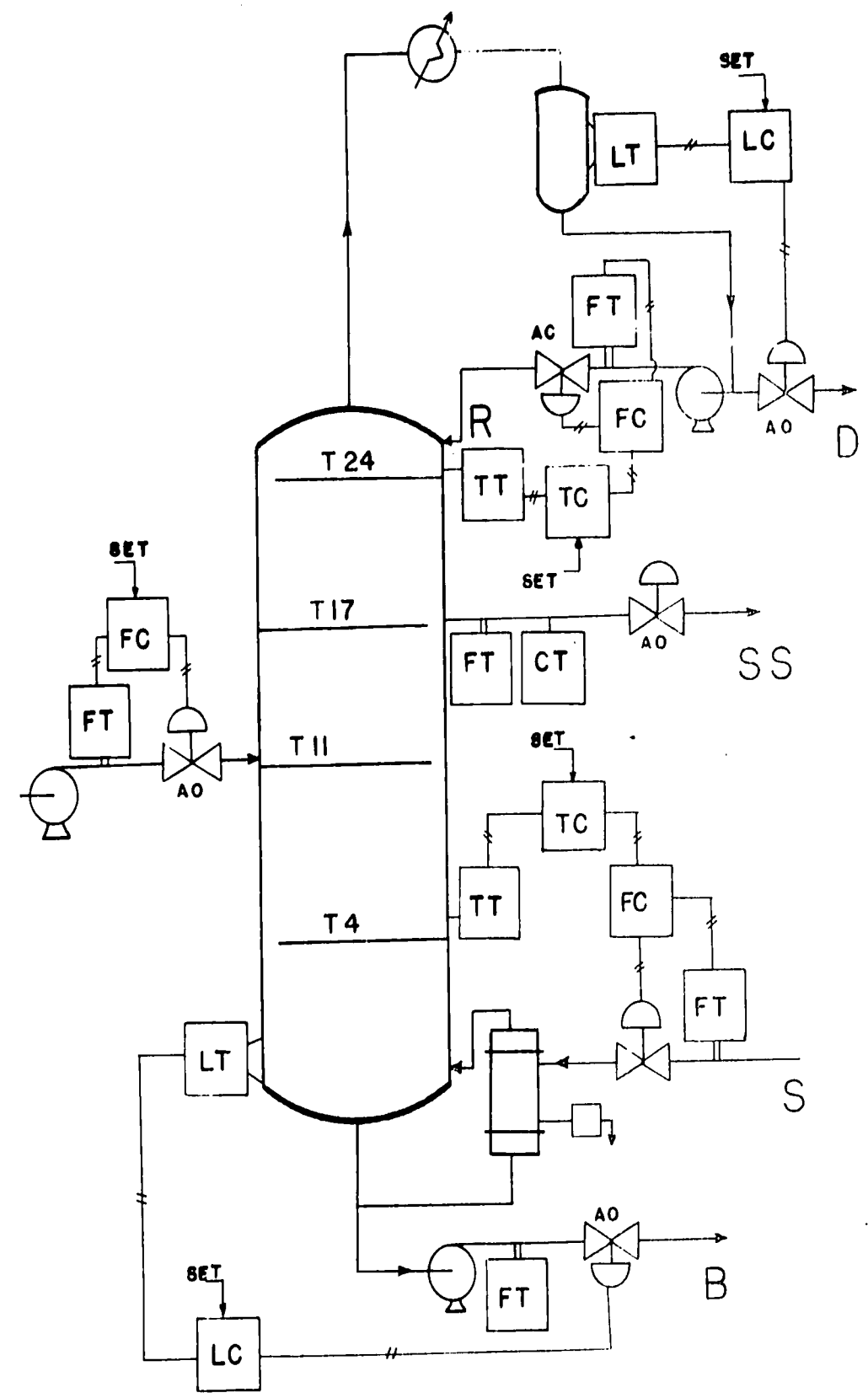
FIGURE 1 - Lehigh Distillation Column, overrides excluded

continuously measured by a Princo Densitrol. Feed, distillate and

bottom compositions were determined by density and temperature

measurements.

TABLE 1 - EQUIPMENT

1. Distillation Column
   Total number of trays   24
   Type   two 3-in. bubble
             cups per tray

   Feed tray   11
   Sidestream trays   15, 17 or 19
   Tray spacing   6 in.
   Weir height   1 in.
   Inside diameter   8 in.

2. Reboiler
   Thermo syphon type
   4 in. OD shell
   Fourteen 4 ft. tubes (0.625 in. OD and 0.065 in. wall thickness)
   Outside area   9.15 sq.ft.

3. Condensers
   Total of three
   4 in. OD shell
   Ten 4 ft. tubes (0.625 in. OD and 0.065 in. wall thickness)
   Double pass arrangement on tube side
   Outside area   6.54 ft.^{2}

4. Reflux tank (vertical cylindrical)
   6 in. OD
   24 in. long
   Both reflux and distillate taken from the bottom.

DESCRIPTION OF THE WORK

The steady-state behavior of a 24 tray methanol-water distillation column with sidestream draw off was studied and the effectiveness of the various variables was investigated for sidestream composition control. For this purpose a mathematical model was developed and some simulations compared with experiments.

Mathematical Model

While developing the model, the following simplifying assumptions were made:

a) Tray efficiencies were different constants for each part of the column (stripping section, between feed and sidestream and at rectifying section). These constants were determined from experimental data.

b) Pressure varied linearly in the column. Since total pressure drop was small no effort was made on calculating tray to tray pressure drops.

c) Calculated heat loss was equally divided between trays.

d) Liquid sidestream was at its equilibrium composition and temperature and it did not contain any vapor. Similarly vapor sidestream was assumed to contain no liquid.

e) Physical property data for methanol-water system was taken from the literature. (10, 13, 14)

9

Derivation

The steady-state model consisted of simultaneous algebraic equations which are derived from:

a) Material balance

b) Component balance

c) Energy balance

at each tray.

In the stripping section for tray m, these balances around envelope I of Figure 2 gives:

Material balance: $L_m = V_{m-1} + B$

Component balance: $L_m X_m = V_{m-1} Y_{m-1} + BX_B$

Energy balance: $Q_B + L_m h_m = Q_{L1} + V_{m-1} H_{m-1} + Bh_B$

For trays between feed and sidestream draw off, balance around envelope II of Figure 2 gives:

Material balance: $F + L_n = V_{n-1} + B$

Component balance: $FX_F + L_n X_n = V_{n-1} Y_{n-1} + BX_B$

Energy balance: $Q_B + Fh_F + L_n h_n = Q_{L2} + V_{n-1} H_{n-1} + Bh_B$

For trays between sidestream and top tray:

Material balance: $L_k + F = V_{k-1} + SS + B$

Component balance: $L_k X_k + FX_F = V_{k-1} Y_{k-1} + SS\ X_S + BX_B$

Energy balance: $Q_B + L_k h_k + Fh_F = V_{k-1} H_{k-1} + SS\ h_S + BX_B + Q_{L3}$

These equations together with physical properties and Murphee tray efficiency equation construct the digital computer program.
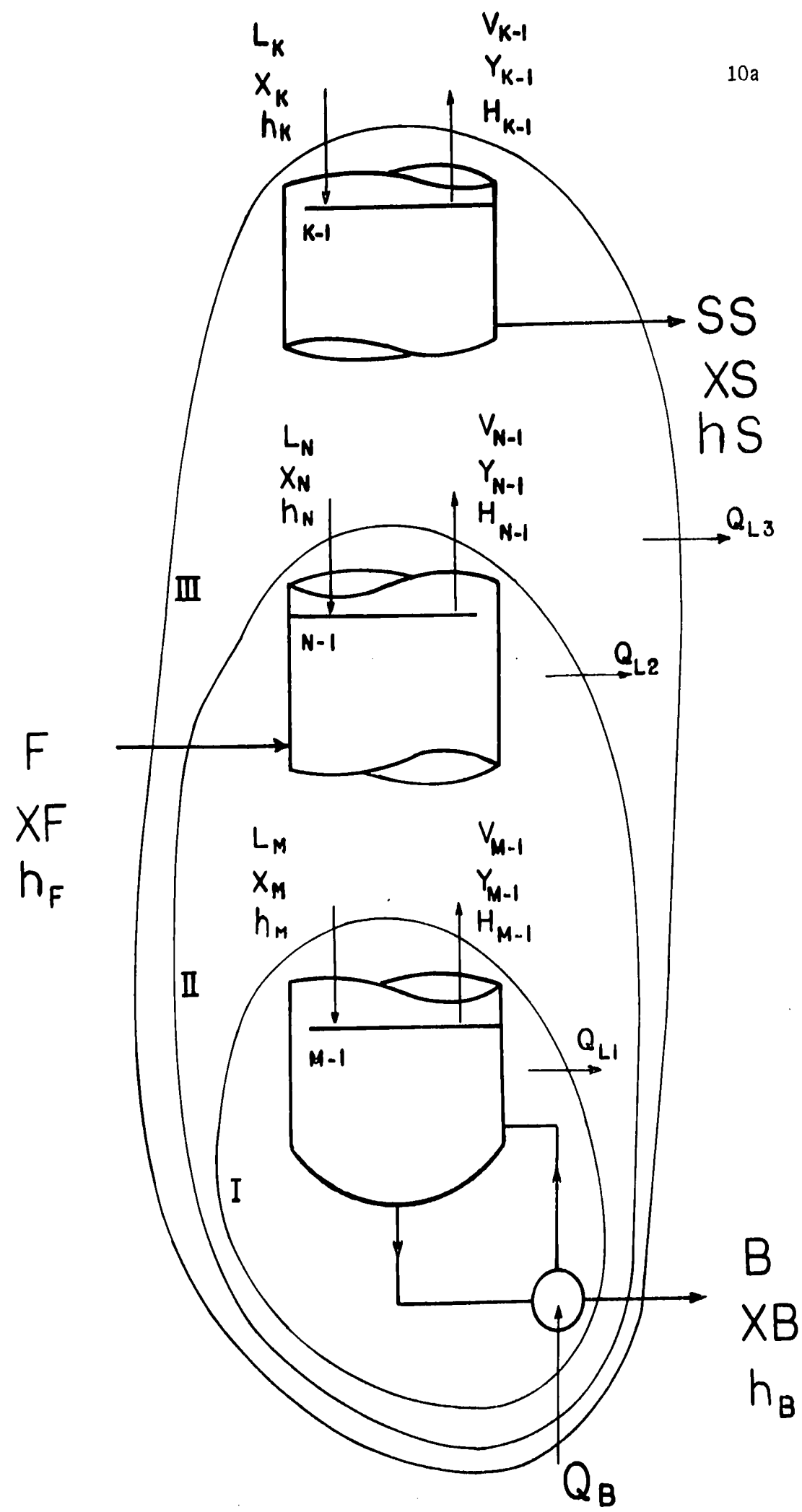
FIGURE 2

The variables that were specified in the program were X_B, X_D, and the sidestream flow rate. A two-variable convergence procedure was used to converge on the unknown variables: X_S and Q_B.

The digital simulation was started by making initial guesses of both sidestream composition and heat input to the reboiler. Overall material and component balances gave values for B and D. Then plate-to-plate calculations up the column gave a top tray vapor composition for the assumed heat input. If this top tray vapor composition did not equal the specified X_D, the heat input was adjusted. After an agreement on X_D is reached, the calculated sidestream tray composition was compared to the initial guess of the sidestream composition. If these did not agree, the guess of X_S was adjusted and the whole process repeated until all convergences were completed. Interval-halving was used in the Q_B convergence loop and false positioning was used in the X_S convergence loop.

Experimental Work

The first phase was to verify the model for a simple distillation column without a sidestream. That way the physical data and the assumptions were checked. The problem was to adjust the efficiencies so that the results from model fitted the experimental data.

The next step was to take the sidestream out of the column. The original column was not designed for sidestream product. There are three circular openings at each tray which are used for necessary temperature sensors and thermocouples. Two of those three holes are in the vapor section of the tray. The sidestream withdrawal line was installed in the middle opening by bending 3/8 in. OD copper tubing

2 in. from the end. The edge of the tube rested on the plate so a liquid sidestream was withdrawn. Because of the elevation difference between the sidestream trays and the product tank and slight pressure inside the column, it was possible to get liquid from the tray to syphon action without using a pump. Trays 19, 17 and 15 were used for sidestream draw off. Measurements are taken at sidestream trays (17 and 19) for several draw off rates.

Five tray temperatures, stream rates and necessary stream temperatures were recorded continuously during the experiments. Sidestream composition was also recorded by use of a densitrol mentioned earlier. Samples were taken to determine the composition of feed, distillate and bottoms. Composition was determined from density measurements at known temperature.

The column was operated in automatic using both top and bottom cascade loops, bottom level control, reflux drum level control, feed rate control (see Figure 1). The only control loop which was not used is the sidestream composition control scheme designed by Treyus (9).

A total of 6 runs were made.

DISCUSSION OF THE RESULTS

a) Steady-State Profile with Sidestream

As we mentioned in previous chapter the only values which were not fixed in the mathematical model was the Murphee tray efficiencies. We adjusted only these parameters to fit the experimental data.

The assumption of constant efficiency in each section of the column was shown to be valid because the model represented the experimental data reasonably well. The predicted values and experimental results are given in Table 2.

TABLE 2

	Predicted value	Experimental result
F	8574.91	8574.
X_F	0.35559	0.3556
D	2237.55	2269.6
X_D	0.93872	0.9387
B	5041.36	5010
X_B	0.01922	0.01922
SS	1296.0	1296
XS	0.65731	0.6369
R	3045.26	3323
T_4	84.50	85.0
T_8	79.62	78.9
T_{10}	78.77	78.6
T_{14}	75.42	76.0
T_{24}	67.0	67.1

13

b) The effect of sidestream draw off rate on sidestream composition

Figure 3 shows predicted effect together with some experimental data points on tray 19, 17 and 15. As we can see the effect of sidestream flow rate is small on composition change. As we move up in the column, this change becomes smaller.

In predictions the distillate and bottom compositions were held constant; but in experiments, even if we adjust the reflux flow and vapor boil up, it was difficult to keep those values constant. The maximum sidestream removal rate was limited by two constraints. The first one of these was when distillate rate dropped to zero. The second restriction occurred when we reached a liquid composition pinch point in the column. For water-methanol system this pinch point always occurred at feed plate. Both these limitations were experienced in the simulations. Moving the feed tray up the column might improve the pinch point situation but this time at low sidestream rates the performance of the column is poor.

So we can summarize that sidestream draw off rate has a minor effect on sidestream composition especially if we are close to the top tray at rectifying section.

But for vapor sidestream in stripping section simulations revealed a different situation. In this case the sidestream removal rate had a greater effect on its composition. Figure 4 shows the effect of sidestream removal rate on the composition.

c) The effect of distillate and bottom composition on sidestream

Higher distillate compositions increase the sidestream purity at rectifying section as expected. Figure 5 shows the simulations
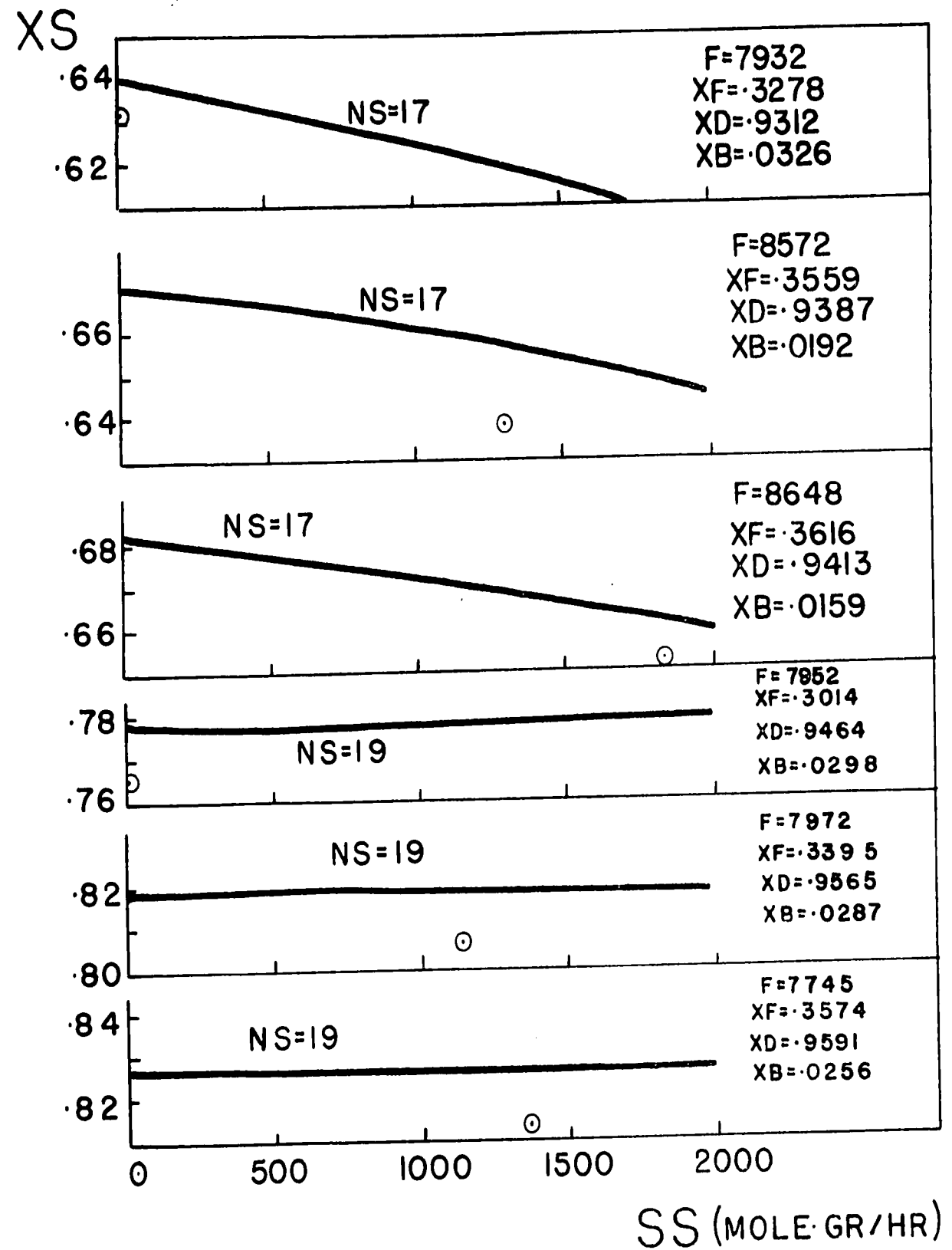
14

FIGURE 3 - Comparison of the experimental data points with simulations for trays 17 and 19
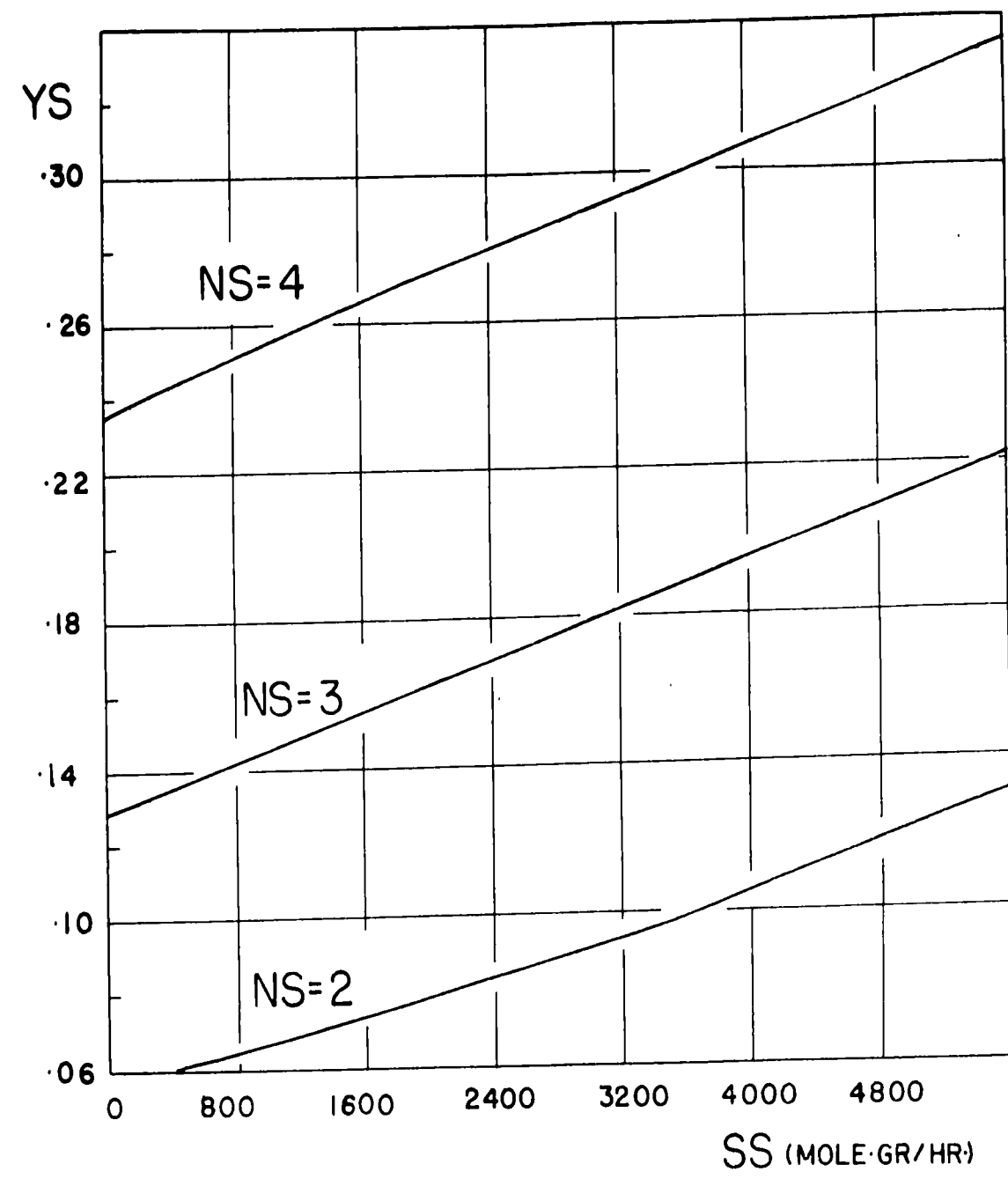
FIGURE 4 - Simulated effect of vapor sidestream drawoff rate on
its composition for three different trays in stripping
section

for four different distillate compositions while bottoms product

composition held constant. As we can see change in sidestream

composition is considerable. One other interesting observation is

that at higher distillate compositions the effect of sidestream rate

decreases; this is more evident in lower trays.

Simulations where bottom composition is changed while

distillate composition held constant are given in Figure 6.

For trays closer to overhead there is almost no effect

for cases X_B = .01 and .001. Sidestream rate versus sidestream

composition curve does not change. At lower trays we can see the

effect. This effect decreases by increasing sidestream rate. But

overall effect of X_B on X_S is minor. The effect of X_D on X_S is

more evident.

On the other hand vapor sidestream at stripping section

shows different results. Bottoms composition change had a big

effect on sidestream composition. This is shown in Figure 7. The

simulations showed that the effect is greater at trays further away

from the bottom tray. In this case distillate composition changes

do not effect the sidestream composition.

d) Feed tray location

This effect was mentioned in part (a) indirectly. There, we

mentioned that by changing the feed tray location for a fixed feed

composition we can improve the pinch point situation in the operation.

When we do not have a sidestream, tray 8 is "optimum feed

tray" for X_F = 0.40. With same feed composition for the case where
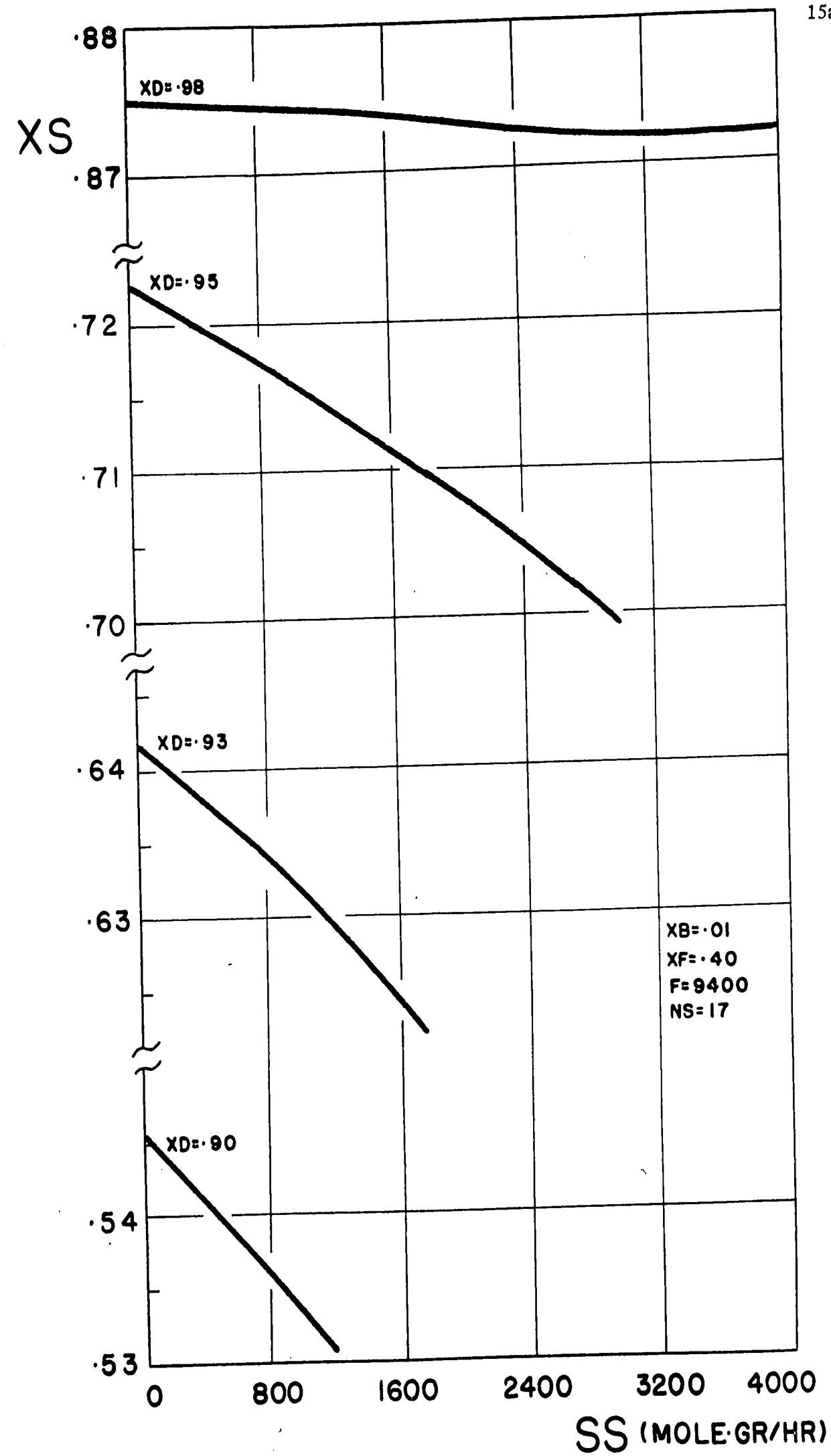
FIGURE 5 - The results of computer simulations for four different distillate compositions
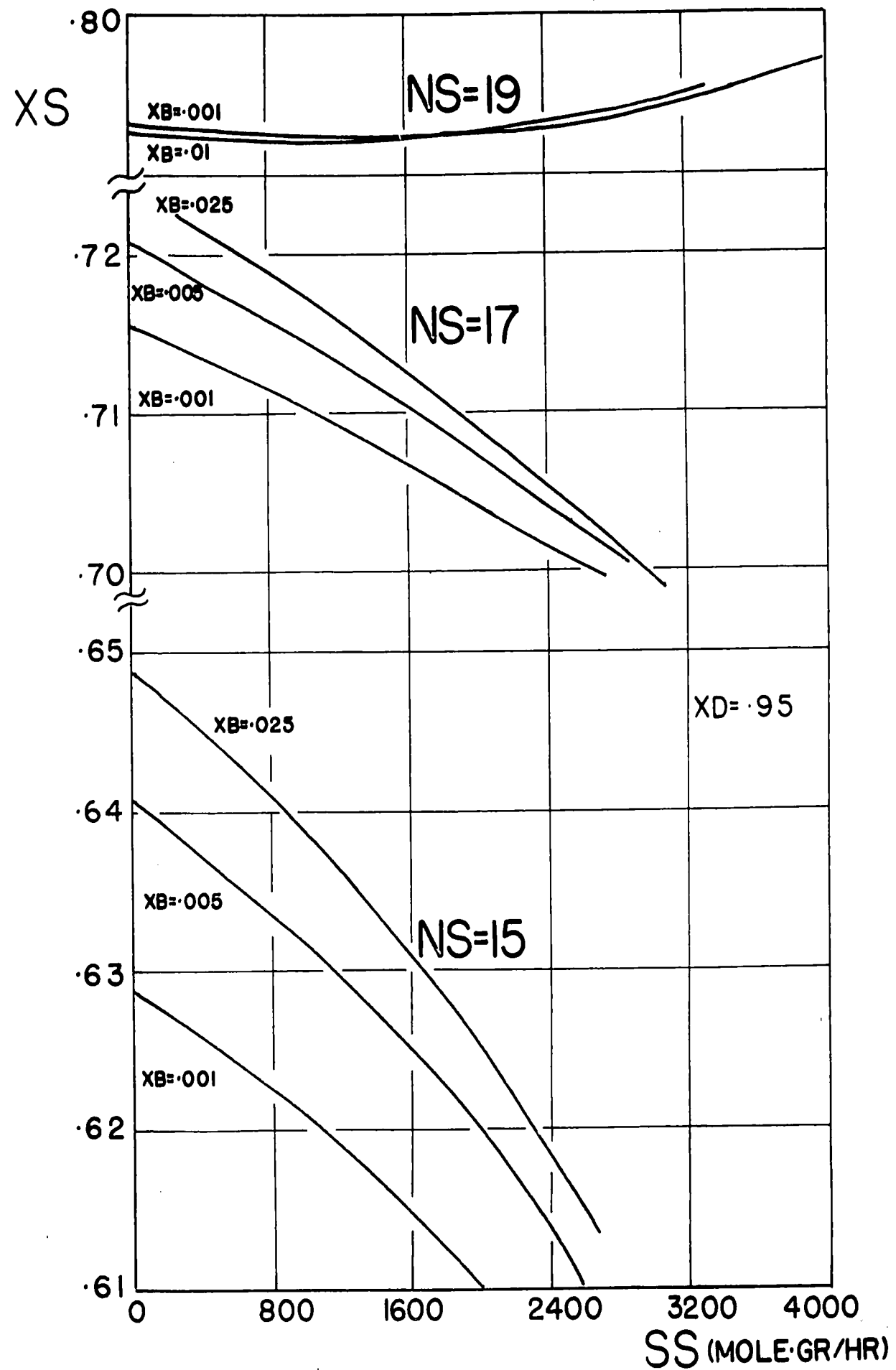
FIGURE 6 - The results of simulations for different bottoms composition
while XD held constant
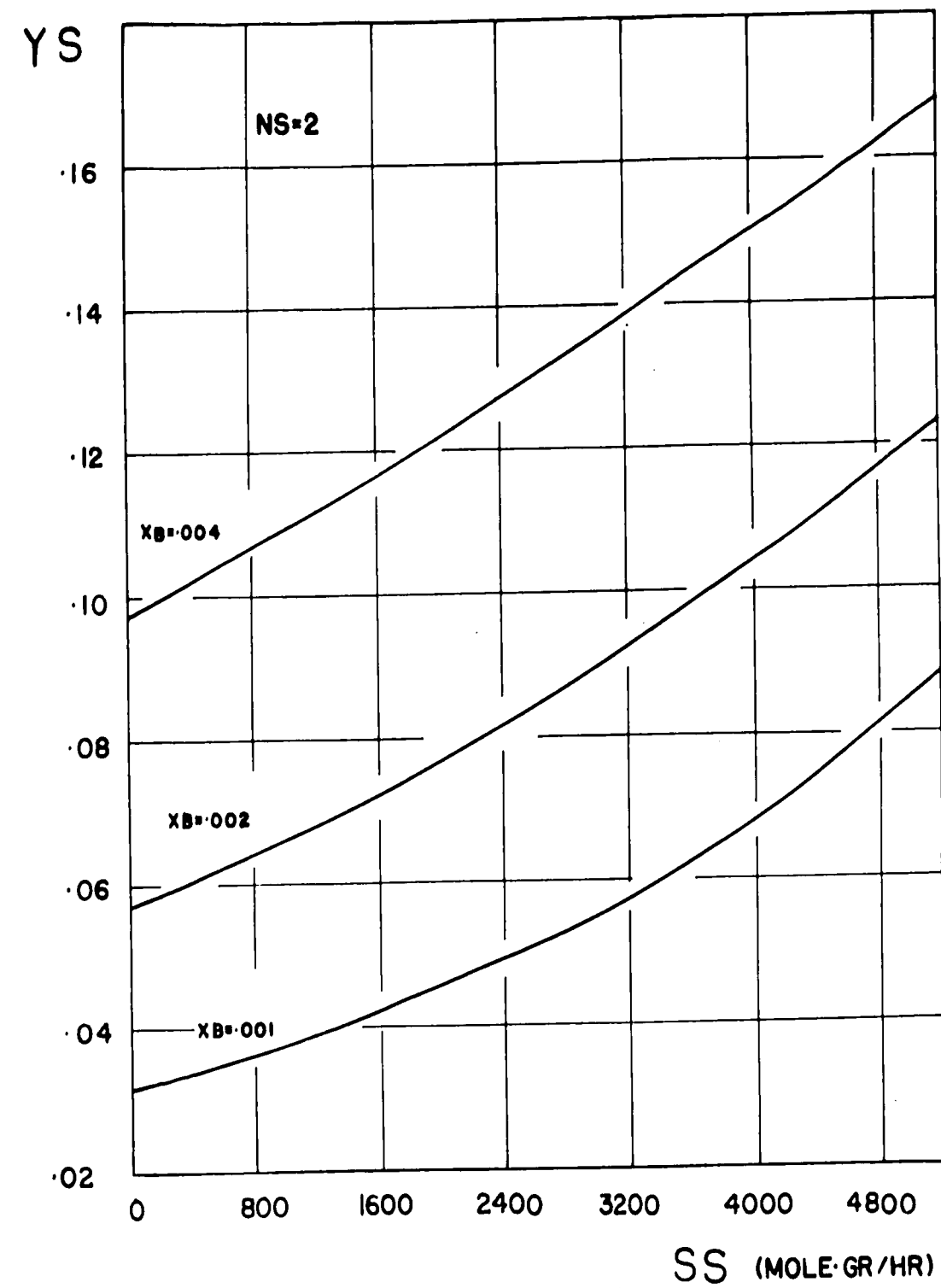
FIGURE 7A - The effect of bottoms composition change on vapor sidestream composition. Figures 7A, 7B and 7C give the simulated results at three different trays.
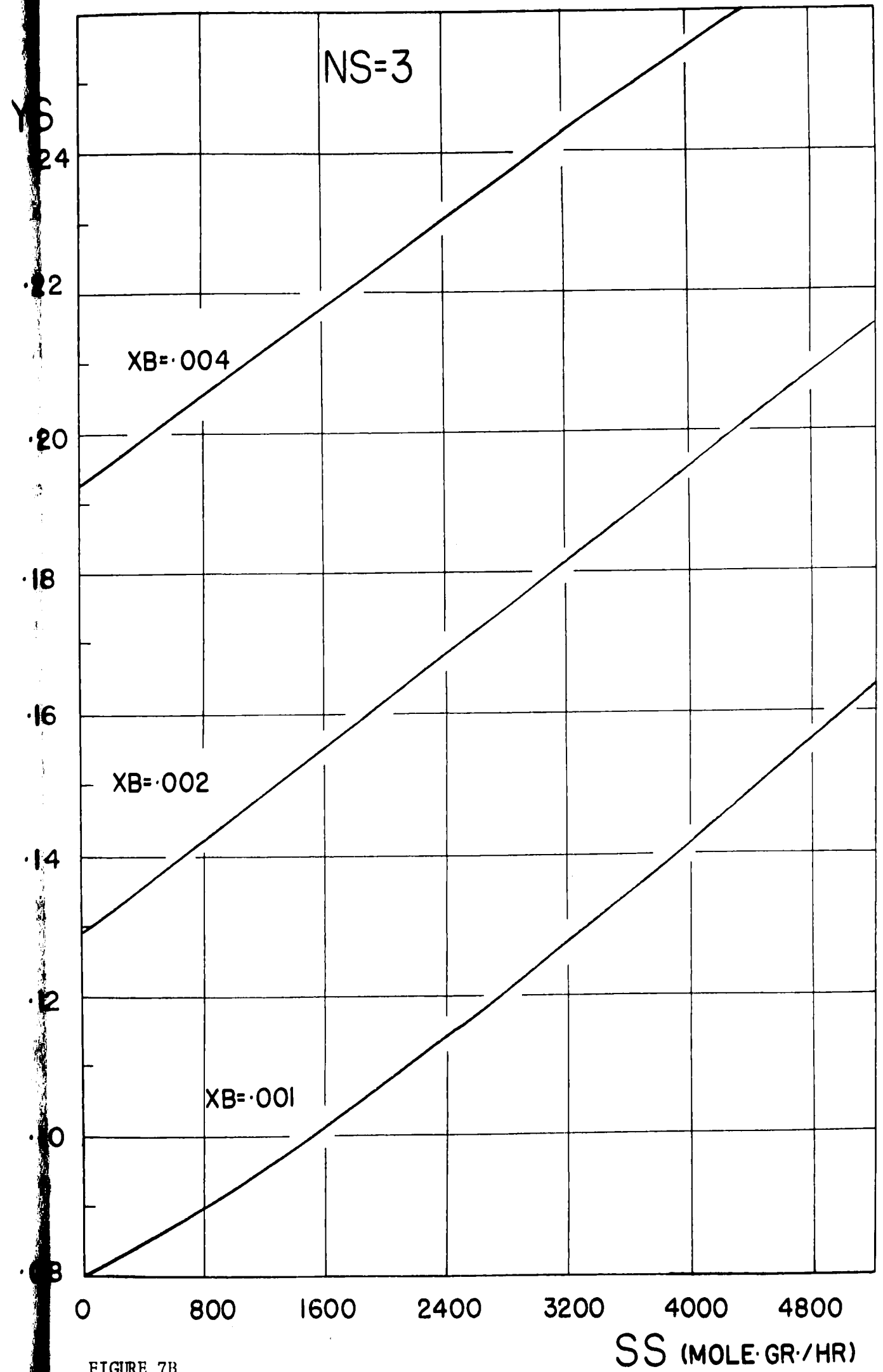
FIGURE 7B
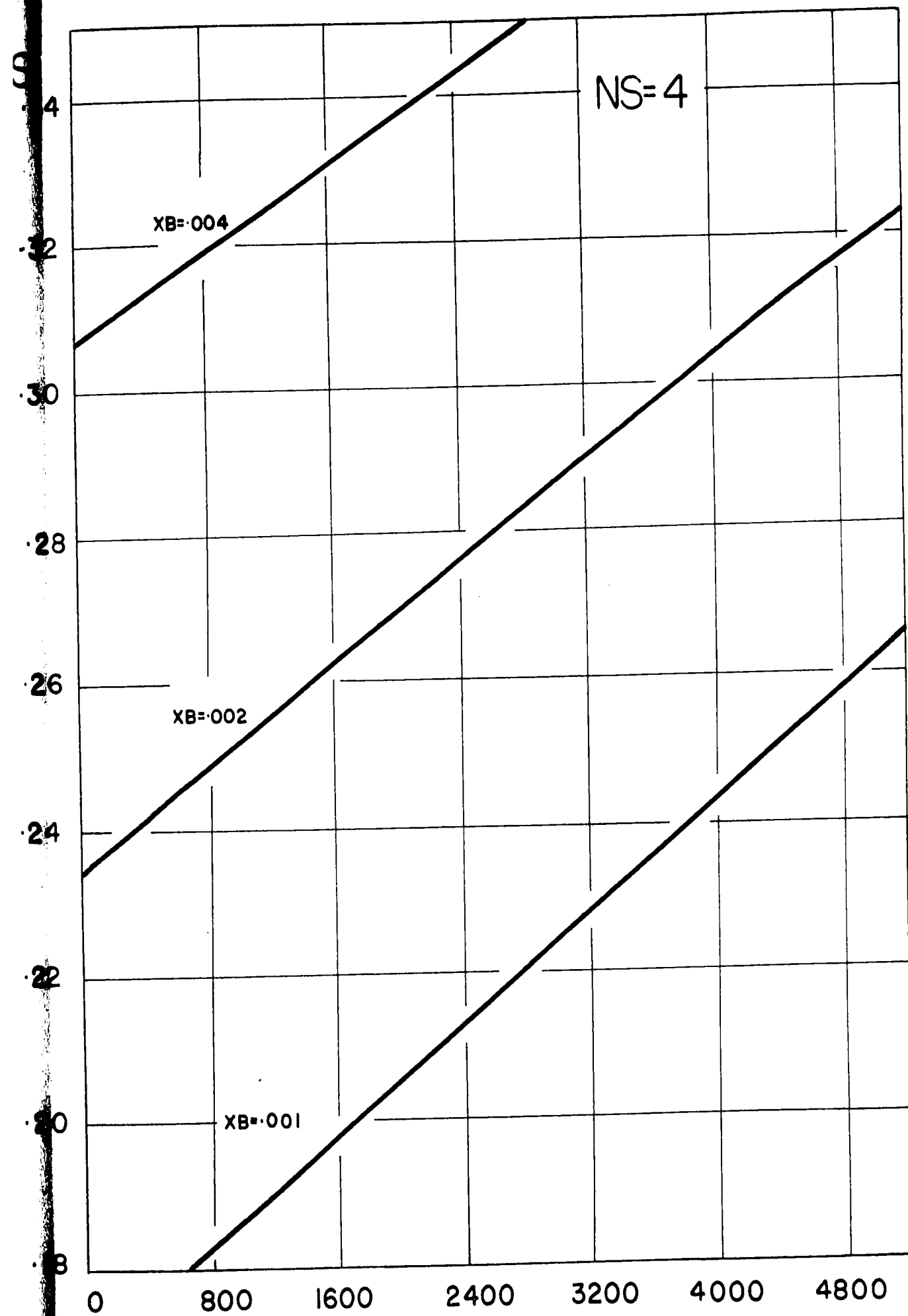
FIGURE 7C

we have a sidestream about 40% of the feed, tray 11 becomes optimum feed tray.

Table 3 shows the effect of the feed tray location where tray 12 and tray 11 compared in simulations. As we can see these are only minor differences in the results. In simulations X_D and X_B held constant. All stream compositions are almost same so are the rates. Major difference is in reflux rate and heat input which favors tray 11.

TABLE 3

	Feed tray 11	Feed tray 12
Distillate rate (mole. gr./hr.)	2216.2	2215.7
Distillate composition	0.950	0.950
Bottoms rate (mole. gr./hr.)	5183.8	5184.2
Bottoms composition	0.008	0.008
Sidestream rate (mole. gr./hr.)	2000.	2000.
Sidestream composition	0.80656	0.80679
Reflux rate (mole. gr./hr.)	4923.	5021.5
Heat input (cal./hr.)	7.457×10^7	7.542×10^7

e) The effect of sidestream tray location

All factors up to this point have little effect on liquid sidestream composition at rectifying section. They do not cover a wide range of composition change. But by moving the sidestream tray, we can cover a wide range of compositions. Figure 8 shows three trays at rectifying section. By examining this figure we see that the

16
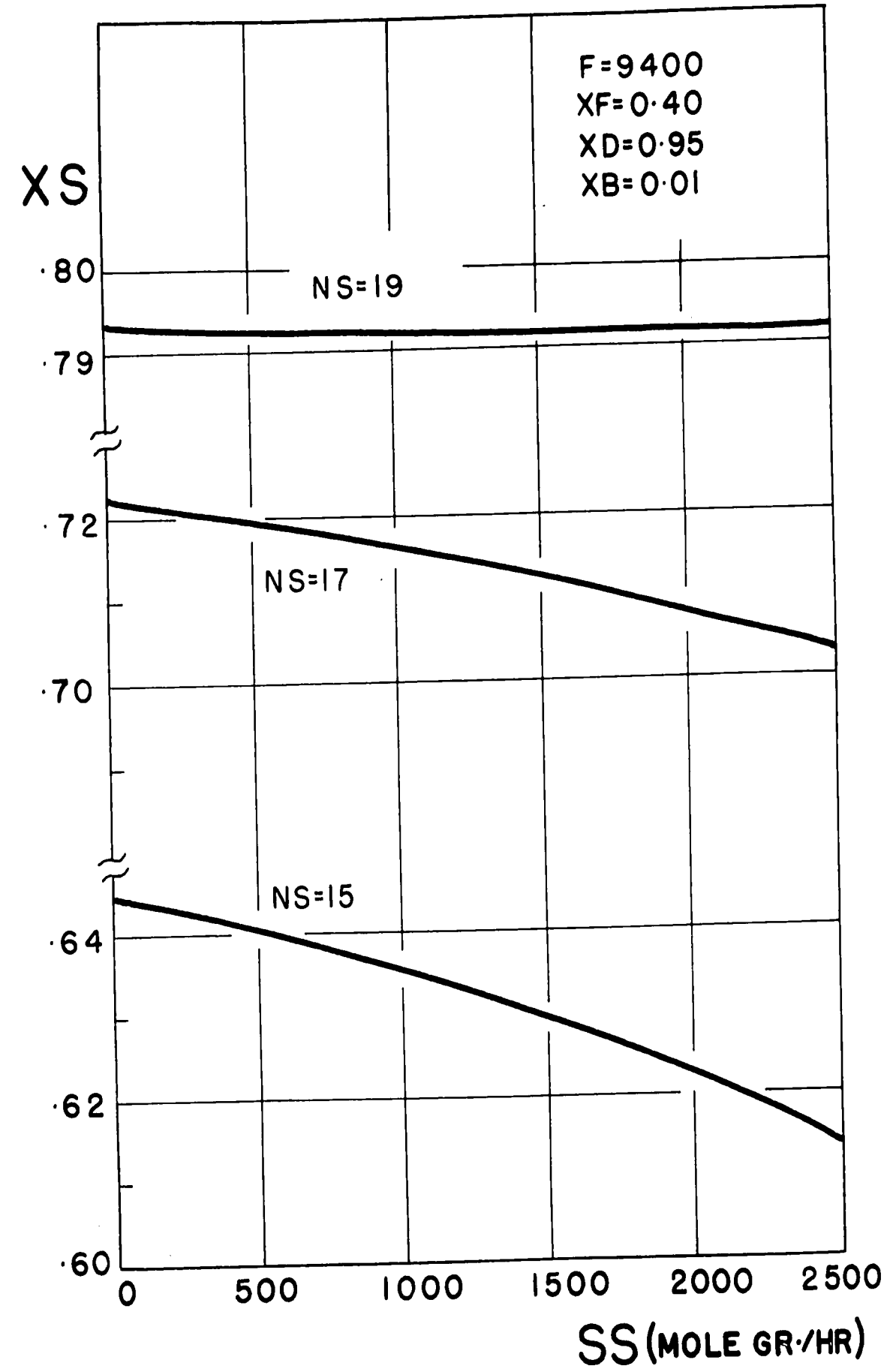
FIGURE 8 – The simulated results of sidestream tray location at rectifying section

location of sidestream also effects the sensitivity of sidestream composition to its draw off rate. We mentioned this point earlier.

Three trays have been simulated in rectifying section, these being 15, 17 and 19 trays.

At stripping section for vapor sidestream Figure 4 shows the results of simulations. For this part of the column tray location gives significant change at sidestream composition but it is not the only major factor.

CONCLUSIONS

Some insight into the dynamics of sidestream columns can
be gained from steady-state considerations. Of course, dynamic
simulations and experiments will give the final answer.

It is always necessary to choose a manipulative variable
which has a considerable effect on controlled variable.

For liquid sidestreams in the rectifying section, simulations
and experiments show that sidestream tray location is the major
factor on sidestream composition. The best scheme, therefore,
should be to take the sidestream from more than one tray and to
control its composition by changing individual stream rates.

Treyus (9) draws this conclusion after dynamic simulations
and experiments. An analog controller monitored the individual rates
for three trays (tray 15, 17 and 19) to keep the overall sidestream
composition at set point.

For vapor sidestream in the stripping section, sidestream
draw off rate promises to be a good manipulative variable to control
the sidestream composition. This conclusion must be verified by
experiments and dynamic simulations.

PHYSICAL DATA

Vapor Pressure

For methanol-water system starting from Clapeyron equation
with simplifying assumptions, we get most widely used and reasonably
accurate equation at low total pressures.

$$\ln p_i = \frac{Ai}{T} + B_i$$

for methanol:

$$A_1 = -4386.934$$
$$B_1 = 12.9848$$

for water:

$$A_2 = -4981.036$$
$$B_2 = 13.3486$$

With these constants and T in $^{\circ}K$ the result p is in atmosphere.

Equilibrium

We might think that at low pressures that we have in our
system, methanol water binary system can be treated as "ideal" so
we can use Raoult's law:

$$Y_i P = X_i p_i$$

But equilibrium data (10) does not fit this expression
accurately.

19

If we assume vapor phase can be treated as ideal gas mixture and nonideality comes from liquid phase, then we can include "activity coefficient." The most common expression to calculate this coefficient is van Laar equation (11). Because it is much simpler than other expressions and gives good prediction for simple systems. Modified van Laar equation (12) is:

$$\ln \gamma_1 = \frac{A^1}{\left[1 = \frac{A^1}{B^1} \frac{X^1}{X^2}\right]^2}$$

$$\ln \gamma_2 = \frac{B^1}{\left[1 + \frac{B^1}{A^1} \frac{X^2}{X^1}\right]^2}$$

A^1 and B^1 are dimensionless constants which can be determined experimentally. Then for equilibrium relationship:

$$Y_i P_t = \gamma_i X_i P_i$$

Table 4 shows experimental data with predictions from Raoult's law and van Laar equation at 1 atmosphere:

TABLE 4

X	Experimental		Raoult's Expression		Van Laar Equation	
	Y	T	Y	T	Y	T
0.0	.0	100	.0	100	.0	100
.02	-	-	-	-	-	-
.04	-	-	-	-	-	-
.10	0.418	87.7	0.27768	93.61	0.41671	87.21
.15	0.517	84.4	0.38085	90.86	0.5029	83.98
.20	0.579	81.7	0.46737	88.34	0.56386	81.57
.30	.665	78.0	0.6037	83.90	0.6501	78.05
.40	0.729	75.3	0.70554	80.08	0.71451	75.39
.50	0.779	73.1	0.78402	76.73	0.76933	73.17
.60	0.825	71.2	0.84596	73.76	0.81933	71.18
.70	.870	69.3	0.89602	71.10	0.86665	69.35
.80	0.915	67.6	0.93702	68.7	0.91227	67.65
.90	0.958	66.0	0.97125	66.51	0.95668	66.03
.95	0.979	65.0	0.98615	65.48	0.97846	65.25

In this table $A^1 = 0.90$ and $B^1 = 0.48$ and two constant vapor pressure equation which was described in previous section were used.

As we can see from this table experimental results agree reasonably well with predictions using van Laar equation. So in simulations equilibrium data is predicted by using van Laar equation.

Enthalpy composition relation

Data from Plewes et. al. (13) is used. They assumed ideal gas phase and neglected the heat of mixing in gas phase. Their data is well represented by linear relation in gas phase and second order polynomial in liquid phase.

In terms of cal./mole. gr., the enthalpies of saturated phases are:

Vapor Phase $\quad\quad H_o = 11440 - 1990\ Y$

Liquid Phase $\quad\quad h_L = 1800 - 2433X + 1753X^2$

For subcooled liquid, constant heat capacities are assumed.

Density-composition-temperature relation

Pure substances densities as a function of temperature were predicted by tables given in American Institute of Physics Handbook (14). For composition dependency it is assumed that the change of specific volumes upon mixing was negligible. Simple mixing relationships gave the densities of liquid solution. These densities are used to convert experimental stream rates (gpm) to mole. gr./hr. to use in simulations.

For liquid water using the data and constructing the central-difference table the following polynomials were reached.

Between 65°C and 105°C:

$$\rho = 0.97185 - 6.24 \times 10^{-4} (t-80) - 2.40 \times 10^{-6} (t-80)^2$$

where
$$\rho \ (gr./cc) \ and \ t \ (°C)$$

The error in predicted densities is less then ± 0.00005.

Between 45°C and 65°C:

$$\rho = 0.98573 - 4.83 \times 10^{-4} (t-55) - 3.0 \times 10^{-6} (t-55)^2$$

with same units as previous one.

The error in predicted densities is less then ± 0.00002.

For pure methanol between the temperatures of 15°C to 94.5°C this polynomial is given in reference:

$$\rho = 0.81015 - 1.0041 \times 10^{-3} t - 1.802 \times 10^{-6} t^2 - 1.657 \times 10^{-8} t^3$$

where
$$\rho \ (gr./cc) \ and \ t \ (°C)$$

DIGITAL SIMULATIONS

The algebraic equations describing the system is found previously under the section "Mathematical Model."

In computer simulations only these equations in more useful form, Murphee efficiency relation and physical properties which is described in Appendix A were used.

Performance of the Program

In this section we will describe the input variables and computed (output) variables.

Total of 13 variables are assumed to be known and used as input. These are:

Feed rate F, Feed composition X_F, Feed temperature T_F, Bottoms composition X_B, Distillate composition X_D, Reflux temperature T_R, Total number of trays NT, Feed tray NF, Sidestream tray NS, Sidestream rate SS, Heat loss Q_L, Tray efficiencies (E_1, E_2, E_3).

Heat input and sidestream composition (Q_B and XS) is guessed to start the calculations. These variables are then adjusted in the program to get the defined value of X_D by tray to tray calculations starting at the bottom.

At the end of each run tray compositions X_n and Y_n, tray temperatures T_n, liquid and vapor flow rates at each tray L_n and V_n,

their enthalpies h_L and H_V, Distillate rate D, Bottom rate B, Reboiler and condenser heat duties Q_B and Q_P and sidestream composition X_S are printed as an output.

Convergence Procedure

In this part we will examine the convergence procedures that are used in our program.

a) Tray Composition Convergence: Computations start by an initial composition and temperature profile assumption. By using enthalpy balance, material balance and component balance equations in succession, we can calculate a new liquid composition and repeat the procedure by substituting this new value in equations until new calculated liquid composition agree with the previous one. This successive substitution technique is adequate because liquid composition tends to converge rather rapidly. Only few substitutions are necessary.

b) Equilibrium vapor composition convergence: For a given liquid composition, we first guess the tray temperature and then find corresponding vapor pressures and activity coefficients. Then we calculate the total pressure and compare this value with actual tray pressure. Temperature is adjusted using Newton-Raphson technique until calculated and actual pressures agree.

The procedure is outlined below:

$$p_i = \text{EXP} \left(\frac{\Lambda}{Tm} + B \right)$$

$$\gamma_i = \text{EXP} \frac{A^1}{\left(1 + \frac{A^1}{B^1} \frac{X_i}{1-X_i}\right)^2}$$

24

$$P_{calc} = \gamma_1 X_1 p_1 + \gamma_2 X_2 p_2$$

$$f = P_{calc} - P$$

$$\frac{\partial f}{\partial T_m} = \gamma_1 X_1 \frac{\partial p_1}{\partial T_m} + \gamma_2 X_2 \frac{\partial p_2}{\partial T_m}$$

where

$$\frac{\partial p_i}{\partial T_m} = p_i \left(\frac{A}{T^2} \right)$$

then

$$T_{m+1} = T_m - \frac{f}{\frac{\partial f}{\partial T}}$$

This Newton-Raphson technique converges to the correct value faster then interval halving technique but there is always a possibility of divergence if the initial temperature guess is away from correct value. So we have to check the temperature by an upper and lower limit. By using this method instead of interval halving we can save considerable computation time.

c) Distillate composition convergence: We proceed the previous tray to tray calculations from bottom to top. While doing this we check some physical limitations; these are:

1) Liquid and vapor rates cannot be negative.

2) Liquid composition cannot be decreasing while moving up the column. (This occurs in simulations and cannot be corrected if we are in "minimum reflux" operation.)

3) Liquid compositions cannot exceed distillate composition.

25

While performing tray to tray calculations, we check these limitations and when one of these occur we adjust the heat input using interval halving technique.

We continue to our tray to tray calculations to the top tray and compare the top tray vapor composition with the given distillate composition. If these two values agree we can proceed with sidestream composition convergence if not, we change the heat input and repeat the procedure.

d) Sidestream composition convergence: To start with overall component and material balance to compute B and D we have to make an initial guess for sidestream composition. After completing the distillate composition convergence, we compare the assumed side-stream composition with liquid composition of sidestream tray (for vapor sidestream at stripping section we compare the initial guess with vapor composition of the sidestream tray).

If these two values agree the simulation is over. If they do not, we have to change the sidestream composition accordingly. For this purpose, it is decided to use "false positioning" technique. Because successive substitution technique oscillates and interval halving method, even though always converges, is a time consuming technique for this purpose. Despite the divergence problems of false positioning technique depending on the initial guess, the method saves valuable computation time and that is why it is accepted over others.

After sidestream composition convergence completed the

simulation terminates and we proceed in same manner for the next case. Except we use the composition and temperature profiles of the previous case as an initial guess.

Digital Computer Program for Steady-State Profile

Figure 10 gives the complete program listing of SSPLDC (Steady State Profile of Lehigh Distillation Column). The program is explained by comments also input data and convergence procedures are expalined in previous sections. Fortran II language is used.

NOMENCLATURE OF THE COMPUTER PROGRAM

B : Bottoms rate (mole. gr./hr.)

C : Constant point in false positioning

D : Distillate rate (mole. gr./hr.)

DMIN : Minimum distillate rate (mole. gr./hr.)

DQB : Step size for adjusting the heat input (cal./hr.)

DS : Step size of the sidestream rate increase (mole. gr./hr.)

E : Tray efficiency at stripper

E1 : Tray efficiency between feed and sidestream plate

E2 : Tray efficiency from sidestream draw off to top plate

FC : Function value of C

FL : Feed rate (mole. gr./hr.)

FLAGM, FLAGP : Constants for adjusting the step size in interval halving

FNX : The value of the defined function in false positioning

GAM1, GAM2 : Activity coefficients

HF : Enthalpy of subcooled feed (cal./ mole. gr.)

HL : Liquid enthalpy (cal./mole. gr.)

HLB : Bottoms product enthalpy (cal./ mole. gr.)

HLSS : Sidestream enthalpy

HR : Enthalpy of subcooled reflux (cal./mole. gr.)

HV : Vapor enthalpy (cal./mole. gr.)

LOOP : Counter for the XD convergence loop

LOOP1 : Counter for the tray convergence loop

LOOPB : Counter for the XS convergence loop

LOOPS : Counter for the sidestream rate increase steps

N : Tray number

NF : Feed plate

NS : Sidestream plate

NT : Total number of trays

P : Pressure (atm.)

QB : Heat duty of reboiler (cal./hr.)

QD : Condenser heat duty (cal./hr.)

QL : Heat loss per tray (cal./hr.)

QLOSS: Total heat loss at any tray N (cal./hr.)

R : Reflux rate (mole. gr./hr.)

RAT : Ratio of sidestream to distillate rate

SS : Sidestream rate (mole. gr./hr.)

T : Temperature (^{o}C)

TB : Bottoms temperature (^{o}C)

TF : Feed temperature (^{o}C)

TR : Reflux temperature (^{o}C)

V : Vapor rate

VANLAR : Subroutine for equilibrium relation

VB : Vapor boil up rate from reboiler (mole. gr./hr.)

X : Liquid composition (mole fraction)

XB : Bottoms composition (mole fraction)

XD : Distillate composition (mole fraction)

XF : Feed composition (mole fraction)

XS : Sidestream composition (mole fraction)

XCALC : Calculated liquid composition on any tray (mole fraction)

Y : Vapor composition (mole fraction)

```
      PROGRAM SSPLOC(INPUT,OUTPUT)
C...
C...   THIS PROGRAM SIMULATES COMPOSITION,TEMPERATURE,LIQUID AND
C      VAPOR RATES PROFILE FOR NONEQUAL MOLAR OVERFLOW BINARY
C      DISTILLATION COLUMN WITH SIDESTREAM PRODUCT. BOTTOMS AND
C      DISTILLATE COMPOSITION,FEED RATE,COMPOSITION AND ITS TEMPERA-
C      TURE IS GIVEN. SIDESTREAM DRAW OFF RATE IS INCREASED BY SMALL
C      STEPS AND THE PROFILES ARE CALCULATED FOR EACH CASE.
C...
000003         DIMENSION X(25),Y(25),HL(25),HV(25),V(25),XL(25),T(25),P(25)
C...   TRAY PRESSURES
000003         DATA P   / 1.13234, 1.09940, 1.09662, 1.09377, 1.09091, 1.08803,
              1    1.08519, 1.08233, 1.07948, 1.07662, 1.07376, 1.07090, 1.06803,
              2    1.06519, 1.06233, 1.05947, 1.05661, 1.05376, 1.05090, 1.04804,
              3    1.04518, 1.04232, 1.03947, 1.03661 /
000003    1    READ 11,XF,FL,TF,XD,XB,TR,,Q9
000027    11   FORMAT(8F10.5)
0J3027         IF(XF,LT.0.)CALL EXIT
000032         SS=0.
000033         LOOPS=0
000034         READ 12,QL,QS,XS,E1,E2,NT,NF,NS
000057    12   FORMAT(5F10.4,3I5)
000057         IF(SS.LT.DS)GO TO 99
000062   103   SS=SS+DS
000064         XS=X(NS )
000066    99   LOOPS=LOOPS+1
000070         LOOPQ=0
000071   101   LOOPQ=LOOPQ+1
000073         IF(LOOPQ.GT.20)GO TO 22
C...   OVERALL MATERIAL BALANCE
000076         B=((XD-XF)*FL-(XD-XS)*SS)/(XD-XB)
0J3105         D=FL-B-SS
C...   FEED AND REFLUX SUBCOOLING
0J3107         TT=TF+25.
000112         CALL VANLAR(XF,TT,YY,P(NF))
000115         HF=HLIQ(XF)-(TT-TF)*(18.*(1.-XF)+22.4*XF)
C...   REFLUX...
0J3130         TT=TD+25.
000132         PR=1.
000134         CALL VANLAR(XD,TT,YY,PR)
0J3137         HR=HLIQ(XD)-(TT-TD)*(18.*(1.-XD)+22.4*XD)
000152         DDD=QD/ 10.
000154         FLAGR=-1.
000155         FLAGP=-1.
0C0156         LOOP=0
000157         HLD=HLIQ(XD)
000161         TD=97.
000163         PD=1.10914
3J0165         CALL VANLAR(XD,TD,YD,PD)
0J0170         YD=XD+E*(YD-XD)
000174         HVD=HVAP(YD)
C...   AFTER THE FIRST SIMULATION IS COMPLETED TAKE THIS PROFILE
C      AS AN INITIAL GUESS FOR NEXT CASE
000176         IF(LOOPS.GT.1)GO TO 100
0J3202         T(1)=TD
000202         X(1)=XD+0.05
C...   MAKE AN INITIAL GUESS FOR TEMPERATURE AND COMPOSITION FOR EACH
```

```
          C     TRAY
000205          DO 5  N=2,NT
000206          X(N)=X(N-1)+0.02
000210     5    T(N)=T(N-1)-1.
000215          T0=T(NT)
000216    100   LOOP=LOOP+1
000220          IF(LOOP.GT.50)GO TO 2
000223          N=1
          C...   INITIALIZE THE HEAT LOSS
000223          QLOSS=0.
000224          LOOP1=0
          C...   TRAY 1 CALCULATIONS
000226    10    LOOP1=LOOP1+1
000230          IF(LOOP1.GT.25)GO TO 21
000233          HL(1)=HLIQ(X(1))
          C...   FROM ENTHALPY BALANCE
000234          XL(1)=(Q3+B*(HVB-HLB))/(HV3-HL(1))
          C...   MATERIAL BALANCE
000243          VB=XL(1)-B
000245          IF(VB.LT.0.)GO TO 70
          C...   COMPONENT BALANCE
000247          XCALC=(Y3*VB+X9*B)/XL(1)
000252          IF(ABS(XCALC-X(1)).LT.1.E-0)GO TO 15
000257          X(1)=XCALC
000260          GO TO 10
000260     15   CALL VANLAR(X(1),T(1),Y(1),P(1))
000263          Y(1)=Y3+E*(Y(1)-YB)
000267          HV(1)=HVAP(Y(1))
          C...   STRIPPING TRAYS CALCULATIONS
000272          DO 30  N=2,NF
000273          QLOSS=QLOSS+QL
000275          LOOP1=0
000276     20   LOOP1=LOOP1+1
000300          IF(LOOP1.GT.25)GO TO 21
000303          HL(N)=HLIQ(X(N))
          C...   ENTHALPY BALANCE FOR STRIPPING SECTION
000307          XL(N)=(Q3-QLOSS+B*(HV(N-1)-HLB))/(HV(N-1)-HL(N))
          C...   MATERIAL BALANCE
000320          V(N-1)=XL(N)-B
          C...   COMPONENT BALANCE
000322          XCALC=(V(N-1)*Y(N-1)+B*XB)/XL(N)
000326          IF(ABS(XCALC-X(N)).LT.1.E-0)GO TO 25
000333          X(N)=XCALC
000334          GO TO 20
000334     25   CALL VANLAR(X(N),T(N),Y(N),P(N))
000340          Y(N)=Y(N-1)+E*(Y(N)-Y(N-1))
000345     30   HV(N)=HVAP(Y(N))
          C...   RECTIFYING TRAYS CALCULATIONS
000353          NFP1=NF+1
000354          NS1=NS-1
000356          DO  50   N=NFP1,NS1
000360          QLOSS=QLOSS+QL
000362          LOOP1=0
000363     40   LOOP1=LOOP1+1
000365          IF(LOOP1.GT.25)GO TO 21
000370          HL(N)=HLIQ(X(N))
          C...   ENTHALPY BALANCE FOR RECTIFYING SECTION
000374          XL(N)=(QB-QLOSS-FL*(HV(N-1)-HF)+B*(HV(N-1)-HLB))/(HV(N-1)-HL(N))
```

```
000712        PRINT 53
000716    53  FORMAT(///,1X,* N          X          Y          T          L          V
         1          HL         HV*)
000716        N=0
000717        PRINT 54,N,XB,YB,TB,B,VB,HLB,HVB
000743    54  FORMAT (1X,I2,4X,2F10.5,10F10.2)
000743        DO 56  N=1,NT
000745    56  PRINT 54,N,X(N),Y(N),T(N),XL(N),V(N),HL(N),HV(N)
000773        PRINT 57,XD,D,TR,R
001006    57  FORMAT(//,5X,12F15.4)
001006        DMIN=DS-100.
001010        IF(D.LT.DMIN)GO TO 1
001013        GO TO 103
         C...
         C...    FOLLOWING IS THE CONVERGENCE PROCEDURE FOR XD AND XS
         C...    INTERVAL HALVING FOR XD CONVERGENCE BY ADJUSTING QB
         C...
001013    69  IF(XD-Y(NT))80,80,70
001017    68  PRINT 168,X(N),N
001027   168  FORMAT(15X,F10.4,10X,*TRAY *,I2)
001027    70  IF(FLAGP.LT.0.)GO TO 71
001031        DQB=DQB*0.5
001032    71  QB=QB+DQB
001034        FLAGM=1.
001036        GO TO 100
001036    80  IF(FLAGM.LT.0.)GO TO 81
001040        DQB=DQB*0.5
001041    81  QB=QB-DQB
001043        FLAGP=1.
001045        GO TO 100
         C...    FALSE POSITIONING TECHNIQUE FOR XS CONVERGENCE
001045    72  IF(LOOPB.GT.1)GO TO 75
         C...    OUR FIRST GUESS WILL BE USED AS THE CONSTANT POINT IN
         C       THE METHOD OF FALSE    POSITION
001051        C=XS+0.01
         C...    WE WILL DEFINE THE FUNCTION...
001052        FC=X(NS)-C
001055        XS=X(NS)
001056        GO TO 101
         C...    WE WANT THE FUNCTION TO BE ZERO AS WE GET THE DESIRED VALUE
         C       OF XS, SO WE DEFINE...
001057    75  FNX=X(NS)-XS
         C...    USING POINT C AND XS WE CAN ESTIMATE A BETTER VALUE FOR XS
         C       USING FALSE POSITION METHOD
001061        XS=(C*FNX-XS*FC)/(FNX-FC)
001067        GO TO 101
         C...    PRINTING STATEMENTS IF ONE OF THE LOOPS DOES NOT CONVERGE
001070     2  PRINT 200
001074   200  FORMAT(5X,*QB LOOP*)
001074        PRINT 201,QB
001102   201  FORMAT(/,5X,E15.5)
001102        RAT=SS/0
001104        PRINT 202,N,XL(N),RAT
001116   202  FORMAT(/,3X,*TRAY *I2,5X,*LIQ. RATE*,F8.2,5X,*SIDE STREAM TO DISTI
         1LLATE RATIO*,F10.4,/)
001116        GO TO 1
001117    21  PRINT 211
001123   211  FORMAT(5X,*TRAY LOOP*)
```

```
001123        PRINT 212,N,T(N),X(N),Q9
001137   212  FORMAT(1X,I2,8X,2F10.5,E15.5)
001137        GO TO 1
001140    22  PRINT 220,XS,SS,C
001152   220  FORMAT(/,5X,* XS DID NOT CONVERGE *,10X,* XS= *,F8.5,5X,* FOR SS=*
             1,F8.1,/,10X,*THE FIRST GUESS WAS *,F8.5,//)
001152        GO TO 103
001153        END


              FUNCTION FUNCTN(T,PP,X)
         C... THIS FUNCTION IS USED IN VANLAR SUBROUTINE TO FIND TRAY TEMP.
         C    AND VAPOR COMPOSITION VIA NEWTON - RAPHSON TECHNIQUE
000006        COMMON/TRANS/GAM1,GAM2,X2,PCALC
000006        COMMON/VP/P1,P2
         C... PREDICTED VAPOR PRESSURE CURVE FOR PUKE MATERIAL( LN(P)=A/(T+273)
         C...                                                   +B  TYPE)
         C... T  IN DEGREE CENTIGRATE , P  IN ATMOSPHERES
         C... DATA FROM PERRY S CHEM. ENGR.HAND BOOK
000006        P1=EXP(-4386.93375/(T+273.15)+12.984856)
000015        P2=EXP(-4981.0357/(T+273.15)+13.349615)
000025        PCALC=GAM1*X*P1+GAM2*X2*P2
000033        FUNCTN=PCALC-PP
000035        RETURN
000035        END


              FUNCTION DF(T,PP,X)
         C... THIS IS THE DERIVATIVE OF THE PREVIOUS FUNCTION WITH RESPECT
         C    TO TEMPERATURE
000006        COMMON/TRANS/GAM1,GAM2,X2,PCALC
000006        COMMON/VP/P1,P2
000006        DP1=P1*(4386.93375/(T+273.)**2)
000011        DP2=P2*(4981.0357/(T+273.)**2)
000014        DF=GAM1*X*DP1+GAM2*X2*DP2
000022        RETURN
000023        END


              SUBROUTINE VANLAR(X,T,YV,PP)
000007        DIMENSION R(51)
000007        COMMON/TRANS/GAM1,GAM2,X2,PCALC
000007        COMMON/VP/P1,P2
         C... THIS SUBROUTINE FINDS VAPOR COMPOSITION AND TEMPERATURE FOR A
         C    GIVEN LIQUID COMPOSITION
000007        X2=1.-X
         C... ACTIVITY COEFFICIENTS USING VAN LAAR EQUATIONS
000010        GAM1=EXP(0.9*X2**2/(0.9*X/0.48+X2)**2)
000023        GAM2=EXP(0.48*X**2/(X+0.48*X2/0.9)**2)
000036        R(1)=T
000037        DO 1  I=1,50
         C... CALCULATE THE TRAY TEMPERATURE AND EQUILIBRIUM VAPOR COMP.
         C    USING NEWTON RAPHSON TECHNIQUE
000041        F=FUNCTN(R(I),PP,X)
000047        R(I+1)=R(I)-F/DF(R(I),PP,X)
```

```
000063    1    IF(ABS(F).LT.1.0E-06)GO TO 20
000070         PRINT 121,R(I),X,GAM1,GAM2,PCALC
000110   121   FORMAT(5X,*NO CONVERGENCE IN VAN LAAR*,3X,4H T= ,F6.2,4(5X,F8.4))
000110         CALL EXIT
000111   20    YV=X*P1*GAM1/PP
000115         T=R(I+1)
000120         RETURN
000121         END


         FUNCTION HLIQ( X )
   C...   LIQUID ENTHALPY - COMPOSITION DATA FITS THIS SECOND ORDER
   C      POLYNOMIAL
   C...   X IN MOLE. FRACTIONS, HLIQ IN CAL/GR.MOLE
000003         HLIQ=1800.-2433.*X+1753.*X**2
000011         RETURN
000011         END


         FUNCTION HVAP( Y )
   C...   VAPOR ENTHALPY - COMPOSITION DATA FITS THIS LINEAR EQUATION
   C...   Y IS VAPOR COMPOSITION IN MOLE.FRACTION, HVAP IN CAL/GR.MOLE.
000003         HVAP=11440.-1990.*Y
000006         RETURN
000007         END
```

TABLE OF REFERENCES

1 - Van Winkle, M. "Distillation" McGraw-Hill 1967

2 - Ruszkay, R. J. "Analog Computer Simulation of a Solvent Recovery
Column" ISAJ 1964

3 - Luyben, W. L. "10 Schemes to Control Distillation Columns with
Sidestream Draw Off" ISAJ July 1966

4 - Buckley, P. S. "Controls for Sidestream Draw Off Columns" CEP 65,
5, 1969

5 - Buckley, P. S. and Cox, R. K. "New Developments in Overrides for
Distillation Columns" ISA Transactions, 10, 4

6 - Luyben, W. L. "Process Modeling, Simulation and Control for
Chemical Engineers" Chapters 3, 5 McGraw-Hill 1973

7 - Franks, R. G. E. "Modeling and Simulation in Chemical Engineering"
Chapter 8, John Wiley and Sons, 1972

8 - Coulson and Richardson. "Chemical Engineering" Vol. 2, Permagon
Press, London, 2nd edition, 1967

9 - Tyréus, B.
Master of Science Degree Thesis Lehigh University 1974

10 - Perry, J. H. "Chemical Engineers' Handbook" McGraw-Hill, 4th
edition, 1963

11 - Van Laar, J. J. 2 Phys. Chem. 185:35 (1929)

12 - Carlson, H. D. and Colburn, A. P. IEC 34, 581 (1942)

13 - Plewes, A. C.; Jardine, D. A.; and Butler, R. M. Canadian
Journal of Technology, 32 (4), 133 (July 1954)

14 - American Institute of Physics Handbook, 3ed edition