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TWOPOT: A Computer Model of the Two-Pot Extraction Distillation Concept for Nitric Acid

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MARTIN MARIETTA ENERGY SYSTEMS, INC.
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ORNL/TM-9241
Dist. Category UC-86

Consolidated Fuel Reprocessing Program

TWOPOT: A COMPUTER MODEL OF THE TWO-POT EXTRACTION DISTILLATION CONCEPT FOR NITRIC ACID

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Date Published: May 1985

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Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
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MARTIN MARIETTA ENERGY SYSTEMS, INC.
for the
U.S. DEPARTMENT OF ENERGY
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TWOPOT: A COMPUTER MODEL OF THE TWO-POT EXTRACTIVE DISTILLATION CONCEPT FOR NITRIC ACID

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ABSTRACT

A mathematical model, TWOPOT, of the "two-pot" extractive distillation concept for nitric acid concentration has been developed. Prediction from a computer simulation using this model shows excellent agreement with the experimental data. This model is recommended for use in the design of large-scale, similar-purpose equipment.

1. INTRODUCTION

The use of high-strength nitric acid (~95 wt %) has been proposed for off-gas scrubbing operations to remove iodine in proposed nuclear fuel reprocessing operations (IODOX process). High-strength nitric acid can be produced by the recycle and concentration of available lower-strength nitric acid streams; however, concentration by simple distillation is complicated by the existence of an azeotrope at a nitric acid concentration of ~68.5 wt %. A major portion of high-strength nitric acid is currently manufactured commercially by extractive distillation using $Mg(NO_3)_2$ as the solvent;[1,2] however, the commercially proven extractive distillation systems do not seem to be appropriate for use in remotely maintained facilities because of maintenance and operational complexity. To avoid the problems of these commercial systems, a simplified system of distillation, called the two-pot process, was developed. The process consists of two major process vessels—an extractive distillation pot (EDP), where high-strength acid is produced from the contact of the feed acid and the solvent $Mg(NO_3)_2$; and a solvent recovery pot (SRP), where the solvent is regenerated for recycle. The two-pot concept offers several advantages such as simplicity and reliability over conventional extractive distillation processes using column-type contactors, making the two-pot process useful for remote operation in a nuclear fuel reprocessing plant.

This process has been successfully tested on a laboratory scale. To aid in understanding the system more fully and in developing the control schemes, a process model, TWOPOT, was formulated and is presented in this report.

2. BACKGROUND

The two-pot extractive distillation scheme using $Mg(NO_3)_2$ is shown in Fig. 2.1. The system consists of two heated vessels (or "pots") operated at different temperatures. Nitric acid at or below the azeotropic composition of ~68.5 wt % is fed to the lower temperature

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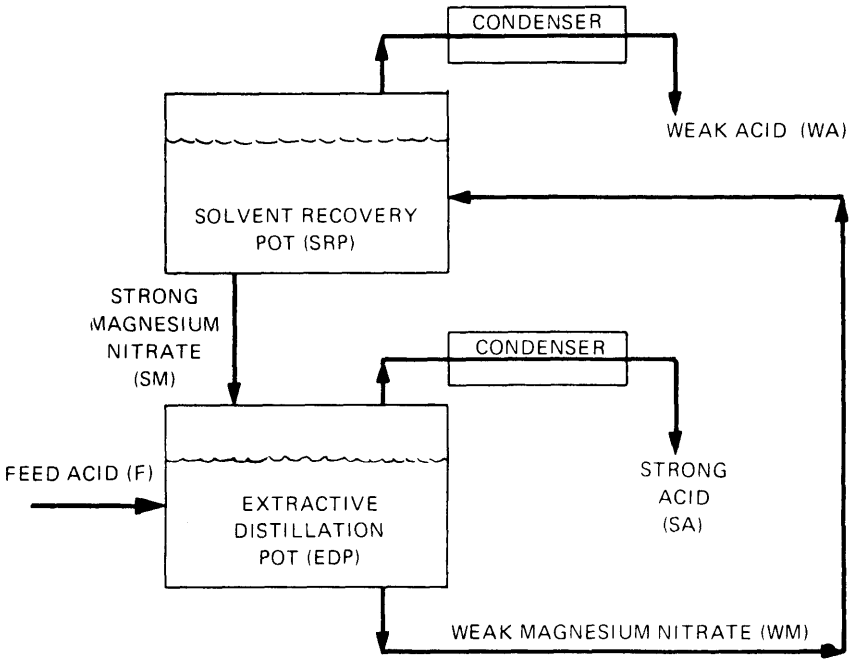

Fig. 2.1. Two-pot scheme.

vessel called the extractive distillation pot (EDP). In this vessel, the nitric acid feed is mixed with a boiling $Mg(NO_3)_2$ solution. Vapor leaving the EDP consists of a strong nitric acid–water mixture, which is totally condensed to form the strong acid (SA) product of the system. The $Mg(NO_3)_2$ is concentrated for recycle in the higher temperature pot, the solvent recovery pot (SRP), by the evaporation of weak acid. Vapor leaving the SRP consists of a weak nitric acid–water mixture, which is also totally condensed to form a weak nitric acid (WA) product.

This equipment was assembled and tested at the Oak Ridge National Laboratory (ORNL) and reported by Counce et al.[3] The Counce report presents data for 33 demonstration runs over a fairly wide range of operating conditions. Counce also attempted to relate the observed values to available vapor-liquid- equilibrium (VLE) data in an attempt to determine operating efficiency. However, at the time the Counce report was written, no suitable VLE model was available over the range of interest.

The equilibrium phase diagram for the nitric acid–water–$Mg(NO_3)_2$ system[4] is shown in Fig. 2.2. The equilibrium information in this diagram is based primarily on the work of

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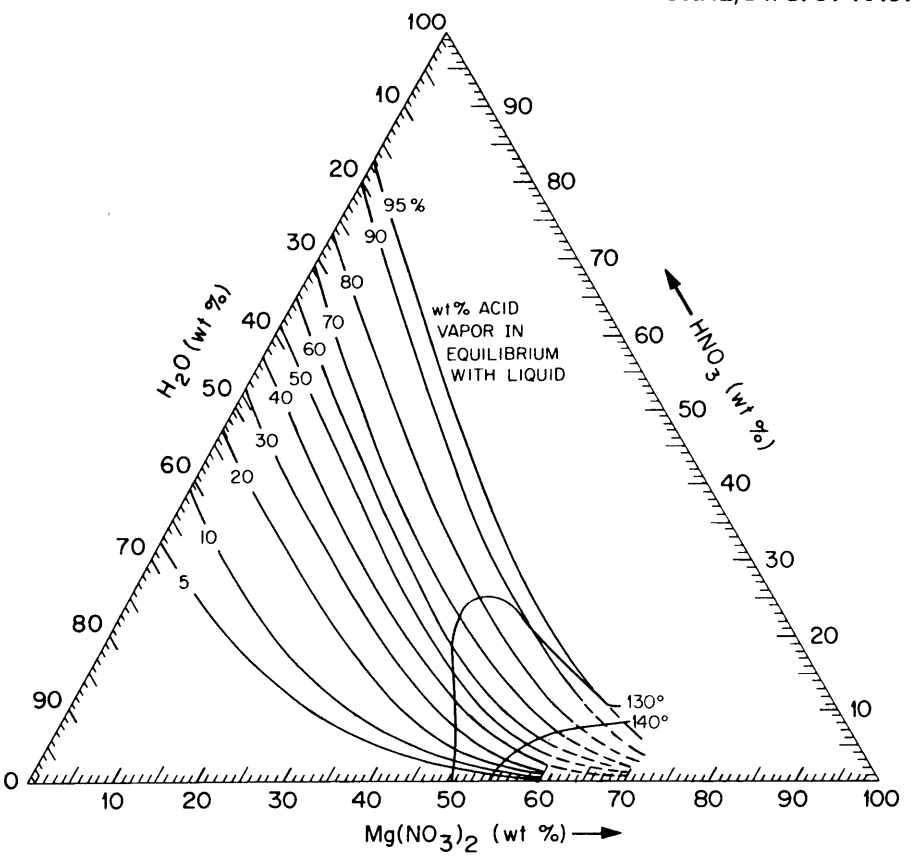

Fig. 2.2. Equilibrium vapor and liquid information with selected boiling isotherms for the nitric acid–water–$Mg(NO_3)_2$ systems; parameters are in weight percent nitric acid–water–$Mg(NO_3)_2$ system boiling isotherms. The liquid composition is located by the axis labels, and the vapor in equilibrium with the liquid is represented by the percent parameter lines passing over the liquid composition (from Ginnow and Clark, who incorporated data from Shneerson et al.). *Source*: R. J. Ginnow and W. E. Clark, *Iodox Recycle Scoping Studies of the Solubility of Iodic Acid and of Vapor-Liquid Equilibria in the System: 60 to 80% $Mg(NO_3)_2$-O to 20% HNO_3-2O to 40% H_2*, ORNL/TM-6398, December 1978.

Shneerson et al.[5] and is presented here for illustration only. Thompson et al.[6] used VLE data from Ginnow and Clark[4] and Shneerson[5] as well as from other sources as a basis for a VLE model of the $Mg(NO_3)_2$-HNO_3-H_2O system. Liquid phase density for the $Mg(NO_3)$-HNO_3-H_2O system is available from the work of Jubin et al.[7] Other useful information is available in a review article by Sloan.[8]

The operating temperatures for the EDP and the SRP were normally in the range 140 to 180°C. The VLE data for this temperature range are incomplete with only a few data points at temperatures >140°C. This region of the SRP and the EDP operating conditions is bounded by the 140°C isotherm of Fig. 2.2, and generally located below and to the right of the 140°C isotherm. Recent work by Thompson et al.[6] produced a simplified dissociation VLE model that appears to model the available data within the accuracy of the data

and is well-behaved up to 200°C, thus covering the range of interest; calculations using the simplified dissociation VLE model are shown in Figs. 2.3 and 2.4.

This modeling effort is, then, an attempt to bring together the proposed VLE model, a material balance program, and the experimental data to produce a tool for the design and better understanding of this two-pot distillation system.

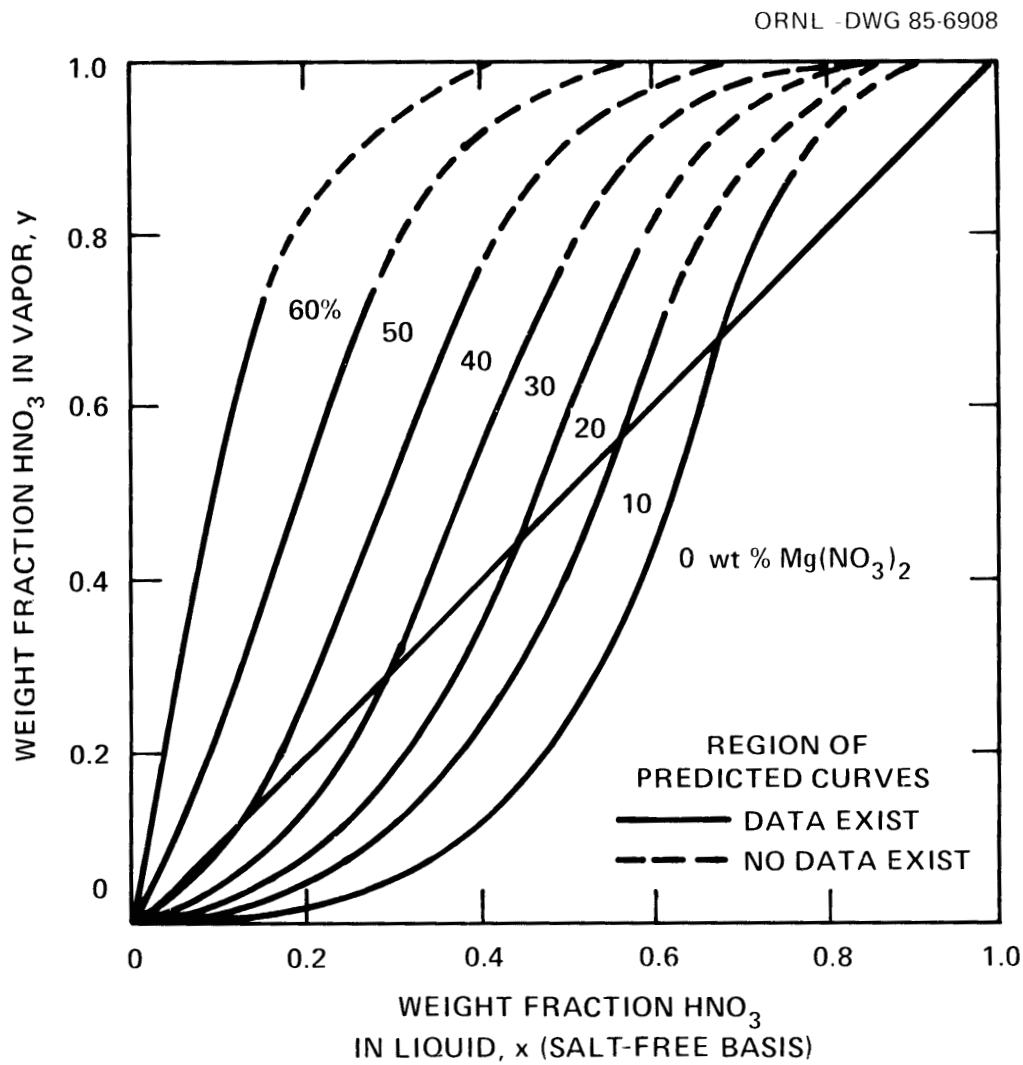

Fig. 2.3. Vapor composition as a function of liquid composition—simplified dissociation model.

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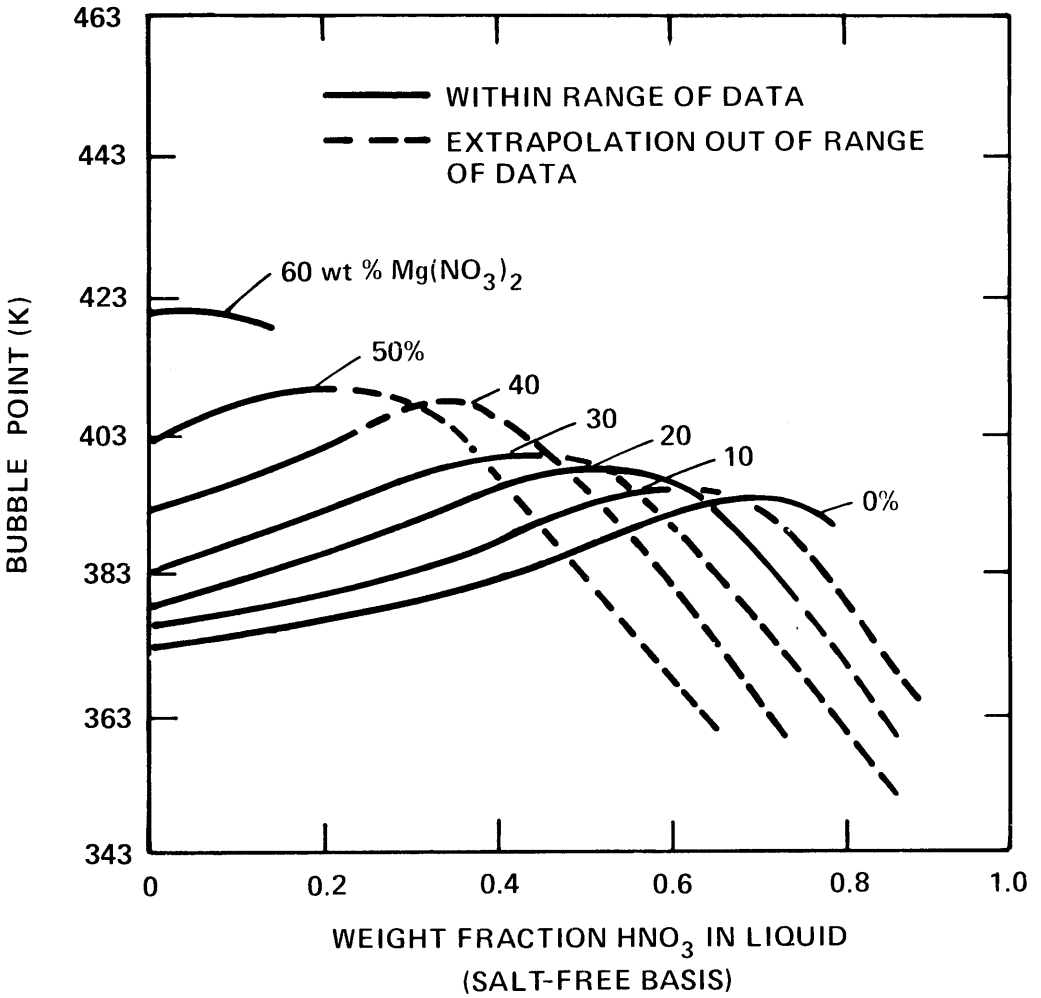

Fig. 2.4. Predicted bubble-point temperature as a function of liquid composition—simplified dissociation model.

3. COMPUTATIONAL PROCEDURES

This methodology uses overall and component steady-state material balances around each vessel and the complete system. From a balance around the complete system, the following mass and nitric acid balances may be obtained.

$$F = WA + SA \ , \tag{1}$$

and

$$F(X_F) = WA(X_{WA}) + SA(X_{SA}) \ , \tag{2}$$

where F, WA, and SA are the mass flow rates of the feed acid, the weak acid product, and the strong acid product, respectively, and X_F, X_{WA}, and X_{SA} are the nitric acid weight fractions of the same streams. Similar balances are obtained from around the solvent recovery pot (SRP).

$$WM = SM + WA \ , \tag{3}$$

and

$$WM(X_{WM}) = SM(X_{SM}) + WA(X_{WA}) \ , \tag{4}$$

where WM and SM are the mass flow rates of the weak and strong magnesium nitrate streams, and X_{WM} and X_{SM} are the nitric acid weight fractions in the respective streams. Assuming that $Mg(NO_3)_2$ is a nonvolatile component, none would therefore be present in either the SA or the WA product. It is assumed that no $Mg(NO_3)_2$ is present in the feed acid stream. The $Mg(NO_3)_2$ balance around the SRP or the EDP can then be described by

$$WM(Z_{WM}) = SM(Z_{SM}) \ , \tag{5}$$

where Z_{WM} and Z_{SM} are the weight fractions of $Mg(NO_3)_2$ in the weak and strong magnesium nitrate streams respectively. Figure 3.1 is a block diagram showing the streams within the two-pot distillation system. The EDP is considered as two blocks, a mixer and a

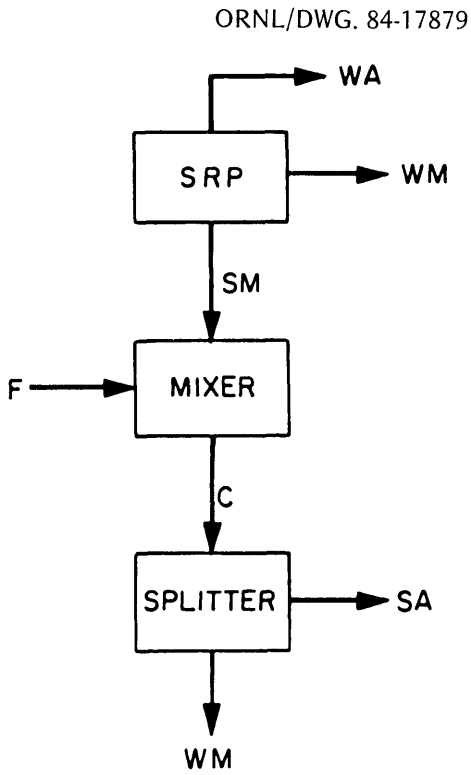

Fig. 3.1. Simplified flow diagram for two-pot system.

splitter. In the mixer, the feed acid (F) and SM solutions are combined to form solution C. If mass is conserved, the points F, SM, and C lie on a straight line if plotted on a triangular diagram (line 1 of Fig. 3.2). The composition of point C can be determined by the inverse lever arm rule. The second block, the splitter, takes stream C and makes the two-component SA stream and the three-component WM stream. These three stream compositions lie on a straight line, line 2. The third block represents the solvent recovery pot, which separates the WM into two streams—the two-component WA and three-component SM solutions. These three points must also lie on a straight line, line 3. The relative amounts of WA and SM can be determined by the inverse lever arm rule, as can SA and WM.

Also note that the overall material balance is represented by the line SA-F-WA on the H_2O axis and that this is a two-component system, while the other equations involved all three components.

This solution thus far has only addressed the material balance aspect of distillation. Equilibrium considerations can be examined by a sample problem.

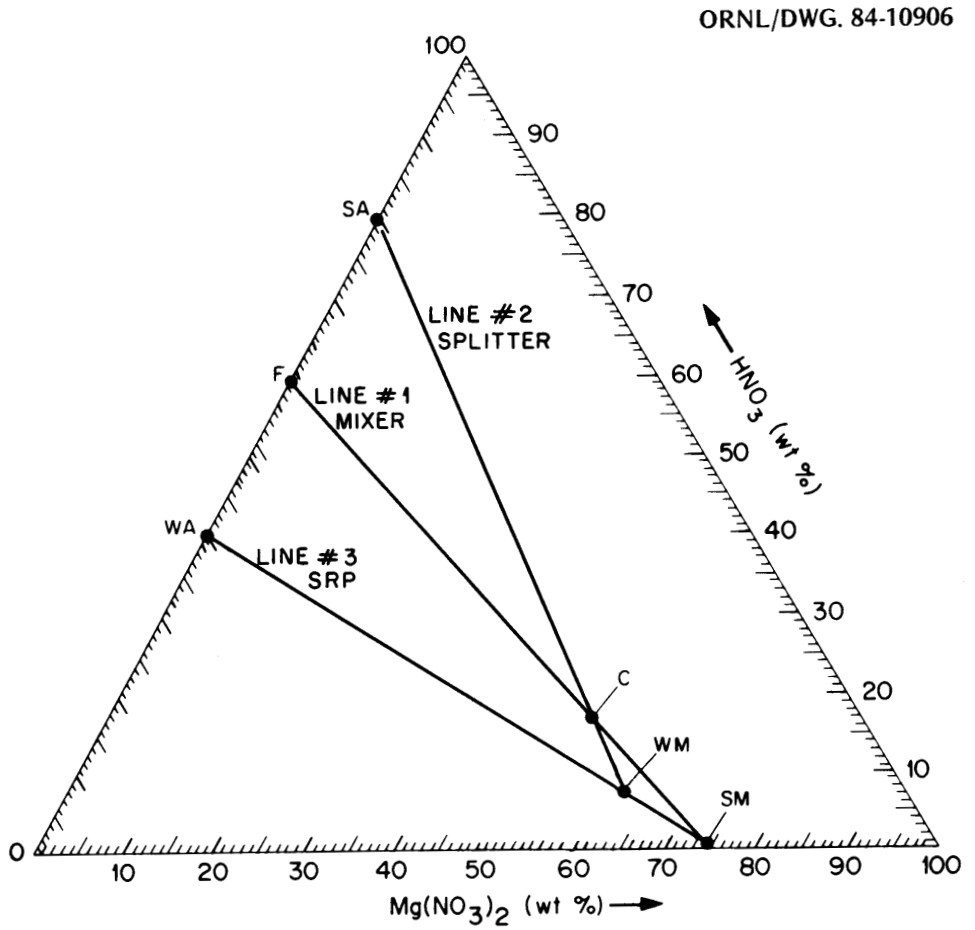

Fig. 3.2. Material balance relationships as determined on triangular diagram.

The composition of the SA and WA streams is assumed to be the vapor composition in equilibrium with streams WM and SM respectively. The composition of these condensed product streams may be calculated by the correlation of Thompson et al.[6] as a function (f) of

$$X_{SA} = f(X_{WM}, Z_{WM}, T_{EDP}) \ ; \tag{6}$$

$$X_{WA} = f(X_{SM}, Z_{SM}, T_{SRP}) \ . \tag{7}$$

It is important to note that Thompson's correlation, which is in the form of a FORTRAN subroutine, provides the user with the acid vapor composition and the total of the vapor pressure of the HNO_3 and H_2O for a given liquid composition and temperature.

Equations (1) through (7) contain 12 variables; thus five degrees of freedom exist in this system of equations. The five variables selected to be user-specified—X, X_F, SA, X_{SA}, T_{EDP}—do not provide the most straightforward approach to solving the system of equations, but they appear to be the most useful in the design mode.

Considering a sample problem in which F = 1.0, SA = 0.5, X_{SA} = 0.80, X_F = 0.60, and T_{EDP} = 140°C, the points X_{SA} and X_F can be located immediately on the diagram in Fig. 3.3. The location of WA can be calculated from the overall material balance [Eq.(1)] and from the acid balance [Eq. (2)]. The coordinates of the point located at the

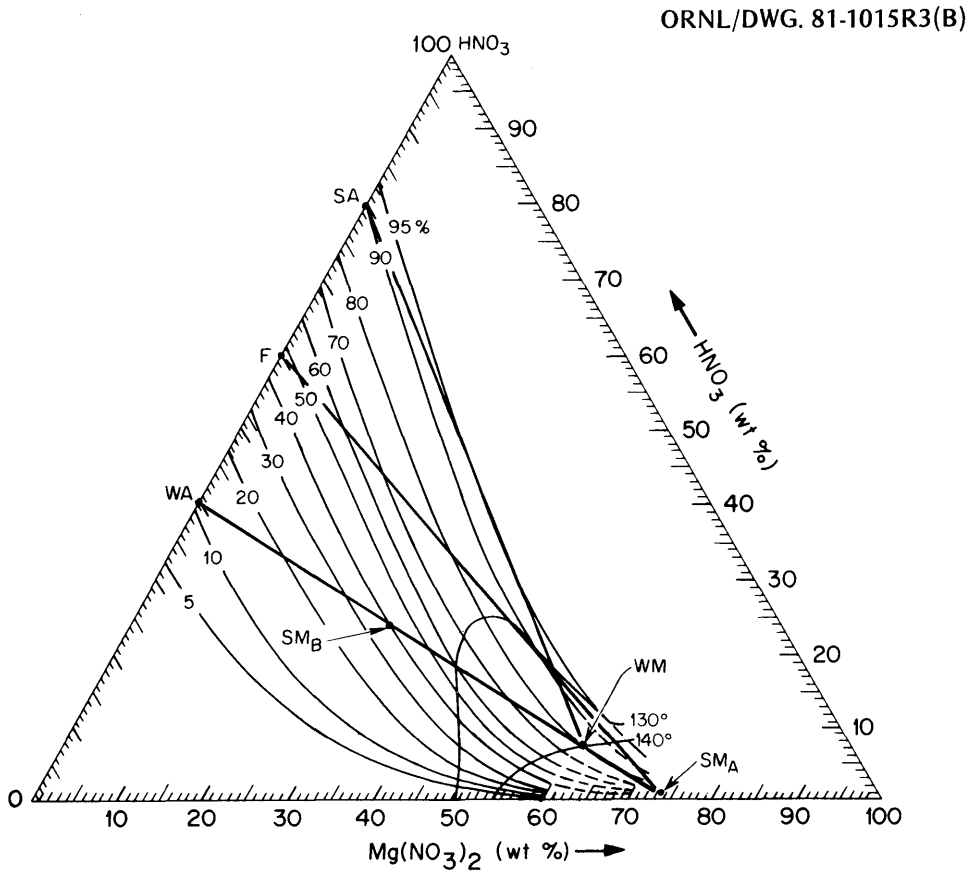

Fig. 3.3. Sample graphic solution.

intersection of the 140°C isotherm and the 80% acid vapor line can be determined using Eq. (6) since the vapor in equilibrium with WM is SA.

Equation (4) requires that WA, WM, and SM lie on a straight line, and equilibrium requires a vapor composition of 40 wt % (i.e., the composition of WA). As shown in Fig. 3.3, there are two possible solutions, SM_A and SM_B, for the location of point SM. The difference is in the boiling point of the two solutions and the liquid composition. The solution to the physical problem at hand requires that the SRP operate with the WM stream split into the SM and WA streams; hence, the point WM must lie on the line between SM and WA. This answer also reflects the physical situation of the SRP operating at a higher temperature than this EDP.

Note that the equilibrium lines below and to the right of the 140°C isotherm cover only a small range of liquid compositions but, on the other hand, cover a wide range of vapor compositions. Graphic solutions become very difficult and inaccurate in this range. Since most operations of the two-pot distillation system require that the SRP operate

between 160 and 180°C, a computer process model is desirable provided that an adequate VLE correlation is available in this region.

The main logic of the process model, TWOPOT, is shown in the flow chart in Fig. 3.4. (The complete code is listed in Appendix A.) There are two main procedures involved in this model. The first, SOLVO, determines the composition of the liquid in the EDP, given the temperature and the vapor composition above it. This is done using the Numerical Algorithms Group (NAG) routine E04JAF to find the calculated solution to the "cost" equation, which sets the total pressure in the system at 760 mm Hg and the calculated vapor composition equal to the given vapor compositions. Checks were required to ensure that the calculated solution had the correct total pressure, since in early runs nondesired local minima were located. When a nondesired minimum was encountered, a new starting point was chosen for E04JAF, and the search procedure was rerun.

This local minima problem generally occurs when the correct composition is found, but the total pressure of the system is in error. The random probes by E04JAF beyond the local area, in nearly all cases, produce a higher "cost" term since the correct solution could be thought of as a very deep but narrow well in the cost surface with many shallow, broad depressions.

The second major calculation procedure is SALVO. This routine returns T_{SRP}, X_{SM}, and Z_{SM} given X_{WA}, Z_{WM}, and X_{WM}. This requires varying all three variables that drive the Thompson correlation. The liquid compositions are determined by the split of the weak $Mg(NO_3)_2$ feed solution to the SRP between the vapor phase and the strong $Mg(NO_3)_2$ stream. In addition, the operating temperature is not known. Once again, the solution is found using E04JAF. Certain constraints must be applied to this routine since two possible solutions exist [i.e., one to the right of the EDP point (the correct one) and one to the left, in which, while it solves the equilibrium equations, the flows are in the wrong directions since the SM would then be the combined stream instead of the WM, as previously described]. In addition, local minima, which are generally at the incorrect pressure, must be dealt with in a similar manner as in SOLVO.

The recognition of nonsolvable cases must also be handled by the model. The first, requiring more acid than available to be in SA, can be detected by the overall material balance. The second case, requiring a strong acid that is weaker than the feed acid, can be detected from the input data. The third case is more insidious. Such a large fraction of the acid reports to the strong acid that the weak acid composition is sufficiently lowered so the line of Eq. (3) contains no point right of WM in equilibrium with the weak acid vapor (Fig. 3.5). That is to say, the vapor lines to the right of the point WM lie below the line WA-WM, and the point SM cannot be located on a 15 wt % vapor line since it is virtually on the $Mg(NO_3)_2$ axis. This type case was successfully detected by the high "cost" associated with the SALVO routine (Table 3.1) in simulation designed to test the TWOPOT model's ability to identify such a case.

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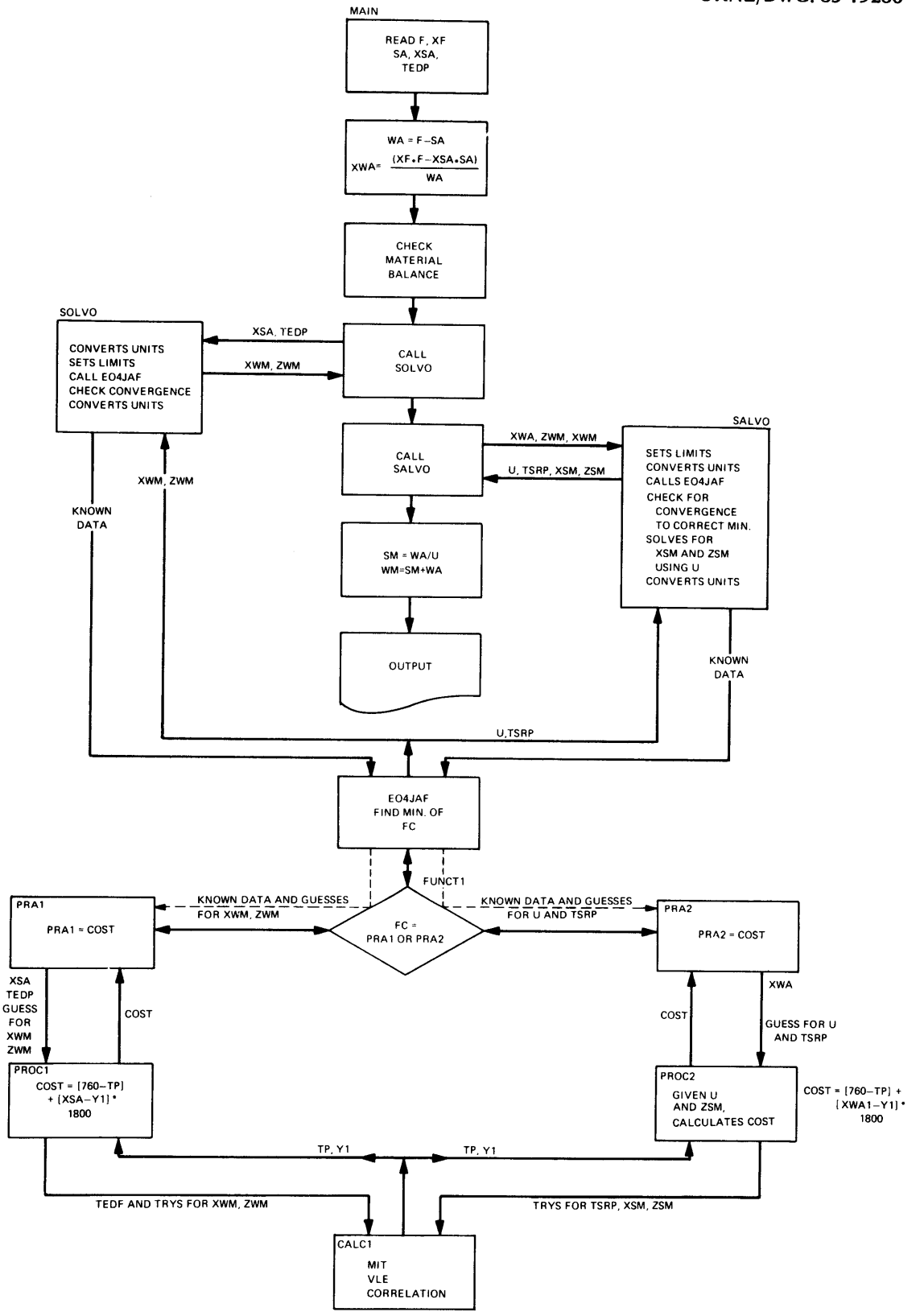

Fig. 3.4. Logic flowchart for TWOPOT model.

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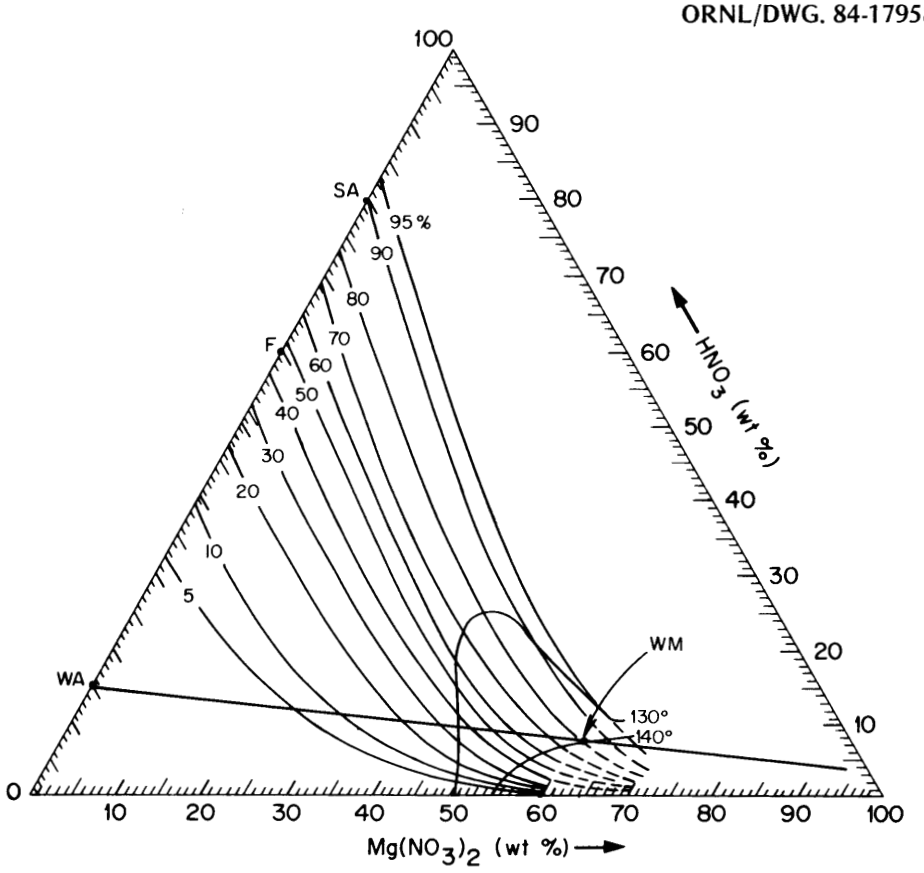

Fig. 3.5. System with no solution.

Table 3.1. Determination of TWOPOT model's behavior over expected range of process conditions

(Variables: SA, X_{SA}, T_{EDP}, X_F; F = 1)

SA→	X_{SA} = 0.75 T_{EDP} = 130°C					X_{SA} = 0.75 T_{EDP} = 140°C					X_{SA} = 0.75 T_{EDP} = 150°C				
X_F↓	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9	0.1	0.3	0.5	0.7	0.9
0.61	+	+	C	C	O	+	+	+	C	O	+	+	+	?	O
0.64	+	+	?	C	O	+	+	+	?	O	+	+	+	+	O
0.67	+	+	+	C	O	+	+	+	+	O	+	+	+	+	O
0.70	+	+	+	+	C	+	+	+	+	C	+	+	+	+	C
	X_{SA} = 0.85 T_{EDP} = 130°C					X_{SA} = 0.85 T_{EDP} = 140°C					X_{SA} = 0.85 T_{EDP} = 150°C				
0.61	+	C	C	O	O	+	+	C	O	O	+	+	+	O	O
0.64	+	?	C	C	O	+	+	+	C	O	+	+	+	C	O
0.67	+	+	C	C	O	+	+	+	C	O	+	+	+	C	O
0.70	+	+	?	C	O	+	+	+	C	O	+	+	+	+	O
	X_{SA} = 0.95 T_{EDP} = 130°C					X_{SA} = 0.95 T_{EDP} = 140°C					X_{SA} = 0.95 T_{EDP} = 150°C				
0.61	+	+	C	O	O	+	+	C	O	O	+	+	+	O	O
0.64	+	+	C	O	O	+	+	?	O	O	+	+	+	O	O
0.67	+	+	C	O	O	+	+	+	O	O	+	+	+	O	O
0.70	+	+	?	O	O	+	+	+	O	O	+	+	+	O	O

Key to symbols: +, solution found; O, material balance problem; C, high cost in SALVO; ?, questionable.
Units: F, volume/time; SA, volume/time; T_{EDP}, °C; X_F, weight fraction HNO_3; X_{SA}, weight fraction HNO_3.

4. TESTING OF THE MODEL

The mathematical model, which is based on the assumption that equilibrium is attained in both the EDP and the SRP and also on the Thompson equations as an accurate description of equilibrium, was tested by comparing certain quantities calculated using the model with experimental values from the results of Counce et al.[3]

Input values for the computer code were the amount of feed acid (F), composition of the feed acid (XF), amount of the strong acid product (SA), composition of the strong acid product (XSA), and temperature of the extractive distillation pot (T_{EDP}). The values for these five quantities were set at the corresponding values for each experimental run; and the computer code was used to generate compositions and flow rates for the weak acid product, the strong magnesium nitrate solution in the SRP, the weak magnesium nitrate solution in the EDP, and the temperature of the SRP.

For each run considered, errors were calculated by comparing the particular quantity predicted by the model with the valve which was determined experimentally. Average errors, based on all of the runs considered, and standard deviations of the errors were also tabulated. A deviation between a quantity predicted by the model and the corresponding experimentally determined quantity could conceivably be caused by one or more of three sources. These are (1) the assumption concerning the attainment of equilibrium in the EDP and SRP could be in error, (2) the calculated VLE relations for the $Mg(NO_3)_2$-HNO_3-H_2O system could be in error, (3) the experimental data for a particular run could be in error.

In order to eliminate deviations between experimental calculated quantities that might be due to erroneous experimental measurements, only those experimental runs in which the overall nitric acid material balances (output compared to input) were within 90% were used in the comparison. Even so, the difficulties in attaining steady-state and in sampling and analyzing the magnesium nitrate streams are such that errors in the experimental results cannot be discounted. The percentage errors [defined as (experimental value—calculated value)/experienced value $\times$ 100] were calculated for the weak acid flow rate, the weak acid concentration, the nitric acid and magnesium nitrate composition of the strong magnesium nitrate solution in the SRP, the flow rate and nitric acid composition and magnesium nitrate composition of the weak magnesium nitrate solution that flows from the EDP to the SRP. An error term [defined as experimental temperature (°C)−calculated temperature (°C)] was calculated based on the temperature of the SRP. Plots of the errors versus levels of the particular variable were made to determine if any trends were apparent in the deviation between experimental and model-predicted quantities. A summary of the mean errors and standard deviations for the model variables is presented in Table 4.1. The average percentage error in the weak acid flow rate was found to be 1.2% based on 26 runs. The standard deviation for the set of data was 6.7. The agreement between model and experiment for this variable seems good. A study of the error pattern in Fig. 4.1 indicates no recognizable trends.

Table 4.1. Model comparison study results

Variable	Mean error	Standard deviation	Number of data points
WAVOL	1.2%	6.7%	26
XWA	−0.6%	11.5%	26
XSM	−96.3%	131.2%	19
ZSM	0.7%	6.2%	19
WMVOL	13.8%	25.9%	26
XWM	−34.5%	33.2%	16
ZWM	3.2%	8.8%	16
SRP	0.5°C	12.2°C	26

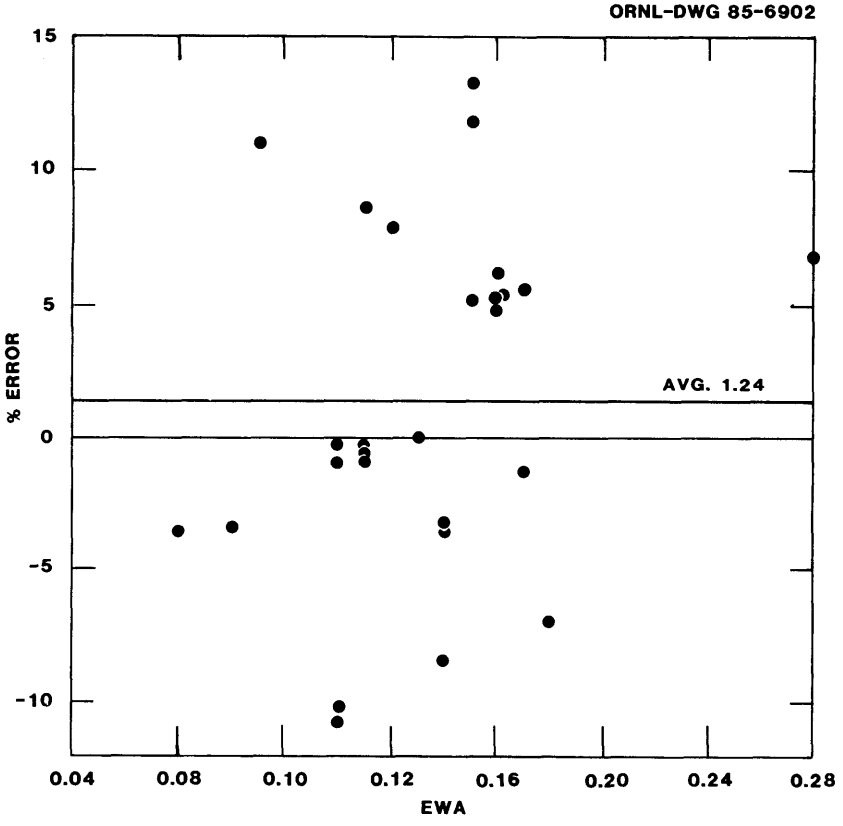

Fig. 4.1. Percentage of error in the weak acid flow versus the experimental weak acid flow [calculated by (experimental value—calculated value)/experimental value × 100].

Examination of the error in the prediction of the nitric acid composition of the weak acid indicates an average percentage error of only 0.6%. However, a standard deviation of 11.5% was obtained for the 26 runs considered.

As can be seen on the flowsheet of the computer model (see Fig. 3.4), the first two steps in the calculational procedure are the calculation of weak acid flow rate and composition assuming steady state. The calculations do not involve the VLE data or the ideal stage assumptions upon which many of the subsequent calculations are based. Thus, the errors associated with both the weak acid flow rate and composition are felt to reflect inconsistency in the experimental data rather than indicating a deficiency in the model.

The average error found in the nitric acid content of the strong magnesium nitrate solution (XSM) was found to be 96.3% for the 19 runs considered. These errors were distributed around the mean with a standard deviation of 131.2. This error seems quite large; however, it should be noted that most of the data were obtained at values of nitric acid concentration of only a few percent. Thus, an error in the acid determination of around 1% will lead to quite large percentage errors.

Another interesting point concerning this set of data (Fig. 4.2) is that most of the errors are negative, indicating experimental quantities lower than predicted by the computer model. Since the sampling of the molten salt streams for subsequent chemical

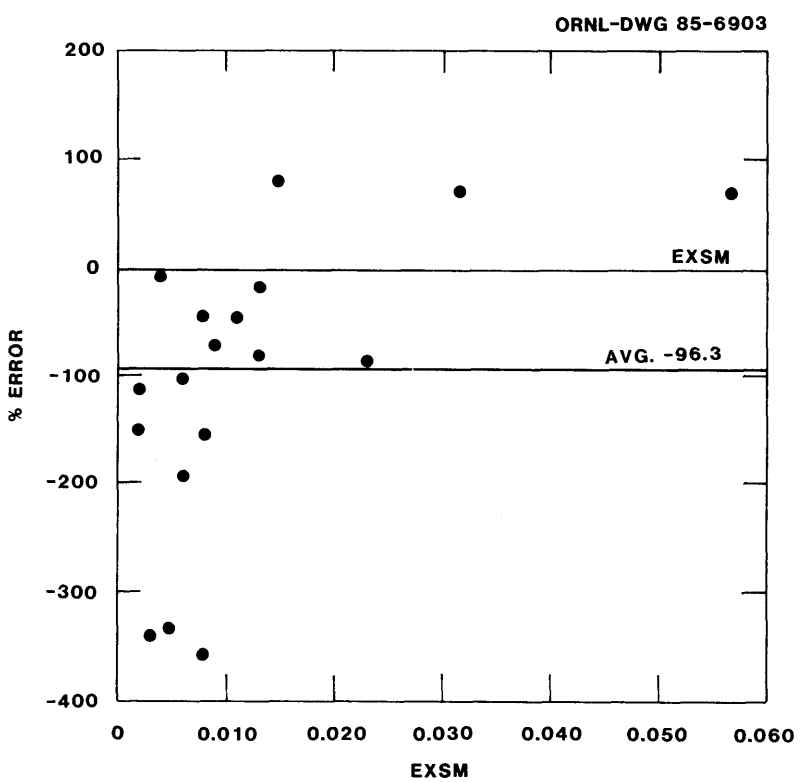

Fig. 4.2. Percentage of error in the nitric acid concentration of the strong magnesium nitrate solution versus the experimentally determined acid concentration [calculated by (experimental value—calculated value)/experimental value × 100].

analysis for HNO_3 is quite difficult and the likelihood of losing some of the acid by vaporization from the hot stream is very real, it is not surprising that the errors seem to be in the negative direction. The model seems to do a better job of predicting the $Mg(NO_3)_2$ composition of the strong magnesium nitrate solution. Of 19 data sets tested, the average error in the magnesium nitrate composition was only 0.7% with a standard deviation of 6.2%. Data for this quantity (Fig. 4.3) are pretty much evenly distributed around the mean.

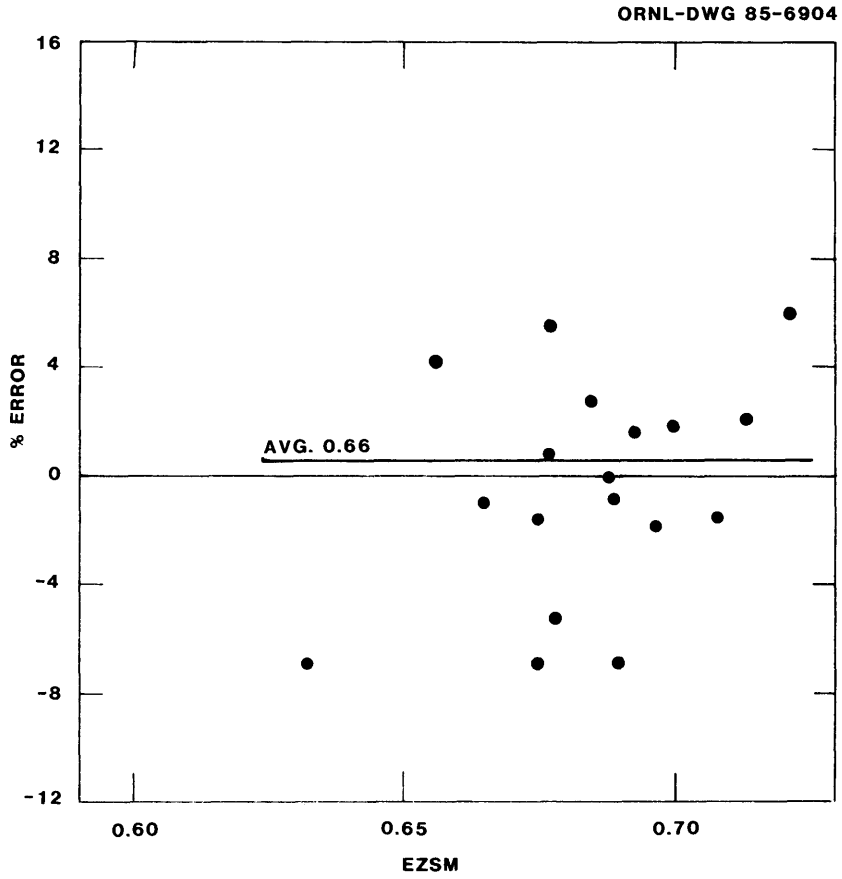

Fig. 4.3. Percentage of error in the $Mg(NO_3)_2$ concentration versus the experimental $Mg(NO_3)_2$ concentration [calculated by (experimental value—calculated value)/experimental value × 100].

The next three quantities involve the weak magnesium nitrate solution. These are the flow rate of the stream, the nitric acid composition and the $Mg(NO_3)_2$ composition of the stream. The average error in the flow rate was 13.8% based on 26 points with a standard deviation of 25.9%. The positive error indicates the computer predicted values are less than the experimentally determined ones.

The error in the HNO_3 in the weak magnesium nitrate solution was found to be −34.6% for the 16 runs tested. The standard deviation was 33.2%. The relatively large error associated with this variable is probably associated with the small HNO_3 composition of the stream and the relatively large effect on the percent error of a small error in the sampling or chemical analysis procedure. Just as was found for the HNO_3 in the strong magnesium nitrate solution, the errors in this solution are negative, indicating the possibility of a loss of HNO_3 in the samples tested.

The $Mg(NO_3)_2$ composition of the weak magnesium nitrate solution had an error of 3.2% based on 16 experimental points. The standard deviation was 8.8%. This is slightly larger than the errors for the strong magnesium nitrate solution but certainly comparable.

The calculated temperature of the SRP was only in error by an average of 0.5°C for the 26 runs considered. However, a rather high standard deviation of 12.2°C indicates there was considerable spread between calculated and measured temperatures on individual runs.

In summary, a rigorous comparison between the computer model and the available experimental data is not possible because of the difficulty in determining whether the source of error lies in the model's assumptions or in experimental procedures. Overall, the model appears to predict reasonable values of most of the variables studied but leads to rather large percentage errors in the HNO_3 concentration of the magnesium nitrate solution streams.

It is believed that the model described should be a useful tool in the design of a nitric acid extractive distillation system. Its use should allow a designer to quickly evaluate the interrelationship of the various variables and perform parametric studies on such a system. Further refinements in the model can only come when more experimental data on this rather difficult-to-operate system is available.

5. TWOPOT MODEL USER'S GUIDE

The TWOPOT model code requires only one line of input consisting of six data fields:

1. RN—run descripter,
2. F—acid feed rate (mL/s),
3. SA—desired strong acid flow rate (mL/s),
4. T_{EDA}—temperature of extractive distillation pot (K),
5. X_F—mass fraction of HNO_3 in feed, and
6. X_{SA}—mass fraction of HNO_3 in strong acid.

The format for this data is A4, 1X, 5F5.2. Additional cases can be run by placing additional lines of data after the first. The program will continue to calculate new cases until no new data are found.

The output from the program generally consists of three parts: (1) a listing of the input parameters; (2) a listing of all stream flow, composition, and densities (this output also includes the input parameters for completeness); and (3) a diagram of the system with the stream parameters listed by the appropriate stream.

Three sample outputs are shown in Figs. 5.1 through 5.3. The conditions used for Fig. 5.1 are the same as those in Fig. 3.3 and represent a unique solution to the problem posed. Figure 5.2 is the output for the case presented in Fig. 3.5 in which equilibrium conditions cannot be met. In this case, a fourth section to the report is generated below the input parameters. This section issues the warning about temperature constraints and convergence errors and provides a listing of internal values used to determine convergence. In the subroutine, SOLVO, the convergence criteria require that total pressure of the system (TP) equals 760 mm Hg and that Y1 = YS for a correct solution where Y1 = X_{SA} and YS is the calculated vapor composition. SALVO requires that TP = 760 mm Hg and that X_{WA} = Y1 where X_{WA} is the weak acid composition as calculated by SOLVO and Y1 is the same term calculated by SALVO. The output of these values allows the user to decide if results are of any value.

The final example, Fig. 5.3, shows the results of requesting conditions that impose impossible material balance constraints. If this condition is detected, the case is aborted and the next case is begun.

ORNL/DWG. 84-17880

RUN NUMBER 1

INPUT VALUES

FEED STREAM FLOWRATE =0.408 GM/SEC
MASS FRACTION OF ACID IN FEED STREAM =0.6000

STRONG ACID STREAM FLOWRATE =0.203 GM/SEC
MASS FRACTION OF ACID IN STRONG ACID STREAM =0.8000

TEMPERATURE OF EXTRACTIVE DISTILLATION POT = 139.8 CELSIUS

****

OUTPUT VALUES

STREAM	FLOW (L/SEC)	MASS FRACTION (ACID)	MASS FRACTION (MAG. NITRATE)	DENSITY (G/CC)
FEED	0.3000	0.6000	0	1.3605
STRONG ACID	0.1400	0.8000	0	1.4480
WEAK MAG. NITRATE	0.5825	0.0923	0.5798	1.5625
WEAK ACID	0.1651	0.4027	0	1.2441
STRONG MAG. NITRATE	0.4260	0.0018	0.7489	1.6543

TEMPERATURE OF EXTRACTIVE DISTILLATION POT = 139.8 CELSIUS
TEMPERATURE SOLVENT RECOVERY POT = 206.3 CELSIUS

CONVERGENCE ERROR FOR SOLVO = 0.000
CONVERGENCE ERROR FOR SALVO = 0.000

Fig. 5.1. Sample output for TWOPOT model showing no equilibrium convergence problems (see continuation on following page).

ORNL/DWG. 84-17880

TEMPERATURES IN DEGREES CELSIUS
DENSITIES IN GRAMS PER CUBIC CENTIMETER
FLOWS IN CUBIC CENTIMETERS PER SECOND
Z S ARE MASS FRACTIONS OF MAG. NITRATE
X S ARE MASS FRACTIONS OF ACID

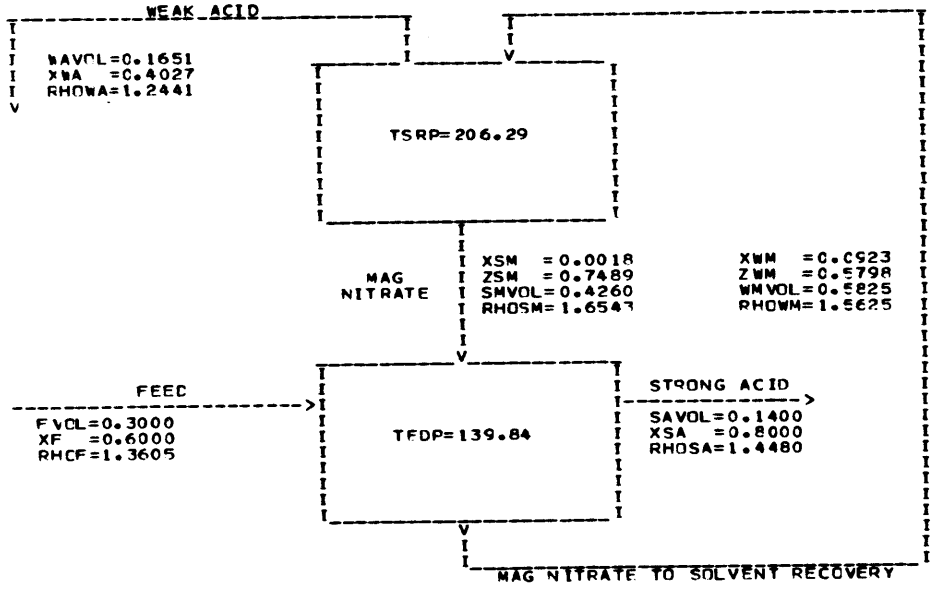

Fig. 5.1 (continued).

```
                                   RUN NUMBER 2

                                   INPUT VALUES

                   FEED STREAM FLOWRATE =0.408 GM/SEC
                 MASS FRACTION OF ACID IN FEED STREAM =0.6000

                  STRONG ACID STREAM FLOWRATE =0.290 GM/SEC
                MASS FRACTION OF ACID IN STRONG ACID STREAM =0.8000

              TEMPERATURE OF EXTRACTIVE DISTILLATION POT = 139.8 CELSIUS

*****************************************************************************************************************************

                                   ***********
                                   * WARNING *
                                   ***********

          TEMPERATURE OF EXTRACTIVE DISTILLATION POT = TEMPERATURE OF SOLVENT RECOVERY POT

                          CONVERGENCE ERROR FOR SALVO= 56.1

                              FACT WAS CHANGED 4. TIMES

 SOLVC                                                  SALVO
P1=0.0621    Y1=0.5335    TP  =760.00                   XSM=0.0621    XWA1=0.0346    X1=0.0621    TP=760.00
                                     ERROR=  0.00                                                              ERROR= 56.13
P2=0.1658    YS=0.5335    TEDF=139.84                   ZSM=0.1658    Y1  =0.5335    P1=0.0000    P2=139.84

*****************************************************************************************************************************
```

OUTPUT VALUES

STREAM	FLOW (L/SEC)	MASS FRACTION (ACID)	MASS FRACTION (MAG. NITRATE)	DENSITY (G/CC)
FEED	0.3000	0.6000	0	1.3605
STRONG ACID	0.2900	0.8000	0	1.4480
WEAK MAG. NITRATE	*******	0.0923	0.5798	1.5625
WEAK ACID	0.1127	0.1115	0	1.0520
STRONG MAG. NITRATE	*******	0.0923	0.5798	1.5625

TEMPERATURE OF EXTRACTIVE DISTILLATION POT = 139.8 CELSIUS

TEMPERATURE SOLVENT RECOVERY POT = 139.8 CELSIUS

Fig. 5.2. Sample output for TWOPOT model showing equilibrium convergence problems (see continuation on following page).

ORNL/DWG. 84-17881

TEMPERATURES IN DEGREES CELSIUS
DENSITIES IN GRAMS PER CUBIC CENTIMETER
FLOWS IN CUBIC CENTIMETERS PER SECOND
Z S ARE MASS FRACTIONS OF MAG. NITRATE
X S ARE MASS FRACTIONS OF ACID

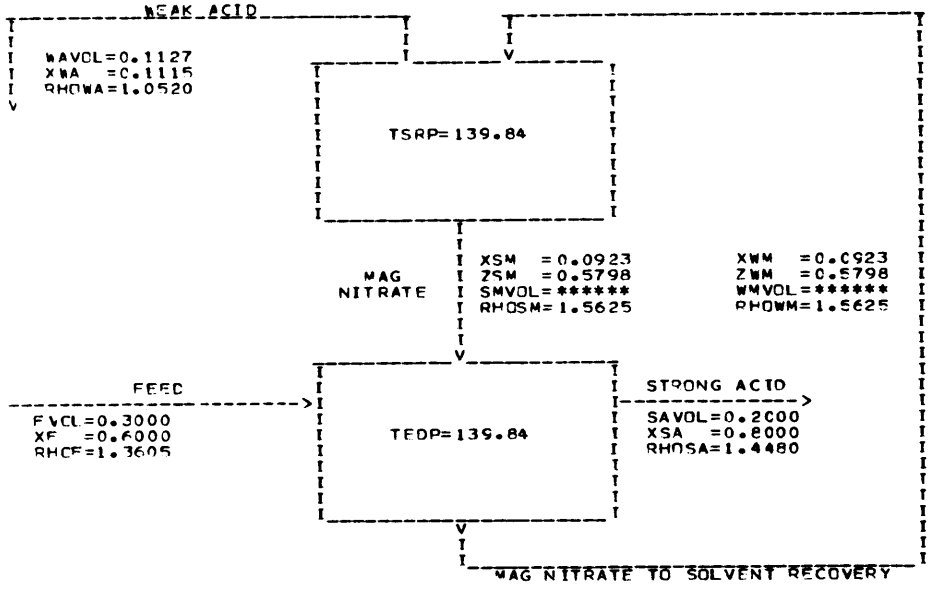

Fig. 5.2 (continued).

ORNL/DWG. 84-17882

```
                    RUN NUMBER 18

            *** IMPOSSIBLE MATERIAL BALANCE ***

                    INPUT VALUES

        FEED STREAM FLOWRATE =0.197 GM/SEC
   MASS FRACTION OF ACID IN FEED STREAM =0.7000

      STRONG ACID STREAM FLOWRATE =0.165 GM/SEC
   MASS FRACTION OF ACID IN STRONG ACID STREAM =0.6200

  TEMPERATURE OF EXTRACTIVE DISTILLATION POT = 139.8 CELSIUS

*****************************************************************************************************************

IHC002I STOP      0
```

Fig. 5.3. Sample output for TWOPOT model for input parameters imposing impossible material balance.

6. NOMENCLATURE

C	Pseudo mixed stream formed within the extractive distillation pot
EDP	Extractive distillation pot
F	Feed acid stream-mass flow
f( )	A function of the terms in parentheses
SA	Strong acid product stream-mass flow
SM	Strong $Mg(NO_3)_2$ stream-mass flow
SRP	Solvent recovery pot
T_{EDP}	Temperature of the extractive distillation pot (K)
TP	Calculated total pressure for boiling solution of given composition and temperature by the MIT correlation
T_{SRP}	Temperature of the solvent recovery pot (K)
U	Ratio of acid in the weak acid stream to the strong $Mg(NO_3)_2$ stream
VLE	Vapor liquid equilibrium
WA	Weak acid product stream-mass flow
WM	Weak $Mg(NO_3)_2$ stream-mass flow
X	Weight fraction nitric acid of subscripted stream
Y	Weight fraction water of subscripted stream
Y1	When used in SOLVO = X_{SA}; when used in SALVO the reaction of acid vapor in equilibrium with a known solution as calculated by the MIT correlation
YS	Used in SALVO, the fraction of acid vapor in equilibrium with a known solution as calculated by the MIT correlation
Z	Weight fraction $Mg(NO_3)_2$ of subscripted stream

Subscripts

A	Alternate solution
B	Alternate solution
CAL	calculated
EXP	experimental
F	Feed stream
SA	Strong acid stream
SM	Strong $Mg(NO_3)_2$ stream
WA	Weak acid stream
WM	Weak $Mg(NO_3)_2$ stream

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9. C. J. King, *Separation Processes*, McGraw-Hill, New York, 1971.

Appendix A

LISTING OF TWOPOT MODEL

```
C        MAIN PROGRAM
C
         IMPLICIT REAL*8(A-H,O-Z)
         COMMON/TRANS1/Y1,TEDPP
         COMMON/F2/FACT
         COMMON/TRANS2/X33,X11,XWA1
         COMMON/OSO/P1,P2,Y11,Y1S,CSTSO,TOTPSO
         COMMON/OSA/P3,P4,XSMSA,XWA1SA,X1SA,TOTPSA,CSTSA,ZSMSA,Y1SA
         COMMON/OUT1/WAVOL,XWA,RHOWA,XSM,ZSM,SMVOL,RHOSM,XWM,ZWM,WMVOL,
     *RHOWM,FVOL,XF,RHOF,SAVOL,XSA,RHOSA,TEDP,TSRP,F,SA,RN
   10    READ(22,20,END=40)RN,F,SA,TEDP,XF,XSA
   20    FORMAT(A4,1X,5F5.2)
C
C F AND SA ARE READ AS VOL FLOWRATE(CC/SEC.).
C
C
C THIS PACKAGE CONVERTS TO MASS FLOWS.
C
         FVOL=F
         SAVOL=SA
         A1=0.0
         TAMB=25.0
         CALL DENSIT(TAMB,XF,A1,RHOF)
         F=FVOL*RHOF
         CALL DENSIT(TAMB,XSA,A1,RHOSA)
         SA=SAVOL*RHOSA
C
C END OF ADJUSTMENTS
C
         WA=F-SA
         TEDP=TEDP-273.16
         XWA=(XF*F-XSA*SA)/WA
         IF(XWA.GT.XF.OR.XWA.LE.0.0) GO TO 30
         CALL SOLVO(XSA,TEDP,XWM,ZWM)
         CALL SALVO(XWA,ZWM,XWM,U,TSRP,XSM,ZSM)
         YW=1-XWM-ZWM
         CALL MAMO(XWM,YW,ZWM,P1,YY,P2)
         CALL CALC1(TEDP,P1,P2,Y1S,TP)
         CSTSO=DABS(760-TP)+DABS((Y1-Y1S)*1800)
         Y11=Y1
         TOTPSO=TP
         P3=U
         P4=TSRP
         YSM=1-XSM-ZSM
         CALL MAMO(XSM,YSM,ZSM,XSMSA,YYY,ZSMSA)
         CALL CALC1(P4,XSMSA,ZSMSA,Y1SA,TOTPSA)
         CSTSA=DABS(760-TOTPSA)+DABS((XWA1-Y1SA)*FACT)
         XWA1SA=XWA1
         X1SA=X11
         SM=WA/U
         WM=SM+WA
         CALL DENSIT(TSRP,XSM,ZSM,RHOSM)
         CALL DENSIT(TEDP,XWM,ZWM,RHOWM)
         WMVOL=WM/RHOWM
         SMVOL=SM/RHOSM
         CALL DENSIT(TAMB,XWA,A1,RHOWA)
```

```
      WAVOL=WA/RHOWA
30    CALL OUTPUT
      GO TO 10
40    STOP
    END
      SUBROUTINE SOLVO(Y,T,WX1,WX3)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/T2/ICON
      COMMON/TRANS1/Y1,TEDP
      COMMON/T3/TP
      COMMON/ERR/ERROR1
      DIMENSION P(2),BL(2),BU(2),IW(4),W(30)
      EXTERNAL PRA1,FUNCT1
      ICON=1
      YW=1-Y
      YS=0.0
      TEDP=T
      CALL MAMO(Y,YW,YS,Y1,Y2,Y3)
C
C     Y1 IS MOLE FRACTION ACID
C
      P(1)=0.10
      P(2)=0.10
      BL(1)=0.0
      BU(1)=0.5
      BL(2)=0.0
      BU(2)=1.0
      ICOUNT=0
      NP=2
      LW=4
      LIW=30
50    IFAIL=1
      CALL E04JAF(NP,0,BL,BU,P,COST,IW,LW,W,LIW,IFAIL)
      IF(COST.LT.5.0) GO TO 70
      DIFF=760.0-TP
      IF(ICOUNT.GE.5) GO TO 70
      IF(DIFF.GT.0.0)GO TO 60
      P(1)=P(1)-0.01
      P(2)=P(2)+0.05
      ICOUNT=ICOUNT+1
      GO TO 50
60    P(1)=P(1)+0.01
      P(2)=P(2)-0.05
      ICOUNT=ICOUNT+1
      GO TO 50
70    ERROR1=COST
      X1=P(1)
      X3=P(2)
      X2=1.0-X1-X3
      CALL MOMA(X1,X2,X3,WX1,WX2,WX3)
      RETURN
    END
```

```
      FUNCTION PRA1(P,NP)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION P(2)
      CALL PROC1 (P,COST)
      PRA1=COST
      RETURN
    END
      SUBROUTINE PROC1(P,COST)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/TRANS1/Y1,TEDP
      COMMON/T3/TP
      DIMENSION P(2)
      CALL CALC1(TEDP,P(1),P(2),Y1S,TP)
      COST=DABS(760-TP)+DABS((Y1-Y1S)*1800.)
      RETURN
    END
      FUNCTION PRA2(P,NP)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION P(2)
      CALL PROC2 (P,COST)
      PRA2=COST
      RETURN
    END
      SUBROUTINE PROC2(P,COST)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/TRANS2/X3,X1,XWA1
      COMMON/F2/FACT
      DIMENSION P(2)
      ZSM=X3*(1.0+P(1))
      XSM=X1+(X1-XWA1)*P(1)
      P2=P(2)*100.0
      CALL CALC1(P2,XSM,ZSM,Y1,TP)
      COST=DABS(760-TP)+DABS((XWA1-Y1)*FACT)
      RETURN
    END
      SUBROUTINE FUNCT1 (N,XC,FC)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION XC(2)
      COMMON/T2/ICON
      IF(ICON.EQ.2)GO TO 80
      FC=PRA1(XC,N)
      GO TO 90
80    FC=PRA2(XC,N)
90    RETURN
    END
      SUBROUTINE CALC1(T,XA,XS,YA,TP)
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 K1
C
C     GIVEN LIQ COMP AND T, CALCULATES Y1 AND TOTAL PRESSURE
C
      DATA ANTAW,ANTBW,ANTCW,ANTAA,ANTBA,ANTCA/7.9492,1657.44,227.1,
```

```
*   7.61628,1486.238,230./
    DATA A1,A2,A3,A4,A5,A6/-2.52,6.21,-3.1,23.83,-24.2,-15.8/
    DATA B1,B2,B3,B4,B5,B6/0.0,-0.17,-3.62,-4.47,-15.38,-28.20/
    K1=0.0015*DEXP(1459/(T+273.))
    A=(1+K1)*XA
    B=XS*2*(1+K1)-K1*XA+K1
    C=-K1-2*K1*XS
    ALPHA=((B*B-4*A*C)**.5-B)/(2*A)
    XAP1=(1-ALPHA)*XA/(1+ALPHA*XA+XS*2)
    XWP1=(1-XA-XS)/(1+ALPHA*XA+XS*2)
    VPW=10.**(ANTAW-ANTBW/(T+ANTCW))
    VPA=10.**(ANTAA-ANTBA/(T+ANTCA))
    GA=DEXP(A1+A2*XA+A3*XA*XA+A4*XS+A5*XS*XS+A6*XA*XS)
    GW=DEXP(B1+B2*XA+B3*XA*XA+B4*XS+B5*XS*XS+B6*XA*XS)
    PPA=GA*XAP1*VPA
    PPW=GW*XWP1*VPW
    TP=PPA+PPW
    YW=PPW/TP
    YA=PPA/TP
    RETURN
  END
    SUBROUTINE MAMO(WX1,WX2,WX3,X1,X2,X3)
    IMPLICIT REAL*8(A-H,O-Z)
C
C   CONVERTS MASS FRACTION TO MOLE FRACTION
C
    DATA C1,C2,C3/63.02,18.02,148.36/
    C4=WX1/C1+WX2/C2+WX3/C3
    X1=WX1/C1/C4
    X2=WX2/C2/C4
    X3=WX3/C3/C4
    RETURN
  END
    SUBROUTINE MOMA(X1,X2,X3,WX1,WX2,WX3)
    IMPLICIT REAL*8(A-H,O-Z)
C
C   CONVERTS MOLE FRACTION TO MASS FRACTION
C
    DATA C1,C2,C3/63.02,18.02,148.36/
    C4=X1*C1+X2*C2+X3*C3
    WX1=X1*C1/C4
    WX2=X2*C2/C4
    WX3=X3*C3/C4
    RETURN
  END
    SUBROUTINE DENSIT(T,X1,X3,RHO)
    IMPLICIT REAL*8(A-H,O-Z)
C
C   RHO CAL'D IN GM/CC WITH X IN MASS FRACTION
C   AND T IN CELSIUS
C
    IF (X3.EQ.0.0) GOTO 100
```

```
      Q1=X1*100
      Q3=X3*100
      Q2=100-X1-X3
      RHO=0.9280+0.01185*Q3+0.006215*Q1-0.0007866*T
      RETURN
100   W=X1*100
      D25=(0.97935/(1-0.0065409*W+3.1194D-05*W**2))
      RHO=1.0789*D25+0.0029366*T-0.0031548*T*D25-0.073416
      RETURN
    END
      SUBROUTINE SALVO(XWA,ZWM,XWM,U,TSRP,XSM,ZSM)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/TRANS1/Y1,TEDP
      COMMON/TRANS2/X3,X1,XWA1
      COMMON/T2/ICON
      COMMON/ER/ERROR2,FACTO
      COMMON/F2/FACT
      DIMENSION P(2),BL(2),BU(2),IW(4),W(30)
      EXTERNAL PRA2,FUNCT1
      FACT=1800
      FACTI=FACT
      ICO=1
      ICON=2
      P(1)=0.15
      P(2)=180.0/100.0
      BL(1)=0.000001
      BU(1)=10.0
      BL(2)=TEDP/100
      BU(2)=2.5
      YWM=1.0-ZWM-XWM
      CALL MAMO(XWM,YWM,ZWM,X1,X2,X3)
      YW=1.0-XWA
      YS=0.0
      CALL MAMO(XWA,YW,YS,XWA1,YW1,YS1)
      NP=2
      LW=4
      LIW=30
110   IFAIL=1
      CALL E04JAF(NP,0,BL,BU,P,COST,IW,LW,W,LIW,IFAIL)
      IF(COST.GT.1.0.AND.ICO.LT.8)GO TO 120
      IF(P(1).EQ.0.0.AND.XWA1.LT.1.0.AND.XWA1.GT.0.0.AND.ICO.LT.8)
     *GO TO 120
      GO TO 130
120   P(1)=0.05*ICO
      P(2)=2.0
      ICO=ICO+1
      GO TO 110
130   ICO=1
      IF(FACT.LT.(FACTI/8))GO TO 140
      FACT=FACT/2
      IF(COST.GT.1.)GO TO 110
140   FACTO=(DLOG(FACTI/FACT))/0.69315
      ERROR2=COST
```

```
      ZSM1=X3*(1.0+P(1))
      XSM1=X1+(X1-XWA1)*P(1)
      YSM1=1.0-ZSM1-XSM1
      CALL MOMA(XSM1,YSM1,ZSM1,XSM,YSM,ZSM)
      U=P(1)
      SMMW=63.02*XSM1+18.02*YSM1+148.36*ZSM1
      WAMW=63.02*XWA1+18.02*YW1+148.36*YS1
      U=U*WAMW/SMMW
      TSRP=P(2)*100.0
      RETURN
    END
      SUBROUTINE OUTPUT
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/OSO/P1,P2,Y11,Y1S,CSTSO,TOTPSO
      COMMON/OSA/P3,P4,XSMSA,XWA1SA,X1SA,TOTPSA,CSTSA,ZSMSA,Y1SA
      COMMON/ERR/ERROR1
      COMMON/ER/ERROR2,FACTO
      COMMON/OUT1/WAVOL,XWA,RHOWA,XSM,ZSM,SMVOL,RHOSM,XWM,ZWM,WMVOL,
     *RHOWM,FVOL,XF,RHOF,SAVOL,XSA,RHOSA,TEDP,TSRP,F,SA,RN
      WRITE(6,150)RN
      IF(XWA.GT.XF.OR.XWA.LE.0.0)WRITE(6,160)
      WRITE(6,170)F,XF,SA,XSA,TEDP
      IF(XWA.GT.XF.OR.XWA.LE.0.0)GO TO 300
      IF((TSRP-TEDP).LT.1.OR.ERROR1.GT.1.OR.ERROR2.GT.1)WRITE(6,180)
      IF((TSRP-TEDP).LT.1)WRITE(6,190)
      IF(ERROR1.GT.1.)WRITE(6,200)ERROR1
      IF(ERROR2.GT.1.)WRITE(6,210)ERROR2,FACTO
      IF((TSRP-TEDP).LT.1.OR.ERROR1.GT.1.OR.ERROR2.GT.1)
     *WRITE(6,220)P1,Y11,TOTPSO,XSMSA,XWA1SA,X1SA,TOTPSA,CSTSO,
     *CSTSA,P2,Y1S,TEDP,ZSMSA,Y1SA,P3,P4
      WRITE(6,230)FVOL,XF,RHOF,SAVOL,XSA,RHOSA,WMVOL,XWM,ZWM,RHOWM,
     *WAVOL,XWA,RHOWA,SMVOL,XSM,ZSM,RHOSM,TEDP,TSRP
      IF(TEDP.NE.TSRP.AND.ERROR1.LE.1.AND.ERROR2.LE.1)WRITE(6,240)
     *ERROR1,ERROR2
      WRITE(6,250)
      WRITE(6,260)
      WRITE(6,270)WAVOL,XWA,RHOWA,TSRP,XSM,XWM
      WRITE(6,280)ZSM,ZWM,SMVOL,WMVOL,RHOSM,RHOWM
      WRITE(6,290)FVOL,SAVOL,XF,TEDP,XSA,RHOF,RHOSA
150   FORMAT('1',60X,'RUN NUMBER ',A4)
160   FORMAT(///,48X,'*** IMPOSSIBLE MATERIAL BALANCE ***'///)
170 FORMAT('0',60X,'INPUT VALUES'/'+',60X,'____________',
     *//51X,'FEED STREAM FLOWRATE =',F5.3,' GM/SEC',
     */46X,'MASS FRACTION OF ACID IN FEED STREAM =',F6.4,
     *//48X,'STRONG ACID STREAM FLOWRATE =',F5.3,' GM/SEC',
     */44X,'MASS FRACTION OF ACID IN STRONG ACID STREAM =',F6.4,
     *//40X,'TEMPERATURE OF EXTRACTIVE DISTILLATION POT =',F6.1,
     *' CELSIUS',/////66('**')/)
180   FORMAT(61X,'***********'/61X,'* WARNING *'/61X,'***********')
190   FORMAT('0',T30,'TEMPERATURE OF EXTRACTIVE DISTILLATION POT =',
     *' TEMPERATURE OF SOLVENT RECOVERY POT')
200   FORMAT('0',48X,'CONVERGENCE ERROR FOR SOLVO =',F5.1)
```

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210   FORMAT('0',48X,'CONVERGENCE ERROR FOR SALVO=',F5.1,//53X,
   *'FACT WAS CHANGED ',F2.0,' TIMES')
220   FORMAT('0',X,'SOLVO',T60,'SALVO'/'+',X,5('_'),T60,5('_')//
   *X,'P1=',F6.4,T15,'Y1=',F6.4,T30,'TP  =',F6.2,T60,'XSM=',F6.4,T75,
   *'XWA1=',F6.4,T90,'X1=',F6.4,T105,'TP=',F6.2//
   *T45,'ERROR=',F6.2,T120,'ERROR=',F6.2//
   *X,'P2=',F6.4,T15,'YS=',F6.4,T30,'TEDP=',F6.2,T60,'ZSM=',F6.4,T75,
   *'Y1  =',F6.4,T90,'P1=',F6.4,T105,'P2=',F6.2////66('**')/)
230 FORMAT('0'///,61X,'OUTPUT VALUES'/'+',60X,'____________',
   *//8X,'STREAM',T40,'FLOW',T62,'MASS FRACTION',T84,'MASS FRACTION',
   *T110,'DENSITY',/37X,'(L/SEC)',T65,'(ACID)',T84,'(MAG. NITRATE)',
   *T111,'(G/CC)',/' ',66('__')//
   *1X,'FEED',T39,F6.4,T65,F6.4,T88,'  0   ',T111,F6.4//
   *1X,'STRONG ACID',T39,F6.4,T65,F6.4,T88,'  0   ',T111,F6.4//
   *1X,'WEAK MAG. NITRATE',T38,F7.4,T65,F6.4,T88.F6.4,T111,F6.4//
   *1X,'WEAK ACID',T39,F6.4,T65,F6.4,T88,'  0   ',T111,F6.4//
   *1X,'STRONG MAG. NITRATE',T38,F7.4,T65,F6.4,T88,F6.4,T111,F6.4/
   *//40X,'TEMPERATURE OF EXTRACTIVE DISTILLATION POT =',F6.1,' CELSIU
   *S',//44X,'TEMPERATURE SOLVENT RECOVERY POT =',F6.1,' CELSIUS'//)
240   FORMAT('0',48X,'CONVERGENCE ERROR FOR SOLVO =',F7.3//
   *49X,'CONVERGENCE ERROR FOR SALVO =',F7.3)
250   FORMAT('1',//,49X,'TEMPERATURES IN DEGREES CELSIUS',//45X
   *,'DENSITIES IN GRAMS PER CUBIC CENTIMETER',//46X
   *,'FLOWS IN CUBIC CENTIMETERS PER SECOND',//46X
   *,'Z S ARE MASS FRACTIONS OF MAG. NITRATE',//50X
   *,'X S ARE MASS FRACTIONS OF ACID',//)
260 FORMAT('0',T41,'WEAK ACID')
270 FORMAT('+',T30,32('_'),7X,33('_')/T30,'I',T61,'I',T69,'I',T101,
   *'I'/T30,'I',T61,'I',T69,'I',T101,'I',/T30,'I',T33,'WAVOL=',F6.4,
   *T54,7('_'),'I',7('_'),'V',7('_'),T101,'I',/T30,'I',T33,'XWA  =',
   *F6.4,T54,'I',T77,'I',T101,'I',/T30,'I',T33,'RHOWA=',F6.4,
   *T54,'I',T77,'I',T101,'I',/T30,'V',T54,'I',T77,'I',T101,'I'/
   *T54,'I',T77,'I',T101,'I'/T54,'I',T60,'TSRP=',F6.2,T77,'I',
   *T101,'I',/4(T54,'I',T77,'I',T101,'I',/),T54,'I',22('_'),'I',
   *T101,'I'/,T65,'I',T101,'I'/T65,'I',T101,'I'/T65,'I',
   *T67,'XSM  =',F6.4,T87,'XWM  =',F6.4,T101,'I')
280 FORMAT(' ',T58,'MAG',T65,'I ZSM  ','=',F6.4,T87,'ZWM  =',
   *F6.4,T101,'I'/T56,'NITRATE',T65,'I',T67,'SMVOL=',F6.4,
   *T87,'WMVOL=',F6.4,T101,'I'/T65,'I',T67,'RHOSM=',F6.4,T87,
   *'RHOWM=',F6.4,T101,'I')
290 FORMAT(' ',T65,'I',T101,'I'/T65,'I',T101,'I'/T54
   *,11('_'),'V',12('_'),T101,'I'/T54,'I',T77,'I',T101,'I'
   */T40,'FEED',T54,'I',T77,'I',T80,'STRONG ACID',
   *T101,'I'/T30,23('-'),'>I',
   *T77,'I',14('-'),'>',T101,'I'/T32,'FVOL=',F6.4,T54,'I
   *',T77,'I',T80,'SAVOL=',F6.4,T101,'I'/T32,'XF  =',F6.4,T54,'I'
   *,T60,'TEDP=',F6.2,T77,'I',T80,'XSA  =',F6.4,T101,'I'/T32,
   *'RHOF=',F6.4,T54,'I',T77,'I',T80,'RHOSA=',F6.4,T101,'I'/,
   *3(T54,'I',T77,'I',T101,'I',/),T54,'I',22('_'),'I',
   *T101,'I'/T65,'V',T101,'I'/T65,'I',T101,'I'/,
   *T65,'I'35('_'),'I'/T68,'MAG NITRATE TO SOLVENT RECOVERY')
300   RETURN
      END
```

Appendix B

VALIDATION STUDIES

RUN NUMBER 7

SOLVC FINAL COST IS 0.00001

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4201	F=	0.4201	
XF=	0.6800	XF=	0.6800	
SA=	0.2341	SA=	0.2341	
XSA=	0.8500	XSA=	0.8500	
WAVOL=	0.1449	EWA=	0.1400	-3.48
XWA=	0.4660	EXWA=	0.5500	15.27
XSM=	0.0031	EXSM=	0.0150	79.29
ZSM=	0.7372	EZSM=	0.6900	-6.84
WMVOL=	0.6257	EWM=	1.0900	42.59
XWM=	0.0899	EXWM=	0.0760	-18.34
ZWM=	0.5989	EZWM=	0.5910	-1.34
EDP=	138.8401	TEDPC=	138.8401	
SRP=	196.3161	ETSRPC=	171.8401	-24.48 (C)
SM=	0.8054			
SMVOL=	0.4884			

CALCULATED DENSITIES

RHCF=	1.4002
RHCSA=	1.4631
RHCWA=	1.2837
RHCSM=	1.6491
RHCWM=	1.5844

EDP HOLLAND EFFICIENCY 0.845

RUN NUMBER 9

SOLVO FINAL COST IS 0.08925

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1960	F=	0.1960	
XF=	0.6800	XF=	0.6800	
SA=	0.0440	SA=	0.0440	
XSA=	0.8600	XSA=	0.8600	
WAVOL=	0.1106	EWA=	0.1200	7.85
XWA=	0.6279	EXWA=	0.6000	-4.66
XSM=	0.0152	EXSM=	0.0090	-69.01
ZSM=	0.6885	EZSM=	0.6880	-0.07
WMVOL=	0.8886	EWM=	1.4100	36.98
XWM=	0.0809	EXWM=	0.0410	-97.26
ZWM=	0.6147	EZWM=	0.6460	4.84
EDP=	139.8401	TECPC=	139.8401	
SRP=	167.6176	ETSRPC=	170.8401	3.22 (C)
SM=	1.2668			
SMVOL=	0.7812			

CALCULATED DENSITIES

RHCF=	1.4002
RHCSA=	1.4657
RHCWA=	1.3750
RHCSM=	1.6215
RHCWM=	1.5967

EDP HOLLAND EFFICIENCY 0.507

RUN NUMBER 10

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4228	F=	0.4228	
XF=	C.7000	XF=	0.7000	
SA=	0.2177	SA=	0.2177	
XSA=	0.8100	XSA=	0.8100	
WAVOL=	0.1517	EWA=	0.1400	-8.38
XWA=	0.5832	EXWA=	0.5300	-10.04
XSM=	0.0176	EXSM=	0.0060	-194.04
ZSM=	0.6717	EZSM=	0.6770	0.79
WMVOL=	1.0089	EWM=	1.0800	6.59
XWM=	0.0910	EXWM=	0.0650	-40.00
ZWM=	0.5846	EZWM=	0.6010	2.73
EDP=	139.8401	TEDPC=	139.8401	
SRP=	163.3997	ETSRPC=	169.8401	6.44 (C)
SM=	1.3761			
SMVOL=	0.8566			

CALCULATED DENSITIES

RHOF=	1.4092
RHCSA=	1.4513
RHCWA=	1.3516
RHCSM=	1.6064
RHCWM=	1.5673

EDP HOLLAND EFFICIENCY 0.714

RUN NUMBER 12

SOLVC FINAL COST IS 0.00000

SALVO FINAL COST IS 0.12130

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1826	F=	0.1826	
XF=	0.6900	XF=	0.6900	
SA=	0.0295	SA=	0.0295	
XSA=	0.8900	XSA=	0.8900	
WAVOL=	0.1104	EWA=	0.1100	-0.41
XWA=	0.6515	EXWA=	0.6600	1.28
XSM=	0.0146	EXSM=	0.0080	-81.90
ZSM=	0.6953	EZSM=	0.6890	-0.91
WMVOL=	0.7515	EWM=	1.0600	29.11
XWM=	0.0957	EXWM=	0.0830	-15.32
ZWM=	0.6067	EZWM=	0.6020	-0.78
EDP=	135.8401	TEDPC=	135.8401	
SRP=	169.1832	ETSRPC=	169.8401	0.66 (C)
SM=	1.0489			
SMVOL=	0.6443			

CALCULATED DENSITIES

RHOF=	1.4047
RHCSA=	1.4729
RHCWA=	1.3867
RHCSM=	1.6278
RHCWM=	1.5995

EDP HOLLAND EFFICIENCY 0.867

RUN NUMBER 13

SOLVO FINAL COST IS 0.00002

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4228	F=	0.4228	
XF=	0.7000	XF=	0.7000	
SA=	0.0586	SA=	0.0586	
XSA=	0.8600	XSA=	0.8600	
WAVOL=	0.2606	EWA=	0.2800	6.94
XWA=	0.6742	EXWA=	0.6300	-7.02
XSM=	0.0366	EXSM=	0.0080	-357.93
ZSM=	0.6394	EZSM=	0.6770	5.55
WMVOL=	0.8734	EWM=	1.0500	16.82
XWM=	0.2130	EXWM=	0.1300	-63.85
ZWM=	0.4626	EZWM=	0.5380	14.02
EDP=	128.8401	TEDPC=	128.8401	
SRP=	152.9679	ETSRPC=	169.8401	16.87 (C)
SM=	0.9522			
SMVOL=	0.5996			

CALCULATED DENSITIES

RHOF=	1.4092
RHCSA=	1.4657
RHCWA=	1.3975
RHCSM=	1.5882
RHCWM=	1.5072

EDP HOLLAND EFFICIENCY 0.610

RUN NUMBER 14

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4113	F=	0.4113	
XF=	0.6200	XF=	0.6200	
SA=	0.2275	SA=	0.2275	
XSA=	0.7300	XSA=	0.7300	
WAVOL=	0.1420	EWA=	0.1500	5.36
XWA=	0.4838	EXWA=	0.4800	-0.80
XSM=	0.0121	EXSM=	0.0060	-100.96
ZSM=	0.6758	EZSM=	0.6320	-6.93
WMVOL=	0.6737	EWM=	1.0800	37.62
XWM=	0.0958	EXWM=	0.0610	-57.09
ZWM=	0.5558	EZWM=	0.6020	7.67
EDP=	139.8401	TEDPC=	139.8401	
SRP=	166.7890	ETSRPC=	169.8401	3.05 (C)
SM=	0.8512			
SMVOL=	0.5303			

CALCULATED DENSITIES

RHCF=	1.3710
RHCSA=	1.4220
RHCWA=	1.2945
RHCSM=	1.6051
RHCWM=	1.5362

EDP HOLLAND EFFICIENCY 0.637

RUN NUMBER 15

SOLVO FINAL COST IS 0.00000

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.2233	F=	0.2233	
XF=	0.6700	XF=	0.6700	
SA=	0.0856	SA=	0.0856	
XSA=	0.7400	XSA=	0.7400	
WAVOL=	0.1002	EWA=	0.1100	8.89
XWA=	0.6265	EXWA=	0.4600	-36.20
XSM=	0.0426	EXSM=	0.0100	-325.66
ZSM=	0.6170	EZSM=	0.6620	6.80
WMVOL=	1.1339	EWM=	1.0000	-13.39
XWM=	0.0884	EXWM=	0.0660	-34.01
ZWM=	0.5685	EZWM=	0.6140	7.41
EDP=	140.8401	TEDPC=	140.8401	
SRP=	149.7926	ETSRPC=	170.8401	21.05 (C)
SM=	1.6151			
SMVOL=	1.0302			

CALCULATED DENSITIES

RHCF=	1.3955
RHCSA=	1.4260
RHCWA=	1.3743
RHCSM=	1.5678
RHCWM=	1.5459

EDP HOLLAND EFFICIENCY 0.746

RUN NUMBER 16A

SOLVO FINAL COST IS 0.00001

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.2120	F=	0.2120	
XF=	0.7100	XF=	0.7100	
SA=	0.0289	SA=	0.0289	
XSA=	0.7900	XSA=	0.7900	
WAVOL=	0.1301	EWA=	0.1500	13.29
XWA=	0.6974	EXWA=	0.5900	-18.20
XSM=	0.1130	EXSM=	0.0880	-28.40
ZSM=	0.5248	EZSM=	0.6600	20.48
WMVOL=	0.5874	EWM=	0.5300	-10.84
XWM=	0.2375	EXWM=	0.1150	-106.55
ZWM=	0.4130	EZWM=	0.5500	24.91
EDP=	129.8401	TEDPC=	129.8401	
SRP=	137.7768	ETSRPC=	170.8401	33.06 (C)
SM=	0.6762			
SMVOL=	0.4473			

CALCULATED DENSITIES

RHCF=	1.4136
RHCSA=	1.4446
RHCWA=	1.4080
RHCSM=	1.5118
RHCWM=	1.4629

EDP HOLLAND EFFICIENCY 0.484

RUN NUMBER 16B

SOLVO FINAL COST IS 0.00012

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.2127	F=	0.2127	
XF=	0.7200	XF=	0.7200	
SA=	0.0295	SA=	0.0295	
XSA=	0.8900	XSA=	0.8900	
WAVOL=	0.1303	EWA=	0.1800	27.60
XWA=	0.6927	EXWA=	0.6800	-1.86
XSM=	0.0218	EXSM=	0.0	
ZSM=	0.6796	EZSM=	0.0	
WMVOL=	0.9433	EWM=	1.1800	20.06
XWM=	0.1035	EXWM=	0.0	
ZWM=	0.5968	EZWM=	0.0	
EDP=	134.8401	TEDPC=	134.8401	
SRP=	162.3156	ETSRPC=	166.8401	4.52 (C)
SM=	1.3199			
SMVOL=	0.8152			

CALCULATED DENSITIES

RHOF=	1.4178
RHOSA=	1.4729
RHOWA=	1.4059
RHOSM=	1.6192
RHOWM=	1.5935

RUN NUMBER 18

SOLVC FINAL COST IS 0.00012

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1973	F=	0.1973	
XF=	0.7000	XF=	0.7000	
SA=	0.1645	SA=	0.1645	
XSA=	0.6200	XSA=	0.6200	
WAVOL=	0.1303	EWA=	0.0300	-334.38
XWA=	1.1016	EXWA=	0.5200	-111.84
XSM=	0.0218	EXSM=	0.0360	39.55
ZSM=	0.6796	EZSM=	0.5840	-16.37
WMVOL=	0.9433	EWM=	0.9800	3.74
XWM=	0.1035	EXWM=	0.0	
ZWM=	0.5968	EZWM=	0.0	
EDP=	139.8401	TEDPC=	139.8401	
SRP=	162.3156	ETSRPC=	171.8401	9.52 (C)
SM=	1.3199			
SMVOL=	0.8152			

CALCULATED DENSITIES

RHCF=	1.4092
RHCSA=	1.3710
RHCWA=	1.4059
RHCSM=	1.6192
RHCWM=	1.5935

RUN NUMBER 19

SOLVO FINAL COST IS 0.00001

SALVC FINAL COST IS 0.00001

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4214	F=	0.4214	
XF=	0.6900	XF=	0.6900	
SA=	0.2172	SA=	0.2172	
XSA=	0.8000	XSA=	0.8000	
WAVOL=	0.1517	EWA=	0.1600	5.17
XWA=	0.5730	EXWA=	0.5800	1.20
XSM=	0.0171	EXSM=	0.0570	70.06
ZSM=	0.6718	EZSM=	0.6650	-1.02
WMVOL=	1.0591	EWM=	0.9800	-8.07
XWM=	0.0854	EXWM=	0.0	
ZWM=	0.5892	EZWM=	0.0	
EDP=	140.8401	TEDPC=	140.8401	
SRP=	163.6804	ETSRPC=	167.8401	4.16 (C)
SM=	1.4570			
SMVOL=	0.9072			

CALCULATED DENSITIES

RHCF=	1.4047
RHCSA=	1.4480
RHCWA=	1.3460
RHCSM=	1.6059
RHCWM=	1.5685

RUN NUMBER 20

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4124	F=	0.4124	
XF=	0.7300	XF=	0.7300	
SA=	0.2745	SA=	0.2745	
XSA=	0.7900	XSA=	0.7900	
WAVOL=	0.1009	EWA=	0.1000	-0.94
XWA=	0.6106	EXWA=	0.5400	-13.07
XSM=	0.0161	EXSM=	0.0110	-46.60
ZSM=	0.6820	EZSM=	0.6930	1.58
WMVOL=	1.6915	EWM=	1.1400	-48.38
XWM=	0.0463	EXWM=	0.0	
ZWM=	0.6474	EZWM=	0.0	
EDP=	149.8401	TEDPC=	149.8401	
SRP=	165.9514	ETSRPC=	169.8401	3.89 (C)
SM=	2.5788			
SMVOL=	1.5961			

CALCULATED DENSITIES

RHCF=	1.4220
RHCSA=	1.4446
RHCWA=	1.3661
RHCSM=	1.6157
RHCWM=	1.6061

RUN NUMBER 21

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1991	F=	0.1991	
XF=	0.7300	XF=	0.7300	
SA=	0.1011	SA=	0.1011	
XSA=	0.7900	XSA=	0.7900	
WAVOL=	0.0702	EWA=	0.0700	-0.34
XWA=	0.6681	EXWA=	0.5100	-30.99
XSM=	0.0215	EXSM=	0.0110	-95.35
ZSM=	0.6755	EZSM=	0.6970	3.08
WMVOL=	1.7870	EWM=	1.0500	-70.19
XWM=	0.0435	EXWM=	0.0	
ZWM=	0.6525	EZWM=	0.0	
EDP=	150.8401	TEDPC=	150.8401	
SRP=	162.0514	ETSRPC=	170.8401	8.79 (C)
SM=	2.7785			
SMVOL=	1.7211			

CALCULATED DENSITIES

RHCF=	1.4220
RHCSA=	1.4446
RHCWA=	1.3946
RHCSM=	1.6144
RHCWM=	1.6096

RUN NUMBER 22

SOLVO FINAL COST IS 0.00000

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4421	F=	0.4421	
XF=	0.7400	XF=	0.7400	
SA=	0.2172	SA=	0.2172	
XSA=	0.8000	XSA=	0.8000	
WAVOL=	0.1605	EWA=	0.1700	5.59
XWA=	0.6820	EXWA=	0.5600	-21.79
XSM=	0.0428	EXSM=	0.0230	-86.05
ZSM=	0.6285	EZSM=	0.6560	4.19
WMVOL=	1.8587	EWM=	1.2100	-53.61
XWM=	0.0923	EXWM=	0.0	
ZWM=	0.5798	EZWM=	0.0	
EDP=	139.8401	TEDPC=	139.8401	
SRP=	150.6399	ETSRPC=	160.8401	10.20 (C)
SM=	2.6793			
SMVOL=	1.6948			

CALCULATED DENSITIES

RHCF=	1.4260
RHCSA=	1.4480
RHCWA=	1.4011
RHCSM=	1.5809
RHCWM=	1.5625

RUN NUMBER 23

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1826	F=	0.1826	
XF=	0.6900	XF=	0.6900	
SA=	0.0437	SA=	0.0437	
XSA=	0.8300	XSA=	0.8300	
WAVOL=	0.1004	EWA=	0.1000	-0.36
XWA=	0.6459	EXWA=	0.6600	2.13
XSM=	0.0233	EXSM=	0.0130	-78.98
ZSM=	0.6661	EZSM=	0.6850	2.75
WMVOL=	0.9403	EWM=	1.1900	20.99
XWM=	0.0814	EXWM=	0.0	
ZWM=	0.6040	EZWM=	0.0	
EDP=	140.8401	TEDPC=	140.8401	
SRP=	160.1061	ETSRPC=	159.8401	-0.27 (C)
SM=	1.3500			
SMVOL=	0.8407			

CALCULATED DENSITIES

RHOF=	1.4047
RHCSA=	1.4574
RHCWA=	1.3840
RHCSM=	1.6059
RHCWM=	1.5835

RUN NUMBER 24

SOLVO FINAL COST IS 0.00003

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1838	F=	0.1838	
XF=	0.7100	XF=	0.7100	
SA=	0.0293	SA=	0.0293	
XSA=	0.8600	XSA=	0.8600	
WAVOL=	0.1102	EWA=	0.1000	-10.25
XWA=	0.6815	EXWA=	0.6200	-9.92
XSM=	0.0217	EXSM=	0.0050	-333.42
ZSM=	0.6776	EZSM=	0.7210	6.01
WMVOL=	1.1882	EWM=	1.1800	-0.70
XWM=	0.0752	EXWM=	0.0	
ZWM=	0.6227	EZWM=	0.0	
EDP=	140.8401	TEDPC=	140.8401	
SRP=	162.1769	ETSRPC=	168.8401	6.66 (C)
SM=	1.7489			
SMVOL=	1.0816			

CALCULATED DENSITIES

RHOF=	1.4136
RHOSA=	1.4657
RHOWA=	1.4009
RHOSM=	1.6169
RHOWM=	1.6018

RUN NUMBER 25

SOLVC FINAL COST IS 0.00001

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1967	F=	0.1967	
XF=	0.6900	XF=	0.6900	
SA=	0.0440	SA=	0.0440	
XSA=	0.8700	XSA=	0.8700	
WAVOL=	0.1106	EWA=	0.1000	-10.59
XWA=	0.6381	EXWA=	0.6100	-4.60
XSM=	0.0133	EXSM=	0.0030	-341.71
ZSM=	0.6979	EZSM=	0.7130	2.12
WMVOL=	1.0836	EWM=	1.0400	-4.19
XWM=	0.0678	EXWM=	0.0	
ZWM=	0.6370	EZWM=	0.0	
EDP=	141.8401	TEDPC=	141.8401	
SRP=	170.7057	ETSRPC=	170.8401	0.13 (C)
SM=	1.5956			
SMVOL=	0.9795			

CALCULATED DENSITIES

RHCF=	1.4047
RHCSA=	1.4682
RHCWA=	1.3801
RHCSM=	1.6290
RHCWM=	1.6134

RUN NUMBER 26

SOLVO FINAL COST IS 0.00000

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4214	F=	0.4214	
XF=	0.6900	XF=	0.6900	
SA=	0.2462	SA=	0.2462	
XSA=	0.8000	XSA=	0.8000	
WAVOL=	0.1323	EWA=	0.1500	11.81
XWA=	0.5355	EXWA=	0.5000	-7.10
XSM=	0.0118	EXSM=	0.0080	-47.25
ZSM=	0.6863	EZSM=	0.6990	1.82
WMVOL=	0.8647	EWM=	0.9300	7.02
XWM=	0.0792	EXWM=	0.0	
ZWM=	0.5979	EZWM=	0.0	
EDP=	141.8401	TEDPC=	141.8401	
SRP=	169.4185	ETSRPC=	170.8401	1.42 (C)
SM=	1.1860			
SMVOL=	0.7342			

CALCULATED DENSITIES

RHOF=	1.4047
RHOSA=	1.4480
RHOWA=	1.3249
RHOSM=	1.6153
RHOWM=	1.5742

RUN NUMBER 27

SOLVC FINAL COST IS 0.00000

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.3640	F=	0.3640	
XF=	0.6800	XF=	0.6800	
SA=	0.2860	SA=	0.2860	
XSA=	0.7500	XSA=	0.7500	
WAVOL=	0.0621	EWA=	0.0600	-3.47
XWA=	0.4235	EXWA=	0.5100	16.95
XSM=	0.0050	EXSM=	0.0020	-149.67
ZSM=	0.7100	EZSM=	0.6970	-1.86
WMVOL=	0.6464	EWM=	1.0900	40.70
XWM=	0.0364	EXWM=	0.0	
ZWM=	0.6566	EZWM=	0.0	
EDP=	153.8401	TEDPC=	153.8401	
SRP=	181.9827	ETSRPC=	170.8401	-11.14 (C)
SM=	0.9611			
SMVOL=	0.5899			

CALCULATED DENSITIES

RHOF=	1.4002
RHOSA=	1.4300
RHOWA=	1.2573
RHOSM=	1.6293
RHOWM=	1.6077

RUN NUMBER 28

SOLVO FINAL COST IS 0.00000

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1680	F=	0.1680	
XF=	0.6800	XF=	0.6800	
SA=	0.1156	SA=	0.1156	
XSA=	0.7900	XSA=	0.7900	
WAVOL=	0.0414	EWA=	0.0400	-3.57
XWA=	0.4376	EXWA=	0.5800	24.54
XSM=	0.0042	EXSM=	0.0040	-5.55
ZSM=	0.7198	EZSM=	0.7090	-1.53
WMVOL=	0.4371	EWM=	0.9300	53.00
XWM=	0.0363	EXWM=	0.0	
ZWM=	0.6665	EZWM=	0.0	
EDP=	153.8401	TEDPC=	153.8401	
SRP=	186.7692	ETSRPC=	169.8401	-16.93 (C)
SM=	0.6553			
SMVOL=	0.4004			

CALCULATED DENSITIES

RHOF=	1.4002
RHOSA=	1.4446
RHOWA=	1.2662
RHOSM=	1.6367
RHOWM=	1.6194

RUN NUMBER 29

SOLVO FINAL COST IS 0.00002

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1954	F=	0.1954	
XF=	0.6700	XF=	0.6700	
SA=	0.0578	SA=	0.0578	
XSA=	0.7900	XSA=	0.7900	
WAVOL=	0.1004	EWA=	0.0900	-11.53
XWA=	0.6196	EXWA=	0.5500	-12.66
XSM=	0.0132	EXSM=	0.0060	-119.70
ZSM=	0.6949	EZSM=	0.6870	-1.15
WMVOL=	2.4354	EWM=	1.1100	-119.41
XWM=	0.0343	EXWM=	0.0	
ZWM=	0.6707	EZWM=	0.0	
EDP=	154.8401	TEDPC=	154.8401	
SRP=	170.2302	ETSRPC=	170.8401	0.61 (C)
SM=	3.8134			
SMVOL=	2.3456			

CALCULATED DENSITIES

RHOF=	1.3955
RHCSA=	1.4446
RHCWA=	1.3708
RHCSM=	1.6258
RHCWM=	1.6223

RUN NUMBER 30

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.3349	F=	0.3349	
XF=	0.6700	XF=	0.6700	
SA=	0.2574	SA=	0.2574	
XSA=	0.7500	XSA=	0.7500	
WAVOL=	0.0623	EWA=	0.0700	11.05
XWA=	0.4044	EXWA=	0.5100	20.70
XSM=	0.0043	EXSM=	0.0020	-112.57
ZSM=	0.7140	EZSM=	0.6790	-5.16
WMVOL=	0.5997	EWM=	0.9900	39.42
XWM=	0.0364	EXWM=	0.0	
ZWM=	0.6566	EZWM=	0.0	
EDP=	153.8401	TEDPC=	153.8401	
SRP=	184.4454	ETSRPC=	169.8401	-14.61 (C)
SM=	0.8867			
SMVOL=	0.5434			

CALCULATED DENSITIES

RHOF=	1.3955
RHCSA=	1.4300
RHCWA=	1.2453
RHCSM=	1.6317
RHCWM=	1.6077

RUN NUMBER 31

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.2056	F=	0.2056	
XF=	0.6200	XF=	0.6200	
SA=	0.0289	SA=	0.0289	
XSA=	0.7900	XSA=	0.7900	
WAVOL=	0.1303	EWA=	0.1300	-0.24
XWA=	0.5922	EXWA=	0.5900	-0.37
XSM=	0.0211	EXSM=	0.0	
ZSM=	0.6623	EZSM=	0.0	
WMVOL=	1.0904	EWM=	1.4300	23.75
XWM=	0.0800	EXWM=	0.0690	-16.00
ZWM=	0.5939	EZWM=	0.6170	3.75
EDP=	141.8401	TECPC=	141.8401	
SRP=	160.4579	ETSRPC=	169.8401	9.38 (C)
SM=	1.5352			
SMVOL=	0.9597			

CALCULATED DENSITIES

RHOF=	1.3710
RHCSA=	1.4446
RHCWA=	1.3564
RHCSM=	1.5997
RHCWM=	1.5699

EDP HOLLAND EFFICIENCY 0.862

RUN NUMBER 32

SOLVO FINAL COST IS 0.00000

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4097	F=	0.4097	
XF=	0.6100	XF=	0.6100	
SA=	0.1585	SA=	0.1585	
XSA=	0.7800	XSA=	0.7800	
WAVOL=	0.1924	EWA=	0.1800	-6.88
XWA=	0.5027	EXWA=	0.5000	-0.54
XSM=	0.0100	EXSM=	0.0	
ZSM=	0.6893	EZSM=	0.0	
WMVOL=	0.9460	EWM=	1.0900	13.21
XWM=	0.0942	EXWM=	0.0690	-36.56
ZWM=	0.5715	EZWM=	0.5700	-0.26
EDP=	139.8401	TEDPC=	139.8401	
SRP=	171.2734	ETSRPC=	168.8401	-2.43 (C)
SM=	1.2186			
SMVOL=	0.7540			

CALCULATED DENSITIES

RHOF=	1.3658
RHCSA=	1.4411
RHCWA=	1.3058
RHCSM=	1.6163
RHCWM=	1.5537

EDP HOLLAND EFFICIENCY 0.732

RUN NUMBER 33

SOLVO FINAL COST IS 0.08925

SALVO FINAL COST IS 0.02581

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4214	F=	0.4214	
XF=	0.6900	XF=	0.6900	
SA=	0.2345	SA=	0.2345	
XSA=	0.8600	XSA=	0.8600	
WAVOL=	0.1449	EWA=	0.1400	-3.48
XWA=	0.4767	EXWA=	0.5800	17.81
XSM=	0.0034	EXSM=	0.0	
ZSM=	0.7350	EZSM=	0.0	
WMVOL=	0.7151	EWM=	1.1100	35.57
XWM=	0.0809	EXWM=	0.0820	1.37
ZWM=	0.6147	EZWM=	0.6020	-2.11
EDP=	139.8401	TEDPC=	139.8401	
SRP=	194.6203	ETSRPC=	169.8401	-24.78 (C)
SM=	0.9550			
SMVOL=	0.5795			

CALCULATED DENSITIES

RHCF=	1.4047
RHCSA=	1.4657
RHCWA=	1.2902
RHCSM=	1.6481
RHCWM=	1.5967

EDP HOLLAND EFFICIENCY 1.014

RUN NUMBER 34

SOLVO FINAL COST IS 0.08925

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1967	F=	0.1967	
XF=	0.6900	XF=	0.6900	
SA=	0.0440	SA=	0.0440	
XSA=	0.8600	XSA=	0.8600	
WAVOL=	0.1105	EWA=	0.1100	-0.47
XWA=	0.6410	EXWA=	0.6300	-1.75
XSM=	0.0169	EXSM=	0.0	
ZSM=	0.6850	EZSM=	0.0	
WMVOL=	0.9326	EWM=	1.1200	16.73
XWM=	0.0809	EXWM=	0.0740	-9.30
ZWM=	0.6147	EZWM=	0.6060	-1.44
EDP=	139.8401	TEDPC=	139.8401	
SRP=	165.9570	ETSRPC=	169.8401	3.88 (C)
SM=	1.3365			
SMVOL=	0.8252			

CALCULATED DENSITIES

RHOF=	1.4047
RHOSA=	1.4657
RHOWA=	1.3816
RHOSM=	1.6196
RHOWM=	1.5967

EDP HOLLAND EFFICIENCY 0.915

RUN NUMBER 35

SOLVC FINAL COST IS 0.00000

SALVC FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4228	F=	0.4228	
XF=	0.7000	XF=	0.7000	
SA=	0.2182	SA=	0.2182	
XSA=	0.8200	XSA=	0.8200	
WAVOL=	0.1521	EWA=	0.1600	4.96
XWA=	0.5720	EXWA=	0.5800	1.37
XSM=	0.0145	EXSM=	0.0	
ZSM=	0.6814	EZSM=	0.0	
WMVOL=	0.9671	EWM=	1.1200	13.65
XWM=	0.0895	EXWM=	0.0920	2.74
ZWM=	0.5897	EZWM=	0.6640	11.19
EDP=	139.8401	TEDPC=	139.8401	
SRP=	166.7926	ETSRPC=	169.8401	3.05 (C)
SM=	1.3161			
SMVOL=	0.8158			

CALCULATED DENSITIES

RHOF=	1.4092
RHOSA=	1.4544
RHOWA=	1.3455
RHOSM=	1.6132
RHOWM=	1.5724

EDP HOLLAND EFFICIENCY 1.028

RUN NUMBER 36

SOLVO FINAL COST IS 0.00002

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1820	F=	0.1820	
XF=	0.6800	XF=	0.6800	
SA=	0.0438	SA=	0.0438	
XSA=	0.8400	XSA=	0.8400	
WAVOL=	0.1005	EWA=	0.1100	8.66
XWA=	0.6293	EXWA=	0.5900	-6.66
XSM=	0.0193	EXSM=	0.0	
ZSM=	0.6746	EZSM=	0.0	
WMVOL=	0.8023	EWM=	1.0200	21.34
XWM=	0.0857	EXWM=	0.0610	-40.48
ZWM=	0.6012	EZWM=	0.6350	5.32
EDP=	139.8401	TEDPC=	139.8401	
SRP=	163.0533	ETSRPC=	170.8401	7.79 (C)
SM=	1.1324			
SMVOL=	0.7028			

CALCULATED DENSITIES

RHCF=	1.4002
RHCSA=	1.4603
RHCWA=	1.3757
RHCSM=	1.6112
RHCWM=	1.5837

EDP HOLLAND EFFICIENCY 0.712

RUN NUMBER 37

SOLVO FINAL COST IS 0.00002

SALVO FINAL COST IS 0.00181

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.4228	F=	0.4228	
XF=	0.7000	XF=	0.7000	
SA=	0.1898	SA=	0.1898	
XSA=	0.8400	XSA=	0.8400	
WAVOL=	0.1722	EWA=	0.1700	-1.27
XWA=	0.5859	EXWA=	0.5500	-6.53
XSM=	0.0134	EXSM=	0.0	
ZSM=	0.6882	EZSM=	0.0	
WMVOL=	1.1643	EWM=	1.0300	-13.04
XWM=	0.0857	EXWM=	0.0820	-4.50
ZWM=	0.6012	EZWM=	0.5820	-3.31
EDP=	139.8401	TEDPC=	139.8401	
SRP=	168.7972	ETSRPC=	168.8401	0.04 (C)
SM=	1.6111			
SMVOL=	0.9951			

CALCULATED DENSITIES

RHCF=	1.4092
RHCSA=	1.4603
RHCWA=	1.3530
RHCSM=	1.6190
RHCWM=	1.5837

EDP HOLLAND EFFICIENCY 0.957

RUN NUMBER 38

SOLVO FINAL COST IS 0.00003

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1979	F=	0.1979	
XF=	0.7100	XF=	0.7100	
SA=	0.0443	SA=	0.0443	
XSA=	0.9100	XSA=	0.9100	
WAVOL=	0.1107	EWA=	0.1100	-0.66
XWA=	0.6523	EXWA=	0.6600	1.17
XSM=	0.0088	EXSM=	0.0320	72.50
ZSM=	0.7209	EZSM=	0.6750	-6.80
WMVOL=	1.0982	EWM=	1.4300	23.20
XWM=	0.0637	EXWM=	0.0590	-7.98
ZWM=	0.6594	EZWM=	0.5710	-15.48
EDP=	139.8401	TEDPC=	139.8401	
SRP=	180.1091	ETSRPC=	169.8401	-10.27 (C)
SM=	1.6464			
SMVOL=	1.0002			

CALCULATED DENSITIES

RHOF=	1.4136
RHOSA=	1.4770
RHOWA=	1.3871
RHOSM=	1.6461
RHOWM=	1.6390

EDP HOLLAND EFFICIENCY 0.926

RUN NUMBER 39

SOLVC FINAL COST IS 0.00001

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.1979	F=	0.1979	
XF=	0.7100	XF=	0.7100	
SA=	0.0295	SA=	0.0295	
XSA=	0.8900	XSA=	0.8900	
WAVOL=	0.1204	EWA=	0.1000	-20.36
XWA=	0.6785	EXWA=	0.6700	-1.27
XSM=	0.0149	EXSM=	0.0210	29.15
ZSM=	0.6990	EZSM=	0.6870	-1.75
WMVOL=	1.2194	EWM=	1.4300	14.73
XWM=	0.0715	EXWM=	0.0610	-17.15
ZWM=	0.6394	EZWM=	0.6420	0.40
EDP=	139.8401	TECPC=	139.8401	
SRP=	169.4564	ETSRPC=	168.8401	-0.62 (C)
SM=	1.8071			
SMVOL=	1.1071			

CALCULATED DENSITIES

RHOF=	1.4136
RHCSA=	1.4729
RHCWA=	1.3995
RHCSM=	1.6323
RHCWM=	1.6201

EDP HOLLAND EFFICIENCY 0.854

RUN NUMBER 40

SOLVO FINAL COST IS 0.00000

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.2202	F=	0.2202	
XF=	0.6300	XF=	0.6300	
SA=	0.0146	SA=	0.0146	
XSA=	0.8500	XSA=	0.8500	
WAVOL=	0.1502	EWA=	0.1600	6.10
XWA=	0.6143	EXWA=	0.5800	-5.92
XSM=	0.0153	EXSM=	0.0130	-17.74
ZSM=	0.6857	EZSM=	0.6750	-1.58
WMVOL=	1.1370	EWM=	1.4300	20.49
XWM=	0.0834	EXWM=	0.0580	-43.81
ZWM=	0.6077	EZWM=	0.6220	2.29
EDP=	139.8401	TEDPC=	139.8401	
SRP=	167.0795	ETSRPC=	169.8401	2.76 (C)
SM=	1.6024			
SMVOL=	0.9900			

CALCULATED DENSITIES

RHCF=	1.3760
RHCSA=	1.4631
RHCWA=	1.3680
RHCSM=	1.6186
RHCWM=	1.5900

EDP HOLLAND EFFICIENCY 0.695

RUN NUMBER 41

SOLVO FINAL COST IS 0.00291

SALVO FINAL COST IS 0.00000

CALCULATED DATA		EXPERIMENTAL DATA		PERCENTAGE ERROR
F=	0.2322	F=	0.2322	
XF=	0.8100	XF=	0.8100	
SA=	0.0148	SA=	0.0148	
XSA=	0.9300	XSA=	0.9300	
WAVOL=	0.1501	EWA=	0.0900	-66.75
XWA=	0.8018	EXWA=	0.7700	-4.13
XSM=	0.0168	EXSM=	0.0450	62.73
ZSM=	0.7178	EZSM=	0.6770	-6.02
WMVOL=	2.7058	EWM=	1.4200	-90.55
XWM=	0.0547	EXWM=	0.0780	29.83
ZWM=	0.6831	EZWM=	0.6500	-5.09
EDP=	139.8401	TEDPC=	139.8401	
SRP=	168.6778	ETSRPC=	168.8401	0.16 (C)
SM=	4.2782			
SMVOL=	2.5830			

CALCULATED DENSITIES

RHCF=	1.4513
RHCSA=	1.4806
RHCWA=	1.4486
RHCSM=	1.6563
RHOWM=	1.6615

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