

27623

NATIONAL LIBRARY  
OTTAWA



BIBLIOTHÈQUE NATIONALE  
OTTAWA

NAME OF AUTHOR..... DENIS JAKEFIELD, RENE LÉON  
TITLE OF THESIS..... MICELLING..... AMINE  
UNITS AND MULTICOLUMN  
SYSTEMS.....  
UNIVERSITY..... UNIVERSITY OF ALBERTA, EDMONTON  
DEGREE FOR WHICH THESIS WAS PRESENTED..... M.Sc.....  
YEAR THIS DEGREE GRANTED..... 1976.....

Permission is hereby granted to THE NATIONAL LIBRARY  
OF CANADA to microfilm this thesis and to lend or sell copies  
of the film.

The author reserves other publication rights, and  
neither the thesis nor extensive extracts from it may be  
printed or otherwise reproduced without the author's  
written permission.

(Signed)..... D. Jakefield.....

PERMANENT ADDRESS:

C/..... Dept. of Chemical Engineering  
University..... of Alberta  
Edmonton, Alta. T6G 2G6

DATED..... Feb. 6<sup>th</sup> 1976

NL-91 (10-68)

~~INFORMATION TO USERS~~

THIS DISSERTATION HAS BEEN  
MICROFILMED EXACTLY AS RECEIVED

This copy was produced from a microfilm copy of the original document. The quality of the copy is heavily dependent upon the quality of the original thesis submitted for microfilming. Every effort has been made to ensure the highest quality of reproduction possible.

PLEASE NOTE: Some pages may have indistinct print. Filmed as received.

Canadian Theses Division  
Cataloguing Branch  
National Library of Canada  
Ottawa, Canada K1A 0N4

AVIS AUX USAGERS

LA THESE A ETE MICROFILMEE  
TELLE QUE NOUS L'AVONS RECUE

Cette copie a été faite à partir d'une microfiche du document original. La qualité de la copie dépend grandement de la qualité de la thèse soumise pour le microfilmage. Nous avons tout fait pour assurer une qualité supérieure de reproduction.

NOTA BENE: La qualité d'impression de certaines pages peut laisser à désirer. Microfilmée telle que nous l'avons reçue.

Division des thèses canadiennes  
Direction du catalogage  
Bibliothèque nationale du Canada  
Ottawa, Canada K1A 0N4

THE UNIVERSITY OF ALBERTA

MODELING OF AMINE UNITS  
AND MULTICOLUMN SYSTEMS

by

(C)

DENTS WAKEFIELD BROWNE

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH  
IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE  
OF MASTER OF SCIENCE

IN

CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING

EDMONTON, ALBERTA

SPRING, 1976

THE UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and  
recommend to the Faculty of Graduate Studies and Research,  
for acceptance, the thesis entitled "MODELLING OF AMINE  
UNITS AND MULTICOLUMN SYSTEMS", submitted by Denis  
Wakefield Browne, in partial fulfilment of the require-  
ments for the degree of Master of Science in Chemical  
Engineering.

.....*Peter A. Mather*.....  
Supervisor

.....*A.E.Mather*.....

.....*T.A. Stell*.....

Date *Feb. 24. 1976*..... 1976

## ABSTRACT

The calculational method for multistage, multi-component separation processes developed by Ishii has been utilized to build a computational model for imine contactors and regenerators. Use of the model is illustrated with test problems typical of columns operating in natural gas processing plants. Two correlations of experimental solubility data are used in the problems and the results are shown to be sensitive to the correlation employed. Some consideration is also given to the use and estimation of stage efficiencies. The incorporation of efficiencies is shown to be important in an accurate design; however the accuracy of calculated values is limited by a paucity of reliable rate data.

In addition, Ishii's method has been extended to produce an algorithm for the solution of multicolumn configurations. The algorithm utilizes the basic block tridiagonal matrix form of the linearized steady state equations and the sparseness of many of the matrices to produce a quick and efficient solution procedure. The algorithm has shown reliability in converging for the three systems tried, namely a thermally coupled distillation system, an extractive distillation system and an amine treating system. However, some problems are encountered with certain column specifications.

#### ACKNOWLEDGEMENTS

The author wishes to express his sincere thanks to Dr. F. D. Otto for his advice, encouragement and personal interest throughout this work.

To AMOCO Ltd. an expression of thanks for supplying a correlation of the solubilities of  $\text{CO}_2$  and gases in amine solutions.

The financial support of the University of Alberta is appreciated.

To Ev, my typist, warm thanks for her diligent preparation of the manuscript.

And special thanks to Judy, who became my wife during the course of the thesis, and who provided the special impetus that makes all the effort worthwhile.

TABLE OF CONTENTS

CHAPTER		PAGE
1.	INTRODUCTION	1
2.	LITERATURE REVIEW	5
	2.1 Design Methods for Alkanolamine Units	6
	2.2 Correlation of Equilibrium Solubility Data For $H_2S$ and $CO_2$ in Alkanolamine Solutions	7
	2.3 Enthalpy Data for Acid Gas-Amine Systems	12
	2.4 Numerical Solution of Stagewise Processes for Multicomponent Mixtures	13
	2.4.1 Algorithms for Equilibrium Stage Calculations	13
	2.4.2 Stage Efficiencies	15
	2.5 Stage Efficiencies for Amine Units	18
	2.6 Multicolumn Calculations	21
	MODELLING AMINE CONTACTORS AND REGENERATORS	25
3.	3.1 Stage Model	25
	3.1.1 Solution Procedure	28
	3.1.2 Initial Assumptions	30
	3.2 Determination of Equilibrium K-ratios	34
	3.3 Determination of Enthalpies	36
	3.4 Development of Partial Derivatives	37

TABLE OF CONTENTS

CHAPTER		PAGE
4.	APPLICATION OF THE MODEL TO THE DESIGN OF AMINE UNITS	43
4.1	Test Problems	43
4.2	Discussion of Test Problems	51
4.3	Dependence of Sweet Gas H <sub>2</sub> S Composition on Lean Amine Residuals	55
4.4	Prediction of Stage Efficiency	58
4.4.1	CO <sub>2</sub> Stage Efficiency	60
4.4.2	H <sub>2</sub> S Stage Efficiency	62
4.4.3	Example Problem No. 5	63
5.	A GENERAL ALGORITHM FOR SOLVING MULTICOLUMN SYSTEMS	66
5.1	Model Equations	66
5.2	Linearized Equations	69
5.3	Matrix Forms	74
5.4	Effect of Problem Specifications on Matrix Elements	85
5.5	Solution Procedure	88
6.	USE OF THE MULTICOLUMN ALGORITHM	94
6.1	Example Problems	94
6.2	Results and Discussion	104
6.2.1	Evaluation of the Algorithm	105
6.2.2	Example Problem 1	108

TABLE OF CONTENTS

CHAPTER	PAGE
6.2.3 Example Problem 2	109
6.2.4 Example Problem 3	112
6.3 Application to the Design of Amine Treating Systems	114
6.3.1 The Split Flow System Option	114
6.3.2 Choice of a Stripping Steam Rate to Achieve a Given Lean Amine Resi- dual	116
7. CONCLUSIONS	121
NOMENCLATURE	124
REFERENCES	130

APPENDIX

1. Enthalpies of Solution of CO <sub>2</sub> and H <sub>2</sub> S in MEA and DEA Solutions	133
2. Constants in Correlations for Ideal Gas Enthalpy and Latent Heat of Vapourization	136
3. Intermediate Partial Derivatives Required in the Derivation of K/x for H <sub>2</sub> S and CO <sub>2</sub>	138
4. Computer Printouts for Amine Contactor and Regenerator Problems	146

TABLE OF CONTENTS

<b>APPENDIX</b>		<b>PAGE</b>
<b>4.1</b>	Test Problem 1 - Nasir Correlation	<b>147</b>
<b>4.2</b>	Test Problem 2 - Nasir Correlation	152
<b>4.3</b>	Test Problem 3 - Nasir Correlation	156
<b>4.4</b>	Test Problem 4 - Nasir Correlation	161
<b>4.5</b>	Test Problem 1 - Amoco Correlation	167
<b>4.6</b>	Test Problem 2 - Amoco Correlation	172
<b>4.7</b>	Test Problem 3 - Amoco Correlation	176
<b>4.8</b>	Test Problem 4 - Amoco Correlation	181
<b>4.9</b>	Test Problem 5 - Nasir Correlation	186
<b>5.</b>	Equilibrium and Enthalpy Data for Extractive Distillation Problem	192
<b>6.</b>	Computer Printouts for Problems Using Linked Column Algorithm	197
<b>6.1</b>	Thermally Coupled Distillation System	198
<b>6.2</b>	Extractive Distillation System	209
<b>6.3</b>	Amine Treating System	225

## TABLE OF TABLE

## TABLE

Page

1	Henry's Law Coefficients (wt. % to fraction) For $\text{CO}_2$ and $\text{H}_2\text{S}$ in Water	65
2	Number of Iterations and CPU Time Required for Test Problems for TW Data Corrections	66
3	Comparison of the Values of Important Design Variables	67
4	Murphree Efficiencies as calculated From Vapourization Efficiencies	67
5	Contribution of Interlinked Streams to Material and Energy Balance Equations	68
6	Terms in Linearized Equations Arising from Interconnected Streams	70
7	Non-zero Off-diagonal Elements in Each Coefficient Matrix	70
8	Convergence Characteristics and CPU Times for Linked Column Example Problems	74
9	Comparison of Runs for Thermally Coupled Distillation Problem	79
10	Comparison of Results Given by Saturated Flow and Conventional Configurations	81
11	$\text{H}_2\text{S}$ and $\text{CO}_2$ Lean Amine Residuals for Different Reboiler Stream Rates and Acid Gas Ratios in the Feed	81

## CONTENTS

FIGURE	PAGE
1 Amine-Sweetening System	29
2 Generalized Stage Model	29
3 Composition of $\text{H}_2\text{S}$ in Sweet Gas Versus $\text{H}_2\text{S}$ Lean Amine Residual	56
4 General Stage in A Multicolumn System	61
5 Example System of 5 Columns	76
6 General Matrix Form	80
7 Thermally Coupled Distillation System	91
8 Extractive Distillation System	96
9 Acid Gas Lean Amine Residuals Versus Acid Gas Feed Ratio at different Steam Rates	113

## 1 - INTRODUCTION

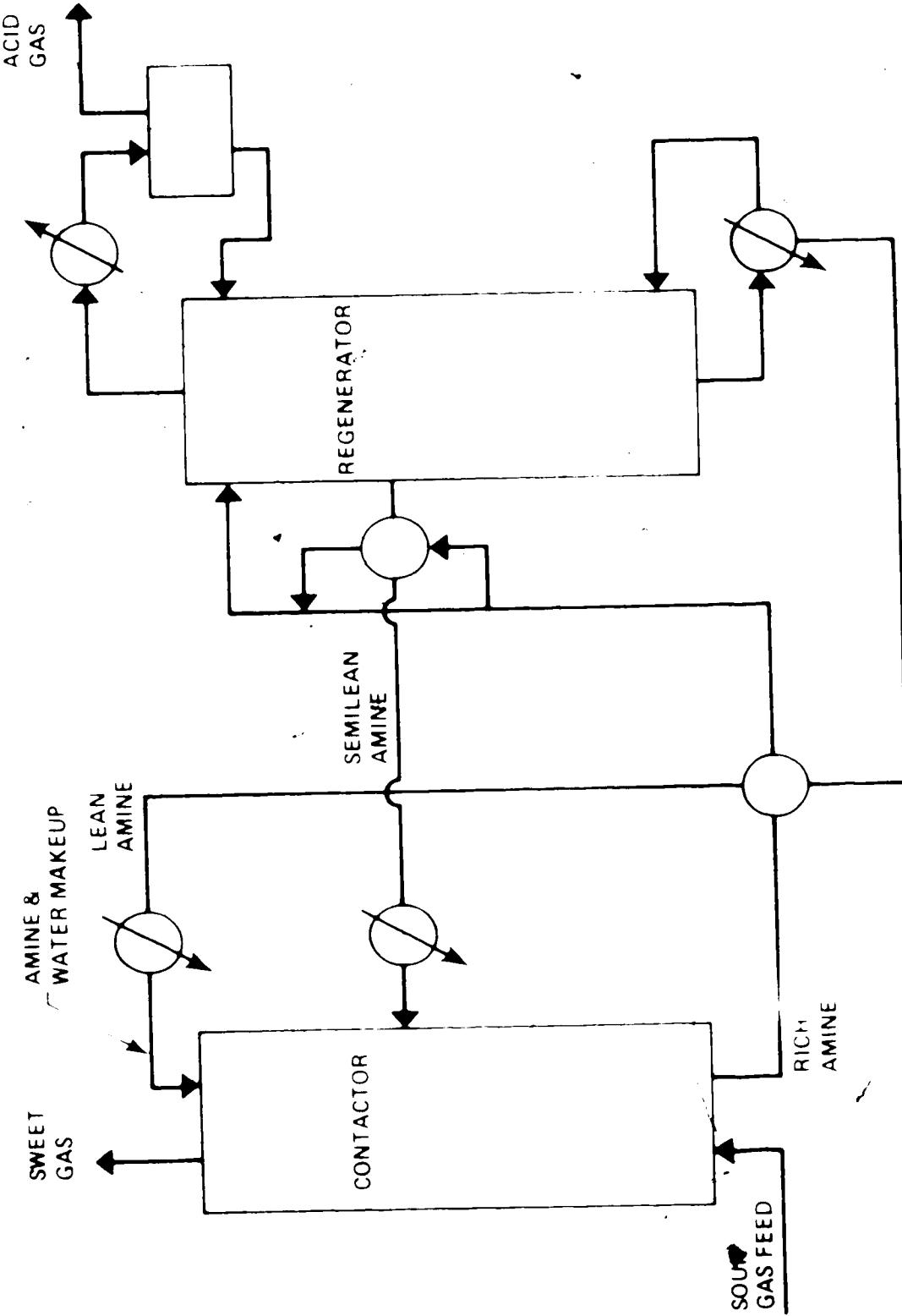
In the gas processing industry the removal of acid gases ( $H_2S$  and  $CO_2$ ) from gas streams is of prime importance. Alkanolamines are widely used to effect this removal, particularly from streams such as the hydrocarbon streams encountered in natural gas processing, in petroleum refining and in the upgrading of bitumen obtained from oil sands. Also, in the production of ammonia alkanolamines are used to remove  $CO_2$  from the synthesis gas stream.

The normal flowsheet configuration of a gas sweetening system using alkanolamines is shown as Figure 1. Sour gas feed is contacted with a lean amine stream containing small quantities of  $H_2S$  and  $CO_2$ . The resulting sweet gas stream contains  $H_2S$  and  $CO_2$  to the extent of some with a typical specification of no more than 0.25 mmol per 100 ml (approximately 1 ppm). This lean amine is fed to a reboiler in which essentially all the acid gas components are removed as overhead product, producing as bottoms product the lean amine which is recycled to the top contactor stage.

A small makeup of amine and water is needed to counter vapourization losses. The semi-lean amine stream is an optional innovation that may reduce operating costs.

In the design of an amine system the important

FIGURE 1: AMINE SWEETENING SYSTEM



information required includes:

- (i) the number of stages in each column
- (ii) type of amine and solution concentration
- (iii) the amine circulation rate
- (iv) steam requirements in the regenerator.

The absorption of  $H_2S$  and  $CO_2$  in alkanolamine solutions is complex in that it involves simultaneous absorption and chemical reaction, and rate and equilibrium data are scarce for such systems. As a result amine systems are most often designed on the basis of "rules-of-thumb" derived from experience. Typical examples are the use of approximately 20 stages in the towers, regenerator steam loads of between 1.0 and 1.2 lb. of steam per gallon of circulating amine, circulation rates based on a pickup of 2.5 SCF acid gas per gallon of amine, and the choice of MEA solution concentration of 15 weight percent. The use of these "rules-of-thumb" no doubt fails to produce an optimum design in many cases. Thus there is a need for a better design procedure.

This study was undertaken to develop a computer oriented design procedure which would make use of recent advances in two areas namely:

- (i) techniques for making stagewise calculations for multicomponent mixtures, based on the equilibrium stage concept.

- (ii) developments in the preparation of thermodynamically based correlations of equilibrium solubility data for  $H_2S$  and  $CO_2$  in alkanolamine solutions.

Considering that the amines have a different selectivity for  $H_2S$  than for  $CO_2$ , the stage efficiency becomes an important consideration in an accurate simulation or design. Thus some attention is given to the use and estimation of stage efficiencies.

An additional aim of the study is to extend the method described by Ishii and Otto<sup>18</sup> for multistage, multi-component equilibrium stage calculations to multicolumn systems. Part of the motivation for this is that amine systems involve recycle streams, in particular the lean amine and the semilean amine. The latter is an option in which a partially regenerated amine stream is recycled from the regenerator to the middle section of the contactor. There is some dispute over the usefulness of this configuration and an adequate model of the system will permit an accurate evaluation to be made.

## 2. LITERATURE REVIEW

### 2.1 Design Methods for Alkanolamine Units

Most current design techniques for alkanolamine units rely heavily on empirical "rules-of-thumb". In particular, it is common practice to use 20 stages for the contactor, and a similar standard number for the regenerator<sup>24</sup>. The circulation rate is estimated from either an assumed acid gas pickup per gallon of amine solution<sup>30</sup>, or from a limit on the acid gas loading in the rich amine, and steam requirements for the regenerator are assigned as a standard quantity of steam per gallon of circulating amine<sup>30</sup>.

The above practices are known to overdesign units and so certain refinements to design procedures have been proposed, primarily by Kohl and Riesenfeld<sup>24</sup> and Maddox<sup>30</sup>. The circulation rate has a considerable effect on capital and operating costs, and both authors attempt to calculate this rate more accurately. The basis is to assume a percentage approach to equilibrium on the bottom stage, with values used lying between 65% and 75%<sup>30</sup>. Equivalently, a minimum circulation rate can be estimated on the assumption of equilibrium existing on the bottom stage, and the actual rate obtained by multiplying this minimum rate by an empirically determined factor<sup>24,29</sup>.

Another major design variable is the reboiler heat requirement. Fitzgerald and Richardson<sup>9</sup> used data from a number of operating MEA plants to prepare a widely used empirical correlation which relates the residual H<sub>2</sub>S in the lean amine solution, the ratio of H<sub>2</sub>S:CO<sub>2</sub> in the feed and the steam rate, expressed in lb/qal. A similar chart exists for the CO<sub>2</sub> lean amine residual.

The so-called "split-stream" process, attributed to Shoeld<sup>40</sup>, has achieved some measure of attention. The process reduces the energy requirements in the reboiler<sup>24</sup>, and is claimed to have particular advantage for gas streams containing more than 30 percent acid gas<sup>30</sup>. However, capital investment in a "split-stream" plant is higher than in a conventional plant, because of added complexity in mechanical design, and added pumping and heat exchange costs.

Selection of the type of amine is dictated somewhat by the presence or absence of COS and CS<sub>2</sub>, which undergo irreversible reactions with MEA<sup>24</sup>. The concentration of the solution is also restricted by corrosion considerations<sup>30</sup>, and this is one major reason for using 15 weight percent MEA.

Most authors regard the complexity of the reactions inside the contactor as sufficient justification for using a standard number of stages. However, Kohl and Riesenfeld<sup>24</sup>

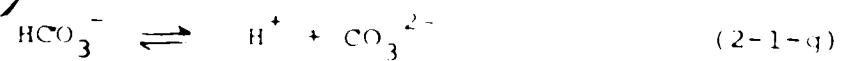
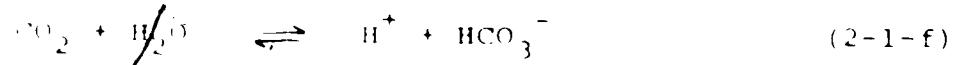
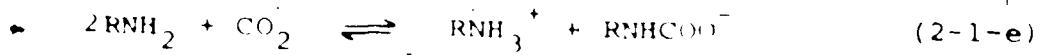
suggest the number of stages can be estimated on the basis of an empirical correlation for the mass transfer coefficient and stage efficiency for  $\text{CO}_2$ . Average values are used for all stages and the presence of  $\text{H}_2\text{S}$  ignored.

One detailed stagewise calculation of an acid-gas absorber has been published, by Rowland and Grens<sup>39</sup>. Solutions with only one acid-gas component are used and a number of simplifying assumptions are made. For example the individual phase mass transfer coefficients are assumed constant on all stages. No detail is given of the method of obtaining equilibrium and enthalpy data. The authors compared stage-to-stage and Thiele-Geddes type calculations and concluded that a stage-to-stage technique is the more effective technique for real stage acid-gas absorbers.

## 2.2 Correlation of Equilibrium Solubility Data

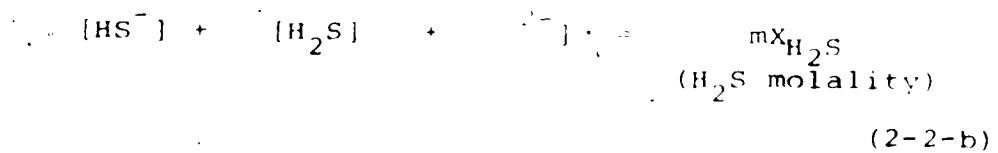
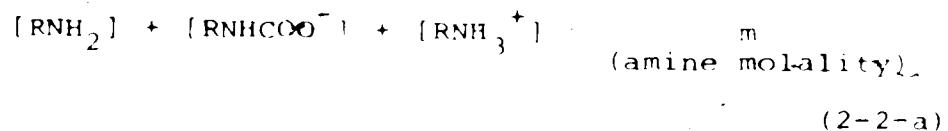
### For $\text{H}_2\text{S}$ and $\text{CO}_2$ in Alkanolamine Solutions.

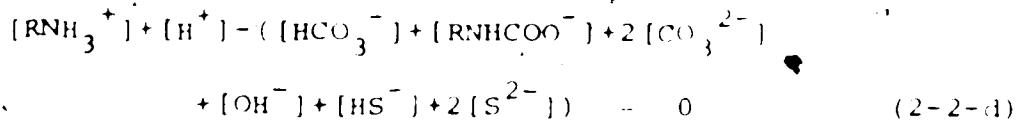
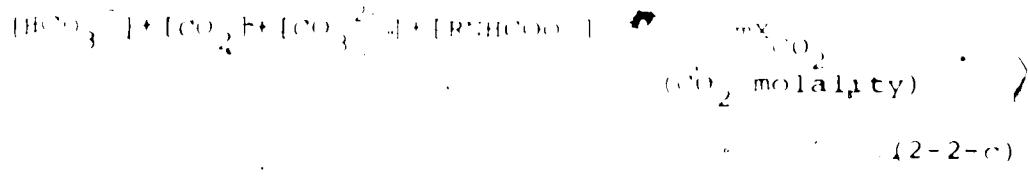
Equilibrium solubility data may be correlated by curve fitting the available data, or alternatively a predictive model can be established based on a suitable set of chemical reactions. For the case of  $\text{H}_2\text{S}$  and  $\text{CO}_2$  in an aqueous amine solution, the following set of reactions can be written<sup>35</sup>:



Where R denotes the group  $-\text{CH}_2-\text{CH}_2-\text{OH}$ . If R-H in the above equations is replaced by R-R, then the equations represent the chemical reactions in the  $\text{H}_2\text{S}-\text{CO}_2$ -DEA-water system.

In addition, three mass balances and an electro-neutrality balance can be written, namely:





Both Klyamer et al.<sup>22</sup> and Nasir<sup>34</sup> have developed models based on this set of equations. In the former model, non-idealities in the liquid phase are accounted for by using activity coefficients. Nasir<sup>35</sup> extended this refinement to include:

- (a) vapour phase fugacities to account for deviations from ideal conditions at low temperatures and high pressures.
- (b) an additional dependence of the activity coefficient on temperature and molality of alkanolamine, rather than just on ionic strength.
- (c) empirical corrections to the partial pressures of H<sub>2</sub>S and CO<sub>2</sub> in the region of very low acid gas loadings, where the predicted values deviate markedly from the experimental values.

For both models the following set of thermodynamic equilibrium constant expressions for equations (2-1-a) to (2-1-i) may be written:

$$K_1 = \frac{2}{a^2} \frac{[RNH_2^+]}{[H_2S]}$$

$$K_w = \frac{2}{a^2} [H^+] [OH^-]$$

$$K_{1c} = \frac{2}{a^2} \frac{[H^+] [HS^-]}{[H_2S]} \quad (2-3-c)$$

$$K_{2c} = \frac{[H^+] [S^{2-}]}{[HS^-]} \quad (2-3-d)$$

$$K_m = \frac{2}{a^2} \frac{[RNH_3^+] [RNHCOO^-]}{[RNH_2]^2 P_{CO_2}} \quad (2-3-e)$$

$$K_{1Y} = \frac{2}{a^2} \frac{[H^+] [HCO_3^-]}{[CO_2]} \quad (2-3-f)$$

$$K_{2Y} = \frac{[H^+] [CO_3^{2-}]}{[HCO_3^-]} \quad (2-3-g)$$

$$H_{CO_2} = \frac{[CO_2]}{[HCO_3^-]^{1/2}} \quad (2-3-h)$$

$$H_{H_2S} = \frac{[H_2S]}{P_{H_2S}} \quad (2-3-i)$$

where:  $\alpha$  is the average coefficient for the ion activity (assumed equal for all ions in solution)

$\alpha$  is the water activity (calculated equal to its molarity)

$a$  is the ratio between the un-ionized ethanolamine activity and the activity of water.

$P_{CO_2}$ ,  $P_{H_2S}$  are the partial pressures of  $CO_2$  and  $H_2S$  in mm Hg.

Equations (2-3-1) and (2-3-1) may be simplified into implicit expressions in  $P_{CO_2}$  and  $P_{H_2S}$  which can be solved numerically. The expressions

$$\frac{P_{H_2S}}{P_{CO_2}} = \frac{K_w}{K_1 K_{1c} \cdot \frac{H_2S}{P_{H_2S}}} \cdot \frac{z^2}{(m - z - A + B)} \quad (2-4)$$

$$\frac{P_{CO_2}}{P_{H_2S}} = \frac{1}{K_m} \cdot \frac{\frac{1}{2} z^2}{\frac{1}{2} m^2} \cdot \frac{z(A+B)}{(m - z - A + B)^2} \quad (2-5)$$

where  $A$  and  $B$  depend on  $P_{H_2S}$  and  $P_{CO_2}$  respectively.

AMOCO<sup>25</sup> derived a solubility model based on a different, but chemically equivalent<sup>35</sup> set of reaction equations (2-1-1) to (2-1-1). Details of the model cannot be disclosed here.

A different approach to the above was taken by Kent and Eisenberg<sup>21</sup>, who combined all the non-idealities into two parameters. These parameters were curve fitted

and irreducible equilibrium data. This is believed best for pure component systems, but shows marked deviations in mixtures.<sup>35</sup>

In the condenser of the regenerator, the liquid phase is essentially all water. Thus a simple Henry's Law model of H<sub>2</sub>S and CO<sub>2</sub> in water may be used. The relevant data taken from Perry<sup>6</sup> are given in Table I.

TABLE I: HENRY'S LAW COEFFICIENT  
(atm/mole fraction)  
FOR CO<sub>2</sub> AND H<sub>2</sub>S IN WATER

t, °C	30	35	40	45	50	60
H <sub>CO<sub>2</sub></sub> × 10 <sup>-3</sup>	1.86	2.09	2.33	2.57	2.83	3.41
H <sub>H<sub>2</sub>S</sub> × 10 <sup>-2</sup>	6.09	6.76	7.43	8.14	8.84	10.3

#### Enthalpy Data for Acid Gas-Amine Systems

The contribution to the liquid or vapour enthalpy of a component with negligible heat of mixing is readily determined using ideal vapour phase enthalpies, modified by latent heats of vapourization for the liquid phase. However, H<sub>2</sub>S and CO<sub>2</sub> have considerable heats of solution and few data are available on these.

on the basis of solubility data, Ben et al.<sup>26,27,28</sup> calculated approximate enthalpies of solution for  $\text{H}_2\text{S}$  and  $\text{CO}_2$  in both MEA and DEA. The values are tabulated in Appendix 1. In all cases the enthalpy of solution is strongly dependent on the acid gas loading, but information to date indicates no temperature dependence and relatively little dependence on solution normality. Kohn and Riesenfeld<sup>24</sup> have published single values for the enthalpies of solution of  $\text{H}_2\text{S}$  and  $\text{CO}_2$  in both MEA and DEA. The values are given in Appendix 1 and are in approximate agreement with those given by Ben et al.<sup>26,27,28</sup>

Pure component enthalpies can be obtained from the API Technical Data Book<sup>1</sup>, latent heats for the amines are found in the Gas Conditioning Fact Book<sup>11</sup>, and for water in Perry<sup>6</sup>.

## 2.4 Numerical Solution of Stagewise Processes for Multicomponent Mixtures

### 2.4.1 Algorithms for Equilibrium Stage Calculations

Many algorithms exist for solving the nonlinear system of equations describing steady state conditions in separation devices. Most of these methods decouple the model equations, that is, the system of equations is split into two or more subsystems which are solved successively

within the outer loop. An alternative approach, namely, one with<sup>10</sup> more computational complexity, is to employ global iteration methods in the light of six decisions that must be made to formulate a solution procedure. It is necessary to be content by Ishii<sup>11</sup>, it is shown that the standard methods are not reliable in that they have difficulties in converging to certain types of problems. There are in addition two other efficient and slower than methods that do not decompose the equations.

An alternative solution approach is to linearize all the model equations and to solve them simultaneously. Although conceptually desirable, this approach may involve an enormous amount of computer storage and time. Thus few algorithms have been proposed, and these can become computationally unwieldy when composition dependent equilibrium and enthalpy data are employed.

Recently, Ishii<sup>12</sup> proposed a new algorithm that overcomes the practical difficulties of total linearization and results in a method that has proven to be both rapid and stable for a wide variety of problems<sup>13</sup>. His approach is to employ only those partial derivatives having a dominant effect on the solution in the linearized equations, thus reducing the matrix structures to terms that can be efficiently manipulated. This computational simplification in no way alters the rigour of the final results.

#### 4.4.2. Estimation of the reference

In the past, much of the modelling of plant growth has concerned the analysis of field experiments that have been designed to estimate the effect of various treatments on plant growth. An important refinement of the field experiment is to include a component to account for the variation in the environment where the effect does not vary from different components and is constant from

Perhaps the most widely used of these is the Marqusee<sup>(1)</sup> vapour transfer function, which is defined by equation (2.6)

$$F_{MV} = \frac{E_{V_1, n} - E_{V_1, n+1}}{E_{V_1, n} + E_{V_1, n+1}} \quad (2.6)$$

where  $E_{V_1, n}$  and  $E_{V_1, n+1}$  are the vapor pressure at the top and bottom of the plant, determined by a plant resistance,  $R_{V_1}$ , and  $E_{V_1, n}$  and  $E_{V_1, n+1}$  are the maximum vapor pressure that is determined by the vapor transfer function,  $\alpha_{V_1}$ , and the vapor pressure at the top of the plant,  $E_{V_1, n}$ .

Another method of estimating these effects is to use the Marqusee<sup>(1)</sup> function, which is achieved by combining a new efficiency, defined by Hall and<sup>(2)</sup>, the efficiency of plant vaporization,  $\eta_{V_1}$ , and is referred by equation (2.7)

$$\eta_{V_1} = E_{V_1} - E_{V_1, n} \quad (2.7)$$

where  $\Delta x_{\text{st}}$  is the distance between stages,  $x_{\text{st}}$  is the liquid mole fraction at the top of stage  $i$ , and  $x_{\text{st}}^{\text{eq}}$  is the equilibrium liquid mole fraction at stage  $i$ .

It is possible to derive an expression for  $\Delta x_{\text{st}}$  in terms of the mass transfer coefficient at the stage,  $K_{\text{act}}$ , and the overall mass transfer coefficient,  $K_{\text{tot}}$ , where  $K_{\text{act}}$  is the product of the liquid hold-up times, where  $\tau = \text{the residence time of the liquid in the column material}$

and  $K_{\text{tot}}$  is

$$\frac{K_{\text{tot}}}{\tau} = \frac{K_{\text{act}}}{1 - (K_{\text{act}} + K_{\text{tot}})S(K_{\text{tot}} + S)^{-1}} \quad (2-8)$$

where:  $\dot{V}_1$  is the vapour flow rate, which is assumed to vary negligibly in the  $z$  direction (moles/hr)

$K_{\text{act}}$  is the overall mass transfer coefficient  
moles/ $\text{ft}^2$  atm hr

$\tau$  is the inter-turbulent contact time, volume of  
column ( $\text{ft}^3$ ) $\text{ft}^{-3}$

$P$  is the pressure in standard units

$S$  is the cross-sectional area of the column, ( $\text{ft}^2$ )

The vapour is assumed to mix totally between stages, i.e. it is to be mixed in passing through the liquid.

Separating the variables in equation (2-8) and integrating across the stages from  $z = 0$  to  $z = z_T$ , the total depth of liquid, gives:

$$\frac{y_{i,j+1}}{y_{i,j}} = \frac{v_i}{K_{i,j} x_{i,j} + v_i} = \frac{(K_{OG} a - P)_{i,j+1}}{v_i} \quad (2-9)$$

This yields:

$$\left\{ \frac{K_{i,j} x_{i,j} + \frac{y_{i,j}}{v_i}}{K_{i,j} x_{i,j} + y_{i,j+1}} \right\} = \frac{v_i}{(K_{OG} a - P)_{i,j+1}} S z_T \quad (2-10)$$

and combining with equation (2-7) gives finally:

$$e_{i,j} = 1 - \exp \left\{ - \frac{(K_{OG} a - P)_{i,j+1}}{v_i} \left[ 1 - \frac{y_{i,j+1}}{K_{i,j} x_{i,j}} \right] \right\} \quad (2-11)$$

This model assumes a well mixed stage. Modifications can be made to accommodate other mixing models<sup>16</sup>.

If the variables in equation (2-11),  $K_{i,j}$ ,  $x_{i,j}$ ,  $y_{i,j+1}$ , and  $P$ , are known from the profiles at each iteration,  $v_i$  (S) is the superficial gas velocity in the column and  $z_T$ , the outlet weir height, is known for a given column design. Thus  $e_{i,j}$  is completely determined if  $(K_{OG} a)_{i,j}$  can be estimated.

For the case of absorption combined with chemical reaction,  $K_{OG} a$  is given by equation (2-12), where  $k_q a$  and  $k_L^0 a$  are the individual gas and liquid phase resistances

In the absence of chemical reaction,  $\alpha$  is the Henry's law coefficient and  $I$  is the enhancement factor.

$$\frac{1}{K_{CO_2}^a} = \frac{1}{k_q^a} + \frac{I}{Ik_L^a} \quad (2-12)$$

The enhancement factor is a measure of how much the rate of absorption is increased by the presence of chemical reaction, and it can be expressed as a function of the reaction rate for a given reaction regime<sup>2</sup>. For example, the penetration theory gives, for the instantaneous reaction regime<sup>2</sup>,

$$I = \left( 1 + \frac{D_2}{D_1} \frac{b_{CO_2}}{q_{CO_2}^a} \right) \sqrt{\frac{D_2}{D_1}} \quad (2-13)$$

#### 2.5 Stage Efficiencies for Amine Units

Little work has been published on efforts to assign values to efficiencies in amine systems. Kohl<sup>23</sup> studied the absorption of CO<sub>2</sub> into MEA solutions. He calculated Murphree vapour stage efficiencies of between 8 and 25%, the low values indicating that the liquid film is controlling. Rowland and Grens<sup>39</sup> found a wide range of efficiency existed over a CO<sub>2</sub>-MEA absorber. Their values were calculated from a fundamental approach, using constant values for k<sub>q</sub><sup>a</sup>, k<sub>L</sub><sup>a</sup> and the liquid holdup, and

ranged from 6.7% at the top to less than 5% at the bottom of the absorber.

Kohl and Pfeiffer<sup>24</sup> have published a correlation for  $K_{OG}^a$  for the absorption of  $\text{CO}_2$  in MEA solutions. The correlation comes from a review of the available data and strictly applies only to a limited range of conditions and to absorption of  $\text{CO}_2$  in the absence of  $\text{H}_2\text{S}$ . The expression is<sup>24</sup>:

$$K_{OG}^a = \left( \frac{V}{z_T} \right) 1.2 \times 10^{-4} / \mu^{0.68} [1 + 1.2 (0.5 - x_{\text{CO}_2}) \ln \left( \frac{1.0067T - 3.4D}{1.0067T + 3.4D} \right)] \quad (2-14)$$

where:  $K_{OG}^a$  = overall mass transfer coefficient

$\frac{1}{\text{lb moles}} / (\text{hr.ft}^3/\text{atm})$

$V$  = actual gas volume

$(\text{ft}^3 / \text{hr.ft}^2 \text{ tray})$

$z_T$  = height of contact zone (ft)

$\mu$  = viscosity (cp)

$x_{\text{CO}_2}$  = concentration of  $\text{CO}_2$  in solution  
(moles/mole MEA)

$m$  = amine concentration in solution (g moles/l)

$T$  = temperature ( $^{\circ}\text{F}$ )

$D$  = partial pressure (atm)

If the temperature is above  $125^{\circ}\text{F}$ ,  $T$  in equation (2-14) is replaced by  $250-T^{23}$ .

Relatively few studies on H<sub>2</sub>S absorption in amine solutions have been published, and no correlations such as equation (2-14) are available. However, K<sub>OG</sub><sup>a</sup> could be estimated from fundamental rate data and equation (2-12). Both Astarita<sup>2</sup> and Danckwerts<sup>7</sup> suggest that H<sub>2</sub>S absorption occurs in the instantaneous reaction regime for the majority of conditions in an amine system. For the simultaneous absorption of H<sub>2</sub>S and CO<sub>2</sub>, Danckwerts and Sharma<sup>8</sup> suggest the following expression for the enhancement factor, I<sub>1</sub>, for H<sub>2</sub>S absorption, assuming the instantaneous reaction regime applies:

$$I_1 = \left[ \frac{1 + \frac{[RNH_2]}{2c'_{o,1}} \frac{D_3}{D_1}}{1 + \frac{2c'_{o,2}}{c'_{o,1}} \frac{D_2}{D_1}} \right] \sqrt{\frac{D_3}{D_1}} \quad (2-15)$$

where: subscripts 1, 2, 3 refer to H<sub>2</sub>S, CO<sub>2</sub> and MEA respectively.

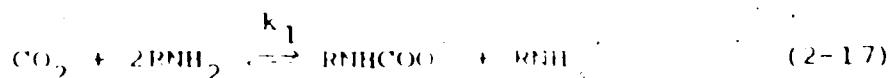
c'\_{o,i} = solubility of i

D<sub>i</sub> = diffusivity of i

Instead of using equation (2-14), K<sub>OG</sub><sup>a</sup> for CO<sub>2</sub> absorption could be calculated from equation (2-12) using the assumption that the reaction is fast regime<sup>2</sup>. In this case the liquid phase coefficient is given by:

$$k_L = ik_L^0 \cdot \sqrt{k_1 p_{CO_2}} \quad (2-16)$$

where  $k_1$  is the pseudo first-order rate constant for the reaction



In general, the limited rate data available on amine systems makes a rigorous determination of stage efficiencies difficult.

## 2.6 Multicolumn Calculations

In most process flowsheet configurations there are a number of recycle streams. Prior to the development of digital computers, these streams made the closure of material balances around a process a job requiring perhaps man-weeks of effort. As computers came into widespread usage, various methods<sup>32, 33, 37, 38</sup> were developed to perform the required iterative calculations far more speedily. Because methods of performing detailed equilibrium stage calculations had not been developed at that stage, each separation device or reaction unit within the system had to be treated in a simplified "black-box" fashion. Therefore, a split was approximated for each component around each device. Such a simplification made the solutions obtained far from rigorous.

More recently a few authors have published methods that solve rigorously the equilibrium stage equations in a system of separation devices. Most of these methods are extensions of previous algorithms developed to handle single columns, and the majority still employ a procedure that decouples the effect of some of the variables.

The "Theta method" has been applied to a number of linked column problems. Initially Tomme and Holland<sup>42</sup> applied the technique to a two column system. They termed the convergence method for systems the "capital" Theta method. A generalization of this procedure was presented by Nartker, Srygley and Holland<sup>34</sup>. Individual units within the system may be any of the conventional separation devices (absorber, reboiled absorber or distillation column) or a special type (mixer, proportional divider, flash unit). The general procedure is based on the calculational procedures for a single column, with the additional use of so-called system thetas, which force simultaneous convergence on all columns in the system. The  $K_b$ -method<sup>15</sup> was used to determine stage temperatures, and the constant composition and Q methods<sup>15</sup> to determine total flow rates. These produced a stable calculational procedure, although the number of iterations increased whenever side heaters or coolers had to be introduced according to the Q method.

13

Later Billingsley<sup>3</sup> presented a simplified formulation of the above procedure. It involves only the theta correction factors used in formulating the equations for a single column, thus making the system thetas redundant. In addition Billingsley notes that in certain cases matrices in the general procedure of Nartker et al.<sup>34</sup> may be nearly singular, in which case gross errors would occur in the material balance around the system. He presents a modification to the equations used which eliminates the difficulty.

Petryschuk and Johnson<sup>36</sup> employed the method of Nartker et al.<sup>34</sup> in the simulation of a complete light ends recovery system. They utilized two other calculation methods - a system block-relaxation method and a sequential iterative method. For a particular recycle loop in the light ends system, a combination of the system theta-method and the block-relaxation method was found to be the superior technique. This combination was up to ten times as fast as the pure block-relaxation method, illustrating the asymptotic approach of the latter to the final solution.

Jelinek et al.<sup>20</sup> found the block-relaxation method superior to the sequential iterative method. The diagonal elements in the material balance matrix, arise from recycle streams between columns, were by a special modification of Gaussian elimination

All of the above methods depend on the material balances from the energy balances, and most would still perform bubble point calculations for the stage temperatures. The desirability of simultaneous solution of all equations has been recognised for some time, but it is only recently that methods have appeared that successfully do this. At present, Harclerode and Gentry<sup>14</sup> are the only authors to have published the application of such a method to a system of columns.

The algorithm is an extension of Gentry's earlier method<sup>12</sup>. In the multiple column case, the matrix equations involve matrices with a limited number of rows and columns that are completely full. Special matrix methods and a modified form of Gaussian elimination are used in the reduction of the matrices to a form where back substitution will yield a solution. Both procedures are specially designed to increase the efficiency of the matrix manipulations and to decrease computing time. One restriction on the method is that the specifications for a column must be symmetrical, i.e. the specification must apply to the same stage as the equation it replaces. The complexity of the matrix manipulations increases markedly when composition dependent equilibrium and enthalpy data are employed.

### 3.1 MODELING AMINE CONTACTORS AND REGENERATORS

#### 3.1.1 Stage Model

A generalized stage model is shown as Figure 3. This model can represent any of the usual separation devices, but in the present context will refer primarily to amine absorbers (contactors) or regenerators.

The steady-state model equations for any stage  $j$  and component  $i$  may be represented as follows:

(1) Phase Relationships:

$$y_{i,j} = e_{i,j} k_{i,j} x_{i,j} \quad (3-1)$$

These reduce to equilibrium relationships if the efficiency factors,  $e_{i,j}$ , are all equal to unity.

(2) Component Material Balances:

$$\begin{aligned} F_j z_{i,j} + L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1} - (L_j + S L_j) x_{i,j} \\ = (V_j + S V_j) y_{i,j} = c_{i,j} \end{aligned} \quad (3-2)$$

(3) Energy Balance:

$$\begin{aligned} F_j H_{F,j} + Q_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1} - (L_j + S L_j) h_j \\ = (V_j + S V_j) H_j = E_j \end{aligned} \quad (3-3)$$

(4) Summation Equation:

$$\sum_{i=1}^{NCP} x_{i,j} = 1.0 = s_j \quad \text{or} \quad \sum_{i=1}^{NCP} y_{i,j} = 1.0 = s_j \quad (3-4)$$

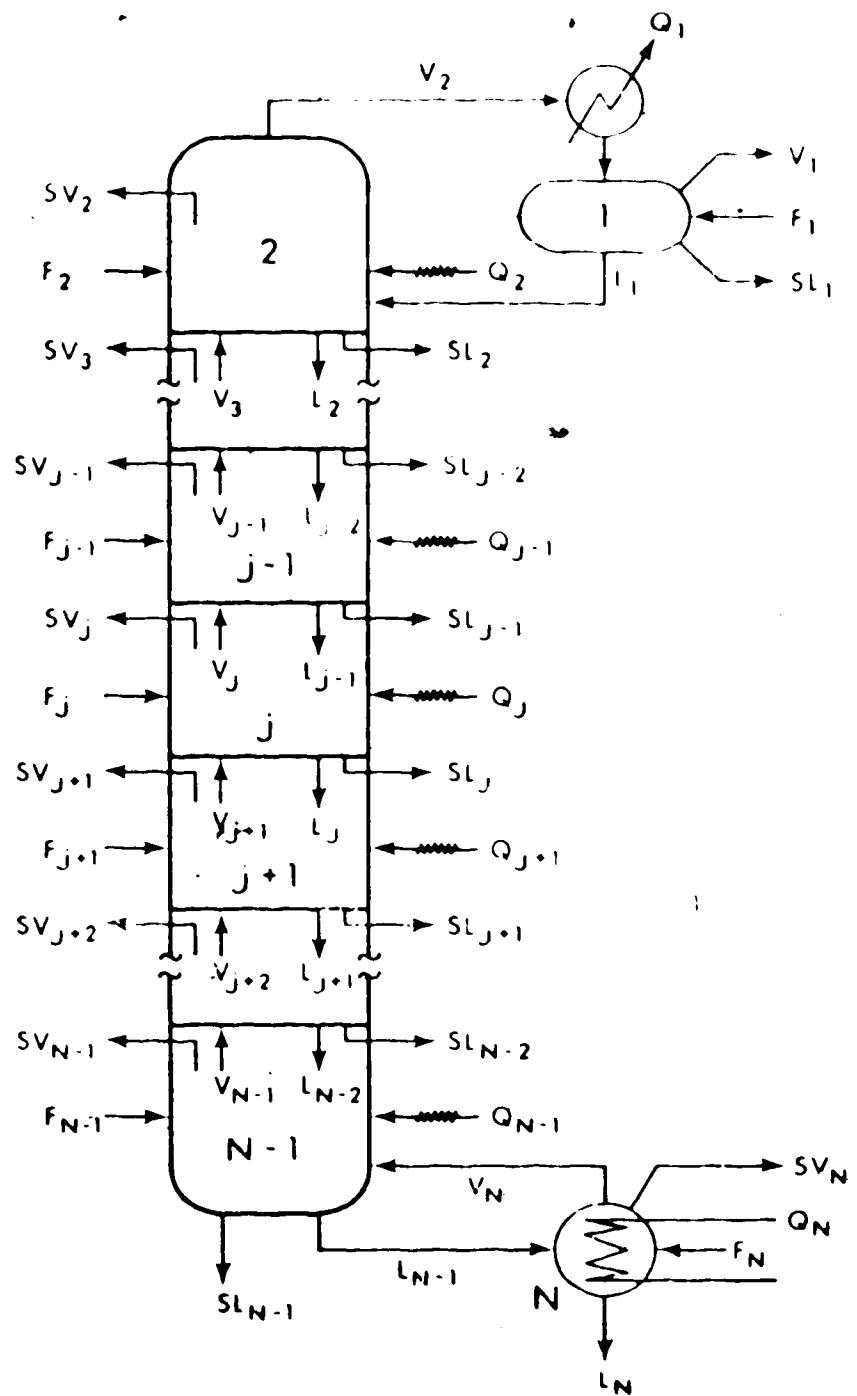


FIGURE 2: GENERALIZED STAGE MODEL

### 3.2 Overall Material Balances

$$F_{1,1} + L_{1,n+1} + V_{1,n+1} - (L_1 \cdot S_{1,1}) - (V_1 \cdot S_{1,1}) = M_1$$

(3-5)

Normally equations (3-2) and (3-3) are combined to give:

$$(L_1 \cdot S_{1,1}) + V_{1,n+1} = (V_1 \cdot S_{1,1}) + F_{1,1} \cdot x_{1,n+1}$$

$$\begin{aligned} & (L_1 \cdot S_{1,1}) \cdot x_{1,n+1} + (V_1 \cdot S_{1,1}) \cdot (1 - x_{1,n+1}) \\ & = C_{1,n+1} \end{aligned} \quad (3-6)$$

The following quantities must be specified in order to match the number of unknowns with the number of independent equations.

- (i) the total number of stages
- (ii) the pressure at each stage
- (iii) the location, total rate, composition and condition of each feed
- (iv) the location and total quantity of each side stream (liquid or vapour)
- (v) the location and heat duty of any intercoolers or heaters (including condenser and reboiler)
- (vi) the values of the vapourization efficiencies.

It should be noted that any of the above specifications may be replaced by an equivalent specification involving another variable. In particular, for regenerator

or a constant value other than zero, the values of the dependent variables are calculated at the next iteration.

Values of the various rate coefficients may be supplied as constants at the start, or calculated by the computer program, or a value can be calculated at each iteration from the current profiles and a knowledge of the dynamics of the tray. The first two equations will

### 3.1.1. Solution Procedure

A solution to the model equations is obtained when a set of values of the temperatures,  $T_i$ 's, the liquid and vapour flow rates,  $L_i$ 's, and  $V_i$ 's, and the phase compositions,  $x_{i,j}$ 's and  $y_{i,j}$ 's, is found which makes all the  $M_{i,j}$ ,  $\epsilon_{i,j}$ ,  $R_i$  and  $S_i$  equal to zero.

The method of solution which forms the basis of this thesis is that developed by Y. Ishii<sup>[1]</sup>. It is essentially a modified Newton-Raphson method, and employs the Taylor approximation procedure in the linearization of the equations.

For the purpose of linearization the  $\epsilon_{i,j}$  are assumed independent of temperature and composition.

The linearized equations are:

#### (1) Component Material Balances:

$$M_{j+1} \cdot S_{1,j+1} + M_{j+1} \cdot S_{2,j+1} + M_{j+1} \cdot S_{3,j+1} = M_j \cdot S_{1,j}$$

$$+ M_{j+1} \cdot S_{1,j+1} + M_{j+1} \cdot S_{2,j+1} + M_{j+1} \cdot S_{3,j+1} = M_j \cdot S_{1,j}$$

$$M_{j+1} \cdot S_{1,j+1} + M_{j+1} \cdot S_{2,j+1} + M_{j+1} \cdot S_{3,j+1} = M_j \cdot S_{1,j}$$

$$+ M_{j+1} \cdot S_{1,j+1} + M_{j+1} \cdot S_{2,j+1} + M_{j+1} \cdot S_{3,j+1} = M_j \cdot S_{1,j}$$

$$+ M_{j+1} \cdot S_{1,j+1} + M_{j+1} \cdot S_{2,j+1} + M_{j+1} \cdot S_{3,j+1} = M_j \cdot S_{1,j}$$

$$+ M_{j+1} \cdot S_{1,j+1} + M_{j+1} \cdot S_{2,j+1} + M_{j+1} \cdot S_{3,j+1} = M_j \cdot S_{1,j}$$

#### (2) Energy Balance:

$$M_{j+1} \cdot \frac{dh}{dT} \Big|_{T_{j+1}} \cdot T_{j+1} = \left[ L_1 \cdot S_{1,j+1} + L_2 \cdot S_{2,j+1} + L_3 \cdot S_{3,j+1} \right] - M_j \cdot h_j$$

$$+ M_{j+1} \cdot \frac{dh}{dT} \Big|_{T_{j+1}} \cdot T_{j+1} = M_j \cdot h_j$$

$$+ M_{j+1} \cdot h_j + M_{j+1} \cdot H_{j+1}$$

#### (3) Overall Material Balance:

$$M_{j+1} + M_{j+1} = M_j + M_j$$

#### (4) Summation Equation:

$$\sum_{i=1}^{NCP} \Delta x_{i,j} = -S_j \quad (i=1 \dots N)$$

It is readily seen that since the absorption of the component material depends upon the identity of the equilibrium case, and thus no different handling methods are necessary in formulating a solution. The solution procedure is the same as that described by Lester<sup>17</sup>. Iterative calculations are continued until a suitable convergence criterion<sup>17</sup> is satisfied.

#### 5.1.2. Initial Assumptions

To begin the iterative solution procedure it is necessary to have initial values of the  $V_j$ 's,  $L_j$ 's,  $T_j$ 's,  $x_{i,j}$ 's and  $y_{i,j}$ 's. A knowledge of the operating characteristics of amine units can be employed to do this.

##### (a) Vapour Flow Rates:

For a contactor all the  $V_j$ 's can be set equal to the quantity of hydrocarbons, nitrogen and hydrogen in the column gas. This is equivalent to assuming most of the absorption occurring on the bottom stages. In a regenerator, however, the vapor rate must be approximated by the quantity of amine, carbon dioxide, nitrogen and light hydrocarbons in the feed to the regenerator. The initial reflux ratio is usually set at 2, and this then gives  $V_2$ . The other  $V_j$ 's are then increased down the column.

tapering off to almost constant molar flowrates in the bottom half.

(b) Liquid Flow Rates:

Once the  $V_j$ 's have been estimated,  $L_j$ 's are obtained from equation (3-5), with  $M_j = 0$ .

(c) Temperature:

For the contactor a linear interpolation between the top and bottom stage temperatures is generally sufficient. The temperature of the top stage can be set equal to the lean amine feed temperature. The bottom stage temperature is more difficult to estimate and depends on the quantity of acid gas being absorbed. If necessary approximate values of the enthalpy of solution of  $H_2S$  and  $CO_2$  can be used to calculate the expected temperature rise in the liquid.

For the reboiler, the condenser temperature is specified and the reboiler temperature will normally be about  $255^{\circ}F$ . The temperature of the feed stage (normally the second) can be approximated as  $30-40^{\circ}F$  above the temperature of the feed. A linear interpolation between this temperature and the reboiler is then used. In the feed stage

is not the second stage, then stages between the condenser and the feed can assume the feed stage temperature.

(d) Liquid Compositions

For the Contactor,

(i) the bottom stage composition for  $H_2S$  and  $CO_2$  is obtained by assuming that all the acid gas, in all feeds, is absorbed into the rich amine. On other stages the respective compositions are equated to the lean amine composition.

(ii) MEA/DEA and water are assumed to remain solely in the liquid.

(iii) other components in the feed, such as hydrogen, nitrogen and light hydrocarbons, are assumed to remain solely in the vapour.

For the Regenerator,

(i) in the condenser the compositions are set equal to the following, where subscripts 1, 2, 3, and 4 refer to  $H_2S$ ,  $CO_2$ , MEA/DEA and  $H_2O$  respectively:

$$x_1 = .001, \quad x_2 = .0002, \quad x_3 = .006,$$

$$x_4 = .9928, \quad x_i = .001 z_i, \quad i = 5 \rightarrow NCP$$

where  $z_i$  is the composition in the rich amine feed. The same values apply for stages between the condenser and the feed stage.

(ii) on the feed stage  $H_2S$ ,  $CO_2$ , MEA/DEA and  $H_2O$  are assigned their respective feed compositions. For other components, their overall composition in the feed is reduced by a factor of 1000 to give the liquid phase compositions.

(iii) for stages between the feed and the reboiler, the  $H_2S$  and  $CO_2$  compositions are linearly interpolated to zero at a fictional stage one below the reboiler (to give a non-zero composition in the reboiler), MEA/DEA and water are assumed to remain solely in the liquid, and other components have their compositions reduced by a factor of 10 on each successive stage.

#### (e) Vapour Compositions

Once liquid phase compositions have been estimated and normalized, K-ratios can be determined. The  $y_{i,j}$ 's are then given by equation (3-1).

### 3.2 Determination of Equilibrium K-ratios

The modified model of Klyamer et al.<sup>22</sup>, as derived by Nasir<sup>35</sup>, was used to predict the partial pressures of H<sub>2</sub>S and CO<sub>2</sub> (see equations 2-4 and 2-5). The equilibrium ratios are then given by equation (3-11), where i represents either H<sub>2</sub>S or CO<sub>2</sub>.

$$K_i = \frac{P_i}{P_T x_i} \quad (3-11)$$

For the condenser, where there is a dilute solution of the acid gas components in water, the K ratios are determined via the Henry's Law coefficients for H<sub>2</sub>S and CO<sub>2</sub>, as tabulated in Table 1. The temperature range of the data in the table covers the normal range of condenser temperatures.

With only a few data points it was deemed sufficiently accurate to use Lagrange interpolating polynomials. These were made to pass through the data points at temperatures of 30, 40, 50 and 60°C, and then slight adjustments made to the coefficients to ensure a good match at temperatures of 35 and 45°C. A third order polynomial was chosen as this produces a curve with a small oscillatory nature.

The equations for the Henry's Law coefficients are then:

(1) For  $\text{H}_2\text{S}$

$$\begin{aligned}
 H = & 0.1717 (T-30)(T-40)(T-50) \\
 & -0.442 (T-30)(T-40)(T-60) \\
 & +0.3725 (T-30)(T-50)(T-60) \\
 & -0.1015 (T-40)(T-50)(T-60) \quad (3-12)
 \end{aligned}$$

(2) For  $\text{CO}_2$

$$\begin{aligned}
 H = & 0.568 (T-30)(T-40)(T-50) \\
 & -1.415 (T-30)(T-40)(T-60) \\
 & +1.165 (T-30)(T-50)(T-60) \\
 & -0.310 (T-40)(T-50)(T-60) \quad (3-13)
 \end{aligned}$$

Finally the K-values are given by the equation

$$K_i = \frac{H_i}{P} \quad (3-14)$$

where: P is the condenser pressure in atmospheres

i refers to either  $\text{H}_2\text{S}$  or  $\text{CO}_2$ .

For other components the Henry's Law coefficients have been curvefitted as a function of temperature. Some of these fits are quite approximate because of the paucity of data for the solubility of hydrocarbons in amine solutions. For simplicity all fractions higher than  $\text{C}_6$  are lumped together.

Raoult's Law is employed to give the partial pressure, and thus the equilibrium K-ratios are given by equation (3-15).

$$K_i = \frac{H_i}{P_T} \quad i = 5 \rightarrow NCP \quad (3-15)$$

where:  $P_T$  is in mm Hg

$H_i$  is in mm Hg/mole fraction.

### 3.3 Determination of Enthalpies

The molar enthalpy of component  $i$  as an ideal gas,  $H_i^0$ , is given by the following cubic equation in temperature,  $^{\circ}\text{R}$ . The coefficients are taken from the API Technical Data Book<sup>1</sup> and are given in Appendix 2.

$$H_i^0 = \{A_i(T/100) + B_i(T/100)^2 + C_i(T/100)^3 + D_i(100/T) + E_i\} XM_i \quad (3-16)$$

The molar enthalpy of the gas phase is then given by equation (3-17)

$$H = \sum_{i=1}^{NCP} y_i H_i^0 \quad (3-17)$$

For non-volatile components, namely MEA/DEA and water, the latent heat of vapourization has been correlated as a quadratic in temperature,  $^{\circ}\text{R}$ .

$$H_{vap,i} = \{AL_i + BL_i T + CL_i T^2\} XM_i \quad (3-18)$$

The coefficients are given in Appendix 2.

The enthalpy of the liquid phase is given by:

$$h = \sum_{i=1}^{NCP} x_i (H_i^0 - H_{vap,i} + \Delta H_{sol}) \quad (3-19)$$

$\Delta H_{sol}$  is the enthalpy of solution of the acid gas components. Values are tabulated in Appendix 1.

### 3.4 Development of Partial Derivatives

Linearization of the model equations introduces a set of partial derivatives that must be evaluated either numerically or analytically at each iteration. In accordance with the findings of Ishii<sup>17</sup>, only those partials with a dominant effect on the solution need be evaluated, namely

$$\frac{\partial K_{i,j}}{\partial T_j}, \frac{\partial K_{i,j}}{\partial x_{i,j}}, \frac{\partial h}{\partial T_j} \text{ and } \frac{\partial h}{\partial T_j}$$

The K-ratios for components other than  $H_2S$  and  $CO_2$  are given by equation (3-15). Then the partial derivatives with respect to  $T$  and  $x$  are:

$$\frac{\partial K_{i,j}}{\partial T_j} = \left\{ \frac{1}{P_T} \frac{\partial H_i}{\partial T} \right\}_j \quad (3-20)$$

$$\frac{\partial K_{i,j}}{\partial x_{i,j}} = 0 \quad (3-21)$$

For  $H_2S$  and  $CO_2$ ,  $\frac{\partial K_{i,j}}{\partial T_j}$  was evaluated numerically using a step size of  $1^\circ F$ .

$\frac{\partial K_{i,j}}{\partial x_{i,j}}$  for these two components can be derived analytically as follows:

The implicit expressions for the partial pressures of  $H_2S$  and  $CO_2$ , are given by equations (2-4) and (2-5) as:

$$P_{H_2S} = \frac{K_w}{K_i K_{1c} H_{H_2S}} \cdot \frac{\gamma^2}{a\alpha} \cdot \frac{A(A+B)}{(m-z-A-B)} \quad (2-4)$$

$$P_{CO_2} = \frac{1}{K_m} \cdot \frac{\gamma^2}{a^2 \alpha^2} \cdot \frac{z(A+B)}{(m-z-A-B)^2} \quad (2-5)$$

Then using equation (3-11) with each of (2-4) and (2-5) in turn, and rearranging yields:

$$(K_i K_{1c} P_T H_{H_2S} a \alpha) K_{H_2S} x_{H_2S} (m-z-A-B) - K_w \gamma^2 A(A+B) = 0 \quad (3-22)$$

$$(K_m P_T a^2 \alpha^2) K_{CO_2} x_{CO_2} (m-z-A-B)^2 - \gamma^2 z (A+B) = 0 \quad (3-23)$$

Both of these equations are of the form

$$F(K_j, x_j) = \text{constant}$$

where  $i$  represents  $H_2S$  or  $CO_2$ .

Then the partial derivative of  $K_j$  with respect to  $x_j$  is given by

$$\frac{\partial K_j}{\partial x_j} = \frac{-\left(\frac{\partial F}{\partial x_j}\right)_{K_j}}{\left(\frac{\partial F}{\partial K_j}\right)_{x_j}} \quad (3-24)$$

(A) For  $H_2S$  (subscript 1 =  $H_2S$ )

$$(i) \left(\frac{\partial F}{\partial x_1}\right)_{K_1} = K_i K_{1C} P_T H_1 a K_1 \left[ x_1(m-z-A-B) + x_1 \left\{ (m-z-A-B) \frac{\partial x_1}{\partial x_1} - z \frac{\partial A}{\partial x_1} \right\} \right] - K_W \left[ \gamma^2 (2A+B) \frac{\partial A}{\partial x_1} + 2 \cdot A (A+B) \frac{\partial A}{\partial x_1} \right] \quad (3-25)$$

$$(ii) \left(\frac{\partial F}{\partial K_1}\right)_{x_1} = K_i K_{1C} P_T H_1 a x_1 \left[ (m-z-A-B) - K_1 \frac{\partial A}{\partial K_1} \right] - K_W \gamma^2 (2A+B) \frac{\partial A}{\partial K_1} \quad (3-26)$$

The partial derivatives required to evaluate

$\partial F / \partial x_1$  and  $\partial F / \partial K_1$  are given in Appendix 3.

(B) For  $\text{CO}_2$  (subscript 2  $\text{CO}_2$ )

$$\begin{aligned}
 \text{(i)} \quad \left( \frac{\partial F}{\partial x_2} \right)_{K_2} &= K_M P_T a^2 K_2 \left[ \alpha^2 (m-z-A-B)^2 \right. \\
 &\quad + x_2 (m-z-A-B)^2 \left( 2z \frac{\partial z}{\partial x_2} \right. \\
 &\quad \left. \left. + 2x_2 (m-z-A-B) \alpha^2 \left( -\frac{\partial z}{\partial x_2} - \frac{\partial B}{\partial x_2} \right) \right] \right. \\
 &\quad - 2yz (A+B) \frac{\partial y}{\partial x_2} - y^2 z \frac{\partial B}{\partial x_2} - y^2 (A+B) \frac{\partial z}{\partial x_2} .
 \end{aligned}$$

(3-27)

$$\begin{aligned}
 \text{(ii)} \quad \left( \frac{\partial F}{\partial K_2} \right)_{x_2} &= K_M P_T a^2 \alpha^2 x_2 \left[ (m-z-A-B)^2 \right. \\
 &\quad + 2K_2 (m-z-A-B) \left( -\frac{\partial z}{\partial K_2} - \frac{\partial B}{\partial K_2} \right) \\
 &\quad \left. - y^2 \left\{ (A+B) \frac{\partial z}{\partial K_2} + z \frac{\partial B}{\partial K_2} \right\} \right] \quad (3-28)
 \end{aligned}$$

where the required partial derivatives are given in Appendix 3.

In the special case of the condenser of the regenerator the partial derivatives are computed by differentiating equations (3-12) and (3-13). Thus:

$$\frac{\partial K_{1,2}}{\partial T_j} = \frac{(15.84 - 1.38T + .0021T^2) - 1.8}{(74.1 - 1.62T + .024T^2) - 1.8} \text{ P for } H_2S \\ (3-29)$$

$$\frac{\partial K_{1,2}}{\partial x_{1,i}} = 0 \quad (3-30)$$

$\frac{\partial H}{\partial T}$  &  $\frac{\partial h}{\partial T}$  are expressed as follow:

$$\frac{\partial H}{\partial T} = \frac{NCP}{x_1} \gamma_1 \frac{\partial H_i^0}{\partial T} \quad (3-31)$$

$$\frac{\partial h}{\partial T} = \frac{NCP}{x_1} \gamma_1 \left[ \frac{\partial H_i^0}{\partial T} + \frac{\partial H_{vap,i}}{\partial T} \right] \quad (3-32)$$

where:

$$\frac{\partial H_i^0}{\partial T} = (A_1 + B_1(T/100) + C_1(T/100)^2) \cdot \frac{V_M}{100} \\ = D_1 (100/T)^2 + \frac{V_M}{100} \quad (3-33)$$

$$\frac{\partial H_{vap,i}}{\partial T} = (BL_1 + 2CL_1 T) \cdot \gamma_1 \quad (3-34)$$

In the region of low acid gas loadings empirical corrections are added to the expressions for the activity coefficient,  $\gamma$ , and to the final expressions for the

partial pressures of liquid and vapor. The dependence of these corrections on liquid composition or temperature is expected to be slight and therefore no corrections are made to the partial derivatives.

## 4. APPLICATION of the Model (III)

### DESIGN OF AMINE UNITS

The intention of this chapter is to demonstrate how the computational model may be used in the design of contactors and regenerators. Four test problems, using both MEA and DEA as solvents, are presented and the results obtained with two different data correlations are given. Other uses of the model are indicated, with detailed attention being focussed on evaluating the relationship between the lean amine residuals of the acid gas components and the sweet gas  $H_2S$  composition. Finally, details are given of a method of predicting the vaporization efficiency of  $H_2S$  and  $CO_2$  in amine units.

#### 4.1 Test Problems

The following four problems are typical of amine contactors and regenerators operating in natural gas processing plants.

##### Example Problem No. 1 - MEA Contactor

The problem specifications and initial assumptions are as follows:

COMPOSITIONS OF ENTERING STREAMS

<u>Component</u>	<u>Sour Gas (moles/time)</u>	<u>Semilean Amine (moles/time)</u>	<u>Lean Amine (moles/time)</u>
H <sub>2</sub> S	18.7	54.3	1.28
CO <sub>2</sub>	2.95	6.3	1.57
MEA	-	250.0	62.05
Water	5.91	2550.0	630.0
Hydrogen	629.47	-	-
Nitrogen	29.53	-	-
Methane	781.55	-	-
Ethane	354.36	0.16	-
Propane	124.02	0.42	-
n-butane	1.97	-	-
i-butane	19.69	-	-

The sour gas is estimated over 10 total acid gas, and both lean and semilean amine streams are 25 weight percent. The lean amine contains 50 grains per gallon gr/gal of both H<sub>2</sub>S and CO<sub>2</sub>, while the semilean amine contains 2200 gr/gal H<sub>2</sub>S and 200 gr/gal CO<sub>2</sub>.

Number of ideal stages = 20

Feed temperatures:

Sour gas = 95°F

Semilean amine = 120°F

Lean amine = 100°F

Semilean amine enters stage 4.

Column pressure = 150 psia.

#### Initial Assumptions

<u>Stage No.</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/time)</u>
1	110	1960
2 + 20	120	1960

#### Example Problem No. 2 - DEA Contactor

This problem corresponds to medium pressure DEA contactors operating in Alberta. Specifications and initial assumptions are:

#### Compositions Of Entering Streams

<u>Component</u>	<u>Sour Gas (moles/day)</u>	<u>Semilean Amine (moles/day)</u>	<u>Lean Amine (moles/day)</u>
H <sub>2</sub> S	6948.0	290.5	36.3
CO <sub>2</sub>	868.4	140.25	28.1
DEA	-	8147.5	5415.0
H <sub>2</sub> O	-	154,650.0	70,260.0
methane*	21,130.6	-	-

\* because the relative compositions of the light hydrocarbon components were unknown, all such components were considered as methane for convenience.

These compositions correspond to 24% H<sub>2</sub>S and 3% CO<sub>2</sub> in the sour gas, a 31 weight percent DEA lean amine solution with 40 grains per gallon each of H<sub>2</sub>S and CO<sub>2</sub>, and a 23.6 weight percent DEA semilean amine solution, containing 160 grains per gallon H<sub>2</sub>S and 100 grains per gallon CO<sub>2</sub>. The flowrates of lean and semilean amine are respectively 150 and 300 gallons per minute.

Number of ideal stages = 4

Feed temperatures:

Sour gas = 100°F

Semilean amine = 145°F

Lean amine = 135°F

Semilean amine enters stage 2

Column pressure = 712 psia.

Initial Assumptions:

<u>Stage No.</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/day)</u>
1	135	21,131
2	140	21,131
3	145	21,131
4	150	21,131

Example Problem No. 3 - MEA Regenerator

The problem specifications and initial assumptions are:

Feed Composition

<u>Component</u>	<u>Feed (moles/time)</u>
H <sub>2</sub> S	1140.2
C <sub>2</sub> S	101.8
MEA	3220.0
H <sub>2</sub> O	32730.0
H <sub>2</sub>	0.67
N <sub>2</sub>	0.04
CH <sub>4</sub>	0.57
C <sub>2</sub> H <sub>6</sub>	0.32
C <sub>3</sub> H <sub>8</sub>	0.34

Number of ideal stages = 14

Feed stage number = 2

Feed conditions: temperature = 200°F

Pressure = 100 psia

Column pressure = 28 psia

Pressure drop per stage = 0.33 psia

Condenser: temperature = 120°F

Pressure = 27 psia

Reboiler duty = 114.11 MM BTU/time.

The rich amine is 25 weight percent MEA containing about 3650 gr/gal H<sub>2</sub>S and 250 gr/gal CO<sub>2</sub>. The reboiler duty corresponds to 1.3 lbs. of 55 psia steam per gallon of amine solution.

Initial Assumptions

<u>Stage No.</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/time)</u>
1	120	1140
2	230	3420
3	240	5000
4	242	5100
5	244	5200
6	246	5300
7	248	5400
8	250	5500
9	252	5600
10	254	5700
11	256	5800
12	258	5900
13	260	6000
14	262	6100

Estimated reflux ratio = 2.0.

Example Problem No. 4 - DEA Regenerator

The problem specifications and initial assumptions are:

<u>Component</u>	<u>Feed Composition</u>	<u>Feed (moles/time)</u>
H <sub>2</sub> S		37.82
CO <sub>2</sub>		123.71
DEA		290.88
H <sub>2</sub> O		6012.4
CH <sub>4</sub>		0.43
C <sub>2</sub> H <sub>6</sub>		0.03
C <sub>3</sub> H <sub>8</sub>		0.01

The DEA solution is 22 weight percent and the reboiler duty corresponds to approximately 1 lb. of 55 psia steam per gallon of amine solution.

Number of ideal stages = 14

Feed stage number = 2

Feed conditions: temperature = 180°F

Pressure = 48 psia

Column pressure = 27 psia

Pressure drop per stage = 0.33 psia

Condenser: temperature = 100°F

pressure = 25 psia

Reboiler duty

16.171 MM BTU/time

Vapourization efficiencies:

$$\left. \begin{array}{l} H_2S = 0.7 \\ CO_2 = 0.3 \end{array} \right\} \text{on all stages}$$

Initial Assumptions

<u>Stage No.</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/time)</u>
1	100	160
2	220	400
3	232	700
4	234	850
5	236	900
6	238	905
7	240	910
8	242	915
9	244	920
10	246	925
11	248	930
12	250	935
13	252	940
14	254	945

Estimated reflux ratio = 1.5

#### 4.2 Discussion of Test Problems

The detailed computer printouts for the test problems are found in Appendix 4. Two different data correlations were used for each problem:

(a) Nasir's<sup>35</sup> modification of the work of Klyamer et al.<sup>22</sup>

(b) the correlation supplied by AMOCO<sup>25</sup>

Table 2 lists a comparison of the number of iterations and CPU times required for each correlation. The computer used was an IBM 360/67. In general fewer iterations are needed when employing the AMOCO correlation, but more CPU seconds per iteration.

TABLE 2: NUMBER OF ITERATIONS AND CPU TIMES  
REQUIRED FOR TEST PROBLEMS FOR TWO  
DATA CORRELATIONS

CORRELATION USED ↓ PROBLEM →	NASIR		AMOCO	
	NO. OF ITERATIONS	CPU TIME (SECONDS)	NO. OF ITERATIONS	CPU TIME (SECONDS)
1 MEA Contactor	6	17.2	6	17.7
2 DEA Contactor	4	1.7	3	1.7
3 MEA Regenerator	6	6.8	5	8.3
4 DEA Regenerator	10	10.3	7	11.3

The latter is largely because in the AMOCO correlation a standard set of 18 components is used and this results in a number of redundant multiplications when any of the 18 are not present.

The different data correlations produce very different results. The comparative values of important design variables for each test problem are given in Table 3. It is obvious from the tabulated values that the results are highly sensitive to the data correlation used.

TABLE 3: COMPARISON OF THE VALUES OF  
IMPORTANT DESIGN VARIABLES.

PROBLEM	VARIABLE	NASIR	AMOCO
MEA Regenerator	Reflux ratio	1.87	1.79
	Moles H <sub>2</sub> S in lean amine	125.1	94.2
	Moles CO <sub>2</sub> in lean amine	59.3	84.3
DEA Regenerator	Reflux ratio	1.33	1.22
	Moles H <sub>2</sub> S in lean amine	2.69	0.47
	Moles CO <sub>2</sub> in lean amine	17.0	12.6
MEA Contactor	ppm H <sub>2</sub> S in sweet gas	10.14	15.82
	ppm CO <sub>2</sub> in sweet gas	0.09	0.22
DEA Contactor	ppm H <sub>2</sub> S in sweet gas	3.18*	1.57
	ppm CO <sub>2</sub> in sweet gas	0.40*	0.10

\* not using empirical corrections to K-ratios at low acid gas loadings.

Nasir's correlation<sup>36</sup> lies closer to published experimental curves than do the other three correlations referenced in this work<sup>21,22,25</sup>. However, his correlation exhibits a limitation at very low acid gas loadings. Namely, the empirical corrections used to force the predicted solubilities to follow the trend of experimental curves for conditions found in the base of the regenerator, encounter a discontinuity at  $x_{H_2S} = 0.0095$ . This is the reason the empirical corrections were not applied in the DEA contactor problem. The discontinuity problem will be encountered when very low partial pressures are achieved in the sweet gas, and particularly in medium and high pressure contactors.

For a given data correlation, the model can be used to determine optimal values of variables that are important cost-wise, particularly the reboiler load and the amine circulation rate.

The reboiler load must be adequate to reduce the quantity of acid gas components in the regenerated amine to acceptably low levels. In addition the entering temperature of the rich amine feed can affect the amount of heat required. Often a hotter feed may significantly lower the reboiler load. The reflux ratio is also dependent on the reboiler load and may be found to exceed the rule-of-thumb criterion of being between 1.0 and 3.0,

if too little, or too much, heat is supplied.

The amine circulation rate can be varied in order to obtain an acceptable  $H_2S$  level in the sweet gas. The option of using a semilean stream can also be investigated using the model. This involves both the composition and quantity, and the entering stage, of the stream. For example, if problem 1 is repeated with 4 ideal stages (using Nasir's model) and the semilean enters on stage 3, the sweet gas contains 14 ppm  $H_2S$ . If instead the semilean enters on stage 2, the sweet gas contains 66 ppm  $H_2S$ .

Incorporating the vapourization efficiencies changes the results obtained. Problem 4 was run twice with a reboiler load of 17.0 MM BTU, and with vapourization efficiencies on all stages of:

- (i) 1.0 for both  $H_2S$  and  $CO_2$
- (ii) 0.7 for  $H_2S$ , 0.3 for  $CO_2$

The calculated reflux ratios were respectively 0.95 and 1.70. In the ideal stage case 4.04 moles  $H_2S$  and 7.71 moles  $CO_2$  remained in the regenerated amine; for case (ii) there were 2.83 moles  $H_2S$  and 16.59 moles  $CO_2$ . The next section illustrates how important accurate estimation of these residuals is in reaching an acceptable  $H_2S$  level in the sweet gas.

Details of calculating vapourization efficiencies from fundamental rate data are considered in Section 4.4.

#### 4.3 Dependence of Sweet Gas H<sub>2</sub>S Composition on Lean Amine Residuals.

The model can be used to obtain information on the relationship between the lean amine residual compositions of H<sub>2</sub>S and CO<sub>2</sub> and the composition of H<sub>2</sub>S in the sweetened gas. Figure 3 shows the results of such an investigation utilizing the model developed by Nasir<sup>35</sup>. In the figure ppm H<sub>2</sub>S in the sweet gas is plotted against grains of H<sub>2</sub>S per gallon of circulating lean amine solution, at various loadings of CO<sub>2</sub> in the lean amine (gr/gal).

The contactor used in the study had the following specifications:

Number of ideal stages = 1

Feed temperatures:

sour gas = 100°F

lean amine = 110°F

Column pressure = 500 psia

The sour gas was 20 percent total acid gas and the acid gas loading in the rich amine was between 0.51 and 0.67 moles per mole of MEA. A 15.3 weight percent solution of MEA was used.

Various ratios of H<sub>2</sub>S:CO<sub>2</sub> in the sour gas feed were used; however for the contactor used the ppm H<sub>2</sub>S in the sweet gas was independent of this ratio at given H<sub>2</sub>S and

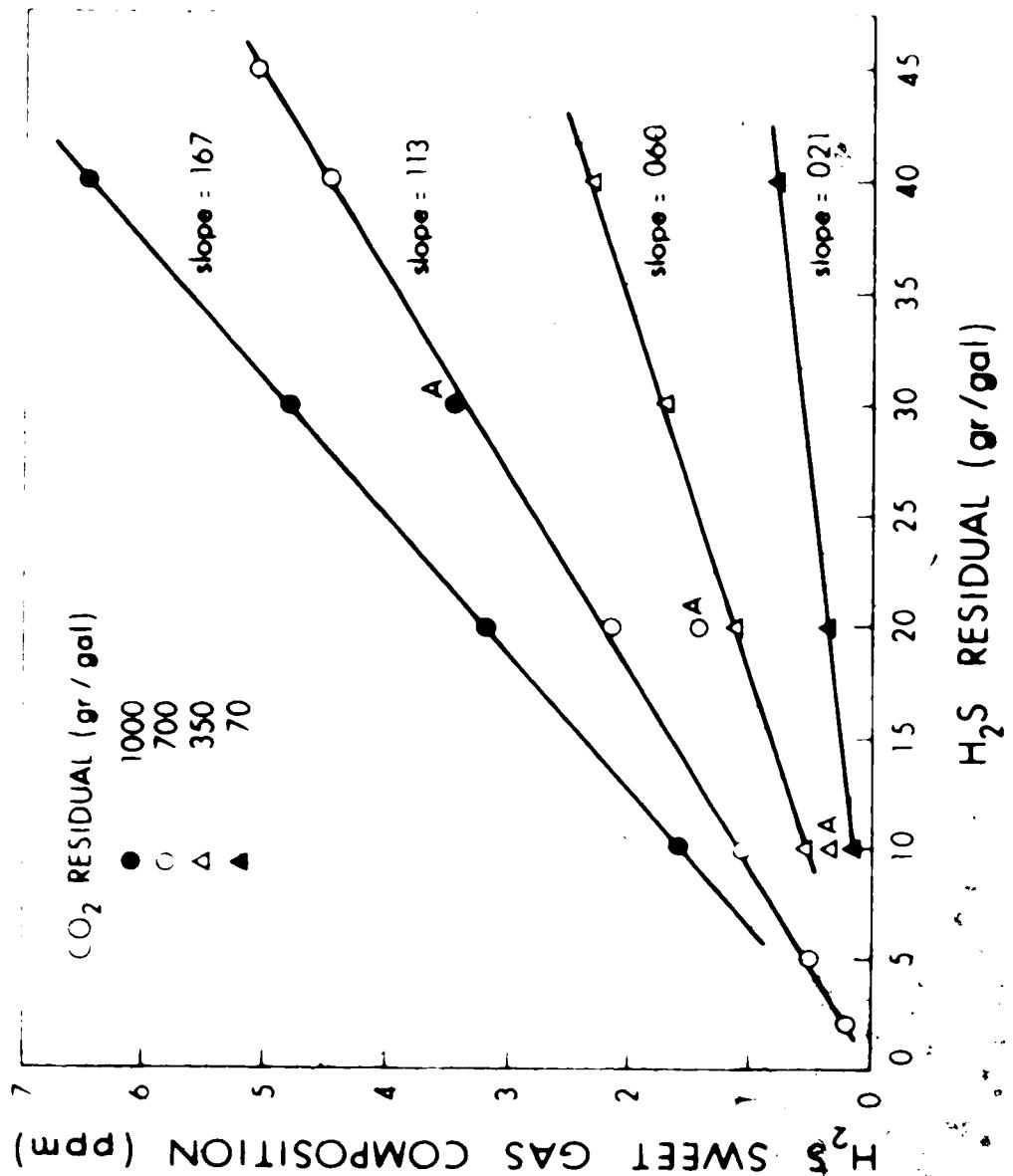


FIGURE 3: COMPOSITION OF  $\text{H}_2\text{S}$  IN SWEET GAS VERSUS  
 $\text{H}_2\text{S}$  LEAN AMINE FLOW (A)

$\text{CO}_2$  lean amine residual. This is evident because the number of ideal stages used is more than adequate. In terms of producing an overheadless sweetening system, the dependence of the  $\text{H}_2\text{S}$  sweet gas composition on the  $\text{H}_2\text{S}$  feed ratio could be determined by repeating the study with a column of fewer ideal stages, say 4 or less.

Four different  $\text{CO}_2$  residual concentrations were used. At a given value of  $\text{CO}_2$  residual, the amount of  $\text{H}_2\text{S}$  in the sweet gas increases linearly with  $\text{H}_2\text{S}$  residual. The presence of  $\text{CO}_2$  affects the degree to which  $\text{H}_2\text{S}$  may be absorbed. The slopes of the straight lines on Figure 3 increase approximately linearly with increasing  $\text{CO}_2$  residual. Thus stripping of the  $\text{CO}_2$  to a low level in the regenerator will facilitate  $\text{H}_2\text{S}$  absorption in the absorber.

In the design of a sweetening system, a prime concern is meeting the pipeline specifications on  $\text{H}_2\text{S}$  in the sweet gas. Knowing the sweetening system can absorb  $\text{H}_2\text{S}$  and  $\text{CO}_2$  simultaneously, the  $\text{H}_2\text{S}$  and  $\text{CO}_2$  residuals in the lean amine that will result in an acceptable level of  $\text{H}_2\text{S}$  in the product. The regenerator must then be designed so as to strip the lean amine to the required degree. This amounts to a multivariable problem because the  $\text{H}_2\text{S}$  and  $\text{CO}_2$  residuals are not independent<sup>30</sup>. According to the plot of Fitzgerald and Richardson<sup>9</sup> the usual range of interest would be  $\text{CO}_2$  residuals of 100

grains per gallon or greater, for feed ratios less than 3 moles of H<sub>2</sub>S per mole of CO<sub>2</sub>. This corresponds to the upper lines in Figure 3. For a reasonable stripper design, the same authors indicate that H<sub>2</sub>S would be stripped to a residual of less than 40 grains per gallon except in cases where the sour gas feed is predominantly H<sub>2</sub>S.

The actual positioning of the points on Figure 3 depends on the equilibrium data correlation employed. To illustrate this, three of the runs were duplicated using the AMOCO correlation. The points are marked with an 'A', and it is seen that the predicted H<sub>2</sub>S compositions in the sweet gas are lower than those given by the other correlation. However, neither correlation can claim greater accuracy than the other as the region covered by Figure 3 lies outside the range of any hitherto published data. For both data correlations the predicted solubilities are therefore an extrapolation of trends in the region of higher H<sub>2</sub>S loadings. Experimental data in the region of very low H<sub>2</sub>S loadings, that is down to 0.01 moles/mole amine or lower, would allow a more accurate evaluation of the dependence of the sweet gas H<sub>2</sub>S composition on the lean amine residuals.

#### 4.4 Prediction of Stage Efficiencies

The stage efficiencies for H<sub>2</sub>S and CO<sub>2</sub> are

calculated from equation (2-11). Of the variables in this equation, the overall mass transfer coefficient,  $K_{OG}^a$ , is the only one not trivially obtained from the current values of the stage variables. For  $\text{CO}_2$   $K_{OG}^a$  will be estimated directly from equation (2-14), which is a general correlation for bubble cap trays given by Kohl and Riesenfeld<sup>24</sup>.  $K_{OG}^a$  for  $\text{H}_2\text{S}$  will be estimated from equation (2-12); thus estimates are required for  $k_g^a$ ,  $k_L^O$ ,  $a$  and  $I$ . Values of the individual phase mass transfer coefficients and interfacial area per volume of plate are estimated via the following formulae given by Danckwerts<sup>7</sup> for bubble cap plates

$$k_g^a = 7 u^{0.25} s^{-0.5} D_g^{0.5} \quad (4-1)$$

$$k_L^O = 11 u^{0.25} s^{-0.5} D_A^{0.5} \quad (4-2)$$

$$I = 0.7 + 0.001833 \quad (4-3)$$

where:  $D_g$  is the diffusivity of  $\text{H}_2\text{S}$  in the gas phase  $\text{cm}^2/\text{s}$ , and can be estimated as given in Treybal<sup>43</sup>

$D_A$  = diffusivity of  $\text{H}_2\text{S}$  in the liquid phase  
( $\text{cm}^2/\text{s}$ )

$u$  = volumetric gas flow rate per unit area of plate ( $\text{cm}/\text{s}$ )

$s$  = volume of liquid on plate per unit area of plate ( $\text{cm}^3/\text{cm}^2$ )

$a''$  = interfacial area per unit area of plate

$$(\text{cm}^2/\text{cm}^2)$$

$k_G$ ,  $k_L^0$  have units of  $\text{cm/s}$ .

The column diameter can be estimated from charts given by Maddox<sup>30</sup>, thus giving the cross-sectional area. The average depth of liquid on the plate,  $z_T$ , can be calculated using standard design techniques<sup>31</sup>. Knowing this enables  $S$  in equations (4-1) to (4-3) above to be calculated. Then the interfacial area per volume of plate is:

$$a = a''/z_T \quad (4-4)$$

Finally  $k_G a$  is given from  $k_G^0$  by the equation

$$k_G a = \frac{k_G^0 a}{RT} \quad (4-5)$$

The enhancement factor  $I$  is estimated from equation (2-1).

#### 4.4.1 CO<sub>2</sub> Stage Efficiency

The various terms in equation (2-14) are calculated as follows:

- (i) Data on the viscosity of amine solutions<sup>11</sup> was approximately curvefitted by the equation:

$$\ln \mu = 0.96 + 0.036(\text{wt} - 0.10) - 0.011T \quad (4-6)$$

where  $\rho_L$  is in gm/cm<sup>3</sup>

wt = weight fraction of amine

T = temperature (°F)

(ii) The values of  $x_{CO_2}$ , T and  $\rho_L$  are given by the current values of the stage variables.

(iii)  $z_T$  is known from Section 4.4, and V can be calculated from the molar flowrate and cross-sectional area.

#### 4.4.2 H<sub>2</sub>S Stage Efficiency

The bulk phase concentration of free amine can be calculated as follows. The concentration of amine at the top of the absorber is given by:

$$[RNH_2]_{top} = 1000 \rho_L (z_3 - 2z_2 - z_1) / XM_{av} \quad (4-7)$$

where:  $z_1$ ,  $z_2$ ,  $z_3$  are respectively the quantities of H<sub>2</sub>S, CO<sub>2</sub> and MEA in the lean amine (mole/mole solution).

$XM_{av}$  is the average molecular weight of the lean amine (g/gmole).

$\rho_L$  is the density of the amine solution (g/cm<sup>3</sup>), and is given approximately by equation (4-8).

$$\begin{aligned} \rho_L &= 1.002 + .052(wt - .10) - .000278(T-68) \\ &+ .001(6 - 20 wt)(T-68)^{0.5} \end{aligned} \quad (4-8)$$

where  $w_t$  and  $T$  are the same as in equation (4-6).

The amount of  $\text{CO}_2$  absorbed above plate  $j$  in the column is given by:

$$(\text{CO}_2)_{\text{abs}} = \frac{1000 \rho_L}{X M_{\text{av}}} \left\{ \frac{V_j}{L_j} Y_{2,j} - \frac{V_1}{L_1} Y_{2,1} \right\} \quad (4-9)$$

Similarly the quantity of  $\text{H}_2\text{S}$  absorbed above plate  $j$  can be calculated. Then, as two moles of amine react with one mole of  $\text{CO}_2$ , the concentration of free amine in solution on plate  $j$  is:

$$[\text{RNH}_2]_j = [\text{RNH}_2]_{\text{top}} - 2 \cdot (\text{CO}_2)_{\text{abs}} - (\text{H}_2\text{S})_{\text{abs}} \quad (4.10)$$

It is necessary to iterate to determine the value of  $K_{OG}^a$  because the interfacial partial pressure is unknown, yet the enhancement factor and hence  $K_{OG}^a$  depend on it.

The iterative procedure is as follows:

- (i) Assume the interfacial partial pressure,  $P_{int}$ .
- (ii) Calculate  $I$  from equation (2-15). The solubilities  $C_{O,1}$  and  $C_{O,2}$  are obtained from a Henry's Law expression and the bulk phase concentration of amine is given by equation (4-10).
- (iii) Calculate  $K_{OG}^a$  from equation (2-12).



(iv) Calculate the mean rate of absorption of  $\text{H}_2\text{S}$  as

$$\bar{V}_a = k_{OG}^a \cdot p_{\text{H}_2\text{S}} \quad (4-11)$$

(v) Calculate the actual interfacial partial pressure as

$$p_{int} = p_{\text{H}_2\text{S}} - \frac{\bar{V}_a}{k_q^a} \quad (4-12)$$

(vi) Repeat steps (i) to (v) until a constant value of  $\bar{V}_a$  is achieved.

#### 4.4.3 Example Problem No. 5

Example problem I was used, with 8 stages and the inclusion of the above methods to calculate vapourization efficiencies for  $\text{H}_2\text{S}$  and  $\text{CO}_2$ . All other efficiencies were set equal to unity. The physical parameters required for the problem are as follows:

$$\begin{array}{ll} \text{Diffusivities} & \\ \text{H}_2\text{S} & 1.2 \\ \text{CO}_2 & 1.4 \\ \text{MEA} & 0.77 \end{array} \left. \right\} \times 10^{-5} (\text{cm}^2/\text{s})$$

$$\begin{aligned} \text{For } \text{H}_2\text{S absorption} & - k_L^O = .033 \text{ cm/s} \\ k_q^a & = 1.0 \times 10^{-6} \text{ g mole/cm}^3 \text{ atm.s} \end{aligned}$$

$$\begin{aligned} a & = 4.3 \text{ cm}^2 \text{ interfacial} \\ & \text{area/cm}^3 \text{ liquid} \end{aligned}$$

$$\text{Column cross-sectional area} = 6900 \text{ cm}^2$$

$$\text{Average depth of liquid on a stage} = 13 \text{ cm}$$

The computer printout for the example is given in Appendix 4.9. The vapourization efficiencies display a definite trend down the column for both  $\text{CO}_2$  and  $\text{H}_2\text{S}$ . They increase between the top stage and the stage on which the semilean amine is introduced, and then display the same trend between the semilean amine feed stage and the bottom.

The efficiencies are much greater than unity on a number of stages, and particularly so for  $\text{CO}_2$ . These numbers may be more familiarly represented by backing out the Murphree vapour efficiencies using the equation derived as follows. The Murphree efficiency is defined as:

$$E_{MVi,j} = \frac{y_{i,j} - y_{i,j+1}}{K_{i,j} x_{i,j} - y_{i,j+1}} \quad (4-13)$$

Substituting for  $K_{i,j} x_{i,j}$  from equation (3-1), that is,  $K_{i,j} x_{i,j} = y_{i,j}/e_{i,j}$  (4-14)

and rearranging, yields

$$E_{MVi,j} = \frac{e_{i,j} \left( \frac{y_{i,j+1}}{y_{i,j}} - 1 \right)}{\left( e_{i,j} \frac{y_{i,j+1}}{y_{i,j}} \right) - 1} \quad (4-15)$$

Table 4 details the Murphree efficiencies for each stage in the column. The values show selective absorption of  $\text{H}_2\text{S}$  over  $\text{CO}_2$  below the semilean feed tray, and in magnitude the efficiencies agree with the rule of thumb values.

of 0.8 for  $H_2S$  and 0.3 for  $CO_2$ . To illustrate the difference between calculating the efficiencies and using ideal stages, the same problem was run with 4 ideal stages, with

TABLE 4: MURPHREE EFFICIENCIES AS CALCULATED  
FROM VAPOURIZATION EFFICIENCIES

Stage	1	2	3	4	5	6	7	8
$H_2S$	0.92	0.84	1.03	0.89	0.84	0.83	0.82	0.82
$CO_2$	1.00	0.96	0.26	0.36	0.36	0.35	0.35	0.33

the semilean amine feeding to stage 3. In the 8-tray case the sweet gas contained 32 ppm  $H_2S$ , while 4 ideal trays reduced the  $H_2S$  to only 14 ppm in the sweet gas. A further distinction between "real" and ideal stages is that absorption occurs over a larger number of trays in the former case than in the latter. This produces a more slowly variant vapour profile up the column for calculations incorporating vapourization efficiencies.

## 5. A GENERAL ALGORITHM FOR SOLVING MULTICOLUMN SYSTEMS.

### 5.1 Model Equations

A general network of columns may be considered a system of columns in which any stage may have, in addition to an external feed stream, one or more feed streams which originated at another stage in the network. Thus any stage in the general network is represented by Figure 4. There are four possible types of interconnected stream, namely a liquid side stream, vapour side stream, bottoms liquid product stream or top vapour product stream. For convenience in the following discussion, the bottom stage of a column in the system will be subscripted with the symbol NB, and the top stage with the symbol NT.

Equations (3-1), (3-3), (3-4), (3-5) and (3-6) represent the model equations for a single column. In a general network of columns, the material and energy balance equations for a stage must be modified to include the sum of the contributions from interconnected streams entering that stage. That is, equations (3-6), (3-3) and (3-5) for stage  $j$  and component  $i$  become as follows:

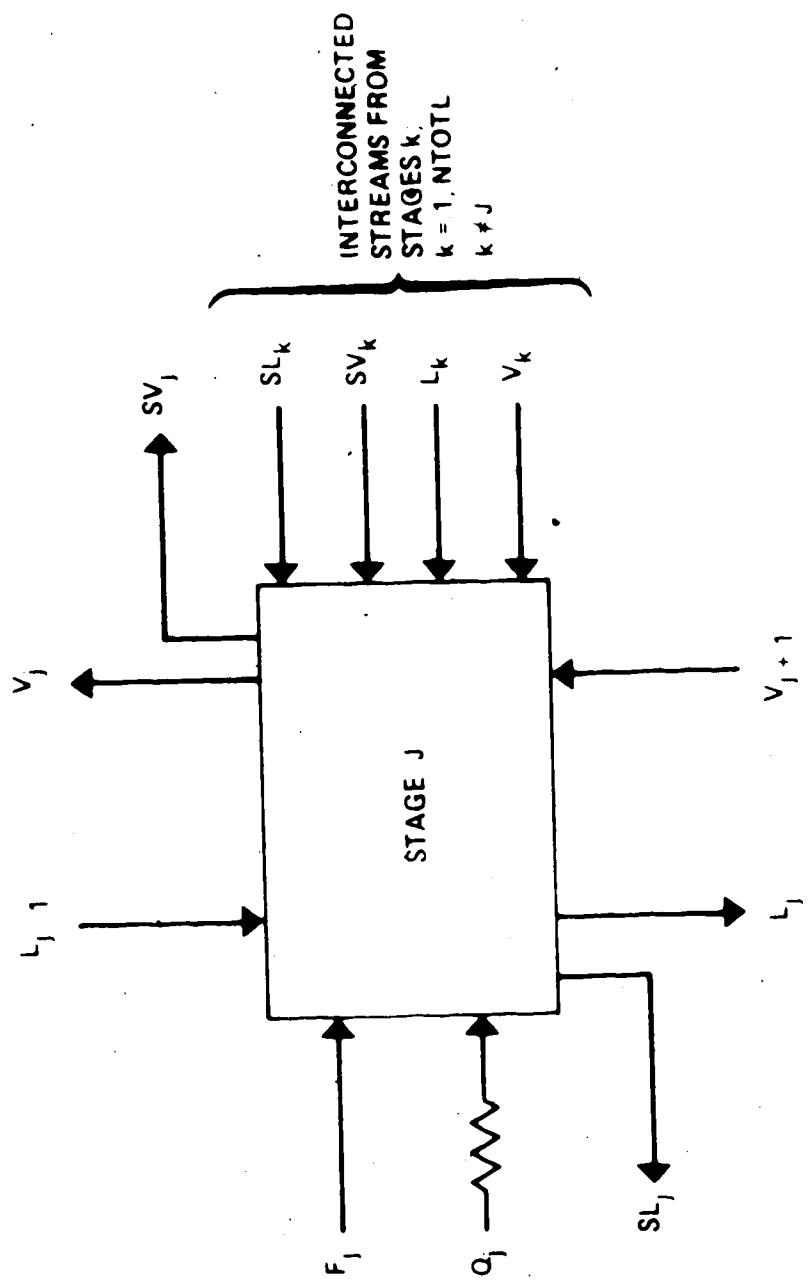


FIGURE 4: GENERAL STAGE IN A MULTICOLUMN SYSTEM

### Component Material Balance

$$\begin{aligned}
 F_j z_{i,j} + L_{j-1} x_{i,j+1} + V_{j+1} e_{i,j+1} K_{i,j+1} x_{i,j+1} \\
 - (L_j + S L_j) x_{i,j} - (V_j + S V_j) e_{i,j} K_{i,j} x_{i,j} \\
 + c_{i,k} - c_{i,j} \quad (5-1)
 \end{aligned}$$

$1 \leq i \leq NCP, \quad 1 \leq j \leq NTOTL$

### Energy Balance

$$\begin{aligned}
 F_j H_{F,j} + Q_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1} - (L_j + S L_j) h_j \\
 - (V_j + S V_j) H_j + \sum_k c_{F,k} E_j \quad (5-2)
 \end{aligned}$$

$1 \leq j \leq NTOTL$

### Overall Material Balance

$$\begin{aligned}
 F_j + L_{j-1} + V_{j+1} - (L_j + S L_j) - (V_j + S V_j) \\
 + \sum_k c_{M,k} M_j \quad (5-3)
 \end{aligned}$$

$1 \leq j \leq NTOTL$

where for the various types of interconnected stream,  $c_{i,k}$ ,  $E_j$  and  $M_j$  are as given in Table 5, with  $k$  denoting the leaving stage of a particular stream. The

phase relation and summation equations remain the same as (3-1) and (3-4).

TABLE 5: CONTRIBUTION OF INTERLINKED STREAMS TO MATERIAL AND ENERGY BALANCE EQUATIONS.

Type of Stream	$\sum_{i=1}^n x_{i,k}$	$\sum_{i=1}^n x_{i,k} h_k$	$\sum_{i=1}^n M_i k$
Liquid side stream	$SL_k x_{1,k}$	$SL_k h_k$	$SL_k$
Vapour side stream	$SV_k e_{1,k} K_{1,k} x_{1,k}$	$SV_k h_k$	$SV_k$
Liquid product	$L_k x_{1,k}$	$L_k h_k$	$L_k$
Vapour product	$V_k e_{1,k} K_{1,k} x_{1,k}$	$V_k h_k$	$V_k$

The summation in equations (5-1) to (5-3) indicates the possibility of more than one interconnected stream entering stage  $j$ .

#### Linearized Equations

The equations are written for each stage in the interconnected system of columns, and then linearized using the same procedure as for individual columns. The linearized equations are:

Component Material Balance:

$$\begin{aligned}
 L_{i-1} \cdot x_{i,j-1} &= \left[ (L_j + S L_{j-1}) + (V_j + S V_{j-1}) e_{i,j-1} \left( \frac{K_{i,j-1}}{x_{i,j-1}} + \frac{x_{i,j-1}}{x_{i,j-1}} \right) \right] \cdot x_{i,j-1} \\
 &+ V_{j+1} e_{i,j+1} \left( \frac{K_{i,j+1}}{x_{i,j+1}} + \frac{x_{i,j+1}}{x_{i,j+1}} \right) \cdot x_{i,j+1} \\
 &+ \sum_k c_{i,j,k} \cdot x_{i,k} = V_{j+1} \cdot \frac{N}{k} \cdot \frac{x_{i,j+1}}{x_{i,j+1}} \cdot x_{i,j+1} \\
 &+ V_{j+1} e_{i,j+1} \cdot x_{i,j+1} \cdot \frac{F_{i,j+1}}{T_{i,j+1}} \cdot T_{j+1} + \sum_k c_{i,j,k} \cdot F_k \\
 &+ x_{i,j-1} \cdot (L_{i-1} - x_{i,j-1}) = Y_{i,j-1} \cdot N \\
 &+ V_{i,j+1} \cdot N = \sum_k c_{i,j,k} \quad (5-4)
 \end{aligned}$$

$N = J - NT$

$$\begin{aligned}
 &+ (L_{NT} + S L_{NT}) + V_{NT} e_{i,NT} \left( \frac{K_{i,NT}}{x_{i,NT}} + \frac{x_{i,NT}}{x_{i,NT}} \right) \cdot x_{i,NT} \\
 &+ V_{NT+1} e_{i,NT+1} \left( \frac{K_{i,NT+1}}{x_{i,NT+1}} + \frac{x_{i,NT+1}}{x_{i,NT+1}} \right) \cdot x_{i,NT+1} \\
 &+ \sum_k c_{i,NT,k} \cdot x_{i,k} = V_{NT} \cdot \frac{N}{k} \cdot \frac{x_{i,NT}}{x_{i,NT}} \cdot T_{NT} \\
 &+ V_{NT+1} e_{i,NT+1} \cdot x_{i,NT+1} \cdot \frac{F_{i,NT+1}}{T_{i,NT+1}} \cdot T_{NT+1} \\
 &+ \sum_k c_{i,NT,k} \cdot T_k = x_{i,NT} \cdot (L_{NT} - Y_{i,NT}) \cdot N = Y_{i,NT} \cdot N + V_{NT+1} \cdot N \\
 &+ \sum_k c_{i,NT,k} = -c_{i,NT} \quad (5-4-a)
 \end{aligned}$$

$\Delta t = J - NB$

$$\begin{aligned}
 L_{NB-1} \Delta x_{1,NB-1} &= [I_{NB} + (V_{NB} + SV_{NB}) e_{1,NB}^T F_{1,NB} + (e_{1,NB}^T \Delta x_{1,NB}) I_{NB}^{-1}] \Delta x_{1,NB} \\
 &\quad + \sum_k e_{k+1,NB-1} \Delta x_{1,k} \\
 &\quad + (V_{NB} + SV_{NB}) e_{1,NB}^T e_{1,NB}^{-1} \Delta x_{1,NB} \\
 &\quad + \sum_k e_{k+1,NB-1} \Delta x_{1,k} - V_{NB} \Delta x_{1,NB} \\
 &\quad + \sum_k e_{k+1,NB-1} \Delta x_{1,k} = -V_{1,NB} \Delta x_{1,NB} \quad (5-4-b)
 \end{aligned}$$

### Energy Balance

$$\begin{aligned}
 L_{j-1} \frac{\Delta h_{j-1}}{\Delta T_{j-1}} + T_{j-1} &= [(L_j + SL_j) \frac{\Delta h_j}{\Delta T_j} + (V_j + SV_j) \frac{\Delta h_j}{\Delta T_j} + P_j \\
 &\quad + V_{j+1} \frac{\Delta h_{j+1}}{\Delta T_{j+1}} + T_{j+1} + \sum_k e_{k+1,NB-1} \Delta T_k + h_{j-1} \Delta L_{j-1} \\
 &\quad - H_{j-1} \Delta E_{j-1} - H_j \Delta V_j + \sum_k e_{k+1,NB-1} \Delta V_{k+1} + \sum_k e_{k+1,NB-1} \Delta E_k] = -E_j \quad (5-5)
 \end{aligned}$$

$\Delta t = J - NT$

$$\begin{aligned}
 &= [(L_{NT} + SL_{NT}) \frac{\Delta h_{NT}}{\Delta T_{NT}} + V_{NT} \frac{\Delta h_{NT}}{\Delta T_{NT}} + P_{NT} \\
 &\quad + V_{NT+1} \frac{\Delta h_{NT+1}}{\Delta T_{NT+1}} + T_{NT+1} + \sum_k e_{k+1,NB-1} \Delta T_k - h_{NT} \Delta L_{NT} - H_{NT} \Delta V_{NT} \\
 &\quad + H_{NT+1} \Delta V_{NT+1} + \sum_k e_{k+1,NB-1} \Delta E_k + Q_{NT} = -E_{NT} \quad (5-5-a)
 \end{aligned}$$

where  $\psi_{NT} = 0$  for an absorber or reboiled absorber.

At  $J = NT$

$$L_{NB-1} \frac{h_{NB-1}}{\psi_{NT-1}} = V_{NB-1} + L_{NB} \frac{h_{NB}}{\psi_{NB}} + (V_{NB} + S V_{NB}) \frac{h_{NB}}{\psi_{NB}} \psi_{NB} \quad (5-5-a)$$

$$\psi_{NB} (\psi_{NB} + h_{NB-1}) L_{NB-1} = h_{NB} L_{NB} = h_{NB} \sum_k M_{k,NB} + \sum_k E_{k,NB} \quad (5-5-b)$$

where  $\psi_{NB} = 0$  for an absorber.

### Overall Material Balance

$$L_{J-1} = L_J = M_J + M_{J+1} + \sum_k M_{k,J} = -M_J \quad (5-6)$$

At  $J = NT$

$$L_{NT} = V_{NT} + V_{NT+1} + \sum_k M_{k,NT} = -M_{NT} \quad (5-6-a)$$

At  $J = NB$

$$L_{NB-1} = L_{NB} = M_{NB} + \sum_k M_{k,NB} = -M_{NB} \quad (5-6-b)$$

The terms in  $\psi$ ,  $\alpha$  and  $\beta$  in equations (5-4) to (5-6) arise from the presence of interconnected streams. For example, the terms  $\psi_{c,i,k}$  in equation (5-1) give rise to the terms  $\psi_{c,i,k}$ ,  $\alpha_{c,k}$  and  $\beta_{c,k}$  in equation (5-4).

TABLE 6: EQUATIONS IN LINEARIZING EQUATIONS ARISING  
FROM INTERCONNECTED STREAMS

Type of Stream	$\frac{dC_{1,k}}{dt}$	$\frac{dC_{2,k}}{dt}$	$\frac{dE_{1,k}}{dt}$	$\frac{dE_{2,k}}{dt}$
Liquid side stream	0	0	$\frac{\partial h_k}{\partial T_k}$	0
Vapour side stream	$SV_k \frac{\partial e_{1,k}}{\partial x_{1,k}}$	$SV_k \frac{\partial e_{1,k}}{\partial x_{1,k}} x_{1,k} \frac{\partial k_{1,k}}{\partial T_k}$	$SV_k \frac{\partial h_k}{\partial T_k}$	0
Liquid product	0	$x_{1,k} \frac{\partial h_k}{\partial T_k}$	$x_{1,k} \frac{\partial h_k}{\partial T_k}$	$x_{1,k} \frac{\partial h_k}{\partial T_k} L_k$
Vapour Product	$v_k \frac{\partial e_{1,k}}{\partial x_{1,k}}$	$v_k \frac{\partial e_{1,k}}{\partial x_{1,k}} x_{1,k} \frac{\partial v_k}{\partial T_k}$	$v_k \frac{\partial h_k}{\partial T_k} x_{1,k} \Delta V_k$	$H_k \Delta V_k$

- A summary of the values of  $c_{i,k}$ ,  $c_{e,k}$ ,  $c_{v,k}$ ,  $F_{e,k}$ ,  $F_{v,k}$  and  $M_{e,k}$  for each possible type of interconnected stream is given in Table 6.

### 5.3 Matrix Forms

In the model for single columns, the matrix form of the linearized equations contains a number of tridiagonal matrices. In particular, the coefficient matrices of  $\bar{A}x_i$  (liquid composition corrections) in the component material balance equations and of  $\bar{\Delta T}$  (temperature corrections) in the energy balance are tridiagonal. The ease of inversion of these matrices facilitates the formulation of a solution.

The linearized equations for a multicol column system (equations (5-4) to (5-6)) may also be represented in matrix form as follows:

$$\bar{A}_i \bar{x}_i + \bar{B}_i \bar{\Delta T} + \bar{D}_i \bar{W} + \bar{F}_i \bar{L} = \bar{C}_i$$

$1 \leq i \leq NCP \quad (5-7)$

$$\bar{P} \bar{\Delta T} + \bar{Q} \bar{W} + \bar{R} \bar{L} = \bar{E} \quad (5-8)$$

$$\bar{G} \bar{W} + \bar{H} \bar{L} = \bar{M} \quad (5-9)$$

However, in this case the presence of interconnected streams introduces off-tridiagonal elements into the

matrices, in particular the coefficient matrices discussed above. Thus, a non-trivial extension of the algorithm used to solve single column systems is required.

The detailed form of the matrices is more clearly understood by considering a particular network of columns, say that shown in Figure 5. The example system consists of three columns, each having 20 stages. There are four interconnected streams:

- (1) a vapour product stream from the top stage of column I to stage 5 of column II
- (2) a bottoms liquid product stream from stage 20 of column I to stage 1 of column III
- (3) a liquid side stream from stage 14 of column II to stage 9 of column III
- (4) a vapour side stream from stage 3 of column III to stage 12 of column I.

In general each coefficient matrix in equations (5-7), (5-8) and (5-9) has the form of the matrix shown in Figure 6. The matrix is basically block tridiagonal, with one diagonal block per separation device. Let the devices in the system be labelled I, II and III, and label the blocks in Figure 6 in the same fashion as elements of a matrix. Then off-tridiagonal elements, arising from the interconnected streams, appear as follows.

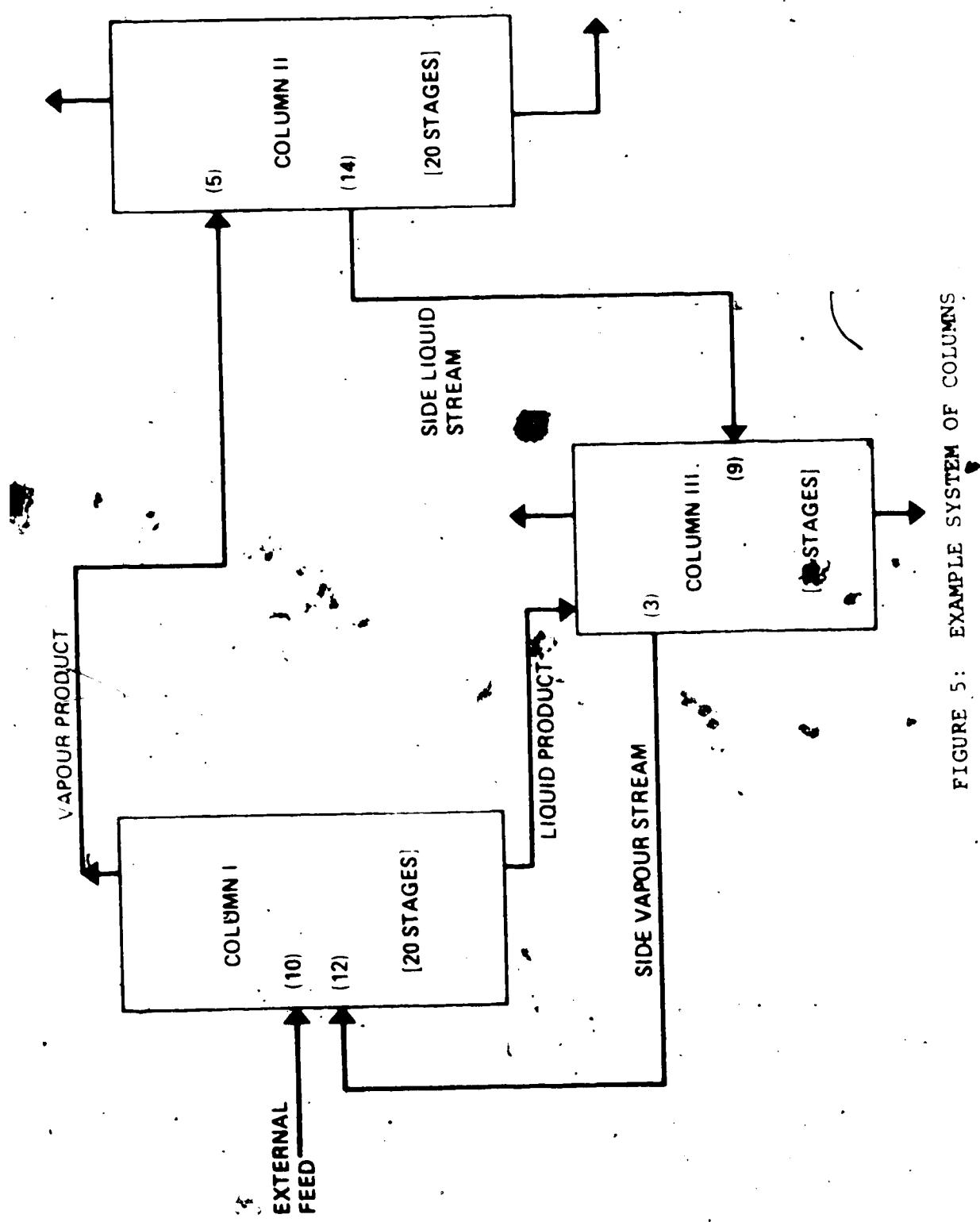


FIGURE 5 : EXAMPLE SYSTEM OF COLUMNS

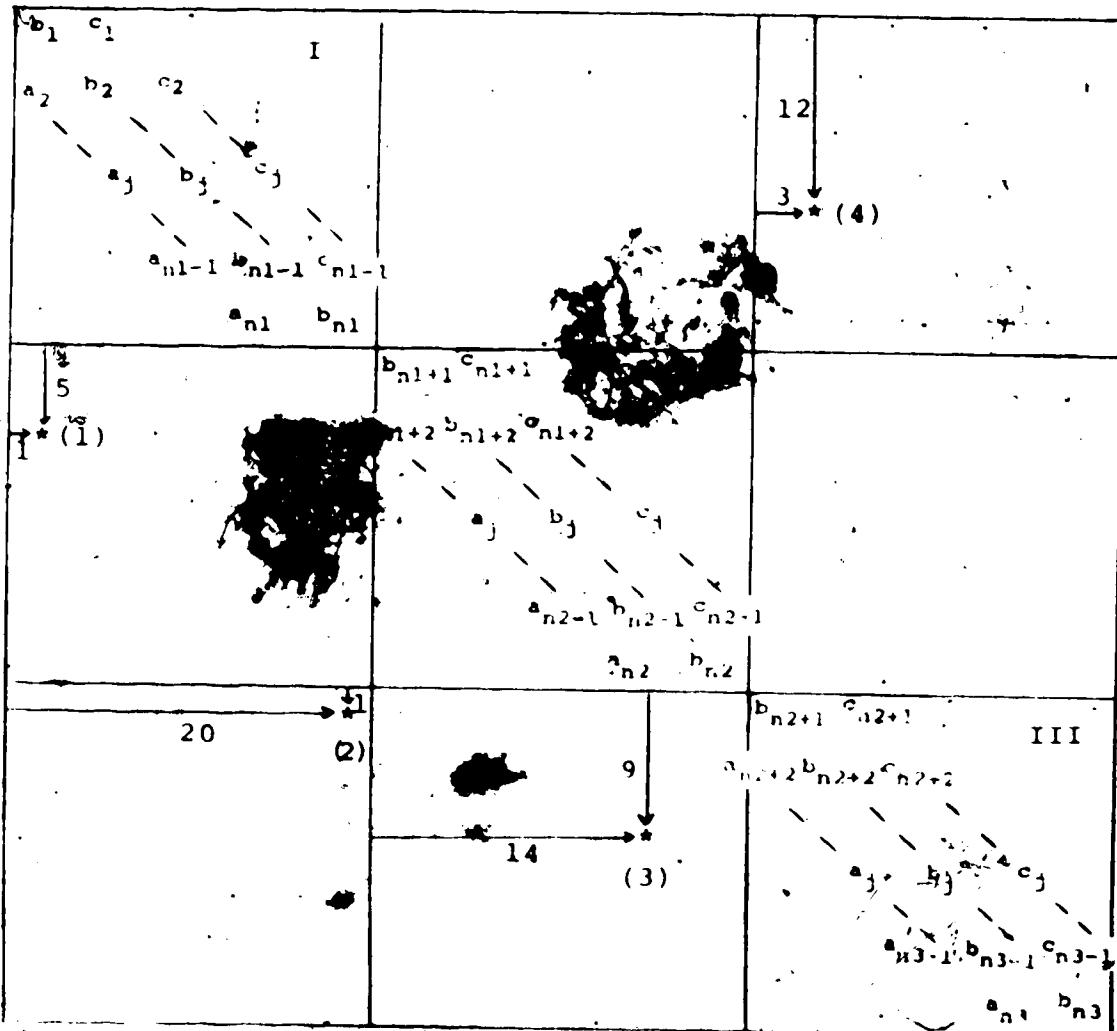


FIGURE 6: GENERAL MATRIX FORM

If an interconnected stream goes from device III to device I, the appropriate off-tridiagonal element appears in block (I,III). The exact position of the element is given by the entering and leaving stages. For example, for stream (4) above it is at position (12,3) inside block (I,III). Other off-tridiagonal elements may occupy the positions indicated on Figure 6. A given off-tridiagonal position in the matrix will represent a unique interconnected stream. Also note that theoretically an off-tridiagonal element could appear in one of the diagonal blocks. This would correspond to a connected stream going between different stages of the same device and is not likely to occur in practice.

Depending on the type of interconnected stream, some off-tridiagonal elements in the coefficient matrices may be zero (see Table 6). For interconnected streams (1) to (4) given above, Table 7 lists which streams will contribute a non-zero element. The value of these non-zero elements can be read off Table 6.

TABLE 3: ~~NON-ZERO OFF-TRIDIAGONAL ELEMENTS~~  
IN EACH COEFFICIENT MATRIX.

<u>Equation</u>	<u><math>\bar{A}x_i</math></u>	Coefficient of:		
		<u><math>\bar{A}T</math></u>	<u><math>\bar{A}V</math></u>	<u><math>\bar{A}L</math></u>
component material balance	1, 2, 3, 4	1, 4	1	2
energy balance	na	1, 2, 3, 4	1	2
overall material balance	na	na	1	2
	na	not applicable		

In each diagonal block the elements  $a_j$ ,  $b_j$  and  $c_j$  will be the same as for a single separation device. Thus, these elements are as follows for the various coefficient matrices in equations (5-7), (5-8) and (5-9).

(1) Matrix  $\bar{A}_i$

$$a_{NT} = 0$$

$$b_{NT} = -(L_{NT} + S_{NT}) - V_{NT} e_{i,NT} (K_{i,NT} + x_{i,NT} \frac{\partial K_{i,NT}}{\partial x_{i,NT}})$$

$$c_{NT} = V_{NT+1} e_{i,NT+1} (K_{i,NT+1} + x_{i,NT+1} \frac{\partial K_{i,NT+1}}{\partial x_{i,NT+1}})$$

$$a_j = L_{j-1}$$

$$b_j = -(L_j + S L_j) - (V_j + SV_j) e_{i,j}^{(K_{i,j} + x_{i,j} \frac{\partial K_{i,j}}{\partial x_{i,j}})}$$

$$c_j = V_{j+1} e_{i,j+1}^{(K_{i,j+1} + x_{i,j+1} \frac{\partial K_{i,j+1}}{\partial x_{i,j+1}})}$$

$j = NT+1 \dots NB-1$

$$a_{NB} = L_{NB-1}$$

$$b_{NB} = -L_{NB} - (V_{NB} + SV_{NB}) e_{i,NB}^{(K_{i,NB} + x_{i,NB} \frac{\partial K_{i,NB}}{\partial x_{i,NB}})}$$

$$a_{NT} = 0$$

(2) ~~matrix B<sub>i</sub>~~

$$a_{NT} = 0$$

$$b_{NT} = -V_{NT} e_{i,NT} x_{i,NT} \frac{\partial K_{i,NT}}{\partial T_{NT}}$$

$$c_{NT} = V_{NT+1} e_{i,NT+1} x_{i,NT+1} \frac{\partial K_{i,NT+1}}{\partial T_{NT+1}}$$

$$a_j = 0$$

$$b_j = -(\nabla_j + SV_j) e_{i,j} x_{i,j} \frac{\partial K_{i,j}}{\partial T_j}$$

$$c_j = V_{j+1} e_{i,j+1} x_{i,j+1} \frac{\partial K_{i,j+1}}{\partial T_{j+1}}$$

$j = NT+1 \dots NB-1$

$$a_{NB} = 0$$

$$b_{NB} = -(v_{NB} + \beta v_{NB}) - c_{1,NB} - x_{1,NB} - t_{NB},$$

$$c_{NB} = 0$$

(3) Matrix D<sub>i</sub>

$$a_j = 0$$

$$b_j = -y_{i,j}$$

$$c_j = y_{i,j+1}$$

$$a_{NB} = 0$$

$$b_{NB} = y_{i,NB}$$

$$c_{NB} = 0$$

(4) Matrix F<sub>i</sub>

$$\left. a_{NT} = 0 \right\}$$

$$b_{NT} = -x_{i,NT}$$

$$c_{NT} = 0$$

$$a_j = x_{i,j-1}$$

$$b_j = -x_{i,j}$$

$$c_j = 0$$

$i = NT+1 \dots NB$

### (5) Matrix P

$$a_{NT} = 0$$

$$b_{NT} = -[(L_{NT} + SL_{NT}) \frac{\partial h_{NT}}{\partial T_{NT}} + (V_{NT} + SV_{NT}) \frac{\partial h_{NT}}{\partial T_{NT}}]$$

$$c_{NT} = V_{NT+1} \frac{\partial h_{NT+1}}{\partial T_{NT+1}}$$

$$a_j = L_{j-1} \frac{\partial h_{j-1}}{\partial T_{j-1}}$$

$$b_j = -[(L_j + SL_j) \frac{\partial h_j}{\partial T_j} + (V_j + SV_j) \frac{\partial h_j}{\partial T_j}]$$

$$c_j = V_{j+1} \frac{\partial h_{j+1}}{\partial T_{j+1}}$$

$j = NT+1 \dots NB-1$

$$a_{NB} = L_{NB-1} \frac{\partial h_{NB-1}}{\partial T_{NB-1}}$$

$$b_{NB} = -[L_{NB} \frac{\partial h_{NB}}{\partial T_{NB}} + (V_{NB} + SV_{NB}) \frac{\partial h_{NB}}{\partial T_{NB}}]$$

$$c_{NB} = 0$$

(6) Matrix Q

$$a_j = 0$$

$$b_j = -h_j$$

$$c_j = h_{j+1}$$

$$j = NT + 1 \rightarrow NB-1$$

$$a_{NB} = 0$$

$$b_{NB} = -h_{NB}$$

$$c_{NB} = 0$$

(7) Matrix R

$$a_{NT} = 0$$

$$b_{NT} = -h_{NT}$$

$$c_{NT} = 0$$

$$a_j = h_{j-1}$$

$$b_j = -h_j$$

$$c_j = 0$$

$$j = NT+1 \rightarrow NB$$

## (8) Matrix G

$$a_1 = 0$$

$$b_1 = 1$$

$$c_1 = +1$$

$$j = NT + NB - 1$$

$$a_{NB} = 0$$

$$b_{NB} = 1$$

$$c_{NB} = 0$$

## (9) Matrix H

$$a_{NT} = 0$$

$$b_{NT} = -1$$

$$c_{NT} = 0$$

$$a_1 = +1$$

$$b_1 = -1$$

$$c_1 = 0$$

$$j = NT + 1 + NB$$

#### 5.4 Effect of Problem Specifications on Matrix Elements

For a specified column with a specified feed, the number of specifications is equal to the number of controllable variables. For a distillation column with a partial condenser these controllable variables are the reboiler and condenser duties, while for a reboiled absorber the reboiler duty is controllable. Thus two variables may be specified for a distillation column, and one for a reboiled absorber.

In the method presented by Bartscherode and Gentry<sup>14</sup>, the calculational procedure is limited to cases involving symmetrical specifications, where a symmetrical specification is one which applies to the same state as the equation it replaces. For example, if the top vapour product is specified instead of the condenser duty, the specification is symmetrical.

With the current algorithm the limitation on specifications is not entirely the symmetrical consideration. Certain symmetrical specifications cannot be handled because the matrix  $\bar{H}$  in equation (5-9) becomes singular. However, one other symmetrical specification, namely that of the bottoms liquid product in a reboiled absorber, also does not work even though no matrices are singular. The reason for this is unclear at present.

The following changes of specification have been successfully incorporated into the algorithms:

- (a) Specification of the reflux ratio and quantity of reboiler vapour for a distillation column.

For the case of a partial condenser,  $V_{NT+1}$  and  $V_{NT}$  are related by the equation

$$V_{NT+1} = (1 + R) V_{NT} \quad (5-10)$$

As  $R$  is fixed it follows that

$$\Delta V_{NT} = \Delta V_{NT+1} / (1 + R) \quad (5-11)$$

Equation (5-11) is used to eliminate  $\Delta V_{NT}$  from equations (5-4-a), (5-5-a) and (5-6-a). In the energy balance equation  $\Delta Q_{NT}$  is non-zero, and this is placed into the position in the  $\bar{A}\bar{V}$  matrix left vacant by the effective removal of  $\Delta V_{NT}$  (by equation (5-11)). The reboiler vapour is fixed, giving  $\Delta V_{NB} = 0$  in equations (5-4-b), (5-5-b) and (5-6-b). Similarly to the above,  $\Delta Q_{NB}$  occupies the position of  $\Delta V_{NB}$ .

Correspondingly, the following matrix elements are altered:

$$\text{in } D_1 \quad D_{NT} - D_{NB} - C_{NB-1} = 0$$

$$C_{NT} = Y_{i,NT+1} - \frac{Y_{i,NT}}{(1+R)}$$

$$\text{in } \bar{Q}, \quad b_{NT} = b_{NB} = 1, 0$$

$$c_{NT} = \frac{H_{NT+1}}{(1+R)} = \frac{H_{NT}}{(1+R)}$$

$$c_{NB-1} = 0$$

$$\text{in } \bar{G}, \quad b_{NT} = b_{NB} = c_{NB-1} = 0$$

$$c_{NT} = \frac{R}{(1+R)}$$

(b) An alternative specification for a distillation column is of condenser temperature and reboiler duty. In this case  $\Delta T_{NT} = 0$  in equations (5-4-1) and (5-5-1a) and  $\Delta Q_{NT}$  occupies the position left vacant by  $\Delta T_{NT}$ . The following changes occur in the matrix elements:

$$\text{in } \bar{B}_i, \quad b_{NT} = 0$$

$$\text{in } \bar{P}, \quad b_{NT} = 1, 0$$

$$a_{NT+1} = 0$$

~~For a reboiled absorber the amount of reboiled vapour may be specified.~~ Then  $\Delta V_{NB} = 0$  and its position is occupied by  $\Delta Q_{NB}$ . Changes in the matrix elements are:

$$\text{in } \bar{D}_i, \quad b_{NB} = c_{NB-1} = 0$$

$$\text{in } \bar{Q}, \quad b_{NB} = 1, 0$$

$$c_{NB-1} = 0$$

$$\text{in } \bar{G}, \quad b_{NB} - c_{NB+1} = 0$$

(d) For a reboiled absorber with reboiler duty specified, or for a distillation column with reboiler and condenser duties specified, no changes are necessary to the matrix elements.

### 5.5 Solution Procedure

The linearized equations (5-4, 5-5 and 5-6) may be expressed in matrix form as:

$$\bar{A}_i \Delta \bar{x}_i + \bar{B}_i \Delta \bar{T} + \bar{D}_i \Delta \bar{V} + \bar{F}_i \Delta \bar{L} = \bar{C}_i \quad (5-7)$$

1 ≤ i ≤ NCP

$$\bar{P} \Delta \bar{T} + \bar{Q} \Delta \bar{V} + \bar{R} \Delta \bar{L} = \bar{E} \quad (5-8)$$

$$\bar{G} \Delta \bar{V} + \bar{H} \Delta \bar{L} = \bar{M} \quad (5-9)$$

In the case of a single column, equation (5-9) can be solved algebraically for the  $\Delta L_j$  in terms of the  $\Delta V_j$ 's. The presence of interconnected streams (i.e. off-tridiagonal elements) precludes this possibility and equation (5-9) must be solved using matrix methods. This is readily done, by setting  $\bar{M}$  equal to the zero matrix.

Assuming a solution to (5-9) has been obtained so that one may write:

$$\mathbf{A}_i^{-1} \mathbf{x}_i + \mathbf{B}_i^{-1} \mathbf{v} = \mathbf{C}_i \quad (5-12)$$

then substitution of equation (5-12) into equations (5-7) and (5-8) reduces them to the form of equations (5-13) and (5-14).

$$\mathbf{A}_i^{-1} \mathbf{x}_i + \mathbf{B}_i^{-1} \mathbf{v} + \mathbf{D}_i^{-1} \mathbf{y} = \mathbf{C}_i \quad (5-13)$$

$\mathbf{1} \leq i \leq NCP$

$$\mathbf{P} \mathbf{M} \mathbf{v} + \mathbf{Q} \mathbf{v} = \mathbf{F} \quad (5-14)$$

These equations are identical in form to those for a single column; however, each matrix may include off-tridiagonal elements. In particular,  $\mathbf{A}_i^{-1}$  has the same number of off-tridiagonal elements as there are connected streams (see section 5.3). The rapidity of the solution procedure relies on easy conversion of  $\bar{\mathbf{A}}_i$  to a unit matrix, hence its pseudo-tridiagonal character is crucial.

Denote  $\bar{\mathbf{A}}_i$  as the sum of two matrices:

$$\bar{\mathbf{A}}_i = \bar{\mathbf{A}}_{T,i} + \bar{\mathbf{A}}_{OD,i} \quad (5-15)$$

where:  $\bar{\mathbf{A}}_{T,i}$  is strictly tridiagonal

$\bar{\mathbf{A}}_{OD,i}$  is a sparse matrix containing all zeros except for the off-tridiagonal elements in  $\bar{\mathbf{A}}_i$ .

The method of solution of (5-13) and (5-14) is then as follows:

(i) Invert  $\bar{A}_{T,i}$  using a suitable algebraic algorithm for tridiagonal matrices. Examples are the Thomas algorithm or the modification derived by Ishii<sup>17</sup>.

(ii) Multiply equation (5-13) by the inverse of  $\bar{A}_{T,i}$ . Using (5-15) this produces:

$$(\bar{I} + (\bar{A}_{T,i})^{-1} \bar{A}_{OD,i}) \bar{E}\bar{x}_i + \bar{B}_i^T \bar{AT} + \bar{D}_i^T \bar{AV} = \bar{C}_i^T \quad (5-16)$$

The matrix  $(\bar{A}_{T,i})^{-1} \bar{A}_{OD,i}$  consists of as many non-zero columns as there are interconnected streams entering different stages; all other columns consisting solely of zeros. Therefore:

(iii) Eliminate each non-zero column in turn by row-wise elimination on the matrix  $(\bar{I} + (\bar{A}_{T,i})^{-1} (\bar{A}_{OD,i}))$ , pivoting around the diagonal element and applying the procedure to all terms in equation (5-16), thus reducing it to the form

$$\bar{E}\bar{x}_i + \bar{B}_i^T \bar{AT} + \bar{D}_i^T \bar{AV} = \bar{C}_i^T \quad (5-17)$$

(iv) Sum equation (5-17) over each component to yield:

$$\bar{I} \bar{E}\bar{x}_i + \bar{B}^T \bar{AT} + \bar{D}^T \bar{AV} = \bar{C} \quad (5-18)$$

Then using equation (5-10) with  $S_j = 0$  reduces equation (5-18) to an equation of the form:

$$\bar{B} \bar{T} + D \bar{V} = C \quad (5-19)$$

(v) Apply the procedure of steps (ii) to (iv) to equation (5-14), reducing it to the form

$$\bar{E} \bar{T} + \bar{Q} \bar{V} = \bar{F} \quad (5-20)$$

(vi) Equations (5-19) and (5-20) are then solved simultaneously to yield  $\bar{T}$  and  $\bar{V}$ ;  $\bar{L}$  is obtained from equation (5-12).

(vii) These values are substituted back into equation (5-7) for each  $i$ , and the equation solved for the  $x_{i,j}$ . This again involves the manipulations of steps (i) to (iii).

(viii) New values of the temperature, vapour, liquid and composition profiles are calculated as follows, where  $t$  is an appropriate weighting factor ( $0 < t \leq 1$ )

$$T_i^{k+1} = T_i^k + t \Delta T_i \quad (5-21)$$

$$V_j^{k+1} = V_j^k + t \Delta V_j \quad (5-22)$$

$$x_{i,j}^{k+1} = x_{i,j}^k + t \Delta x_{i,j} \quad (5-23)$$

$$y_{i,j} = k_{i,j} x_{i,j} \quad (5-24)$$

and the new  $L_j$ 's are evaluated from the overall material balance equation (5-3) with  $M_j = 0$ . This avoids truncation errors associated with computing the new  $L_j$ 's from the old values and the corrections "L".

- (ix) The  $x_{1,j}$ 's are normalized to avoid truncation error, and then  $K_{1,j}$ ,  $H_{1,j}$ ,  $h_{1,j}$ ,  $\frac{F_{1,j}}{\Delta T_j}$ ,  $\frac{K_{1,j}V}{\Delta x_{1,j}}$ ,  $\frac{H_j}{\Delta T_j}$  and  $\frac{h_j}{\Delta T_j}$  calculated.

The elements of the matrices are obtained using these values and the updated values of the stage variables.

- (x) Calculations are continued until the following convergence criterion is satisfied:

$$\frac{[\text{CRIT}]}{N_{\text{TOTL}}} \leq \text{tolerance} \quad (5-25)$$

where [CRIT] is defined as

$$[\text{CRIT}] = \frac{N_{\text{TOTL}}}{\sum_{j=1}^{N_{\text{TOTL}}} \left[ \left( \frac{y_{1,j}}{y_{1,j+1}} - 1.0 \right)^2 + \left( \frac{E_j / (F_j H_{F,j}) + O_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1} + \frac{V_j}{k} E_{j,k}}{V_{j+1} H_{j+1} + \frac{V_j}{k} E_{j,k}} \right)^2 \right]} \quad (5-26)$$

Experience has shown that tightening the convergence criterion (that is reducing the tolerance in equation (5-25)) does not result in any significant change in the final values of the temperatures, liquid and vapour flowrates and compositions.

The weighting factor  $t$  used in step (viii) is chosen as follows<sup>17</sup>. First an initial value of  $t$ ,  $t^{(1)}$ , is chosen as the smallest value of  $t$  (less than or equal to unity) which satisfies both equations (5-27) and (5-28):

$$T_j^k - \Delta T_{lim} < T_j^k + t \Delta T_j < T_j^k + \Delta T_{lim} \quad (5-27)$$

$$0.5 V_j^k - V_j^k + t V_j < 2.0 V_j^k \quad (5-28)$$

where  $\Delta T_{lim}$  is chosen by the user with a default value of  $60^{\circ}\text{F}$ . If  $t^{(1)}$  does not satisfy the condition that

$$[\text{CRIT}]^{k+1} = [\text{CRIT}]^k \quad (5-29)$$

then a second weighting factor  $t^{(2)} = 0.5t^{(1)}$  is used.

Generally this procedure produces monotonic convergence.

## 6. USE OF THE MULTICOLUMN ALGORITHM

Application of the algorithm discussed in chapter 5 will be demonstrated with examples involving three different systems of columns. Limitations of the algorithm will be identified.

### 6.1 Example Problem

Problem No. 1 is a thermal binary column distillation system which is depicted in Figure 1. A hydrocarbon feed is split into three products: a  $C_2 + C_3$  fraction, a  $C_4$  fraction and a  $C_5^+$  fraction. The problem specifications and initial assumptions are:

<u>Component</u>	<u>Feed (moles/time)</u>
ethane	32.7
propane	2156.1
i-butane	400.5
n-butane	715.3
i-pentane	251.2
n-pentane	267.1
hexane	141.8
octane	110.3

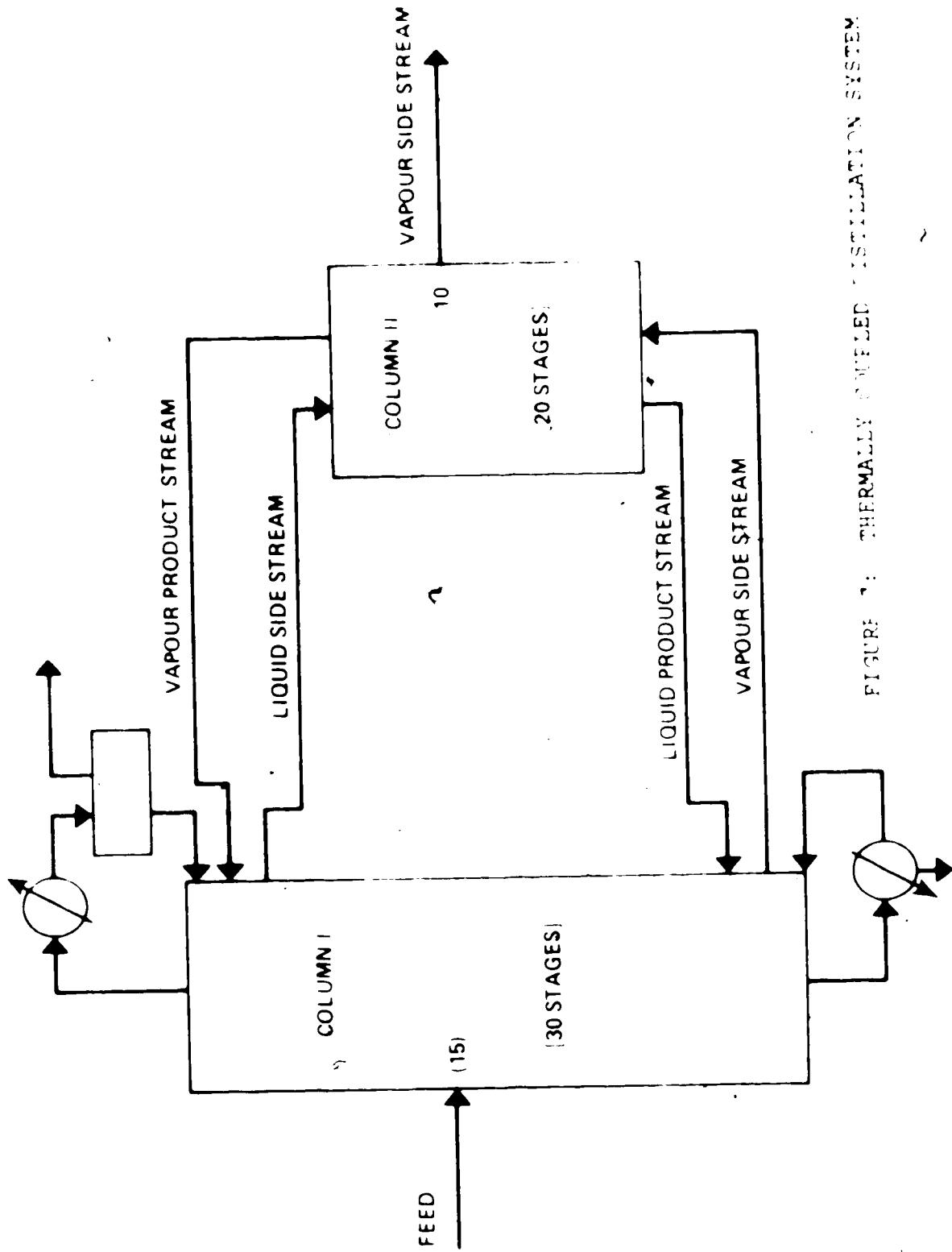


FIGURE 1: THERMALLY COUPLED DISTILLATION SYSTEM

Various side stream leaves stage 40 (stage 10 of  
of column II)

Quantity 1209.6 moles

The interlinked streams are as follows (see Figure 7).

Type of Stream	Leaving Stage Number	Entering Stage Number	Quantity (moles/time)
Input sidestream	5	31	2500
Vapour sidestream	25	50	3000
Vapour product	31		a variable
Liquid product	50		a variable

For column 1 the additional specifications are:

Reboiler vapour 6850 moles/time

Reflux ratio = 2.50

### Partial condenser

Equilibrium and enthalpy data were obtained using the Chao-Saeder correlation<sup>5</sup>. Details of the evaluation of the required partial derivatives have been given by Ishii<sup>17</sup>.

The initial assumptions are as follows:

<u>Stage</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/time)</u>
1	122	2207.2
2	124	7725.4
3	126	7650
4	130	7600
5	134	7550
6	138	5000
7	142	5000
8	144	5000
9	146	5000
10	148	5000
11	150	5000
12	152	5000
13	154	5000
14	156	5000
15	164	5000
16	172	4800
17	180	4800
18	188	4800
19	196	4800
20	204	4800
21	212	4800
22	220	4800
23	228	4800
24	240	4800
25	252	4800
26	264	7500
27	276	7500
28	288	7500
29	300	7500
30	325	6850
31	137	2200
32	145	2200
33	153	2200
34	161	2200
35	173	2200
36	185	2200
37	197	2200
38	205	2200
39	213	2200
40	221	2200
41	229	3100
42	237	3100

## Problem No. 1

Stage	Temperature (°C)	Vapour Rate (mole/time)
43	24.2	3100
44	24.4	3100
45	24.6	3100
46	24.8	3100
47	25.0	3100
48	25.2	3100
49	25.4	3100
50	25.6	3100

## Problem No. 2

This problem concerns extraction of cellulose system which generates an acetone-acetonitrile mixture and solvent is solvent. The system is represented in Figure 8. The extraction column is taken from a paper by Ishikawa and Murata<sup>19</sup>. Solvent circulation, feed and suitable values for the reflux ratio, number of stages and amount of reboiler energy such that the solvent is removed from a single tower, motivated the use of two solvent recovery towers. Detailed description of the problem are:

Component	Solvent Circulation Rate (mole/time)	Feed Rate (mole/time)
Acetone	—	90.0
Acetonitrile	—	10.0
Water	200.0	—

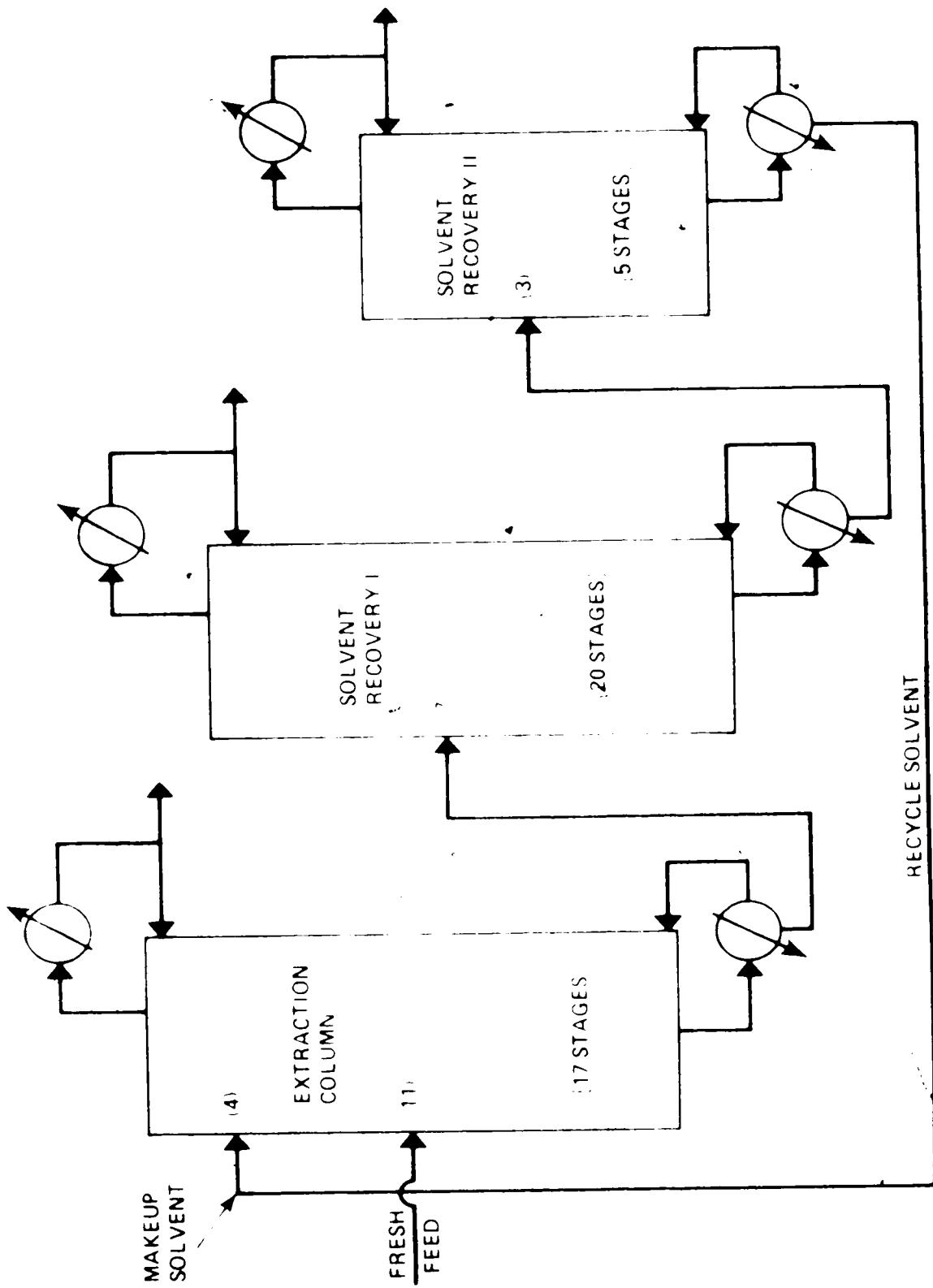


FIGURE 8: EXTRACTIVE DISTILLATION SYSTEM

	Extraction column	Solvent Recovery Towers	
		I	II
Number of equilibrium stages	17	20	5
Column pressure (psia)	14.7	14.7	14.7
Pressure drop per stage (psia)	0.0	0.0	0.0
Reflux ratio	3.0	2.0	10.0
Reboiler vapour (moles/time)	185.0	135.0	95.0
Condenser	total	total	total

Fresh feed stage = 11

Feed conditions: bubble point temperature

pressure = 14.7 psia

Type of Interlinked Stream	Leaving Stage Number	Entering Stage Number	Quantity
Liquid product	17	24	variable
Liquid product	37	40	variable
Liquid product	4.	4	variable

Equilibrium K-ratios are provided by vapour pressures and activity coefficients, the latter being given by Margules third order equations. Enthalpy data is evaluated using average specific heats and latent heats of vapourization. Details of the above evaluations and of the calculation of partial derivatives are given in Appendix 5.

The initial assumptions are as follows:

<u>Stage No.</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/time)</u>
1	134	0
2	135	200
3	136	200
4	137	200
5	138	200
6	139	200
7	140	200
8	141	200
9	142	200
10	143	200
11	144	200
12	145	200
13	146	200
14	147	200
15	148	200
16	149	200
17	150	185
18	138	0
19	143	165
20	148	165
21	153	165
22	158	165
23	163	165
24	166	165
25	168	165
26	170	165
27	172	165
28	180	165
29	180	165
30	180	165
31	180	165
32	180	165
33	180	165
34	185	165
35	190	165
36	195	165
37	200	135
38	150	0
39	180	110
40	200	110
41	205	110
42	210	95

**Problem No. 3**

This problem involves a typical amine sweetening system, using MEA as solvent. The system is the same as that depicted in Figure 1. Problem specifications are:

### **Composition of Feed**

<u>Component</u>	<u>Sour Gas (moles/time)</u>
H <sub>2</sub> S	35.7
CO <sub>2</sub>	39.5
MEA	-
H <sub>2</sub> O	5.0
hydrogen	500.0
nitrogen	5000.0
methane	4000.0
ethane	2500.0
propane	900.0
n-butane	89.0
i-butane	89.0

Babaiyan, due to - 13.9.2014, page 10

**AMOUNT OF AMINO ACID CONCENTRATION** (M)

Solution strength (wt. pct.) = 15.3

Total flowrate of semilean

amine stream = 2550 moles/time

Semilean stream goes from stage 17 to stage 5

Rich amine enters stage 12

<u>Stream</u>	<u>Entering Temperature (°F)</u>	<u>Entering Pressure (psia)</u>
Sour gas feed	90	250
Lean amine	110	250
Rich amine	190	100
Semilean amine	100	250

Equilibrium and enthalpy data were provided by the correlation of Nasir<sup>35</sup>.

Initial assumptions for the stage variables are:

<u>Stage No.</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/time)</u>
1	100	13090
2	100	13090
3	100	13090
4	100	13090
5	100	13090
6	100	13090
7	100	13090
8	100	13090
9	100	13090
10	110	13090
11	120	80
12	230	240
13	232	500
14	234	600
15	236	615
16	238	630

(continued)

<u>Stage No.</u>	<u>Temperature (°F)</u>	<u>Vapour Rate (moles/time)</u>
17	240	645
18	242	660
19	244	675
20	246	690
21	248	705
22	250	720
23	252	735
24	254	750

Estimated reflux ratio = 2.0

6.2 Results and Discussion

Computer printouts for the example problems are given in Appendix 6. Convergence-characteristics and CPU times for each problem are summarized in Table 8.

TABLE 8: CONVERGENCE CHARACTERISTICS AND  
CPU TIMES FOR LINKED COLUMN  
EXAMPLE PROBLEMS

Thermally Coupled Distillation System		Extractive Distillation System		Amine Treating System	
Iter. No.	[CRIT]	Iter. No.	[CRIT]	Iter. No.	[CRIT]
0	2.32	0	14.64	0	0.16
1	$0.62 \cdot 10^{-2}$	1	26.89	1	$0.19 \cdot 10^{-1}$
2	$0.24 \cdot 10^{-2}$	4	0.49	2	$0.49 \cdot 10^{-2}$
3	$0.13 \cdot 10^{-2}$	7	0.12	3	$0.42 \cdot 10^{-2}$
4	$0.75 \cdot 10^{-3}$	10	$0.30 \cdot 10^{-1}$	4	$0.17 \cdot 10^{-2}$
5	$0.11 \cdot 10^{-3}$	13	$0.23 \cdot 10^{-2}$	5	$0.44 \cdot 10^{-4}$
6	$0.53 \cdot 10^{-4}$	16	$0.46 \cdot 10^{-3}$	6	$0.20 \cdot 10^{-4}$
7	$0.55 \cdot 10^{-5}$	19	$0.20 \cdot 10^{-3}$		
		21	$0.15 \cdot 10^{-4}$		
CPU Time (secs)		CPU Time (secs)		CPU Time (secs)	
24.1 <sup>+</sup>		21.2 <sup>+</sup>		4.7 <sup>+</sup>	

+ On an Amdahl 470 V/6

### 6.2.1 Evaluation of the Algorithm

Important factors in evaluating the linked column algorithm include: ease and rate of convergence, limitations of the algorithm and the computer storage and time requirements.

The example problems show that with reasonable initial assumptions the program is able to converge. However, experience has shown that more iterations may be needed where the assumptions are far removed from solution. This is not usually so in the solution of individual columns. In addition, convergence is not always monotonic with the linked column algorithm (see especially iterations 0 and 1 for the extractive distillation problem in Table 8). Non-monotonic behaviour occurs mostly in the early iterations and when large corrections to temperatures, vapour flow rates and liquid compositions are generated. More work on the choice of the weighting factor used in equations (5-21) to (5-23) may then help to increase the rate of convergence. Despite the non-monotonic behaviour, the program has demonstrated robustness in converging for a wide range of initial assumptions.

One limitation of the algorithm is that it encounters difficulty in converging with some specifications. The specifications that present problems are the following:

- (i) reflux ratio and total amount of top product  
(distillation)
- (ii) reflux ratio and total amount of bottom product  
(distillation)
- (iii) total amount of top product (reboiled absorber)
- (iv) total amount of bottom product (reboiled absorber)

Cases (i) and (ii) are specifications made in place of the condenser duty and reboiler duty, and cases (iii) and (iv) are those made instead of the reboiler duty.

The difficulties encountered with the above specifications are mostly related to the occurrence of a singular matrix in the linearized material balance equation (cases (i), (ii) and (iv)). It is unclear why case (iii) does not work, although Harclerode and Gentry<sup>14</sup> indicate their algorithm is restricted to cases where symmetrical specifications are made, and this restriction could also apply to case (iii). On the other hand, both cases (ii) and (iv) are symmetrical, yet neither works. Thus restrictions on the present algorithm differ from those given by Harclerode and Gentry<sup>14</sup>, as some of both symmetrical (cases (ii) and (iv)) and non-symmetrical (cases (i) and (iii)) specifications do not produce a converged solution. Note that the difficulties just discussed only arise for the linked column program.

In summary, specifications that are successfully handled are the following, where one each of (a) and (b) is selected for a distillation column, and one of (b) for a reboiled absorber:

- (a) reflux ratio, condenser temperature, condenser duty
- (b) amount of reboiler vapour, reboiler duty.

For a given number of stages, more computer storage and CPU time per iteration are required by the algorithm than for the solution of a single column. Most of the increase in CPU time requirements is related to the elimination of the  $\bar{A}L$  matrix from the linearized equations and to the handling of off-tridiagonal elements. No special techniques were introduced to make the matrix manipulations more efficient; thus some savings in the times quoted in Table 8 could be achieved by utilizing more fully the block tridiagonal nature of the matrices. In particular, a number of multiplications by zero can be eliminated without the need for time consuming comparisons. Even without any refinements to the handling of the matrix equations the CPU times required per iteration are very favourable.

Finally, the handling of intercooling or heating of interlinked streams is a useful capability. Change of phase in the heating or cooling is not presently

accounted for, but theoretically this could be readily incorporated as the additional requirement is merely a flash calculation on the entering stream to determine its condition and enthalpy.

#### 6.2.2 Example Problem 1

The configuration used for the thermally coupled problem differs from that suggested by Stupin and Lockhart<sup>41</sup> in that the feed enters the reboiled column and the side vapour product leaves the other column rather than the reverse being true. For the number of stages, reboiler duty and quantities of interlinked side vapour and side liquid streams, the configuration used in the example produced a better separation of the feed into the desired product fractions.

Four runs were performed of Problem 1, with essentially the same reboiler duty and using different specifications on the reboiled column. Both system configurations were used. A brief comparison of the results is given in Table 9, where 'a' denotes the present configuration and 'b' that used by Stupin and Lockhart<sup>41</sup>. A fuller analysis of the thermally coupled system would involve determination of the energy savings it offers over the conventional system of employing a reboiler on both columns.

TABLE 9: COMPARISON OF RUNS FOR THERMALLY  
COUPLED DISTILLATION PROBLEM.

Configuration	Specified Variables	Percent Recovery of C <sub>3</sub>	C <sub>4</sub>	C <sub>5</sub> 's	Reflux Ratio	Condenser Temp (°F)	No. of Iterations
a	Q <sub>NB</sub> , R	98.1	93.4	75.3	2.5	121.78	7
c	Q <sub>NB</sub> , T <sub>NT</sub>	98.1	91.5	75.6	2.51	121.71	5
b	Q <sub>NB</sub> , T <sub>NT</sub>	77.6	65.4	99.5	3.53	121.71	5
e	Q <sub>NB</sub> , R	80.7	64.1	84.5	2.5	137.71	4

### 6.2.3 Example Problem 2

For the extractive distillation problem, some changes were made to the equations presented in Chapter 5 to account for the makeup solvent stream. If n is the entering stage number and NB the leaving stage number of the recycle solvent, the following changes are made to the equations about stage n.

- (i) In equation (5-1),  $\psi_{C,i,k}$  for component i in the solvent equals  $L'_{NB} x'_{i,NB}$
- (ii) In equation (5-2),  $\psi_{E,k}$  for the solvent equals  $L'_{NB} h'_{NB}$
- (iii) In equation (5-3),  $\psi_{M,k}$  is  $L'_{NB}$  for the solvent

where:  $L'_{NB} = L_{NB} + \text{makeup solvent}$

$$x'_{i,NB} = \frac{L_{NB} x_{i,NB}}{L'_{NB}} \quad i = 1 \dots NCP$$

$i \neq ns$

$$x'_{ns,NB} = \frac{\text{solvent circulation rate}}{L'_{NB}}$$

$h'_{NB}$  is evaluated at the specified entering temperature of the solvent for liquid compositions  $x'_{i,NB}$ .

$L'_{NB}$  is calculated as a known quantity at each iteration from the equation

$$L'_{NB}^{(k+1)} = [L_{NB}^{(k)} + (L_{NB}^{(k)})^* (1 - x'_{ns,NB})]$$

+ (specified) solvent circulation rate (6-1)

Then in the linearized equations, namely (5-4), (5-5) and (5-6), no terms in  $x_{i,NB}$ ,  $L_{NB}$  or  $T_{NB}$  appear in the equations around stage n.

In the final solution the required makeup of solvent equals the difference between the circulation rate (moles/time) and the moles of solvent in the stream leaving stage NB. The makeup of water in problem 2 is then 19.5 moles/time.

Alternatively to the above procedure, the makeup of solvent could be calculated at each iteration as the

total amount of solvent lost in streams leaving the system. Then  $L'_{NB}$  is given directly from the sum of  $L_{NB}$  and the makeup solvent. The methods produce equivalent results, although in the former a check should be made that the solvent material balance around the system closes. This is so for the example problem, to the accuracy of the printed results.

In the linearized equations, the partial derivatives with respect to composition were set equal to zero, even though the equilibrium K-ratios are strongly composition dependent. This did not prevent a converged solution being reached. In fact, when the partials were included, a solution was not achieved for the example problem. The omission of the partials does not affect the rigour of the solution as the K-ratios are calculated exactly as functions of composition at each iteration.

For a solvent recovery tower, it is difficult to choose appropriate values for the number of stages, the reflux ratio and the amount of reboiler vapour such that the desired separation of the solvent from other components is achieved. This difficulty largely motivated the use of two solvent recovery towers, as a number of attempts at using a single recovery tower failed to produce a converged result. The separation achieved in problem 2 appears quite reasonable as the top product from

The extraction column (6-2) acetone and contains only 90 ppm acetonitrile, while 95% of the acetonitrile is recovered in the top product of solvent recovery tower 1. The second solvent recovery tower removes the remaining acetonitrile and produces an overhead product containing 0.26% acetonitrile and only 2 ppm acetone.

In addition the use of two solvent recovery towers demonstrates that the algorithm can solve systems of more than two columns.

#### 6.2.4 Example Problem 3

In the case of the amine system, modifications to the linearized equations are needed because the quantities of amine and water in the lean amine are specified. The changes are the same in form as those for the extraction problem, with the quantities  $L_{NB}^{(k+1)}$ ,  $x_{1,NB}^{(k+1)}$  and  $x_{4,NB}^{(k+1)}$  being calculated as follows, where subscripts 1 and 4 denote amine and water respectively.

$$L_{NB}^{(k+1)} = L_{NB}^{(k)} + \frac{L_{NB}^{(k)}}{x_{1,NB}^{(k)}} (1 - x_{3,NB}^{(k)} - x_{4,NB}^{(k)}) \quad (6-2)$$

+ (moles amine + moles water) in the  
lean amine

(6-2)

$$x_{1,NB}^{(k+1)} = \frac{L_{NB}^{(k)} x_{1,NB}^{(k)}}{L_{NB}^{(k)}} \quad i = 1, 2, 3 + NCP \quad (6-2-a)$$

$$x'_{3,NB} = \frac{\text{moles amine in lean amine}}{L'_{NB}} \quad (6-2-b)$$

$$x'_{4,NB} = \frac{\text{moles water in lean amine}}{L'_{NB}} \quad (6-2-c)$$

Moles water in lean amine  
 $= (\text{moles amine in lean amine}) \left( \frac{XM_3}{XM_4} \right) \left( \frac{100-wt}{wt} \right)$

(6-2-d)

where wt = weight percent of amine in solution,

and  $XM_i$  is the molecular weight of i.

$h'_{NB}$  is evaluated at the specified lean amine temperature for liquid compositions  $x'_{i,NB}$ .

The required makeup of amine and water is then the difference between the specified moles of each in the lean amine and the moles in the bottoms liquid product from the regenerator. For problem 3 the makeups are 0.10 moles amine and 14.3 moles water.

Each interlinked stream undergoes heat exchange before entering its destined stage. It is usual to control the entering temperatures of the lean, semilean and rich amine streams<sup>30</sup>; thus the entering temperatures are specified. If the stream leaves stage k and enters stage n, no terms in  $\Delta T_k$  appear in the linearized enthalpy balance equation (5-5) around stage n.

### 6.3 Application to the Design of Amine Treating Systems

It is the intention of this section to very briefly demonstrate two particular design considerations that can be investigated using the linked column algorithm, namely the option of using a split flow system and the determination of a suitable reboiler steam rate to achieve a desired lean amine residual.

#### 6.3.1 The Split Flow System Option

This option is claimed to have particular advantages for feed streams containing over 30 percent acid gas<sup>30</sup>. Thus a feed containing 30% H<sub>2</sub>S and 70% was used. The basic system is the same as that depicted in Figure 1, with the omission of the semilean stream for the non-split flow case. Specifications for the columns are the same as in problem 3, except for the following changes:

#### Sour Gas Feed

<u>Component</u>	<u>Feed (moles/time)</u>
H <sub>2</sub> S	1500
CO <sub>2</sub>	150
H <sub>2</sub> O	5
N <sub>2</sub>	1000
CH <sub>4</sub>	1500
C <sub>2</sub> H <sub>6</sub>	800
C <sub>3</sub> H <sub>8</sub>	45

	<u>Non-Split Flow</u>	<u>Split Flow</u>
Amount of amine in lean		
amine stream (moles/time)	3760	2500
Reboiler duty (MM BTU/time)	225	195
Total amount of semilean amine		
stream (moles/time)		30,000

The total quantity of amine in the system is then the same for the two cases. Table 10 lists the sweet gas inlet and outlet compositions; the quantities of acid gas in the regenerated lean amine and the regenerator reflux ratio for the split flow and non-split flow (conventional) problem. The split flow configuration produces the sweeter overheads product while using less steam in the reboiler.

Thus the results of this example support the contention that for gas streams with a high acid gas content, a split flow system is advantageous because of the saving in operation costs resulting from reduced heat requirements in the reboiler. In a similar fashion the linked linear algorithm can be used to determine whether the divariant rule holds for feeds with other acid gas contents.

TABLE 10

COMPARISON OF RESULTS GIVEN BY SPLIT FLOW  
AND CONVENTIONAL CONFIGURATIONS

VARIABLE		CONVENTIONAL	SPLIT FLOW
Sweet Gas Composition	H <sub>2</sub> S (ppm)	19.2	16.0
Lean Amine Residuals (moles/time)	CO <sub>2</sub>	0.21	0.19
Reflux Ratio	H <sub>2</sub> S	137.6	83.1
Reboiler Duty (MM BTU/time)	CO <sub>2</sub>	62.5	42.1
		2.25	1.37
		225	195

6.3.2 Choice of a Stripping Stream Rate to Achieve a Given Lean Amine Residual

Fitzgerald and Richardson<sup>9</sup> used data from a number of operating units to prepare plots relating the lean amine residuals of H<sub>2</sub>S and CO<sub>2</sub> to the H<sub>2</sub>S/CO<sub>2</sub> feed ratio and to the steam rate in the reboiler. The program can

be used to generate similar information subject to limitations or inaccuracies in the equilibrium data and stage efficiencies.

To demonstrate this use of the program, a number of runs were made using the same operating conditions as in example problem 3, with the reboiler duty and  $H_2S/CO_2$  feed ratio as variables. In all cases the total quantity of acid gas in the sour gas feed was 75.2 moles. An effective quantity of circulating amine, which includes the quantity in both the lean and semilean amine streams, was used. This was in order to account for the split-flow configuration.

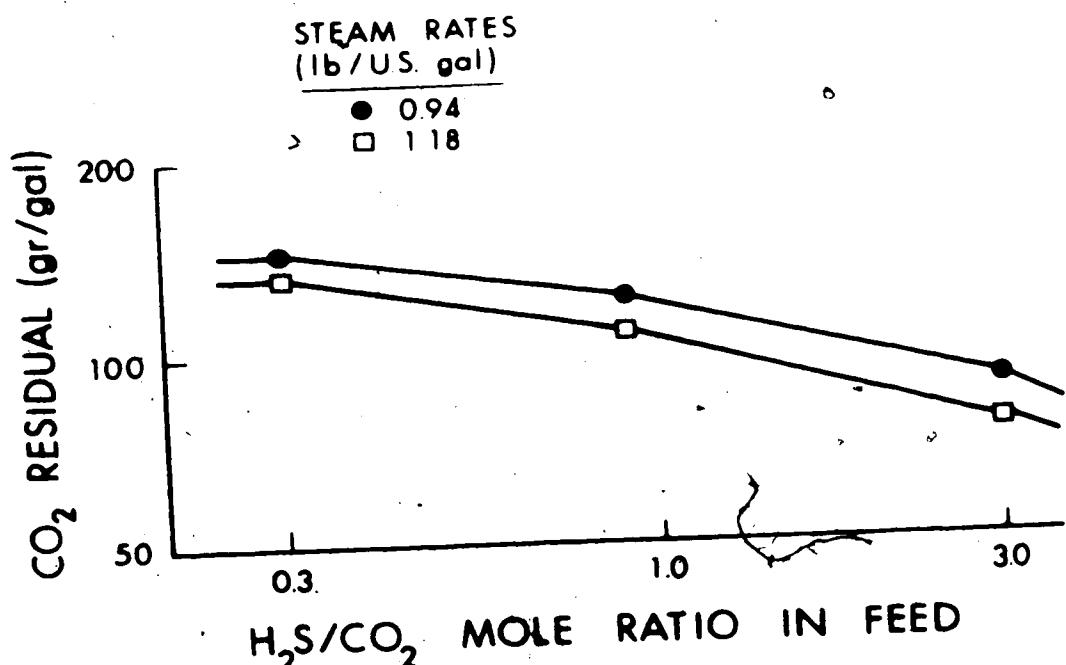
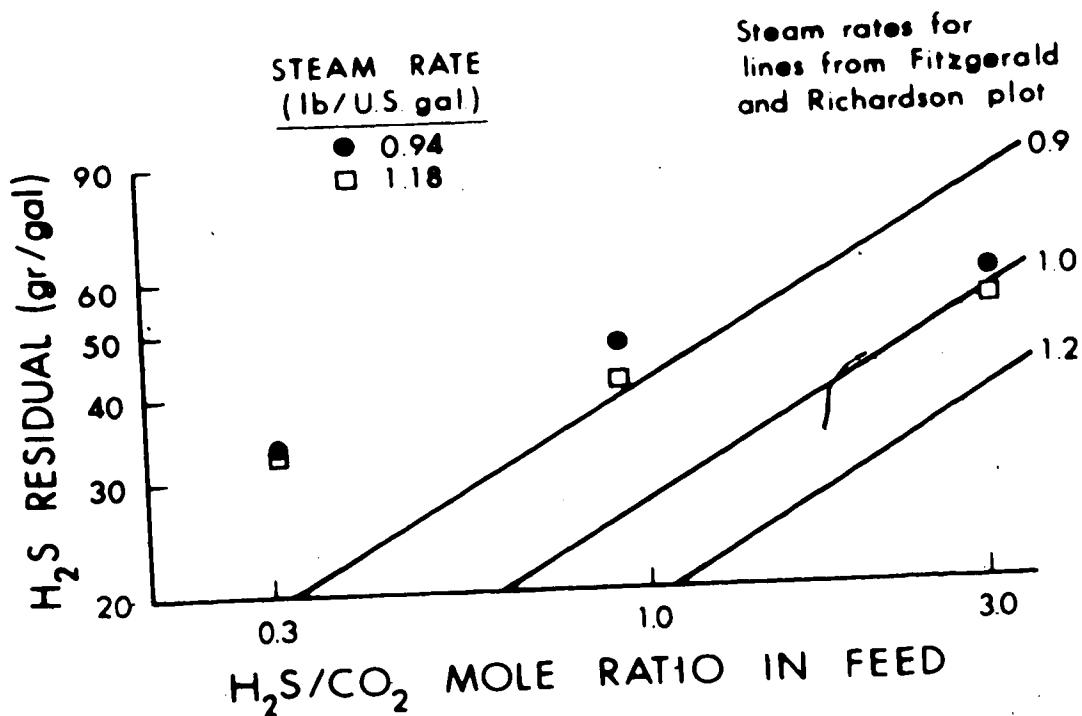
Two steam rates and three  $H_2S/CO_2$  feed ratios were used. The resulting  $H_2S$  and  $CO_2$  residuals in the lean amine are given in Table 11.

TABLE 11:  $H_2S$  AND  $CO_2$  LEAN AMINE RESIDUALS FOR DIFFERENT REBOILER STEAM RATES AND ACID GAS RATIOS IN THE FEED.

$H_2S/CO_2$ MOLE RATIO IN FEED	$H_2S$ RESIDUALS*		$CO_2$ RESIDUALS*	
	STEAM RATE + 0.94	1.18	STEAM RATE + 0.94	1.18
0.3	32.8	31.8	140.7	127.7
0.9	46.7	40.9	120.6	105.4
3.0	58.2	52.5	91.4	83.8

\* grains per gallon of amine in the system

+ lbs. of 55 psia steam per gallon of amine in the system.



The points are plotted on log-log plots as shown in Figure 9. For comparison the straight lines published by Fitzgerald and Richardson<sup>9</sup> are shown on the H<sub>2</sub>S plot. The experimental points lie above those given by interpolating between the lines. Thus the program predicts poorer stripping than indicated by Fitzgerald and Richardson<sup>9</sup>.

In the case of CO<sub>2</sub> the points lie well below the published curves, which give residuals of between about 450 and 1000 gr/gal for the range of acid gas feed ratios used here. However, the same trend is displayed, namely a decreasing CO<sub>2</sub> residual with increasing acid gas feed ratio. The displacement is largely the result of inadequacies in equilibrium data and the use of equilibrium stages rather than actual stages (which incorporate stage efficiencies).

It is postulated that if an adequate set of stage efficiencies were used, the experimental lines would lie much closer to those of Fitzgerald and Richardson<sup>9</sup>. In fact a possible means of estimating the stage efficiencies could be the choice of a set of values that causes the predicted points to lie on the published lines. It should be remembered however, that the published lines represent smoothed data from a number of operating plants. Therefore it seems more reasonable to concentrate on improvements to the fundamental estimation of stage efficiencies rather

than to rely on empirical fitting.

A combination of plots such as Figure 9 and Figure 3 provides a method for the estimation of the steam rate required in the regenerator to meet a given overheads specification in the sweet gas. This is a very useful application of the linked column algorithm.

## 7. CONCLUSIONS

The computational model that has been developed is fast and efficient in providing design data for amine contactors and regenerators. The model can handle data from any given correlation of the solubilities of  $H_2S$  and  $CO_2$  in amine solutions. Use of the model provides values for important design variables, such as the regenerator steam load and the amine circulation rate. In addition the desirability of using a semilean amine stream in the contactor can be determined.

The incorporation of vapourization stage efficiencies into the model equations has been discussed. These efficiencies can be calculated from fundamental rate data and the values obtained indicate that the consideration of efficiencies is important for an accurate design. However, there is a need for more work to obtain better rate data on the absorption process before reliable estimates of the vapourization efficiencies can be made.

The extension of the single column computational model to the solution of systems of columns has been formulated, and the algorithm successfully tested on three systems, namely a thermally coupled distillation system, an extractive distillation system and an amine treating system. Convergence is not dependent on the accuracy of

the initial assumptions, although the rate of convergence may differ. More work is suggested to clarify the influence of the weighting factor on the rate of convergence.

The partial derivatives with respect to composition may be omitted for some problems without affecting convergence. However they must be employed for amine problems.

Some specifications will not work with the algorithm. In most cases this is a result of singular matrices occurring in the solution process. In other cases, the reason is unclear, but it may be related to the restriction quoted by Harclerode and Gentry, which demands that specifications be symmetrical.

For a given size of problem, computer storage and CPU time requirements are larger than for the single column algorithm, but are still favourable. Improvements in the efficiency of the matrix handling routines will reduce the time requirement.

The use of the linked column algorithm in the simultaneous design of contactor and regenerator can provide data on a complete design that meets given requirements on the sweet gas.

Further work on the algorithm is suggested in the following areas:

- (i) application to configurations involving lean oil absorbers
- (ii) a full determination of where  $\delta K/\delta x$  is necessary and where not
- (iii) the incorporation of vapourization efficiencies in the design of complete amine systems.

## NOMENCLATURE

$\alpha$	ratio of the un-ionized alkanolamine activity to the activity of water
$a$	interfacial area per volume of column
$a, b, c$	elements in matrix
$a''$	interfacial area per area of tray
$A, B$	functions in equations (2-4) and (2-5)
$A, B, C, D, E$	constants in ideal gas enthalpy correlation
$\bar{A}, \bar{B}$	matrices
$AL, BL, CL$	constants in latent heat correlation
$b_0$	bulk phase concentration
$c$	component material imbalance function, defined by equations (3-2) and (5-1)
$c_o$	interfacial concentration
$\bar{c}$	column vector
CRIT	convergence criterion, defined by equation (5-26)
D	diffusivity
$\tilde{D}$	matrix
e	vapourization stage efficiency
E	energy imbalance function, defined by equations (3-3) and (5-2)
$E_{MV}$	Murphree vapour stage efficiency

NOMENCLATURE (continued)

F	molar feed rate
F, G, H	matrices
h	enthalpy of liquid
hc	average heat capacity
H	enthalpy of vapour
H	Henry's Law coefficient
h <sub>sol</sub>	enthalpy of solution
I	enhancement factor
I'	identity matrix
k <sub>g</sub> <sup>a</sup>	gas phase mass transfer coefficient
k <sub>G</sub>	gas phase mass transfer coefficient, defined by equation (4-1)
k <sub>L</sub> , k <sub>L</sub> <sup>o</sup>	liquid phase mass transfer coefficients, with and without chemical reaction.
K	equilibrium K-ratio, or equilibrium constant
K <sub>OC</sub>	overall mass transfer coefficient
L	molar liquid flow rate
$\bar{L}$	column vector containing corrections to molar liquid flow rates
m	amine molality or molarity
M	overall material imbalance function, defined by equations (3-5) and (5-3)

NOMENCLATURE (continued)

M	column vector
$n_1, n_2, n_3$	bottom stage numbers of successive columns in three column system
NB	bottom stage of a column
NCP	number of components
NT	top stage of a column
NTOTL	total number of stages in a system of columns
P	pressure
$P_{CO_2}$	$CO_2$ partial pressure
$P_{H_2S}$	$H_2S$ partial pressure
P	matrix
$\alpha$	stoichiometric coefficient
Q	heat duty
Q	matrix
R	gas constant
R	reflux ratio
R	matrix
S	summation imbalance, defined by equation (3-4)
S	cross sectional area of column, or volume of liquid on tray per area of tray
SL	molar flow rate of liquid side stream
SV	molar flow rate of vapour side stream
t	weighting factor

NOMENCLATURE (continued)

T	temperature
$\bar{T}$	column vector containing temperature corrections .
$\dot{V}$	volumetric gas flow per area of tray
$\dot{v}$	molar vapour flow rate
$\bar{\dot{v}}$	column vector containing corrections to molar vapour flow rates
$\bar{V}_a$	mean rate of absorption
wt	weight percent of amine in solution
$\bar{x}$	liquid composition
$\bar{\bar{x}}$	column vector containing corrections to liquid compositions
$x_{CO_2}$	moles $CO_2$ per mole alkanolamine
$x_{H_2S}$	moles $H_2S$ per mole alkanolamine
$M$	molecular weight
y	vapour composition
$\bar{x}_f$	feed composition
$z$	function in equations (2-4) and (2-5), or depth of liquid in tray

NOMENCLATURE (continued)

Greek Letters

- $\alpha$  activity coefficient of water
- $\bar{\alpha}$  average activity coefficient of an ion
- $\Delta$  "new value minus old value"
- $\delta$  composition dependent term in linearized equations arising from interconnected stream, defined in Table 6
- $\eta$  viscosity
- $\vartheta$  temperature dependent term in linearized equations arising from interconnected stream, defined in Table 6
- $\rho$  density
- $\psi$  overall molar flow rate dependent term in linearized equations arising from interconnected stream, defined in Table 6
- $\zeta$  contribution to material and energy balance equations from interlinked stream, defined in Table 5

## NOMENCLATURE (continued)

### Subscripts

A	liquid phase
C	refers to component material balance
E	refers to energy balance
F	feed
G	gas phase
i	component number
int	interfacial value
j	stage number
k	leaving stage number of interlinked stream
lim	limit
L	liquid
M	refers to overall material balance
ns	component number of solvent
NB	bottom stage
NT	top stage
OD	containing off-tridiagonal elements (refers to a matrix)
T	total, or tridiagonal
vap	vapourization

### Superscripts

e	equilibrium condition
k	iteration number
o	pure component, or ideal state

## REFERENCES

1. American Petroleum Institute, "Technical Data Book - Petroleum Refining", 2nd ed., Washington, D.C. (1970).
2. Astarita, G., "Mass Transfer with Chemical Reaction", Elsevier, N.Y., (1967).
3. Billingsley, D.S., Can. J. Chem. Eng., 49, 672, (1971).
4. Carnahan, B., Luther, H.A. and Wilkes, J.O., "Applied Numerical Methods", John Wiley and Sons, N.Y., (1969).
5. Chao, K.C. and Saeder, J.D., AIChE Journal, 7, 598, (1961).
6. Chemical Engineers' Handbook, C. Perry ed., 4th ed., McGraw-Hill, N.Y., (1963).
7. Danckwerts, P.V., "Gas Liquid Reactions", McGraw-Hill, N.Y., (1970).
8. Danckwerts, P.V. and Sharma, M.M., Chem. Engr., 202, 244, Oct. (1966).
9. Fitzgerald, K.A. and Richardson, J.A., Oil and Gas Journal, 64, (43), 110, (1966)
10. Friday, J.R. and Smith, B.D., AIChE Journal, 10, 698, (1964).
11. Gas Conditioning Fact Book, The Dow Chemical Company, Midland, Michigan (1962).
12. Gentry, J.W., Can. J. Chem. Eng., 48, 451, (1970).
13. Hala, E., Wichterle, I., Polak, J. and Boublik, T., "Vapor Liquid Equilibrium Data at Normal Pressures", Pergamon Press, (1968).
14. Harclerode, H. and Gentry, J.W., Can. J. Chem. Eng., 50, 253, (1972).
15. Holland, C.D., "Multicomponent Distillation", Prentice-Hall, Englewood Cliffs, N.J., (1963).

16. Holland, C.D., "Fundamentals and Modeling of Separation Processes", Prentice-Hall, Englewood Cliffs, N.J., (1975).
17. Ishii, Y., M.Sc. Thesis, University of Alberta, (1973).
18. Ishii, Y. and Otto, F.D., Can. J. Chem. Eng., 51, 601, (1973).
19. Ishikawa, T. and Hirata, M., J. of Chem. Enq., of Japan, 5, 125, (1972).
20. Jelinek, J., Hlavacek, V. and Krivsky, Z., Chem. Eng. Sci., 28, 1833, (1973).
21. Kent, R.L. and Eisenberg, B. "Equilibrium of  $H_2S$  and  $CO_2$  with MEA and DEA Solutions", Report presented at Gas Conditioning Conference, (1975).
22. Klyamer, S.D., Kolesnikova, T.L. and Rodin, Yu.A., Gazov. Prom., 18, (2), 44, (1973).
23. Kohl, A.L., AIChE Journal, 2, 264, (1956).
24. Kohl, A.L. and Riesenfeld, F.C., "Gas Purification", 2nd ed., Gulf Publishing Co., Houston, Texas, (1974).
25. Lawson, J.D., private communication.
26. Lee, J.I., Otto, F.D. and Mather, A.E., J. Chem. and Eng. Data, 17, 465, (1972).
27. idem, J. Chem. and Eng. Data, 18, 71, (1973).
28. idem, Can. J. Chem. Eng., 52, 803, (1974).
29. idem, Report presented at the CNGPA Research Seminar, Calgary, Alberta, (1972).
30. Maddox, R.N., "Gas and Liquid Sweetening", 2nd ed., John Campbell Press, (1974).
31. Murphree, E.V., Ind. Eng. Chem., 17, 747, (1925).

32. Nagiev, M.F., Chem. Eng. Progr., 53, (6), 297, (1957).
33. Naphtali, L.M., Chem. Eng. Progr., 60, (9), 70, (1964).
34. Nartker, T.A., Skrygley, J.M. and Holland, C.D., Can. J. Chem. Eng., 44, 217, (1966).
35. Nasir, P., M.Sc. Thesis, University of Alberta, (1975).
36. Petryschuk, W.F. and Johnson, A.I., Can. J. Chem. Eng., 46, 348, (1968).
37. Ravicz, A.E. and Norman, R.L., Chem. Eng. Progr. 60, (5), 71, (1964).
38. Rosen, E.M., Chem. Eng. Progr., 58, (10), 69, (1962).
39. Rowland, C.H. and Grens, E.A. II, Hydro. Proc., 50, (9), 201, (1971).
40. Shoeld, M., U.S. Patent 1,971,798 (1934).
41. Stupin, W.J. and Lockhart, F.J., Chem. Eng. Progr., 68, (10), 71, (1972).
42. Tomme, W.J. and Holland, C.D., Hydro. Proc. and Pet. Ref., 41, (6), 145, (1962).
43. Treybal, R.E., "Mass Transfer Operations", 2nd ed., McGraw-Hill, N.Y., (1968).

**APPENDIX 1**

**ENTHALPIES OF SOLUTION OF CO<sub>2</sub> AND H<sub>2</sub>S IN**

**MEA AND DEA SOLUTIONS**

**(KJ/MOLE GAS)**

APPENDIX 1

Enthalpies of Solution of CO<sub>2</sub> and H<sub>2</sub>S In  
MEA And DEA Solutions. (KJ/Mole Gas)

(a) MEA<sup>28</sup>

Acid Gas	Moles Acid Gas/Mole MEA							
	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
CO <sub>2</sub>	85.4	66.0	50.7	38.6	29.5	23.1	-	-
H <sub>2</sub> S	48.5	47.6	46.3	42.5	24.6	16.8	12.6	11.0

(b) DEA<sup>26, 27</sup>

Acid Gas	Normality of Solution	Moles Acid Gas/Mole DEA						
		0.2	0.4	0.6	0.8	1.0	1.2	1.4
CO <sub>2</sub>	0.5	57.7	53.0	44.3	37.3	31.5	27.2	23.5
	2.0	67.2	59.5	47.5	38.8	32.0	27.2	23.5
	3.5	76.3	65.4	50.3	40.0	32.4	27.3	23.5
	5.0	84.3	70.5	52.6	40.9	32.7	27.4	23.5
	6.5	90.7	73.7	54.2	41.5	32.9	27.4	23.5
	8.0	96.2	76.3	55.5	41.8	33.0	27.4	23.5
H <sub>2</sub> S	2.0, 3.5	47.7	43.5	40.0	31.9	16.4	12.5	11.0

(c) Values of Kohl and Riesenfeld<sup>24</sup>:

	<u>MEA</u>	<u>DEA</u>
CO <sub>2</sub>	84.5	66.9
H <sub>2</sub> S	63.7	40.5

**APPENDIX 2**

**CONSTANTS IN CORRELATIONS FOR  
IDEAL GAS ENTHALPY AND LATENT  
HEAT OF VAPOURIZATION**

## APPENDIX 2 \*

## CONSTANTS FOR IDEAL GAS ENTHALPY

COMPONENT	A	B	C	D	E
H2S	-0.25844E+02	0.35672E+00	-0.9410CE-03	-0.19442E+02	0.0
CO2	0.149C1E+02	0.67C27L+00	-0.675C5E-02	-0.85736L+01	0.0
NEA	0.63910E+01	0.2551CE+01	-0.2801CE-01	0.0	0.50000E+03
DEA	0.7627CE+00	0.2906CE+01	-0.4592DE-01	0.0	0.50000E+03
WATER	0.49832E+02	0.3671CE+00	0.61600E-03	0.34424E+02	0.10000E+04
HYDROGEN	0.34135E+03	-0.17541E+00	0.23314E-01	-0.12957E+03	0.0
NITROGEN	0.2370CE+02	0.9764CE-01	0.5949CE-03	0.15603E+02	0.0
METHANE	0.36817E+02	0.20062E+01	-0.38240E-02	0.46138E+02	0.10080E+02
ETHANE	0.14029E+02	0.31357E+01	-0.30512E-01	0.43453E+02	0.10617E+03
PROPANE	0.80382E+01	0.349C7E+01	-0.39606E-01	0.27530E+02	0.10617E+03
NBUTANE	0.82935E+01	0.3460CE+01	-0.4211E-01	0.30351E+02	0.153C4E+03
TBUTANE	0.65259E+01	0.35927E+01	-0.43014E-01	0.20257E+01	0.15569E+03
C-5 <sup>13</sup>	0.60231E+01	0.34488E+01	-0.40567E-01	0.21828E+02	0.14921E+03
C-6 <sup>15</sup>	0.76175E+01	0.34444E+01	-0.40883E-01	0.18712E+02	0.14398E+03
C-7 <sup>17</sup> S <sub>4</sub>	0.75021E+01	0.33421E+01	-0.39902E-01	0.14124E+02	0.14134E+03

## CONSTANTS FOR LATENT HEAT CORRELATION

COMPONENT	AL	BL	CL
NEA	0.6590CE+02	-0.37230E+00	0.0
DEA	0.5320CE+03	-0.3250CE+00	0.0
WATER	0.11622E+04	0.10015E+00	-0.57198E-03

APPENDIX 3

INTERMEDIATE PARTIAL DERIVATIVES  
REQUIRED IN THE DERIVATION OF  
 $\partial K/\partial x$  FOR  $H_2S$  AND  $CO_2$

## APPENDIX B

## Intermediate Partial Derivatives Required In The Derivation of $\frac{\partial K}{\partial x}$ For $\text{H}_2\text{S}$ And $\text{CO}_2$

(1) For  $\text{H}_2\text{S}$  (see equations (3-25) and (3-26))

$$(A) \quad \alpha_1 = \frac{-x_4}{x_4 + x_3 (1 + \frac{x_1}{x_3} + \frac{x_2}{x_3})} = -x_4$$

$$\alpha_1 = \frac{-x_4}{[x_4 + x_3 (1 + \frac{x_1}{x_3} + \frac{x_2}{x_3})]} = -\frac{x_4}{2}$$

(A 3-1)

$$(b) \quad A = m x_1 + P_1 - H_1$$

$$m x_1 = (P_1 - K_1 - x_2) H_1$$

$$\frac{A}{x_1} = m = P_T - K_1 - H_1 \quad (A3-2)$$

$$\left(\begin{array}{c} t \\ \times 1 \end{array}\right) = \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right) + \left(\begin{array}{cc} -\frac{1}{2} & 0 \\ 0 & 1 \end{array}\right) \quad (\text{A3-3})$$

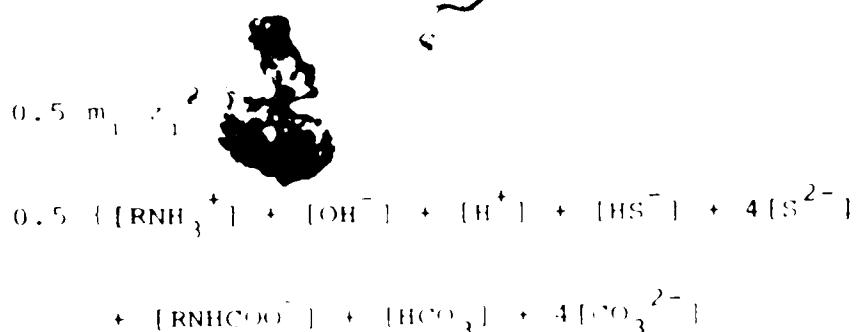
(1)

$$\frac{t_2}{t_1} = \begin{cases} 0.9023 - 1.996\alpha + 0.068e^{-\alpha} & (\alpha < 0, 1) \\ 0.3991 - 3.384 \times 10^{-3}\alpha + 0.3242e^{-\alpha} & (\alpha > 0, 1-\text{MEA}) \\ 0.3664 - 1.598 \times 10^{-2}\alpha + 0.3444e^{-\alpha} & (\alpha > 0, 1-\text{DEA}) \end{cases}$$

$$\frac{t_2}{t_1} = \begin{cases} -1.996 + 0.068e^{-\alpha} & (\alpha < 0, 1) \\ -3.384 \times 10^{-3} - 0.3242e^{-\alpha} & (\alpha > 0, 1-\text{MEA}) \\ -1.598 \times 10^{-2} - 0.3444e^{-\alpha} & (\alpha > 0, 1-\text{DEA}) \end{cases}$$

d  
(A 3-4)

(11)

where  $[\text{HS}^-] = \Delta_{\text{pH}} - [\text{RNHCOO}^-]$ and  $[\text{H}^+]$  and  $[\text{S}^{2-}]$  can be neglected.

$$\frac{t_2}{t_1} = 0.5 \left\{ \frac{\partial [\text{RNH}_3^+]}{\partial x_1} + \frac{\partial [\text{OH}^-]}{\partial x_1} + \frac{\partial \Delta_{\text{pH}}}{\partial x_1} + \frac{\partial z}{\partial x_1} + \frac{\partial [\text{HCO}_3^-]}{\partial x_1} \right. \\ \left. + 4 \frac{\partial [\text{CO}_3^{2-}]}{\partial x_1} \right\} \quad (\text{A 3-5})$$

Now  $\frac{[\text{RNH}_3^+]}{[\text{x}_1]} = \frac{A}{B}$   
 $\frac{[\text{HCO}_3^-]}{[\text{x}_1]} = \frac{B}{z}$

$$\text{Thus } \frac{\frac{[\text{RNH}_3^+]}{[\text{x}_1]}}{\frac{[\text{HCO}_3^-]}{[\text{x}_1]}} = \frac{\frac{A}{B}}{\frac{z}{[\text{x}_1]}} \quad (\text{A3-6})$$

$$\frac{[\text{RNH}_3^+]}{[\text{HCO}_3^-]} = \frac{A}{z} \quad (\text{A3-7})$$

as  $A/B$  is independent of  $x_1$ .

$$\frac{[\text{RNH}_3^+]}{[\text{HCO}_3^-]} = \frac{A}{z} + 0.5 \frac{[\text{OH}^-]}{[\text{x}_1]} + 2 \frac{[\text{C}_3^-]}{[\text{x}_1]} \quad (\text{A3-8})$$

Now  $[\text{OH}^-] = \frac{K_1 \cdot z}{2} \frac{(m-z-A-B)}{(A+B)}$

$$\frac{[\text{RNH}_3^+]}{[\text{HCO}_3^-]} = \frac{1}{\frac{z}{(A+B)}} \left\{ (m-z-A-B) - 2K_1 \cdot z \cdot \frac{1}{[\text{x}_1]} \right\}$$

$$= K_1 \cdot z \left[ \frac{z}{[\text{x}_1]} + \frac{A}{[\text{x}_1]} \right]$$

$$+ \frac{(K_1 \cdot z)^2}{z^2} \frac{(m-z-A-B)}{(A+B)} \left\{ -\frac{2}{z} \frac{z}{[\text{x}_1]} - \frac{1}{(A+B)} \frac{A}{[\text{x}_1]} \right\}$$

(A3-9)

(2)

$$\begin{aligned} [\text{CO}_3^{2-}] &= \frac{\kappa_{2Y} [\text{HCO}_3^-]}{[\text{H}^+]} \\ &= \frac{\kappa_{2Y} [\text{OH}^-] [\text{HCO}_3^-]}{K_w} \end{aligned}$$

$$\begin{aligned} \therefore \frac{[\text{CO}_3^{2-}]}{[\text{x}_1]} &= \frac{\kappa_{2Y}}{K_w} \left\{ -\frac{1}{1} [\text{OH}^-] \frac{z}{[\text{x}_1]} + \frac{1}{1} [\text{HCO}_3^-] \frac{[\text{OH}^-]}{[\text{x}_1]} \right. \\ &\quad \left. + [\text{OH}^-] [\text{HCO}_3^-] \left( \frac{1}{1} \frac{f}{[\text{x}_1]} - \frac{1}{2} \frac{A}{[\text{x}_1]} \right) \right\} \end{aligned}$$

(A3-10)

$$\text{or } \frac{[\text{HCO}_3^-]}{[\text{x}_1]} = z - \frac{z}{[\text{x}_1]} \text{ from equation (A3-7)}$$

solution for  $(\frac{f}{[\text{x}_1]})$  in iteration.

$$(3) \quad A = m - z - B - Sz / (B - z)$$

$$\text{where } S = K_1 K_{1Y} H_1 / K_w K_M \alpha$$

$$f(z) = (m - z - A - B) (z - B) + Sz = 0 \quad (\text{A3-11})$$

$$\frac{z}{[\text{x}_1]} = - \frac{(\cdot f / [\text{x}_1])_z}{(\cdot f' / z) [\text{x}_1]} \quad (\text{A3-12})$$

$$(1) \quad \left( \frac{f}{[\text{x}_1]} \right)_z = (B - z) \frac{A}{[\text{x}_1]} \quad (\text{A3-13})$$

(ii)

$$\left(\frac{\partial f}{\partial z}\right)_{x_1} = m - A + S - 2z$$

(A 3-14)

(e)

$$\left(\frac{\partial A}{\partial K_1}\right) = - P_T x_1 H_1$$

(A 3-15)

(f)

$$\left(\frac{\partial z}{\partial K_1}\right) = - \frac{(\partial f / \partial K_1)_z}{(\partial f / \partial z)_{K_1}}$$

(A 3-16)

(i)

$$\left(\frac{\partial f}{\partial K_1}\right)_z = (B - z) \left(\frac{\partial A}{\partial K_1}\right)$$

(A 3-17)

(ii)

$$\left(\frac{\partial f}{\partial z}\right)_{K_1} = m - A + S - 2z$$

(A 3-18)

(2) For  $\text{CO}_2$  (see equations (3-27) and (3-28))

$$(a) \quad \frac{\partial t}{\partial x_2} =$$

$$\frac{-x_4}{\{x_4 + x_3 (1 + \frac{x_1 + x_2}{x_3})\}^2}$$

(A 3-19)

$$(b) \quad B = mx_2 - P_T K_2 x_2 H_2$$

$$\frac{\partial B}{\partial x_2}$$

$$= m - P_T K_2 H_2$$

(A 3-20)

$$(c) \quad \frac{\partial Y}{\partial x_2}$$

$$= \left(\frac{\partial Y}{\partial \mu}\right) \left(\frac{\partial \mu}{\partial x_2}\right)$$

(A 3-21)

$$(i) \quad \frac{\partial \gamma}{\partial \mu} - \text{see equation (A3-4)}$$

(ii) Using equation (A3-5) with  $x_1$  replaced by  $x_2$ , and the relations:

$$\frac{\partial [\text{RNH}_3^+]}{\partial x_2} = \frac{\partial B}{\partial x_2}$$

and

$$\frac{\partial [\text{HCO}_3^-]}{\partial x_2} = \frac{\partial B}{\partial x_2} + \frac{\partial z}{\partial x_2}$$

one obtains -

$$\frac{\partial \mu}{\partial x_2} = \frac{\partial B}{\partial x_2} + 0.5 \frac{\partial [\text{OH}^-]}{\partial x_2} + \frac{1}{2} \frac{\partial [\text{CO}_3^{2-}]}{\partial x_2}$$

(A3-22)

$$\begin{aligned} \text{Now } (1) \quad \frac{\partial [\text{OH}^-]}{\partial x_2} &= \frac{1}{\gamma^2 (A+B)} \left\{ (m-z-A-B) 2K_i \alpha \alpha \frac{\partial \alpha}{\partial x_2} \right. \\ &\quad \left. - K_i \alpha \alpha^2 \left[ \frac{\partial z}{\partial x_2} + \frac{\partial B}{\partial x_2} \right] \right\} \\ &\quad + \frac{K_i \alpha \alpha^2}{\gamma^2 (A+B)} (m-z-A-B) \left\{ - \frac{2}{\gamma} \frac{\partial \gamma}{\partial x_2} - \frac{1}{(A+B)} \frac{\partial B}{\partial x_2} \right\} \end{aligned} \quad (\text{A3-23})$$

$$(2) \quad \frac{\partial [\text{CO}_3^{2-}]}{\partial x_2} = \frac{K_w}{K_2 \gamma} \left\{ \frac{1}{\alpha} [\text{OH}^-] \left( \frac{\partial B}{\partial x_2} - \frac{\partial z}{\partial x_2} \right) \right.$$

$$\left. + \frac{1}{\alpha} [\text{HCO}_3^-] \frac{\partial [\text{OH}^-]}{\partial x_2} \right\}$$

$$+ [OH^-][HCO_3^-] \left( \frac{1}{\alpha} \frac{\partial \alpha}{\partial x_2} - \frac{1}{\alpha^2} \frac{\partial \alpha}{\partial x_2} \right) \}$$

(A3-24)

- (d) Using equation (A3-11) and equation (A3-13)  
with  $x_1$  replaced by  $x_2$ :

$$\left( \frac{\partial f}{\partial x_2} \right)_z = (A-m+2B) \frac{\partial B}{\partial x_2} \quad (A3-25)$$

and

$\left( \frac{\partial f}{\partial z} \right)_{x_2}$  is the same as in equation (A3-14)

$$(e) \left( \frac{\partial B}{\partial K_2} \right) = - P_T x_2 H_2 \quad (A3-26)$$

- (f) Using equation (A3-11) and equation (A3-17)  
with  $K_1$  replaced by  $K_2$ :

$$\left( \frac{\partial f}{\partial K_2} \right)_z = (A-m+2B) \frac{\partial B}{\partial K_2} \quad (A3-27)$$

and

$\left( \frac{\partial f}{\partial z} \right)_{K_2}$  is the same as in equation (A3-18).

**APPENDIX 4**

**COMPUTER PRINTOUTS FOR  
AMINE CONTACTOR AND  
REGENERATOR PROBLEMS**

## APPENDIX 4.1 -- TEST PROBLEM 1 -- NASIR CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

## TYPE OF COLUMN

NO. OF PLATES 20

PRESSURE AT TOP PLATE (PSIA) 150.00

PRESSURE DROP PER PLATE (PSIA) 0.0

NO. OF FEEDS 3

ENTERING PLATE OF FEED 1 1

FEED QUANTITY 0.69583E+03

PRESSURE OF FEED 150.00

TEMPERATURE OF FEED (F) 100.00

ENTERING PLATE OF FEED 2 4

FEED QUANTITY 0.28612E+04

PRESSURE OF FEED 150.00

TEMPERATURE OF FEED (F) 120.00

ENTERING PLATE OF FEED 3 20

FEED QUANTITY 0.19686E+04

PRESSURE OF FEED 150.00

TEMPERATURE OF FEED (F) 95.00

## \*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

0 SUM OF SQUARES OF RESIDUALS 0.10760E+02

TEMPERATURE  
 0.56960F+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03  
 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03  
 0.57960E+03 0.57960F+03 0.57960E+03 0.57960P+03 0.57960E+03  
 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03 0.57960E+03

VAPOUR FLOW RATE  
 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04 0.19600E+04  
 0.19600E+04 0.19600E+04 0.19600E+04 0.19600F+04 0.19600F+04  
 0.19600F+04 0.19600F+04 0.19600E+04 0.19600E+04 0.19600E+04  
 0.19600E+04 0.19600F+04 0.19600E+04 0.19600F+04 0.19600F+04

1 SUM OF SQUARES OF RESIDUALS 0.48618E-01

TEMPERATURE  
 0.59037E+03 0.60638E+03 0.61723E+03 0.56538F+03 0.56538E+03  
 0.56537E+03 0.56537E+03 0.56537E+03 0.56537F+03 0.56537F+03  
 0.56537E+03 0.56537F+03 0.56537E+03 0.56536E+03 0.56537E+03  
 0.56523E+03 0.56490F+03 0.56376E+03 0.55992F+03 0.54670F+03

VAPOUR FLOW RATE  
 0.19656E+04 0.19768P+04 0.19830E+04 0.19533E+04 0.19532F+04  
 0.19532E+04 0.19532E+04 0.19532E+04 0.19532F+04 0.19532F+04  
 0.19532E+04 0.19532E+04 0.19532E+04 0.19532F+04 0.19532F+04  
 0.19531E+04 0.19529P+04 0.19523E+04 0.19501E+04 0.19438E+04

2 SUM OF SQUARES OF RESIDUALS 0.10229E-01

TEMPERATURE  
 0.56636E+03 0.56294F+03 0.55723E+03 0.57477E+03 0.57477F+03  
 0.57477E+03 0.57477E+03 0.57477E+03 0.57477E+03 0.57477E+03  
 0.57477E+03 0.57476E+03 0.57475E+03 0.57471E+03 0.57461E+03  
 0.57435E+03 0.57370E+03 0.57237E+03 0.57081E+03 0.57608E+03

VAPOUR FLOW RATE  
 0.19506E+04 0.19365E+04 0.19149E+04 0.19592E+04 0.19590E+04  
 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04  
 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04 0.19590E+04  
 0.19588E+04 0.19586E+04 0.19579E+04 0.19569E+04 0.19565E+04

3 SUM OF SQUARES OF RESIDUALS 0.25122E-02

TEMPERATURE  
 0.56618E+03 0.57807E+03 0.59692E+03 0.58306E+03 0.58306E+03  
 0.58306E+03 0.58306E+03 0.58306E+03 0.58306E+03 0.58306E+03  
 0.58306E+03 0.58305E+03 0.58304E+03 0.58301E+03 0.58294E+03  
 0.58281E+03 0.58259E+03 0.58230E+03 0.58186F+03 0.57905E+03

VAPOUR FLOW RATE  
 0.19549E+04 0.19593E+04 0.19644E+04 0.19643E+04 0.19642E+04  
 0.19642E+04 0.19642E+04 0.19642E+04 0.19642E+04 0.19642E+04  
 0.19642E+04 0.19642E+04 0.19641P+04 0.19641F+04 0.19641E+04  
 0.19640E+04 0.19638E+04 0.19634E+04 0.19630E+04 0.19638E+04

## 4 SUM OF SQUARES OF RESIDUALS 0.22373E-03

## TEMPERATURE

0.57459E+03	0.58010E+03	0.57874E+03	0.57944E+03	0.57944E+03
0.57949E+03	0.57949E+03	0.57949E+03	0.57949E+03	0.57949E+03
0.57949E+03	0.57949E+03	0.57947E+03	0.57943E+03	0.57937E+03
0.57949E+03	0.57948E+03	0.57947E+03	0.57943E+03	0.57937E+03
0.57926E+03	0.57907E+03	0.57882E+03	0.57842E+03	0.57549E+03

## VAPOUR FLOW RATE

0.19583E+04	0.19618E+04	0.19585E+04	0.19630E+04	0.19628E+04
0.19628E+04	0.19628E+04	0.19628E+04	0.19628E+04	0.19628E+04
0.19628E+04	0.19628E+04	0.19628E+04	0.19628E+04	0.19628E+04
0.19627E+04	0.19626E+04	0.19624E+04	0.19623E+04	0.19621E+04

## 5 SUM OF SQUARES OF RESIDUALS 0.52480E-04

## TEMPERATURE

0.57064E+03	0.57502E+03	0.58019E+03	0.57984E+03	0.57984E+03
0.57984E+03	0.57984E+03	0.57984E+03	0.57984E+03	0.57984E+03
0.57984E+03	0.57983E+03	0.57982E+03	0.57980E+03	0.57977E+03
0.57971E+03	0.57960E+03	0.57937E+03	0.57867E+03	0.57597E+03

## VAPOUR FLOW RATE

0.19567E+04	0.19589E+04	0.19620E+04	0.19631E+04	0.19629E+04
0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04
0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04
0.19628E+04	0.19628E+04	0.19626E+04	0.19623E+04	0.19621E+04

## 6 SUM OF SQUARES OF RESIDUALS 0.51550E-05

## TEMPERATURE

0.57177E+03	0.57817E+03	0.57988E+03	0.57978E+03	0.57978E+03
0.57978E+03	0.57978E+03	0.57978E+03	0.57978E+03	0.57977E+03
0.57977E+03	0.57977E+03	0.57976E+03	0.57975E+03	0.57972E+03
0.57967E+03	0.57956E+03	0.57927E+03	0.57856E+03	0.57590E+03

## VAPOUR FLOW RATE

0.19573E+04	0.19607E+04	0.19619E+04	0.19631E+04	0.19629E+04
0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04
0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04	0.19629E+04
0.19628E+04	0.19628E+04	0.19626E+04	0.19623E+04	0.19621E+04

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 6

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FUEL

0.150E+03 PSIA	0.100E+03 F	0.290E+07 BTU	1.0
0.150E+03 PSIA	0.120E+03 F	0.119E+08 BTU	1.0
0.150E+03 PSIA	0.950E+02 F	0.128E+08 BTU	1.0

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP F	LIQUID FLOW LB MOL/TIME	VAPOUR FLOW LB MOL/TIME	HEAT DUTY BTU/TIME
1	150.00	112.17	0.69917E+03	0.19573E+04	0.0
2	150.00	118.57	0.70036E+03	0.19607E+04	0.0
3	150.00	120.28	0.70154E+03	0.19619E+04	0.0
4	150.00	120.18	0.35626E+04	0.19631E+04	0.0
5	150.00	120.18	0.35626E+04	0.19629E+04	0.0
6	150.00	120.18	0.35626E+04	0.19629E+04	0.0
7	150.00	120.18	0.35626E+04	0.19629E+04	0.0
8	150.00	120.18	0.35626E+04	0.19629E+04	0.0
9	150.00	120.18	0.35626E+04	0.19629E+04	0.0
10	150.00	120.18	0.35626E+04	0.19629E+04	0.0
11	150.00	120.17	0.35626E+04	0.19629E+04	0.0
12	150.00	120.17	0.35626E+04	0.19629E+04	0.0
13	150.00	120.16	0.35626E+04	0.19629E+04	0.0
14	150.00	120.15	0.35625E+04	0.19629E+04	0.0
15	150.00	120.12	0.35625E+04	0.19629E+04	0.0
16	150.00	120.07	0.35624E+04	0.19628E+04	0.0
17	150.00	119.96	0.35623E+04	0.19628E+04	0.0
18	150.00	119.67	0.35619E+04	0.19636E+04	0.0
19	150.00	118.96	0.35618E+04	0.19623E+04	0.0
20	150.00	116.30	0.35683E+04	0.19621E+04	0.0

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS

	PLATE NO. 1	PLATE NO. 4		
	LB MOL/TIME	MOL FRAC	LB MOL/TIME	MOL FRAC
H2S	0.12800E+01	0.18395E-02	0.54300E+02	0.14978E-01
CO2	0.15700E+01	0.22563E-02	0.63000E+01	0.22019E-02
MEA	0.62050E+02	0.89174E-01	0.25000E+03	0.87377E-01
WATER	0.63093E+03	0.90673E+00	0.25500E+04	0.89124E+00
HYDROGEN	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0
METHANE	0.0	0.0	0.0	0.0
ETHANE	0.0	0.0	0.0	0.0
PROPANE	0.0	0.0	0.16000E+00	0.56921E-04
N-BUTANE	0.0	0.0	0.42000E+00	0.14679E-03
I-BUTANE	0.0	0.0	0.0	0.0
TOTAL	0.69583E+03		0.28612E+04	

	PLATE NO. 20	PLATE NO.	LB MOL/TIME	MOL FRAC
	LB MOL/TIME	MOL FRAC	LB MOL/TIME	MOL FRAC
H2S	0.18700E+02	0.44989E-02		
CO2	0.29500E+01	0.14985E-02		
MEA	0.0	0.0		
WATER	0.59100E+01	0.30021E-02		
HYDROGEN	0.62997E+03	0.32000E+00		
NITROGEN	0.29530E+03	0.15000E-01		
METHANE	0.78155E+03	0.39700E+00		
ETHANE	0.35436E+03	0.18000E+00		
PROPANE	0.12402E+03	0.62997E-01		
N-BUTANE	0.19700E+01	0.10007E-02		
I-BUTANE	0.19690E+02	0.10002E-01		
TOTAL	0.19686E+04			

## PRODUCTS

	TOP PRODUCT	BOTTOM PRODUCT		
	LB MOL/TIME	MOL FRAC	LB MOL/TIME	MOL FRAC
H2S	0.19845E-01	0.10139E-04	0.74261E+02	0.20811E-01
CO2	0.18589E-03	0.94969E-07	0.10820E+02	0.30322E-02
MEA	0.38791E-01	0.19818E-04	0.31201E+03	0.87439E-01
WATER	0.16185E+02	0.82690E-02	0.31707E+04	0.88856E+00
HYDROGEN	0.62983E+03	0.32178E+00	0.16366E+00	0.45865E-04
NITROGEN	0.29525E+02	0.15084E-01	0.54184E-02	0.15185E-05
METHANE	0.78127E+03	0.39915E+00	0.26851E+00	0.75250E-04
ETHANE	0.35443E+03	0.18108E+00	0.91760E-01	0.25715E-04
PROPANE	0.12439E+03	0.63548E-01	0.35321E-01	0.98984E-05
N-BUTANE	0.19699E+01	0.10064E-02	0.32667E-04	0.91548E-08
I-BUTANE	0.19689E+02	0.10059E-01	0.32651E-03	0.91502E-07
TOTAL	0.19573E+04		0.35683E+04	

## APPENDIX 4.2 -- TEST PROBLEM 2 -- NASH CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE OF COLUMN	1
NO. OF PLATES	4
PRESSURE AT TOP PLATE (PSIA)	712.00
PRESSURE DROP PER PLATE (PSIA)	.01
NO. OF FEEDS	3
ENTERING PLATE OF FEED 1	1
FEED QUANTITY	0.757394+05
PRESSURE OF FEED	712.00
TEMPERATURE OF FEED (F)	135.00
ENTERING PLATE OF FEED 2	2
FEED QUANTITY	0.163238+06
PRESSURE OF FEED	712.00
TEMPERATURE OF FEED (F)	145.
ENTERING PLATE OF FEED 3	4
FEED QUANTITY	0.289475+05
PRESSURE OF FEED	712.00
TEMPERATURE OF FEED (F)	100.00

\*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

1. SUM OF SQUARES OF RESIDUALS = 2.13961E+1  
 TEMPERATURE  
 $0.59440E+03 \quad 0.59960E+03 \quad 0.60460E+03 \quad 0.60960E+03$   
 VAPOUR FLOW RATE  
 $0.21131E+05 \quad 0.21131E+05 \quad 0.21131E+05 \quad 0.21131E+05$

2. SUM OF SQUARES OF RESIDUALS = 2.16303E+02  
 TEMPERATURE  
 $0.59511E+03 \quad 0.58438E+03 \quad 0.58479E+03 \quad 0.58931E+03$   
 VAPOUR FLOW RATE  
 $0.21010E+05 \quad 0.21050E+05 \quad 0.21181E+05 \quad 0.21333E+05$

3. SUM OF SQUARES OF RESIDUALS = 2.26640E+03  
 TEMPERATURE  
 $0.59522E+03 \quad 0.60178E+03 \quad 0.60305E+03 \quad 0.62211E+03$   
 VAPOUR FLOW RATE  
 $0.21029E+05 \quad 0.21110E+05 \quad 0.21239E+05 \quad 0.21564E+05$

4. SUM OF SQUARES OF RESIDUALS = 2.38484E+04  
 TEMPERATURE  
 $0.59551E+03 \quad 0.60172E+03 \quad 0.60357E+03 \quad 0.62151E+03$   
 VAPOUR FLOW RATE  
 $0.21025E+05 \quad 0.21111E+05 \quad 0.21249E+05 \quad 0.21542E+05$

5. SUM OF SQUARES OF RESIDUALS = 2.53383E+07  
 TEMPERATURE  
 $0.59552E+03 \quad 0.60179E+03 \quad 0.60484E+03 \quad 0.62151E+03$   
 VAPOUR FLOW RATE  
 $0.21035E+05 \quad 0.21111E+05 \quad 0.21250E+05 \quad 0.21932E+05$

## \*\*\*\*\* COMPARISON TABLE \*\*\*\*\*

## NUMBER OF ITERATIONS = 4

## COMPUTED TEMPERATURE, ENTALPY AND LIQUID FRACTION PROFILE

PLATE	PRESSURE	THERM	LIQUID FLOW	VAPOR FLOW	HEAD	WY
1	712.00	135.9	0.758163+05	0.210351+05	-	-
2	712.00	142.10	0.39138+06	0.211118+05	-	-
3	712.00	148.20	0.390667+06	0.212508+05	-	-
4	712.00	154.30	0.466885+06	0.213328+05	-	-

## \*\*\* PAGE MARKERS \*\*\*

PLATE	PRESSURE	THERM	LIQUID FLOW	VAPOR FLOW	HEAD	WY
1	712.00	135.9	0.758163+05	0.210351+05	-	-
2	712.00	142.10	0.39138+06	0.211118+05	-	-
3	712.00	148.20	0.390667+06	0.212508+05	-	-
4	712.00	154.30	0.466885+06	0.213328+05	-	-

\*\*\* - 2 - \*\*\*

三

•

DATA - NO.		
10	1.7574E+00	1.0L FRM
11	1.4742E+03	1.7121E-13
12	1.7121E+00	1.7121E-13
13	1.7245E+00	1.7245E-11
14	1.7226E+00	1.7226E-12
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		
25		
26		
27		
28		
29		
30		
31		
32		
33		
34		
35		
36		
37		
38		
39		
40		
41		
42		
43		
44		
45		
46		
47		
48		
49		
50		
51		
52		
53		
54		
55		
56		
57		
58		
59		
60		
61		
62		
63		
64		
65		
66		
67		
68		
69		
70		
71		
72		
73		
74		
75		
76		
77		
78		
79		
80		
81		
82		
83		
84		
85		
86		
87		
88		
89		
90		
91		
92		
93		
94		
95		
96		
97		
98		
99		
100		
101		
102		
103		
104		
105		
106		
107		
108		
109		
110		
111		
112		
113		
114		
115		
116		
117		
118		
119		
120		
121		
122		
123		
124		
125		
126		
127		
128		
129		
130		
131		
132		
133		
134		
135		
136		
137		
138		
139		
140		
141		
142		
143		
144		
145		
146		
147		
148		
149		
150		
151		
152		
153		
154		
155		
156		
157		
158		
159		
160		
161		
162		
163		
164		
165		
166		
167		
168		
169		
170		
171		
172		
173		
174		
175		
176		
177		
178		
179		
180		
181		
182		
183		
184		
185		
186		
187		
188		
189		
190		
191		
192		
193		
194		
195		
196		
197		
198		
199		
200		
201		
202		
203		
204		
205		
206		
207		
208		
209		
210		
211		
212		
213		
214		
215		
216		
217		
218		
219		
220		
221		
222		
223		
224		
225		
226		
227		
228		
229		
230		
231		
232		
233		
234		
235		
236		
237		
238		
239		
240		
241		
242		
243		
244		
245		
246		
247		
248		
249		
250		
251		
252		
253		
254		
255		
256		
257		
258		
259		
260		
261		
262		
263		
264		
265		
266		
267		
268		
269		
270		
271		
272		
273		
274		
275		
276		
277		
278		
279		
280		
281		
282		
283		
284		
285		
286		
287		
288		
289		
290		
291		
292		
293		
294		
295		
296		
297		
298		
299		
300		
301		
302		
303		
304		
305		
306		
307		
308		
309		
310		
311		
312		
313		
314		
315		
316		
317		
318		
319		
320		
321		
322		
323		
324		
325		
326		
327		
328		
329		
330		
331		
332		
333		
334		
335		
336		
337		
338		
339		
340		
341		
342		
343		
344		
345		
346		
347		
348		
349		
350		
351		
352		
353		
354		
355		
356		
357		
358		
359		
360		
361		
362		
363		
364		
365		
366		
367		
368		
369		
370		
371		
372		
373		
374		
375		
376		
377		
378		
379		
380		
381		
382		
383		
384		
385		
386		
387		
388		
389		
390		
391		
392		
393		
394		
395		
396		
397		
398		
399		
400		
401		
402		
403		
404		
405		
406		
407		
408		
409		
410		
411		
412		
413		
414		
415		
416		
417		
418		
419		
420		
421		
422		
423		
424		
425		
426		
427		
428		
429		
430		
431		
432		
433		
434		
435		
436		
437		
438		
439		
440		
441		
442		
443		
444		
445		
446		
447		
448		
449		
450		
451		
452		
453		
454		
455		
456		
457		
458		
459		
460		
461		
462		
463		
464		
465		
466		
467		
468		
469		
470		
471		
472		
473		
474		
475		
476		
477		
478		
479		
480		
481		
482		
483		
484		
485		
486		
487		
488		
489		
490		
491		
492		
493		
494		
495		
496		
497		
498		
499		
500		
501		
502		
503		
504		
505		
506		
507		
508		
509		
510		
511		
512		
513		
514		
515		
516		
517		
518		
519		
520		
521		
522		
523		
524		
525		
526		
527		
528		
529		
530		
531		
532		
533		
534		
535		
536		
537		
538		
539		
540		
541		
542		
543		
544		
545		
546		
547		
548		
549		
550		
551		
552		
553		
554		
555		
556		
557		
558		
559		
560		
561		
562		
563		
564		
565		
566		
567		
568		
569		
570		
571		
572		
573		
574		
575		
576		
577		
578		
579		
580		
581		
582		
583		
584		
585		
586		
587		
588		
589		
590		
591		
592		
593		
594		
595		
596		
597		
598		
599		
600		
601		
602		
603		
604		
605		
606		
607		
608		
609		
610		
611		
612		
613		
614		

Ergonomics

	DE	DELT	DE	DELT
1.25	1.86924E+01	1.31415E+01		
C.	1.345E+01	1.34650E+01		
DEA	1.92296E+01	1.24544E+01		
WACER	9.71579E+01	1.34240E+02		
WEDAW	1.20964E+02	1.19464E+02		
TOTAL	1.21235E+02			

L	STATE	N	STATE	N	STATE	N
1.	9.01	-7.74	1.	12.12	8.84	1.
2.	2.47	5.92	+ 7.3	2.	17.79	2.72
3.	1.14	2.55	+ 2.2	3.	4.5	4.23
4.	1.14	7.55	+ 0.4	4.	4.42	1.15
5.	1.54	6.54	+ 7.5	5.	4.4	7.4
6.	1.43	2.32	+ 0.0	6.	1.	1.

PLATE NO. 1  
IN THE TIME OF PEAC

## APPENDIX 4.3 -- TEST PROFILE 3 -- MASTERSHEETATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE OF COOLER

NO. OF PLATES 14

PRESSURE AT CONDENSER (PSIA) 17.0

PRESSURE AT TOP PLATE (PSIA) 18.0

PRESSURE DROP PER PLATE (PSIA) 0.3333

NO. OF FEEDS 1

ENTERING PLATE OF FEED 1 2

FEED QUANTITY 0.37194E+05

PRESSURE OF FEED 100.00

TEMPERATURE OF FEED (F) 100.00

NO. OF INTEC COOLERS OR HEATERS 1

PLATE NO. OF INTEC COOLER OR HEATER 1 14  
HEAT LOAD OF INTEC COOLER OR HEATER 0.11411E+04

## \*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

\* NEGATIVE PARTIAL PRESSURE (S) CALCULATED ARE  
 $\text{H}_2\text{S} = -0.238291\text{E}+01$        $\text{CO}_2 = -0.270499\text{E}-01$

\* NEGATIVE PARTIAL PRESSURE (S) CALCULATED ARE  
 $\text{H}_2\text{S} = -0.254442\text{E}-01$        $\text{CO}_2 = -0.282249\text{E}-02$

0 SUM OF SQUARES OF RESIDUALS = 0.73409E-01

## TEMPERATURE

0.579E+03	0.68960E+03	0.69960E+03	0.72160E+03	0.73360E+03
0.70560E+03	0.70760E+03	0.70960E+03	0.71160E+03	0.71360E+03
0.71560E+03	0.71760E+03	0.71960E+03	0.72160E+03	

## VAPOUR FLOW RATE

0.11400E+04	0.34200E+04	0.50000E+04	0.51000E+04	0.52000E+04
0.53000E+04	0.54000E+04	0.55500E+04	0.56000E+04	0.57000E+04
0.54000E+04	0.59000E+04	0.60000E+04	0.61000E+04	

1 SUM OF SQUARES OF RESIDUALS = 0.15207E-01

## TEMPERATURE

0.57960E+03	0.68725E+03	0.69580E+03	0.72105E+03	0.73422E+03
0.70621E+03	0.70757E+03	0.70895E+03	0.71226E+03	0.71401E+03
0.71532E+03	0.71648E+03	0.71750E+03	0.71814E+03	

## VAPOUR FLOW RATE

0.10800E+04	0.28545E+04	0.46959E+04	0.51882E+04	0.54343E+04
0.55555E+04	0.56241E+04	0.62446E+04	0.61653E+04	0.62699E+04
0.63250E+04	0.64314E+04	0.66211E+04	0.63888E+04	

2 SUM OF SQUARES OF RESIDUALS = 0.65676E-02

## TEMPERATURE

0.57965E+03	0.69145E+03	0.69962E+03	0.72332E+03	0.72561E+03
0.70726E+03	0.70855E+03	0.70961E+03	0.71197E+03	0.71349E+03
0.71463E+03	0.71558E+03	0.71642E+03	0.71803E+03	

## VAPOUR FLOW RATE

0.11317E+04	0.35505E+04	0.50906E+04	0.55470E+04	0.57753E+04
0.59341E+04	0.60839E+04	0.60150E+04	0.61485E+04	0.63430E+04
0.64456E+04	0.65344E+04	0.66400E+04	0.67125E+04	

3 SUM OF SQUARES OF RESIDUALS = 0.16728E-02

## TEMPERATURE

0.57960E+03	0.68678E+03	0.69545E+03	0.70054E+03	0.70362E+03
0.70567E+03	0.70747E+03	0.71067E+03	0.71246E+03	0.71373E+03
0.71475E+03	0.71564E+03	0.71650E+03	0.71809E+03	

## VAPOUR FLOW RATE

0.11238E+04	0.29125E+04	0.45638E+04	0.51074E+04	0.54324E+04
0.56340E+04	0.62236E+04	0.59381E+04	0.61748E+04	0.63117E+04
0.64104E+04	0.64907E+04	0.65449E+04	0.65932E+04	

4 SUM OF SQUARES OF RESIDUALS: 0.24386E+03

TEMPERATURE

0.579E+03	0.6894E+03	0.6976E+03	0.7220E+03	0.7247E+03
0.70663E+03	0.7080E+03	0.7109E+03	0.7125E+03	0.7138E+03
0.71479E+03	0.71568E+03	0.71653E+03	0.71809E+03	

VAPOUR FLOW RATE

0.11295E+04	0.33298E+04	0.49012E+04	0.53376E+04	0.55966E+04
0.57781E+04	0.57800E+04	0.60276E+04	0.62240E+04	0.63453E+04
0.64307E+04	0.64966E+04	0.65574E+04	0.66131E+04	

5 SUM OF SQUARES OF RESIDUALS: 0.76442E+04

TEMPERATURE

0.57960E+03	0.68743E+03	0.69582E+03	0.70077E+03	0.72382E+03
0.70589E+03	0.70739E+03	0.71064E+03	0.71246E+03	0.71373E+03
0.71475E+03	0.71566E+03	0.71652E+03	0.71809E+03	

VAPOUR FLOW RATE

0.11250E+04	0.31005E+04	0.46488E+04	0.51566E+04	0.54719E+04
0.56564E+04	0.58512E+04	0.59855E+04	0.62083E+04	0.63346E+04
0.64217E+04	0.64921E+04	0.65541E+04	0.66071E+04	

6 SUM OF SQUARES OF RESIDUALS: 0.79214E+05

TEMPERATURE

0.57960E+03	0.68842E+03	0.69666E+03	0.70133E+03	0.70421E+03
0.70619E+03	0.70766E+03	0.71074E+03	0.71251E+03	0.71376E+03
0.71477E+03	0.71566E+03	0.71652E+03	0.71808E+03	

VAPOUR FLOW RATE

0.11302E+04	0.32464E+04	0.48199E+04	0.52678E+04	0.55429E+04
0.57375E+04	0.58466E+04	0.60085E+04	0.62193E+04	0.63422E+04
0.64284E+04	0.64972E+04	0.65577E+04	0.66109E+04	

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 6

REFFLUX RATIO 1.87243

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

0.100E+03 PSIA 0.200E+03 F 0.207E+09 BTU 1.0

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP F	LIQUID FLOW LB MOL/TIME	VAPOUR FLOW LB MOL/TIME	HEAT DUTY BTU/TIME
1	27.00	120.00	0.21162E+04	0.11302E+04	-0.41422E+08
2	28.00	228.82	0.40884E+05	0.32464E+04	0.0
3	28.33	237.06	0.41332E+05	0.48199E+04	0.0
4	28.67	241.73	0.41607E+05	0.52678E+04	0.0
5	29.00	244.61	0.41801E+05	0.55429E+04	0.0
6	29.33	246.59	0.41910E+05	0.57375E+04	0.0
7	29.67	248.06	0.42072E+05	0.58466E+04	0.0
8	30.00	251.14	0.42283E+05	0.60085E+04	0.0
9	30.33	252.91	0.42406E+05	0.62193E+04	0.0
10	30.67	254.15	0.42492E+05	0.63422E+04	0.0
11	31.00	255.17	0.42561E+05	0.64284E+04	0.0
12	31.33	256.06	0.42621E+05	0.64972E+04	0.0
13	31.67	256.92	0.42675E+05	0.65577E+04	0.0
14	32.00	258.48	0.36064E+05	0.66109E+04	0.11411E+04

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS

	PLATE NO.	LB MOL/TIME	MOL FRAC	PLATE NO.	LB MOL/TIME	MOL FRAC
H2S	2	0.11402E+04	0.30656E-01			
CO2		0.10180E+03	0.27370E-02			
MEA		0.32200E+04	0.96573E-01			
WATER		0.32730E+05	0.87998E+00			
HYDROGEN		0.67000E+00	0.18014E-04			
NITROGEN		0.40000E-01	0.10754E-05			
METHANE		0.57000E+00	0.15325E-04			
ETHANE		0.32000E+00	0.86036E-05			
PROPANE		0.34000E+00	0.91413E-05			
TOTAL		0.37194E+05				

## PRODUCTS

	TOP PRODUCT		BOTTOM PRODUCT	
	LB MOL/TIME	MOL FRAC	LB MOL/TIME	MOL FRAC
H2S	0.10151E+04	0.89818E+00	0.12507E+03	0.34679E-02
CO2	0.42485E+02	0.37590E-01	0.59326E+02	0.16450E-02
MEA	0.12591E-01	0.11141E-04	0.32200E+04	0.89286E-01
WATER	0.70643E+02	0.62505E-01	0.32659E+05	0.90560E+00
HYDROGEN	0.66997E+00	0.59279E-03	0.24524E-30	0.68002E-35
NITROGEN	0.39998E-01	0.35390E-04	0.14811E-31	0.41069E-36
METHANE	0.56998E+00	0.50431E-03	0.20497E-30	0.56835E-35
ETHANE	0.31999E+00	0.28312E-03	0.11647E-30	0.32297E-35
PROPANE	0.33999E+00	0.30082E-03	0.12432E-30	0.34471E-35
TOTAL	0.11302E+04		0.36064E+05	

## APPENDIX 4.4 -- TEST PROBLEM 4 -- NASTR CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE	COLUMN	3
NO. OF PLATES	14	
PRESSURE OF CONDENSER (PSIA)		25.00
PRESSURE AT TOP PLATE (PSIA)		27.00
PRESSURE DROP PER PLATE (PSIA)		0.3333
NO. OF FEEDS	1	
ENTERING PLATE OF FEED 1	2	
FEED QUANTITY	0.64652E+04	
PRESSURE OF FEED	48.00	
TEMPERATURE OF FEED (F)	180.00	
NO. OF INTER COOLERS OR HEATERS	1	
PLATE NO. OF INTER COOLER OR HEATER 1	14	
HEAT LOAD OF INTER COOLER OR HEATER	0.16171E+08	

## \*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

0 SUM OF SQUARES OF RESIDUALS 0.13119E+01

TEMPERATURE  
 0.55960E+03 0.67960E+03 0.69160E+03 0.69360E+03 0.69560E+03  
 0.69760F+03 0.69960E+03 0.70160E+03 0.70360E+03 0.70560E+03  
 0.70760E+03 0.70960E+03 0.71160E+03 0.71360F+03

VAPOUR FLOW RATE  
 0.16000E+03 0.40000E+03 0.70000E+03 0.85000E+03 0.90000E+03  
 0.90500E+03 0.91000E+03 0.91500E+03 0.92000E+03 0.92500E+03  
 0.93000E+03 0.93500E+03 0.94000E+03 0.94500E+03

1 SUM OF SQUARES OF RESIDUALS 0.60658E+00

TEMPERATURE  
 0.55960E+03 0.68083E+03 0.70406E+03 0.71532E+03 0.71772E+03  
 0.71510E+03 0.71142E+03 0.70892E+03 0.70802E+03 0.70846E+03  
 0.70929E+03 0.71061E+03 0.71219E+03 0.71382E+03

VAPOUR FLOW RATE  
 0.15811E+03 0.40919E+03 0.11628E+04 0.17000E+04 0.17940E+04  
 0.15993E+04 0.13649E+04 0.11829E+04 0.10692E+04 0.10334E+04  
 0.97892E+03 0.95271E+03 0.95045E+03 0.96213E+03

2 SUM OF SQUARES OF RESIDUALS 0.40929E-01

TEMPERATURE  
 0.55960F+03 0.68274E+03 0.70159E+03 0.71046E+03 0.71284E+03  
 0.71108E+03 0.70955E+03 0.70954E+03 0.71032E+03 0.71106E+03  
 0.71181E+03 0.71262E+03 0.71348E+03 0.71433E+03

VAPOUR FLOW RATE  
 0.14895E+03 0.41116E+03 0.79477E+03 0.85000E+03 0.93640E+03  
 0.10469E+04 0.11254E+04 0.11478E+04 0.11187E+04 0.10569E+04  
 0.99671E+03 0.96144E+03 0.96219E+03 0.98713E+03

3 SUM OF SQUARES OF RESIDUALS 0.30413E-01

TEMPERATURE  
 0.55960E+03 0.67193E+03 0.69525E+03 0.70264E+03 0.70619E+03  
 0.70738E+03 0.70826E+03 0.70920E+03 0.71010E+03 0.71091E+03  
 0.71169E+03 0.71244E+03 0.71313E+03 0.71417E+03

VAPOUR FLOW RATE  
 0.15120E+03 0.25868E+03 0.60126E+03 0.79191E+03 0.85373E+03  
 0.90686E+03 0.93104E+03 0.93041E+03 0.92620E+03 0.93081E+03  
 0.93116E+03 0.93446E+03 0.94412E+03 0.95226E+03

4 SUM OF SQUARES OF RESIDUALS 0.11390E-01

TEMPERATURE

0.55960E+03	0.69421E+03	0.70902E+03	0.70736E+03	0.70743E+03
0.70822E+03	0.70893E+03	0.70967E+03	0.71041E+03	0.71112E+03
0.71181E+03	0.71248E+03	0.71316E+03	0.71422E+03	

VAPOUR FLOW RATE

0.15218E+03	0.43760E+03	0.10774E+04	0.10142E+04	0.10226E+04
0.94482E+03	0.91686E+03	0.91574E+03	0.91948E+03	0.92328E+03
0.92856E+03	0.93587E+03	0.94154E+03	0.94372E+03	

5 SUM OF SQUARES OF RESIDUALS 0.10163E-01

TEMPERATURE

0.55960E+03	0.68785E+03	0.70613E+03	0.70605E+03	0.70694E+03
0.70783E+03	0.70862E+03	0.70941E+03	0.71017E+03	0.71091E+03
0.71162E+03	0.71232E+03	0.71304E+03	0.71416E+03	

VAPOUR FLOW RATE

0.14345E+03	0.32820E+03	0.83056E+03	0.93827E+03	0.94255E+03
0.91527E+03	0.90542E+03	0.90866E+03	0.91426E+03	0.91987E+03
0.92618E+03	0.93307E+03	0.93886E+03	0.94314E+03	

6 SUM OF SQUARES OF RESIDUALS 0.49111E-02

TEMPERATURE

0.55960E+03	0.68023E+03	0.70188E+03	0.70433E+03	0.70624E+03
0.70746E+03	0.70843E+03	0.70930E+03	0.71009E+03	0.71086E+03
0.71160E+03	0.71232E+03	0.71305E+03	0.71416E+03	

VAPOUR FLOW RATE

0.14794E+03	0.30456E+03	0.69042E+03	0.90918E+03	0.92664E+03
0.92673E+03	0.92603E+03	0.92887E+03	0.93509E+03	0.94009E+03
0.94510E+03	0.94930E+03	0.95216E+03	0.95401E+03	

7 SUM OF SQUARES OF RESIDUALS 0.63528E-03

TEMPERATURE

0.55960E+03	0.67499E+03	0.69641E+03	0.70291E+03	0.70588E+03
0.70735E+03	0.70841E+03	0.70929E+03	0.71010E+03	0.71087E+03
0.71161E+03	0.71234E+03	0.71306E+03	0.71416E+03	

VAPOUR FLOW RATE

0.15119E+03	0.33342E+03	0.64897E+03	0.87725E+03	0.90757E+03
0.92076E+03	0.92451E+03	0.92883E+03	0.93164E+03	0.93576E+03
0.93979E+03	0.94338E+03	0.94667E+03	0.94931E+03	

453

3 SUM OF SQUARES OF RESIDUALS 0.10255E+03

TEMPERATURE

0.55960E+03	0.67626E+03	0.69710E+03	0.70315E+03	0.70600E+03
0.70744E+03	0.70848E+03	0.70935E+03	0.71015E+03	0.71091E+03
0.71164E+03	0.71237E+03	0.71308E+03	0.71418E+03	

VAPOUR FLOW RATE

0.14975E+03	0.33970E+03	0.69809E+03	0.87492E+03	0.89789E+03
0.90970E+03	0.91465E+03	0.91937E+03	0.92362E+03	0.92841E+03
0.93315E+03	0.93773E+03	0.94222E+03	0.94605E+03	

4 SUM OF SQUARES OF RESIDUALS 0.18993E-04

TEMPERATURE

0.55960E+03	0.67806E+03	0.69781E+03	0.70341E+03	0.70612E+03
0.70752E+03	0.70853E+03	0.70939E+03	0.71017E+03	0.71092E+03
0.71165E+03	0.71236E+03	0.71307E+03	0.71416E+03	

VAPOUR FLOW RATE

0.14807E+03	0.35130E+03	0.73334E+03	0.87051E+03	0.89044E+03
0.90239E+03	0.90875E+03	0.91414E+03	0.91962E+03	0.92497E+03
0.93048E+03	0.93593E+03	0.94112E+03	0.94581E+03	

10 SUM OF SQUARES OF RESIDUALS 0.62679E-05

TEMPERATURE

0.55960E+03	0.67745E+03	0.69751E+03	0.70331E+03	0.70607E+03
0.70748E+03	0.70849E+03	0.70935E+03	0.71013E+03	0.71088E+03
0.71160E+03	0.71232E+03	0.71304E+03	0.71415E+03	

VAPOUR FLOW RATE

0.14794E+03	0.34532E+03	0.71843E+03	0.86818E+03	0.89197E+03
0.90486E+03	0.91128E+03	0.91685E+03	0.92227E+03	0.92776E+03
0.93315E+03	0.93834E+03	0.94315E+03	0.94720E+03	

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 10

REFLUX RATIO 1.33415

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

6.480E+02 PSIA 6.182E+03 F 3.373E+03 BTU 1.0

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP F	LIQUID FLOW LB MOL/TIME	VAPOUR FLOW LB MOL/TIME	HEAT DUTY BTU/TIME
1	25.00	100.00	0.19738E+03	0.14794E+03	-0.25199E+07
2	27.00	217.85	0.70357E+04	0.34532E+03	0.0
3	27.33	237.91	0.71855E+04	0.71843E+03	0.0
4	27.67	243.71	0.72093E+04	0.86818E+03	0.0
5	28.00	246.47	0.72221E+04	0.89197E+03	0.0
6	28.33	247.88	0.72286E+04	0.90486E+03	0.0
7	28.67	248.89	0.72341E+04	0.91128E+03	0.0
8	29.00	249.75	0.72395E+04	0.91685E+03	0.0
9	29.33	250.53	0.72450E+04	0.92227E+03	0.0
10	29.67	251.28	0.72504E+04	0.92776E+03	0.0
11	30.00	252.00	0.72556E+04	0.93315E+03	0.0
12	30.33	252.72	0.72604E+04	0.93834E+03	0.0
13	30.67	253.44	0.72645E+04	0.94315E+03	0.0
14	31.00	254.55	0.63173E+04	0.94720E+03	0.16171E+08

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS

	PLATE NO. 1 / LB. MOL/TIME	MOL FRAC	PLATE NO. LB. MOL/TIME	MOL FRAC
H2S	0.37820E+02	0.58498E-01		
CO2	0.12371E+03	0.19135E-01		
DEA	0.29038E+03	0.44991E-01		
WATER	0.60124E+04	0.92995E+00		
METHANE	0.43000E+03	0.66510E-04		
ETHANE	0.30000E-01	0.46402E-05		
PROPANE	0.10000E-01	0.15467E-05		
TOTAL	0.64652E+04			

## PRODUCTS

	TOP PRODUCT LB. MOL/TIME	MOL FRAC	BOTTOM PRODUCT LB. MOL/TIME	MOL FRAC
H2S	0.35121E+02	0.23739E+00	0.26943E+01	0.42649E-03
CO2	0.10672E+03	0.72138E+00	0.16376E+02	0.26872E-02
DEA	0.49738E+03	0.33613E-10	0.29088E+03	0.46045E-01
WATER	0.56298E+01	0.38054E-01	0.60067E+04	0.95084E+01
METHANE	0.42992E+00	0.29060E-02	0.11638E-27	0.18423E-31
ETHANE	0.29995E-01	0.20274E-03	0.34490E-29	0.13375E-32
PROPANE	0.99982E-02	0.57581E-04	0.28948E-29	0.45824E-33
TOTAL	0.14794E+03		0.63173E+04	

## APPENDIX G.1 - ELEMENT PROBLEMS 1 - TANKAGE CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE OF COLUMN 1

NO. OF PLATES 20

PRESSURE AT TOP PLATE (PSIA) 150.00

PRESSURE DROP PER PLATE (PSIA)

NO. OF FEEDS 3

ENTERING PLATE OF FEED 1	1
FEED QUANTITY	0.69583E+03
PRESSURE OF FEED	150.00
TEMPERATURE OF FEED (F)	100.00

ENTERING PLATE OF FEED 2	4
FEED QUANTITY	0.23612E+04
PRESSURE OF FEED	150.00
TEMPERATURE OF FEED (F)	120.00

ENTERING PLATE OF FEED 3	20
FEED QUANTITY	0.39686E+04
PRESSURE OF FEED	150.00
TEMPERATURE OF FEED (F)	95.00

## \*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

3. SUM OF SQUARES OF RESIDUALS = 6.107E-13E+00

## TEMPERATURE

0.5690CE+03	0.5700E+03	0.5700E+03	0.5700E+03	0.5700E+03	0.5700E+03
0.5790CE+03	0.5790E+03	0.5790E+03	0.5790E+03	0.5790E+03	0.5790E+03
0.5790CE+03	0.5790E+03	0.5790E+03	0.5790E+03	0.5790E+03	0.5790E+03
0.5790CE+03	0.5790E+03	0.5790E+03	0.5790E+03	0.5790E+03	0.5790E+03

## VAPOUR FLOW RATE

0.1961CE+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04
0.1961CE+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04
0.1961CE+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04
0.1961CE+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04	0.19600E+04

1. SUM OF SQUARES OF RESIDUALS = 6.48444E-01

## TEMPERATURE

0.56920E+03	0.56912E+03	0.56912E+03	0.56912E+03	0.56912E+03	0.56912E+03
0.56931E+03	0.56931E+03	0.56931E+03	0.56931E+03	0.56931E+03	0.56931E+03
0.56931E+03	0.56931E+03	0.56931E+03	0.56930E+03	0.56931E+03	0.56931E+03
0.56931E+03	0.56931E+03	0.56931E+03	0.56931E+03	0.56931E+03	0.56931E+03

## VAPOUR FLOW RATE

0.19654E+04	0.19765E+04	0.19628E+04	0.19533E+04	0.19532E+04	0.19532E+04
0.19532E+04	0.19532E+04	0.19532E+04	0.19532E+04	0.19532E+04	0.19532E+04
0.19532E+04	0.19532E+04	0.19532E+04	0.19532E+04	0.19532E+04	0.19532E+04
0.19531E+04	0.19529E+04	0.19528E+04	0.19528E+04	0.19528E+04	0.19528E+04

2. SUM OF SQUARES OF RESIDUALS = 6.16473E-01

## TEMPERATURE

0.56619E+03	0.56268E+03	0.56692E+03	0.57490E+03	0.57640E+03	0.57490E+03
0.57490E+03	0.57490E+03	0.57490E+03	0.57490E+03	0.57490E+03	0.57490E+03
0.57490E+03	0.57490E+03	0.57488E+03	0.57485E+03	0.57474E+03	0.57474E+03
0.57448E+03	0.57382E+03	0.57247E+03	0.57080E+03	0.57636E+03	0.57636E+03

## VAPOUR FLOW RATE

0.19505E+04	0.19364E+04	0.19151E+04	0.19595E+04	0.19597E+04	0.19597E+04
0.19597E+04	0.19597E+04	0.19597E+04	0.19597E+04	0.19597E+04	0.19597E+04
0.19597E+04	0.19597E+04	0.19596E+04	0.19596E+04	0.19596E+04	0.19596E+04
0.19595E+04	0.19591E+04	0.19585E+04	0.19574E+04	0.19580E+04	0.19580E+04

3. SUM OF SQUARES OF RESIDUALS = 6.26886E-02

## TEMPERATURE

0.56643E+03	0.57893E+03	0.59404E+03	0.58226E+03	0.58326E+03	0.58326E+03
0.58326E+03	0.58326E+03	0.58326E+03	0.58325E+03	0.58325E+03	0.58325E+03
0.58325E+03	0.58325E+03	0.58323E+03	0.58320E+03	0.58313E+03	0.58313E+03
0.58299E+03	0.58278E+03	0.58254E+03	0.58223E+03	0.57896E+03	0.57896E+03

## VAPOUR FLOW RATE

0.1950CE+04	0.19595E+04	0.19646E+04	0.19651E+04	0.19649E+04	0.19649E+04
0.19649E+04	0.19649E+04	0.19649E+04	0.19649E+04	0.19649E+04	0.19649E+04
0.19649E+04	0.19649E+04	0.19649E+04	0.19649E+04	0.19649E+04	0.19649E+04
0.19647E+04	0.19645E+04	0.19643E+04	0.19639E+04	0.19642E+04	0.19642E+04



## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

## NUMBER OF PREPARATIONS

## PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID REACTION IN PPSI

1.150E+03 PSIA	1.177E+13 F	1.246E+07 BTU	1.1
1.150E+03 PSIA	1.120E+13 F	1.148E+07 BTU	1.1
1.150E+03 PSIA	1.048E+13 F	1.124E+07 BTU	1.1

## \*\*\* SEAGE VARIATION \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP F	Liquid FLOW LB/HOUR/TIME	VAPOR FLOW LB/HOUR/TIME	HEAT DUTY BTU/HOUR/TIME
1	150.00	110.32	0.35627E+04	0.19574E+04	
2	150.00	110.32	0.35627E+04	0.19631E+04	
3	150.00	120.77	0.35629E+04	0.19622E+04	
4	150.00	120.77	0.35629E+04	0.19634E+04	
5	150.00	120.27	0.35629E+04	0.19632E+04	
6	150.00	120.27	0.35629E+04	0.19632E+04	
7	150.00	120.27	0.35629E+04	0.19632E+04	
8	150.00	120.27	0.35629E+04	0.19632E+04	
9	150.00	120.27	0.35629E+04	0.19632E+04	
10	150.00	120.27	0.35629E+04	0.19632E+04	
11	150.00	120.26	0.35629E+04	0.19632E+04	
12	150.00	120.26	0.35629E+04	0.19632E+04	
13	150.00	120.25	0.35629E+04	0.19632E+04	
14	150.00	120.24	0.35629E+04	0.19632E+04	
15	150.00	120.21	0.35628E+04	0.19632E+04	
16	150.00	120.15	0.35627E+04	0.19632E+04	
17	150.00	120.15	0.35625E+04	0.19631E+04	
18	150.00	119.72	0.35622E+04	0.19529E+04	
19	150.00	118.77	0.35619E+04	0.19625E+04	
20	150.00	116.24	0.35683E+04	0.19623E+04	

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS

	PLATE NO.	1
	LB MOL/TIME	MOL FRAC
H2S	0.12800E+01	0.18395E-02
CO2	0.15700E+01	0.22563E-02
MEA	0.62000E+02	0.89174E-01
H2O	0.63043E+03	0.90671E+02
HYDROGEN	0.0	0.0
NITROGEN	0.0	0.0
METHANE	0.0	0.0
ETHANE	0.0	0.0
PROPANE	0.0	0.0
NBUTANE	0.0	0.0
IBUTANE	0.0	0.0
TOTAL	0.639583E+03	

	PLATE NO.	4
	LB MOL/TIME	MOL FRAC
H2S	0.54300E+02	0.18978E-01
CO2	0.63000E+01	0.22219E-02
MEA	0.25000E+03	0.87377E-01
H2O	0.25500E+04	0.84124E+00
HYDROGEN	0.0	0.0
NITROGEN	0.0	0.0
METHANE	0.0	0.0
ETHANE	0.0	0.0
PROPANE	0.0	0.0
NBUTANE	0.0	0.0
IBUTANE	0.0	0.0
TOTAL	0.28612E+04	

	PLATE NO.	20
	LB MOL/TIME	MOL FRAC
H2S	0.18700E+02	0.944989E-11
CO2	0.22500E+01	0.14985E-02
MEA	0.0	0.0
H2O	0.59100E+01	0.30121E-02
HYDROGEN	0.629978E+03	0.32022E+00
NITROGEN	0.29530E+02	0.15037E-01
METHANE	0.78155E+03	0.39700E+00
ETHANE	0.35436E+03	0.18000E+00
PROPANE	0.12402E+03	0.62997E-01
NBUTANE	0.19700E+01	0.10007E-02
IBUTANE	0.19690E+02	0.10002E-01
TOTAL	0.12686E+04	

	PLATE NO.	
	LB MOL/TIME	MOL FRAC

## PRODUCTS

	TOP PRODUCT	
	LB MOL/TIME	MOL FRAC
H2S	0.30962E-01	0.15818E-04
CO2	0.42326E-03	0.21624E-06
MEA	0.38818E-01	0.19832E-04
H2O	0.16195E+02	0.82738E-02
HYDROGEN	0.62984E+03	0.32178E+00
NITROGEN	0.29525E+02	0.15084E-01
METHANE	0.78126E+03	0.39914E+00
ETHANE	0.35443E+03	0.18108E+00
PROPANE	0.12438E+03	0.63544E-01
NBUTANE	0.19699E+01	0.10064E-02
IBUTANE	0.19689E+02	0.10059E-01
TOTAL	0.19574E+04	

	BOTTOM PRODUCT	
	LB MOL/TIME	MOL FRAC
H2S	0.74242E+02	0.20808E-01
CO2	0.10820E+02	0.30321E-02
MEA	0.31201E+03	0.87439E-01
H2O	0.3107E+04	0.88856E+00
HYDROGEN	0.16365E+00	0.45862E-04
NITROGEN	0.54187E-02	0.15186E-05
METHANE	0.26857E+00	0.75264E-04
ETHANE	0.91769E-01	0.25718E-04
PROPANE	0.35337E-01	0.99030E-05
NBUTANE	0.32656E-04	0.91517E-08
IBUTANE	0.32640E-03	0.91471E-07
TOTAL	0.35683E+04	

## APPENDIX 4.0 -- TEST PROBLEM 2 -- AMOCO CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE OF COLUMN 1

NO. OF PLATES 4

PRESSURE AT TOP PLATE (PSIA) 712.00

PRESSURE DROP PER PLATE (PSIA) 0.0

NO. OF FEEDS 3

ENTERING PLATE OF FEED 1 1

FEED QUANTITY 0.75739E+05

PRESSURE OF FEED 712.00

TEMPERATURE OF FEED (F) 135.00

ENTERING PLATE OF FEED 2 2

FEED QUANTITY 0.16923E+06

PRESSURE OF FEED 712.00

TEMPERATURE OF FEED (F) 145.00

ENTERING PLATE OF FEED 3 3

FEED QUANTITY 0.28947E+05

PRESSURE OF FEED 712.00

TEMPERATURE OF FEED (F) 100.00

\*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

0 SUM OF SQUARES OF RESIDUALS 0.13973E+01

TEMPERATURE

0.59460E+03 0.59960E+03 0.60460E+03 0.60960E+03

VAPOUR FLOW RATE

0.21131E+05 0.21131E+05 0.21131E+05 0.21131E+05

1 SUM OF SQUARES OF RESIDUALS 0.16778E-01

TEMPERATURE

0.59510E+03 0.58437E+03 0.58478E+03 0.58931E+03

VAPOUR FLOW RATE

0.21010E+05 0.21049E+05 0.21180E+05 0.21235E+05

2 SUM OF SQUARES OF RESIDUALS 0.17026E-02

TEMPERATURE

0.59522E+03 0.60177E+03 0.60273E+03 0.62211E+03

VAPOUR FLOW RATE

0.21039E+05 0.21110E+05 0.21138E+05 0.21613E+05

3 SUM OF SQUARES OF RESIDUALS 0.10453E-05

TEMPERATURE

0.59551E+03 0.60173E+03 0.60379E+03 0.62151E+03

VAPOUR FLOW RATE

0.21043E+05 0.21109E+05 0.21241E+05 0.21690E+05

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 3

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

0.712E+03 PSIA	0.135E+03 F	0.453E+09 BTU	1.0
0.712E+03 PSIA	0.145E+03 F	0.924E+09 BTU	1.0
0.712E+03 PSIA	0.100E+03 F	0.154E+09 BTU	0.0

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP F	LIQUID FLOW LB MOLE/TIME	VAPOUR FLOW LB MOLE/TIME	HEAT DUTY BTU/TIME
1	712.00	135.91	0.75816E+05	0.2413E+05	0.0
2	712.00	142.13	0.23918E+06	0.23918E+05	0.0
3	712.00	144.19	0.23963E+06	0.23963E+05	0.0
4	712.00	161.91	0.24688E+06	0.2700E+05	0.0

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS

	PLATE NO.	LB MOL/TIME	MOL FRAC	PLATE NO.	LB MOL/TIME	MOL FRAC
H2S	1	0.36300E+02	0.47928E-03	2	0.29050E+01	0.17797E-02
CO2		0.28130E+02	0.37101E-03		0.14225E+03	0.85923E-03
DEA		0.54150E+04	0.71495E-01		0.81475E+04	0.49915E-01
H2O		0.70260E+05	0.92765E+00		0.15465E+06	0.94745E+00
METHANE		0.0	0.0		0.0	0.0
TOTAL		0.75739E+05			0.16323E+06	

	PLATE NO.	LB MOL/TIME	MOL FRAC
H2S	4	0.69480E+02	0.24002E+00
CO2		0.86840E+03	0.30000E-01
DEA		0.0	0.0
H2O		0.0	0.0
METHANE		0.21131E+05	0.72998E+00
TOTAL		0.28947E+05	

## PRODUCTS

	TOP PRODUCT	LB MOL/TIME	MOL FRAC
H2S	1	0.33056E-01	0.15716E-05
CO2		0.20321E-02	0.96614E-07
DEA		0.52450E-03	0.24937E-07
H2O		0.71196E+02	0.33850E-02
METHANE		0.20962E+05	0.99661E+00
TOTAL		0.21033E+05	

	BOTTOM PRODUCT	LB MOL/TIME	MOL FRAC
H2S	2	0.72748E+04	0.29467E-01
CO2		0.10367E+04	0.41994E-02
DEA		0.13563E+05	0.54935E-01
H2O		0.22484E+06	0.91072E+00
METHANE		0.162E+03	0.68332E-03
TOTAL		0.2462E+06	

## APPENDIX 4.7 -- TEST PROBLEM 3 -- AMOCO CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE OF COLUMN

NO. OF PLATES 14

PRESSURE OF CONDENSER (PSIA) 27.00

PRESSURE AT TOP PLATE (PSIA) 28.00

PRESSURE DROP PER PLATE (PSIA) 0.3333

NO. OF FEEDS 1

ENTERING PLATE OF FEED 1 2

FEED QUANTITY 0.37194E+05

PRESSURE OF FEED 100.00

TEMPERATURE OF FEED (F) 200.00

NO. OF INTER COOLERS OR HEATERS 1

PLATE NO. OF INTER COOLER OR HEATER 1 14

HEAT LOAD OF INTER COOLER OR HEATER 0.11411E+09

## \*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

0 SUM OF SQUARES OF RESIDUALS 1.26205E+00

## TEMPERATURE

0.57960E+03	0.68960E+03	0.69060E+03	0.70160E+03	0.70360E+03
0.70560E+03	0.70760E+03	0.70960E+03	0.71160E+03	0.71360E+03
0.71560E+03	0.71760E+03	0.71960E+03	0.72160E+03	

## VAPOUR FLOW RATE

0.11400E+04	0.34200E+04	0.50000E+04	0.51000E+04	0.52000E+04
0.53000E+04	0.54000E+04	0.55000E+04	0.56000E+04	0.57000E+04
0.58000E+04	0.59000E+04	0.60000E+04	0.61000E+04	

1 SUM OF SQUARES OF RESIDUALS 0.37847E-01

## TEMPERATURE

0.57960E+03	0.68950E+03	0.70042E+03	0.70641E+03	0.70980E+03
0.71150E+03	0.71240E+03	0.71303E+03	0.71368E+03	0.71444E+03
0.71532E+03	0.71627E+03	0.71723E+03	0.71801E+03	

## VAPOUR FLOW RATE

0.0779E+04	0.31658E+04	0.56570E+04	0.63350E+04	0.65563E+04
0.63747E+04	0.65053E+04	0.64120E+04	0.63447E+04	0.63257E+04
0.63654E+04	0.64685E+04	0.66388E+04	0.68862E+04	

2 SUM OF SQUARES OF RESIDUALS 0.89532E-03

## TEMPERATURE

0.57960E+03	0.69033E+03	0.70034E+03	0.70531E+03	0.70815E+03
0.70990E+03	0.71115E+03	0.71217E+03	0.71309E+03	0.71396E+03
0.71481E+03	0.71565E+03	0.71651E+03	0.71815E+03	

## VAPOUR FLOW RATE

0.11328E+04	0.35037E+04	0.50716E+04	0.55503E+04	0.58848E+04
0.61111E+04	0.62559E+04	0.63459E+04	0.64048E+04	0.64498E+04
0.64927E+04	0.65428E+04	0.66162E+04	0.66775E+04	

3 SUM OF SQUARES OF RESIDUALS 0.13085E-03

## TEMPERATURE

0.57960E+03	0.68717E+03	0.69784E+03	0.70375E+03	0.70706E+03
0.70916E+03	0.71067E+03	0.71189E+03	0.71294E+03	0.71389E+03
0.71479E+03	0.71565E+03	0.71652E+03	0.71814E+03	

## VAPOUR FLOW RATE

0.11318E+04	0.30258E+04	0.46829E+04	0.53552E+04	0.57438E+04
0.59709E+04	0.61153E+04	0.62168E+04	0.62956E+04	0.63626E+04
0.64239E+04	0.64829E+04	0.65409E+04	0.66001E+04	

4 SUM OF SQUARES OF RESIDUALS 0.15614E+04

TEMPERATURE

0.57960E+03	0.68870E+03	0.69870E+03	0.71420E+03	0.70731E+03
0.70931E+03	0.71077E+03	0.71195E+03	0.71298E+03	0.71393E+03
0.71482E+03	0.71568E+03	0.71655E+03	0.71815E+03	

VAPOUR FLOW RATE

0.11429E+04	0.32854E+04	0.48773E+04	0.54393E+04	0.57764E+04
0.59785E+04	0.61118E+04	0.62108E+04	0.62912E+04	0.63608E+04
0.64239E+04	0.64833E+04	0.65419E+04	0.65982E+04	

5 SUM OF SQUARES OF RESIDUALS 0.39864E+05

TEMPERATURE

0.57960E+03	0.68781E+03	0.69806E+03	0.70387E+03	0.70714E+03
0.70921E+03	0.71071E+03	0.71191E+03	0.71295E+03	0.71390E+03
0.71479E+03	0.71566E+03	0.71653E+03	0.71814E+03	

VAPOUR FLOW RATE

0.11360E+04	0.31703E+04	0.47453E+04	0.53621E+04	0.57343E+04
0.59538E+04	0.60956E+04	0.61983E+04	0.62805E+04	0.63512E+04
0.64154E+04	0.64765E+04	0.65366E+04	0.65942E+04	

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 5

REFLUX RATIO 1.79674

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

0.100E+03 PSIA 0.200E+3 F 0.2075E+09 BTU 1.0

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP F	LIQUID FLOW LB MOLE/TIME	VAPOR FLOW LB MOLE/TIME	HEAT DUE Y BTU/TIME
1	27.00	120.00	0.20343E+04	0.11360E+04	-0.41285E+08
2	28.00	228.21	0.40803E+05	0.31703E+04	0.0
3	28.33	238.46	0.41420E+05	0.47453E+04	0.0
4	28.67	244.27	0.41792E+05	0.53621E+04	0.0
5	29.00	247.54	0.42012E+05	0.57343E+04	0.0
6	29.33	249.61	0.42154E+05	0.59538E+04	0.0
7	29.67	251.11	0.42256E+05	0.60956E+04	0.0
8	30.00	252.31	0.42338E+05	0.61983E+04	0.0
9	30.33	253.35	0.42409E+05	0.62805E+04	0.0
10	30.67	254.30	0.42473E+05	0.63512E+04	0.0
11	31.00	255.19	0.42534E+05	0.64154E+04	0.0
12	31.33	256.06	0.42595E+05	0.64765E+04	0.0
13	31.67	256.93	0.42652E+05	0.65366E+04	0.0
14	32.00	258.54	0.36058E+05	0.65366E+04	0.11411E+09

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS

	PLATE NO.		PLATE NO.	
	LB MOLE/TIME	MOL FRAC	LB MOLE/TIME	MOL FRAC
H <sub>2</sub> S	0.11402E+04	0.32656E-11		
CO <sub>2</sub>	0.10180E+03	0.27379E-02		
MEA	0.32200E+00	0.86573E-01		
H <sub>2</sub> O	0.32730E+05	0.87998E+00		
HYDROGEN	0.67000E+00	0.18014E-04		
NITROGEN	0.40000E+01	0.10754E-05		
METHANE	0.57000E+00	0.15325E-04		
ETHANE	0.30000E+00	0.46036E-05		
PROPANE	0.34000E+00	0.91413E-05		
TOTAL	0.37194E+05			

## PRODUCTS

	TOP PRODUCT		BOTTOM PRODUCT	
	LB MOLE/TIME	MOL FRAC	LB MOLE/TIME	MOL FRAC
H <sub>2</sub> S	0.10460E+04	0.92072E+02	0.94226E+02	0.26132E+02
CO <sub>2</sub>	0.17478E+02	0.15385E-01	0.84338E+02	0.23389E+02
MEA	0.12464E+01	0.10972E-04	0.32200E+04	0.89302E-01
H <sub>2</sub> O	0.70616E+01	0.62162E-01	0.32659E+05	0.90575E+00
HYDROGEN	0.66999E+00	0.58478E-03	0.36649E-28	0.10164E-32
NITROGEN	0.39999E+01	0.35211E-04	0.20464E-29	0.56753E-34
METHANE	0.56999E+00	0.50175E-03	0.33366E-28	0.92535E-33
ETHANE	0.31999E+00	0.28168E-03	0.18012E-28	0.49954E-33
PROPANE	0.33999E+00	0.29929E-03	0.18419E-28	0.51082E-33
TOTAL	0.11360E+04		0.36158E+05	

## APPENDIX A.2 -- TEST PROBLEM 1 -- AMECO CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE OF COLUMN	3
NO. OF PLATES	14
PRESSURE OF CONDENSER (PSIA)	15.0
PRESSURE AT TOP PLATE (PSIA)	27.00
PRESSURE DROP PER PLATE (PSIA)	.3332
NO. OF FEEDS	1
ENTERING PLATE OF FEED 1	0
FEED QUANTITY	6.64652E+04
PRESSURE OF FEED	48.00
TEMPERATURE OF FEED (F)	180.00
NO. OF INTER COOLERS OR HEATERS	1
PLATE NO. OF INTER COOLER OR HEATER 1	14
HEAT LOAD OF INTER COOLER OR HEATER	1.16171E+08

## \*\*\* RATE OF CONVERGENCE FITTING ITERATION NO. \*\*\*

SUM OF SQUARES OF RESIDUALS = 0.119723E+1

## TEMPERATURE

0.55960E+03	0.67760E+03	0.71608E+03	0.79367E+03	0.70296E+03
0.64766E+03	0.69962E+03	0.73160E+03	0.77367E+03	0.71367E+03
0.70267E+03	0.73365E+03	0.77162E+03	0.77360E+03	

## VAPOUR FLOW RATE

0.16300E+03	0.40000E+03	0.71008E+03	0.85000E+03	0.90000E+03
0.90500E+03	0.91000E+03	0.91500E+03	0.92000E+03	0.93000E+03
0.93000E+03	0.93500E+03	0.94000E+03	0.94500E+03	

1 SUM OF SQUARES OF RESIDUALS = 0.46926E+00

## TEMPERATURE

0.55960E+03	0.67795E+03	0.70076E+03	0.71303E+03	0.71973E+03
0.71886E+03	0.71594E+03	0.71272E+03	0.71057E+03	0.71970E+03
0.71066E+03	0.71101E+03	0.71235E+03	0.71389E+03	

## VAPOUR FLOW RATE

0.16293E+03	0.31846E+03	0.10727E+04	0.16067E+04	0.14000E+04
0.17063E+04	0.15056E+04	0.13008E+04	0.11473E+04	0.14898E+04
0.99322E+03	0.96599E+03	0.95767E+03	0.96398E+03	

2 SUM OF SQUARES OF RESIDUALS = 0.43449E+01

## TEMPERATURE

0.55960E+03	0.67970E+03	0.69903E+03	0.70864E+03	0.71371E+03
0.71378E+03	0.71207E+03	0.71081E+03	0.71054E+03	0.71120E+03
0.71176E+03	0.71260E+03	0.71346E+03	0.71438E+03	

## VAPOUR FLOW RATE

0.15497E+03	0.38493E+03	0.86282E+03	0.81475E+03	0.95102E+03
0.97660E+03	0.10015E+04	0.10030E+04	0.10024E+04	0.99370E+03
0.97864E+03	0.96679E+03	0.96767E+03	0.98765E+03	

3 SUM OF SQUARES OF RESIDUALS = 0.36742E+00

## TEMPERATURE

0.55960E+03	0.67421E+03	0.69542E+03	0.70229E+03	0.71587E+03
0.70757E+03	0.70826E+03	0.70889E+03	0.70970E+03	0.71157E+03
0.71143E+03	0.71225E+03	0.71305E+03	0.71422E+03	

## VAPOUR FLOW RATE

0.15331E+03	0.31629E+03	0.65657E+03	0.81270E+03	0.84425E+03
0.88024E+03	0.90572E+03	0.92346E+03	0.92999E+03	0.93134E+03
0.93359E+03	0.93771E+03	0.94532E+03	0.95267E+03	

4 SUM OF SQUARES OF RESIDUALS 0.11725E-02

TEMPERATURE

0.55960E+03	0.6784CE+03	0.69825E+03	0.70407E+03	0.70815E+03
0.70745E+03	0.70848E+03	0.70935E+03	0.71015E+03	0.71092E+03
0.71167E+03	0.71241E+03	0.71316E+03	0.71430E+03	

VAPOUR FLOW RATE

0.15575E+03	0.36490E+03	0.80808E+03	0.95032E+03	0.96431E+03
0.96117E+03	0.95860E+03	0.95150E+03	0.94699E+03	0.94598E+03
0.94716E+03	0.94958E+03	0.95119E+03	0.95078E+03	

5 SUM OF SQUARES OF RESIDUALS 0.71906E-04

TEMPERATURE

0.55960E+03	0.67569E+03	0.69612E+03	0.70293E+03	0.70550E+03
0.70700E+03	0.70813E+03	0.70907E+03	0.70993E+03	0.71074E+03
0.71153E+03	0.71231E+03	0.71309E+03	0.71426E+03	

VAPOUR FLOW RATE

0.15444E+03	0.33694E+03	0.69902E+03	0.86897E+03	0.91187E+03
0.92344E+03	0.92873E+03	0.93028E+03	0.93220E+03	0.93525E+03
0.93901E+03	0.94309E+03	0.94656E+03	0.94865E+03	

6 SUM OF SQUARES OF RESIDUALS 0.16010E-04

TEMPERATURE

0.55960E+03	0.67545E+03	0.69547E+03	0.70248E+03	0.70531E+03
0.70691E+03	0.70807E+03	0.70904E+03	0.70992E+03	0.71075E+03
0.71154E+03	0.71233E+03	0.71311E+03	0.71426E+03	

VAPOUR FLOW RATE

0.15483E+03	0.34149E+03	0.70823E+03	0.86014E+03	0.90241E+03
0.91520E+03	0.92123E+03	0.92634E+03	0.93100E+03	0.93532E+03
0.93936E+03	0.94311E+03	0.94649E+03	0.94903E+03	

7 SUM OF SQUARES OF RESIDUALS 0.10801E-04

TEMPERATURE

0.55960E+03	0.67563E+03	0.69577E+03	0.70267E+03	0.70543E+03
0.70699E+03	0.70813E+03	0.70909E+03	0.70995E+03	0.71077E+03
0.71156E+03	0.71233E+03	0.71311E+03	0.71427E+03	

VAPOUR FLOW RATE

0.15476E+03	0.34281E+03	0.72096E+03	0.87085E+03	0.90667E+03
0.91626E+03	0.92123E+03	0.92532E+03	0.92939E+03	0.93355E+03
0.93772E+03	0.94176E+03	0.94549E+03	0.94839E+03	

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 7

PEFLUX RATIO 1.21519

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FRED

0.480E+02 PSIA 0.180E+03 °F 0.373E+08 BTU 1.0

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP °F	LIQUID FLOW LB MOLE/TIME	VAPOUR FLOW LB MOLE/TIME	HEAT DUTY BTU/TIME
1	25.00	100.00	0.18806E+03	0.15476E+03	-0.23475E+07
2	27.00	216.03	0.70314E+04	0.34281E+03	0.0
3	27.33	236.17	0.71813E+04	0.72096E+03	0.0
4	27.67	243.07	0.72471E+04	0.87085E+03	0.0
5	28.00	245.83	0.72267E+04	0.90667E+03	0.0
6	28.33	247.39	0.72317E+04	0.91626E+03	0.0
7	28.67	248.53	0.72358E+04	0.92123E+03	0.0
8	29.00	249.49	0.72399E+04	0.92532E+03	0.0
9	29.33	250.35	0.72440E+04	0.92939E+03	0.0
10	29.67	251.17	0.72482E+04	0.93355E+03	0.0
11	30.00	251.96	0.72522E+04	0.93772E+03	0.0
12	30.33	252.73	0.72559E+04	0.94176E+03	0.0
13	30.67	253.51	0.72588E+04	0.94549E+03	0.0
14	31.00	254.67	0.63104E+04	0.94839E+03	0.16171E+08

185

\*\*\* MATERIAL BALANCES \*\*\*

FEEDS

	PLATE NO.	2	PLATE NO.	
	LB MOL/TIME	MOL PRAC	LB MOL/TIME	MOL PRAC
H2S	0.37820E+02	0.58498E-02		
CO2	0.12371E+03	0.19135E-01		
DEA	0.29088E+03	0.44991E-01		
H2O	0.60124E+04	0.92995E+00		
METHANE	0.43000E+00	0.66510E-04		
ETHANE	0.30000E-01	0.46402E-05		
PROPANE	0.10000E-01	0.15467E-05		
TOTAL	0.64652E+04			

PRODUCTS

	TOP- PRODUCT		BOTTOM PRODUCT	
	LB MOL/TIME	MOL PRAC	LB MOL/TIME	MOL PRAC
H2S	0.37343E+02	0.24130E+00	0.47220E+00	0.74829E-04
CO2	0.11109E+03	0.71784E+00	0.12605E+02	0.19975E-02
DEA	0.51058E-08	0.32993E-10	0.29088E+03	0.46095E-01
H2O	0.58535E+01	0.37824E-01	0.60065E+04	0.95183E+00
METHANE	0.42994E+00	0.27782E-02	0.39749E-27	0.62990E-31
ETHANE	0.29996E-01	0.19383E-03	0.25954E-28	0.41129E-32
PROPANE	0.99987E-02	0.64609E-04	0.81276E-29	0.12880E-32
TOTAL	0.15476E+03		0.63104E+04	

## APPENDIX 4.9 -- TEST PROBLEM 5 -- NASIR CORRELATION

## \*\*\*\*\* PROBLEM STATEMENT \*\*\*\*\*

TYPE OF COLUMN	1
NO. OF PLATES	8
PRESSURE AT TOP PLATE (PSIA)	150.00
PRESSURE DROP PER PLATE (PSIA)	0.0
NO. OF FEEDS	3
ENTERING PLATE OF FEED 1	1
FEED QUANTITY	0.69583E+03
PRESSURE OF FEED	150.00
TEMPERATURE OF FEED (F)	100.00
ENTERING PLATE OF FEED 2	3
FEED QUANTITY	0.28612E+04
PRESSURE OF FEED	150.00
TEMPERATURE OF FEED (F)	120.00
ENTERING PLATE OF FEED 3	8
FEED QUANTITY	0.19686E+04
PRESSURE OF FEED	150.00
TEMPERATURE OF FEED (F)	95.00

## PHYSICAL PARAMETERS

KGA = 0.100E-05 KLO = 0.330E-01 AS(CH<sub>2</sub>/CH<sub>3</sub>) = 0.430E+01  
 XSECT AREA(CH<sub>2</sub>) = 0.690E+04 WEIR HEIGHT(CM) = 0.130E+02

\*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

0 SUM OF SQUARES OF RESIDUALS  $2.38013E+01$

TEMPERATURE

$0.56960E+03$   $0.57960E+03$   $0.57960E+03$   $0.57960E+03$   $0.57960E+03$   
 $0.57960E+03$   $0.57960E+03$   $0.57960E+03$

VAPOUR FLOW RATE

$0.19600E+04$   $0.19600E+04$   $0.19600E+04$   $0.19600E+04$   $0.19600E+04$   
 $0.19600E+04$   $0.19600E+04$   $0.19600E+04$

H2S EFFICIENCY

$0.94167E+00$   $0.90612E+00$   $0.25987E+01$   $0.25987E+01$   $0.25987E+01$   
 $0.25987E+01$   $0.21026E+02$   $0.20494E+02$

CO2 EFFICIENCY

$0.41079E+01$   $0.23695E+01$   $0.42008E+02$   $0.42008E+02$   $0.42008E+02$   
 $0.42008E+02$   $0.56385E+02$   $0.47435E+04$

1 SUM OF SQUARES OF RESIDUALS  $0.35561E-01$

TEMPERATURE

$0.59328E+03$   $0.61111E+03$   $0.56416E+03$   $0.56408E+03$   $0.56381E+03$   
 $0.56291E+03$   $0.55992E+03$   $0.54587E+03$

VAPOUR FLOW RATE

$0.19669E+04$   $0.19795E+04$   $0.19526E+04$   $0.19524E+04$   $0.19523E+04$   
 $0.19518E+04$   $0.19495E+04$   $0.19706E+04$

H2S EFFICIENCY

$0.85137E+00$   $0.81081E+00$   $0.81510E+00$   $0.81513E+00$   $0.81515E+00$   
 $0.81523E+00$   $0.10892E+01$   $0.44576E+01$

CO2 EFFICIENCY

$0.48516E+00$   $0.36059E+00$   $0.26116E+00$   $0.26091E+00$   $0.26004E+00$   
 $0.25713E+00$   $0.63609E+02$   $0.17565E+04$

2 SUM OF SQUARES OF RESIDUALS  $0.76671E-02$

TEMPERATURE

$0.56327E+03$   $0.55701E+03$   $0.57553E+03$   $0.57545E+03$   $0.57540E+03$   
 $0.57593E+03$   $0.58099E+03$   $0.57777E+03$

VAPOUR FLOW RATE

$0.19469E+04$   $0.19244E+04$   $0.19592E+04$   $0.19590E+04$   $0.19590E+04$   
 $0.19591E+04$   $0.19611E+04$   $0.19624E+04$

H2S EFFICIENCY

$0.99165E+00$   $0.26609E+01$   $0.90759E+00$   $0.90695E+00$   $0.90163E+00$   
 $0.11319E+01$   $0.12313E+01$   $0.19680E+01$

CO2 EFFICIENCY

$0.90456E+00$   $0.81149E+00$   $0.38273E+00$   $0.38122E+00$   $0.37441E+00$   
 $0.43676E+02$   $0.22173E+03$   $0.21577E+03$

3 SUM OF SQUARES OF RESIDUALS 0.17042E-02

TEMPERATURE  
0.57182E+03 0.59192E+03 0.58210E+03 0.58217E+03 0.58243E+03  
0.58311E+03 0.58320E+03 0.57829E+03

VAPOUR FLOW RATE  
0.19569E+04 0.19629E+04 0.19638E+04 0.19637E+04 0.19638E+04  
0.19648E+04 0.19672E+04 0.19684E+04

H2S EFFICIENCY  
0.11050E+01 0.16033E+01 0.94064E+00 0.93923E+00 0.97432E+00  
0.10425E+01 0.13188E+01 0.19516E+01

CO2 EFFICIENCY  
0.37752E+00 0.53995E+00 0.48877E+00 0.48475E+00 0.19473E+02  
0.15075E+03 0.16290E+03 0.21065E+03

4 SUM OF SQUARES OF RESIDUALS 0.89964E-04

TEMPERATURE  
0.47295E+03 0.57706E+03 0.57926E+03 0.57947E+03 0.58005E+03  
0.58080E+03 0.58029E+03 0.57538E+03

VAPOUR FLOW RATE  
0.19579E+04 0.19588E+04 0.19627E+04 0.19627E+04 0.19633E+04  
0.19649E+04 0.19657E+04 0.19668E+04

H2S EFFICIENCY  
0.15378E+01 0.21714E+01 0.99759E+00 0.10075E+01 0.10297E+01  
0.11132E+01 0.13750E+01 0.20678E+01

CO2 EFFICIENCY  
0.74607E+00 0.10933E+01 0.67922E+00 0.15311E+02 0.12567E+03  
0.14979E+03 0.20011E+03 0.25155E+03

5 SUM OF SQUARES OF RESIDUALS 0.20732E-04

TEMPERATURE  
0.57134E+03 0.57856E+03 0.57967E+03 0.58007E+03 0.58077E+03  
0.58101E+03 0.58044E+03 0.57576E+03

VAPOUR FLOW RATE  
0.19572E+04 0.19613E+04 0.19630E+04 0.19631E+04 0.19642E+04  
0.19648E+04 0.19657E+04 0.19668E+04

H2S EFFICIENCY  
0.17583E+01 0.21306E+01 0.99555E+00 0.10040E+01 0.10272E+01  
0.10992E+01 0.13565E+01 0.20535E+01

CO2 EFFICIENCY  
0.87513E+00 0.12371E+01 0.10332E+02 0.87733E+02 0.10923E+03  
0.15374E+03 0.20500E+03 0.24767E+03

6 . SUM OF SQUARES OF RESIDUALS 0.78246E-05

TEMPERATURE

0.57249E+03 0.57775E+03 0.57961E+03 0.58011E+03 0.58043E+03  
0.58070E+03 0.58016E+03 0.57556E+03

VAPOUR FLOW RATE

0.19577E+04 0.19609E+04 0.19630E+04 0.19639E+04 0.19640E+04  
0.19646E+04 0.19655E+04 0.19668E+04

H2S EFFICIENCY

0.16945E+01 0.21532E+01 0.99901E+00 0.10065E+01 0.10255E+01  
0.10961E+01 0.13627E+01 0.20614E+01

CO2 EFFICIENCY

0.87018E+00 0.14533E+02 0.60327E+02 0.77045E+02 0.11192E+03  
0.15726E+03 0.20648E+03 0.25011E+03

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 6

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

0.150E+03 PSIA	0.100E+03 F	0.290E+07 BTU	1.0
0.150E+03 PSIA	0.120E+03 F	0.119E+08 BTU	1.0
0.150E+03 PSIA	0.950E+02 F	0.128E+08 BTU	0.0

## \*\*\* STAGE VARIABLES \*\*\*

STAGE	PRESSURE PSIA	TEMP F	LIQUID FLOW LB/MOL/TIME	VAPOR FLOW LB/MOL/TIME	HEAT DUTY BTU/TIME
0.					
1	150.00	112.89	0.69897E+02	0.577E+04	0.0
2	150.00	118.16	0.70110E+02	0.609E+04	0.0
3	150.00	120.02	0.35628E+02	0.630E+04	0.0
4	150.00	120.51	0.35633E+02	0.49635E+04	0.0
5	150.00	120.83	0.35639E+02	0.49640E+04	0.0
6	150.00	121.10	0.35648E+02	0.196462E+04	0.0
7	150.00	120.56	0.35661E+02	0.19655E+04	0.0
8	150.00	115.96	0.35679E+02	0.19668E+04	0.0

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS.

	PLATE NO. 1	PLATE NO. 3		
	LB MOL/TIME	MOL PRAC	LB MOL/TIME	MOL PRAC
H2S	0.12800E+01	0.18395E-02	0.54300E+02	0.18978E-07
CO2	0.15700E+01	0.22563E-02	0.63000E+01	0.22019E-02
MEA	0.62050E+02	0.89174E-01	0.25000E+03	0.87377E-01
WATER	0.63093E+03	0.90673E+00	0.25500E+04	0.89124E+00
HYDROGEN	0.0	0.0	0.0	0.0
NITROGEN	0.0	0.0	0.0	0.0
METHANE	0.0	0.0	0.0	0.0
ETHANE	0.0	0.0	0.16000E+00	0.55921E-04
PROPANE	0.0	0.0	0.42000E+00	0.14679E-03
N-BUTANE	0.0	0.0	0.0	0.0
I-BUTANE	0.0	0.0	0.0	0.0
TOTAL	0.69583E+03		0.28612E+04	

	PLATE NO. 8	PLATE NO.		
	LB MOL/TIME	MOL PRAC	LB MOL/TIME	MOL PRAC
H2S	0.18700E+02	0.94989E-02		
CO2	0.29500E+01	0.14985E-02		
MEA	0.0	0.0		
WATER	0.59100E+01	0.30021E-02		
HYDROGEN	0.62997E+03	0.32000E+00		
NITROGEN	0.29530E+02	0.15000E-01		
METHANE	0.78155E+03	0.39700E+00		
ETHANE	0.35436E+03	0.18000E+00		
PROPANE	0.12402E+03	0.62997E-01		
N-BUTANE	0.19700E+01	0.10007E-02		
I-BUTANE	0.19690E+02	0.10002E-01		
TOTAL	0.19686E+04			

## PRODUCTS:

	TOP PRODUCT	BOTTOM PRODUCT		
	LB MOL/TIME	MOL PRAC	LB MOL/TIME	MOL PRAC
H2S	0.63932E-01	0.32656E-04	0.74221E+02	0.20802E-01
CO2	0.22796E-03	0.11644E-06	0.10823E+02	0.30335E-02
MEA	0.39981E-01	0.20422E-04	0.31201E+03	0.87448E-01
WATER	0.16523E+02	0.84399E-02	0.31703E+04	0.88856E+00
HYDROGEN	0.62983E+03	0.32172E+00	0.16325E+00	0.45756E-04
NITROGEN	0.29525E+02	0.15081E-01	0.54106E-02	0.15165E-05
METHANE	0.78127E+03	0.39907E+00	0.26842E+00	0.75231E-04
ETHANE	0.35443E+03	0.18104E+00	0.91658E-01	0.25689E-04
PROPANE	0.12438E+03	0.63533E-01	0.35386E-01	0.99176E-05
N-BUTANE	0.19699E+01	0.10062E-02	0.32513E-04	0.91125E-08
I-BUTANE	0.19689E+02	0.10057E-01	0.32496E-03	0.91079E-07
TOTAL	0.19577E+04		0.35679E+04	

**APPENDIX 5.**

**EQUILIBRIUM AND ENTHALPY DATA FOR  
EXTRACTIVE DISTILLATION PROBLEM**

## APPENDIX 5

### Equilibrium and Enthalpy Data for Extractive Distillation Problem

#### (a) Equilibrium K-ratios

At low pressures, far from critical conditions, the K-value of component  $\text{C}_i$  may be expressed by:

$$K_i = \gamma_i \frac{P_i}{P_T} \quad (\text{A5-1})$$

where:

$\gamma_i$  is the activity coefficient

$P_i$  is the intrinsic vapour pressure  
of the pure component

$P_T$  is the total pressure.

For a three component system, a third order Marqules' expression may be used, namely equation (A5-2).

By cyclically altering subscripts, similar expressions are obtained for  $\ln \gamma_2$  and  $\ln \gamma_3$ .

$$\begin{aligned} \ln \gamma_1 &= x_2^2 (a_{12} + 2x_1 (a_{21} - a_{12})) + (x_3^2 (a_{13} + 2x_1 (a_{31} - a_{13}))) \\ &\quad + x_2 x_3 (0.5(a_{12} + a_{21} + a_{13} + a_{31} - a_{23} - a_{32})) \\ &\quad + x_1 (a_{21} - a_{12} + a_{31} - a_{13}) + (x_2 - x_3) (a_{23} - a_{32}) - (1 - 2x_1) c_{123} \end{aligned} \quad (\text{A5-2})$$

The third order constants are as follows<sup>13</sup>, with subscripts 1, 2, 3 denoting acetone, acetonitrile and water respectively.

$$a_{12} = 0.0482 \quad a_{23} = 0.8145 \quad a_{31} = 0.6867$$

$$a_{21} = -0.0447 \quad a_{32} = 0.7375 \quad a_{13} = 0.8484$$

$$c_{123} = 0.3462$$

The intrinsic vapour pressure of component  $i$  is given by Antoine's equation<sup>13</sup>:

$$\log p_i = A_i - \frac{B_i}{(T_c + C_i)} \quad (A5-3)$$

where  $T_c$  is the temperature ( $^{\circ}\text{C}$ )

$A_i, B_i, C_i$  are Antoine's constants. For the

system acetone-acetonitrile-water they are<sup>13</sup>:

Component, $i$	$A_i$	$B_i$	$C_i$
acetone	7.23967	1279.870	237.5
acetonitrile	7.24299	1397.929	238.894
water	7.96681	1668.210	228.0

The partial derivatives of  $K_i$  with respect to  $T$  and  $x_i$  are given by equations (A5-4) and (A5-5):

$$\frac{\partial K_i}{\partial T} = \frac{Y_i}{P_T} \frac{\partial P_i}{\partial T} + \frac{P_i}{P_T} \frac{\partial Y_i}{\partial T} \quad (A5-4)$$

$$\frac{\partial K_1}{\partial x_1} = \frac{P_1}{P_T} \cdot \frac{\partial Y_1}{\partial x_1} \quad (A5-5)$$

However, for the purposes of linearization,  $\frac{\partial Y_1}{\partial T}$  is considered negligible and  $\frac{\partial K_1}{\partial T}$  approximated as:

$$\frac{\partial K_1}{\partial T} = \frac{Y_1}{P_T} \frac{\partial P_1}{\partial T} \quad (A5-6)$$

From equation (A5-2),  $\frac{\partial Y_1}{\partial x_1}$  is given by the following:

$$\begin{aligned} \frac{\partial Y_1}{\partial x_1} &= Y_1 [2x_2^2(a_{21} - a_{12}) + 2x_3^2(a_{31} - a_{13}) \\ &\quad + x_2 x_3 [(a_{21} - a_{12} + a_{31} - a_{13}) + 2c_{123}]] \end{aligned} \quad (A5-7)$$

Similar expressions apply for  $\frac{\partial Y_2}{\partial x_2}$  and  $\frac{\partial Y_3}{\partial x_3}$ .

### (b) Enthalpy Data

Liquid and vapour enthalpy are given by the following:

$$h = \sum_{i=1}^{NCP} h_{ci} x_i x_{M,i} (T - T_{ref}) \quad (A5-8)$$

$$H = \sum_{i=1}^{NCP} y_i x_{M,i} [h_{ci}(T - T_{ref}) + h_{vap,i}] \quad (A5-9)$$

where  $hc_i$ ,  $XM_i$ ,  $h_{vap,i}$  are respectively the average heat capacity, molecular weight and average heat of vaporization of component  $i$ ,  $T$  is the temperature ( $^{\circ}\text{C}$ ), and  $T_{ref}$  is the reference temperature, conveniently chosen as  $0^{\circ}\text{C}$ . Values of  $hc_i$ ,  $XM_i$  and  $h_{vap,i}$  are as follows:

	<u>Heat Capacity (cal/g<math>^{\circ}\text{C}</math>)</u>	<u>Molecular Weight</u>	<u>Heat of Vapour- ization (cal/g)</u>
acetone	0.54	58.08	120.0
acetonitrile	0.54	41.05	120.0
water	1.00	18.02	550.0

Finally, the partial derivatives of the liquid and vapour enthalpies with respect to temperature are:

$$\frac{\partial h}{\partial T} = \frac{NCP}{1.8} \sum_{i=1}^{NCP} hc_i x_i XM_i \quad (\text{A5-10})$$

$$\frac{\partial H}{\partial T} = \frac{NCP}{1.8} \sum_{i=1}^{NCP} hc_i y_i XM_i \quad (\text{A5-11})$$

where  $T$  is in  $^{\circ}\text{R}$ .

**APPENDIX 6**

**COMPUTER PRINTOUTS FOR  
EXAMPLE PROBLEMS USING  
LINKED COLUMN ALGORITHM**

## APPENDIX 6.1 -- THERMALLY COUPLED DISTILLATION SYSTEM

## \*\* PROBLEM STATEMENT \*\*

COLUMN NO 1 IS DISTILLATION COL.

NO OF PLATES= 30

COL PRESSURE 235.00 PSIA

PRESSURE DROP 0.0 PER PLATE

REFOILER VAPOUR 6850.00 MOLES

REFLUX RATIO 2.500

COLUMN NO 2 IS ABSORPTION COL.

NO OF PLATES= 20

COL PRESSURE 235.00 PSIA

PRESSURE DROP 0.0 PER PLATE

NO. OF FEEDS 1

FEED 1 IS ON TO PLATE 15

QUANTITY 0.4000E+04

PRESSURE 235.00

TEMP (F) 150.00

ENTHALPY 0.6310E+07

NO. OF LIQUID SIDE STREAMS 1

STREAM 1 LEAVES PLATE 5

QUANTITY 0.2500E+04

NO. OF VAPOUR SIDE STREAMS 2

STREAM 1 LEAVES PLATE 25

QUANTITY 0.3000E+04

STREAM 2 LEAVES PLATE 40

QUANTITY 0.12096E+04

NO. OF INTERCOOLERS OR HEATERS 1

INTERCOOLER OR HEATER 1 IS ON PLATE 30

HEAT LOAD IS A VARIABLE

## \*\*\* STREAM CONNECTIONS \*\*\*

LEAVING STREAM NO	LEAVING STAGE NO	STREAM FLUID	ENTERING FRACTION	ENTERING STREAM NO	ENTERING STAGE NO
1	5	1	1.00	3	31
2	25	2	1.00	4	50
3	31	4	1.00	1	5
4	50	3	1.00	2	25

STREAM FLUID 1=LIQUID SIDE STREAM 2=VAPOUR SIDE STREAM  
3=LIQUID PRODUCT 4=VAPOUR PRODUCT

\*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

1. SUM OF SQUARES OF RESIDUALS 0.23241E+01  
 (MAT. BAL. 0.23161E+01 HEAT BAL. 0.79483E-02).

TEMPERATURE (F)

0.5816CE+03 0.58260E+03 0.5856CE+03 0.58960F+03 0.59360E+03  
 0.5976CE+03 0.60160P+03 0.60360E+03 0.60560P+03 0.60760E+03  
 0.6096CE+03 0.61160F+03 0.61360E+03 0.6156CE+03 0.62368F+03  
 0.6316CE+03 0.63960E+03 0.64760E+03 0.65560E+03 0.6636CE+03  
 0.6716CE+03 0.67960F+03 0.68760E+03 0.69960F+03 0.71160E+03  
 0.72360E+03 0.73560E+03 0.74760E+03 0.75960F+03 0.78460E+03  
 0.5966CE+03 0.60465P+03 0.61260E+03 0.62060F+03 0.63260E+03  
 0.64860E+03 0.65660E+03 0.6646CE+03 0.67260E+03 0.68060E+03  
 0.68860E+03 0.69660P+03 0.70160E+03 0.70360F+03 0.70560E+03  
 0.70760E+03 0.70960E+03 0.71160E+03 0.71360E+03 0.71560E+03

VAPOR FLOW RATE

0.42072E+04 0.77252F+04 0.76500E+04 0.76000E+04 0.75500E+04  
 0.50000E+04 0.50000E+04 0.50000E+04 0.50000E+04 0.50000E+04  
 0.50000E+04 0.50000E+04 0.50000E+04 0.50000E+04 0.50000E+04  
 0.48000CE+04 0.48000E+04 0.48000E+04 0.48000E+04 0.48000E+04  
 0.48000CE+04 0.48000E+04 0.48000E+04 0.48000E+04 0.48000E+04  
 0.48000CE+04 0.48000E+04 0.48000E+04 0.48000E+04 0.48000E+04  
 0.75000E+04 0.75000E+04 0.75000E+04 0.75000E+04 0.69500E+04  
 0.22000CE+04 0.22000E+04 0.22000E+04 0.22000E+04 0.22000E+04  
 0.22000CE+04 0.22000E+04 0.22000E+04 0.22000E+04 0.22000E+04  
 0.31000CE+04 0.31000E+04 0.31000E+04 0.31000E+04 0.31000E+04  
 0.31000E+04 0.31000F+04 0.31000E+04 0.31000F+04 0.31000F+04

1. SUM OF SQUARES OF RESIDUALS 0.62283E-02

(MAT. BAL. 0.56247E-02 HEAT BAL. 0.60354E-03)

TEMPERATURE (F)

0.58038E+03 0.58283E+03 0.58494E+03 0.58766F+03 0.591C1E+03  
 0.59504E+03 0.59898E+03 0.60228E+03 0.60509F+03 0.60745F+03  
 0.60949E+03 0.61144F+03 0.61370E+03 0.61703F+03 0.62436E+03  
 0.62945E+03 0.63646E+03 0.64461E+03 0.65352E+03 0.66256F+03  
 0.67123E+03 0.67963E+03 0.68862E+03 0.69962E+03 0.71320F+03  
 0.72438E+03 0.73648E+03 0.74841E+03 0.76300E+03 0.78661E+03  
 0.59215E+03 0.59578E+03 0.60061E+03 0.60718E+03 0.61585E+03  
 0.62575E+03 -0.63698E+03 0.64901E+03 0.66154E+03 0.67367F+03  
 0.67946E+03 0.68527E+03 0.68948E+03 0.69302E+03 0.69628E+03  
 0.69929E+03 0.70205F+03 0.70459E+03 0.70702E+03 0.70970F+03

VAPOR FLOW RATE

0.21304E+04 0.74562F+04 0.74474E+04 0.74143F+04 0.73749E+04  
 0.50942E+04 0.50502E+04 0.50148E+04 0.49791E+04 0.49451E+04  
 0.49110E+04 0.48736E+04 0.48250E+04 0.47495F+04 0.45881E+04  
 0.48476E+04 0.48367E+04 0.48526E+04 0.48727E+04 0.48943E+04  
 0.49116E+04 0.49143E+04 0.48978E+04 0.48615E+04 0.48454E+04  
 0.78188E+04 0.77288E+04 0.76495E+04 0.74069E+04 0.68500E+04  
 0.22550E+04 0.22347E+04 0.22279E+04 0.22170E+04 0.22011E+04  
 0.21831E+04 0.21498E+04 0.20887E+04 0.20264E+04 0.19870E+04  
 0.32030E+04 0.31609E+04 0.31549E+04 0.31451F+04 0.31330E+04  
 0.31210E+04 0.31082E+04 0.30934E+04 0.30742E+04 0.3045CE+04

2 SUM OF SQUARES OF RESIDUALS 0.24420E-02  
 (SAT. BAL. 0.87044E-01 HEAT BAL. 0.15720F-02)

## TEMPERATURE (F)

0.58068E+03 0.58232E+03 0.58409E+03 0.58635E+03 0.58932E+03  
 0.59384E+03 0.59733E+03 0.60070E+03 0.60347E+03 0.60573E+03  
 0.60766E+03 0.60950E+03 0.61167E+03 0.61490E+03 0.62205E+03  
 0.62689E+03 0.63316E+03 0.64103E+03 0.65006E+03 0.65958E+03  
 0.66893E+03 0.67840E+03 0.68904E+03 0.70255E+03 0.71962E+03  
 0.73267E+03 0.74453E+03 0.75541E+03 0.76903E+03 0.79298E+03  
 0.59230E+03 0.59686E+03 0.60442E+03 0.61506E+03 0.62913E+03  
 0.64460E+03 0.65857E+03 0.66902E+03 0.67648E+03 0.68417E+03  
 0.69144E+03 0.69819E+03 0.70420E+03 0.70914E+03 0.71281E+03  
 0.74529E+03 0.78166E+03 0.71727E+03 0.71753E+03 0.71793E+03

## VAPOUR FLOW RATE

0.22376E+04 0.77614E+04 0.77150E+04 0.76572E+04 0.75697E+04  
 0.50758E+04 0.50184E+04 0.49648E+04 0.49266E+04 0.48975E+04  
 0.48741E+04 0.48513E+04 0.48218E+04 0.47722E+04 0.46586E+04  
 0.48349E+04 0.47881E+04 0.47400E+04 0.47093E+04 0.47037E+04  
 0.47290E+04 0.47631E+04 0.47722E+04 0.47408E+04 0.46821E+04  
 0.76089E+04 0.75720E+04 0.75307E+04 0.73592E+04 0.68500E+04  
 0.24021E+04 0.23788E+04 0.23429E+04 0.22980E+04 0.22580E+04  
 0.22330E+04 0.22259E+04 0.22153E+04 0.21883E+04 0.21334E+04  
 0.32678E+04 0.32132E+04 0.31732E+04 0.31431E+04 0.31214E+04  
 0.31063E+04 0.30942E+04 0.30832E+04 0.30713E+04 0.30534E+04

3 SUM OF SQUARES OF RESIDUALS 0.12793E-02  
 (SAT. BAL. 0.26290E-03 HEAT BAL. 0.10074F-02)

## TEMPERATURE (R)

0.58150E+03 0.58380E+03 0.58638E+03 0.58969E+03 0.59383E+03  
 0.59943E+03 0.60419E+03 0.60784E+03 0.61050E+03 0.61244E+03  
 0.61396E+03 0.61541E+03 0.61720E+03 0.62002E+03 0.62641E+03  
 0.63440E+03 0.64430E+03 0.65542E+03 0.66631E+03 0.67566E+03  
 0.68324E+03 0.69008E+03 0.69798E+03 0.70868E+03 0.72257E+03  
 0.73393E+03 0.74470E+03 0.75541E+03 0.76898E+03 0.79332E+03  
 0.59718E+03 0.60225E+03 0.60974E+03 0.61974E+03 0.63145E+03  
 0.64348E+03 0.65473E+03 0.66466E+03 0.67386E+03 0.68415E+03  
 0.69256E+03 0.69947E+03 0.70492E+03 0.70905E+03 0.71206E+03  
 0.71423E+03 0.71583E+03 0.71708E+03 0.71823E+03 0.71968E+03

## VAPOUR FLOW RATE

0.22237E+04 0.77828E+04 0.77422E+04 0.76823E+04 0.76060E+04  
 0.52512E+04 0.51907E+04 0.51457E+04 0.51121E+04 0.50838E+04  
 0.50621E+04 0.50370E+04 0.50404E+04 0.49513E+04 0.48309E+04  
 0.50466E+04 0.50475E+04 0.50643E+04 0.51060E+04 0.51620E+04  
 0.52041E+04 0.52019E+04 0.51394E+04 0.50178E+04 0.48747E+04  
 0.77406E+04 0.76681E+04 0.75960E+04 0.74032E+04 0.68500E+04  
 0.22649E+04 0.22381E+04 0.21957E+04 0.21386E+04 0.20709E+04  
 0.20040E+04 0.19571E+04 0.19499E+04 0.19792E+04 0.19756E+04  
 0.31490E+04 0.31057E+04 0.30656E+04 0.30351E+04 0.30163E+04  
 0.30080E+04 0.30081E+04 0.30127E+04 0.30178E+04 0.30176E+04

4 SUM OF SQUARES OF RESIDUALS 0.75071E-03  
 (HAT. BAL. 0.13282E-03 HEAT BAL. 0.61788E-03)

## TEMPERATURE (P)

0.58140E+03	0.58361E+03	0.58605E+03	0.58910E+03	0.59288E+03
0.59700E+03	0.60066E+03	0.60366E+03	0.60605E+03	0.60795E+03
0.60959E+03	0.61120E+03	0.61319E+03	0.61628E+03	0.62320E+03
0.62889E+03	0.63634E+03	0.64553E+03	0.65565E+03	0.66545E+03
0.67823E+03	0.68239E+03	0.69135E+03	0.70290E+03	0.71788E+03
0.73011E+03	0.74176E+03	0.75326E+03	0.76743E+03	0.79214E+03
0.59809E+03	0.60594E+03	0.61690E+03	0.63004E+03	0.64311E+03
0.65393E+03	0.66200E+03	0.66847E+03	0.67512E+03	0.68364E+03
0.69097E+03	0.69707E+03	0.70190E+03	0.70554E+03	0.70819E+03
0.71011E+03	0.71538E+03	0.71286E+03	0.71373E+03	0.71510E+03

## VAPOUR FLOW RATE

0.22180E+04	0.77632E+04	0.77089E+04	0.76334E+04	0.75397E+04
0.50778E+04	0.50109E+04	0.49622E+04	0.49282E+04	0.49042E+04
0.48847E+04	0.48644E+04	0.48364E+04	0.47884E+04	0.46732E+04
0.48199E+04	0.47311E+04	0.46409E+04	0.45900E+04	0.46053E+04
0.46747E+04	0.47519E+04	0.47902E+04	0.47743E+04	0.47284E+04
0.76657E+04	0.76330E+04	0.75821E+04	0.73969E+04	0.68500E+04
0.23554E+04	0.23212E+04	0.22780E+04	0.22378E+04	0.22132E+04
0.22045E+04	0.21978E+04	0.21802E+04	0.21439E+04	0.20894E+04
0.32287E+04	0.31772E+04	0.31429E+04	0.31207E+04	0.31061E+04
0.30946E+04	0.30841E+04	0.30737E+04	0.30605E+04	0.30413E+04

5 SUM OF SQUARES OF RESIDUALS 0.11433E-03

(HAT. BAL. 0.91650E-04 HEAT BAL. 0.22675E-04)

## TEMPERATURE (R)

0.58120E+03	0.58331E+03	0.58562E+03	0.58856E+03	0.59225E+03
0.59721E+03	0.60151E+03	0.60494E+03	0.60756E+03	0.60958E+03
0.61126E+03	0.61289E+03	0.61486E+03	0.61789E+03	0.62460E+03
0.63122E+03	0.63952E+03	0.64914E+03	0.65904E+03	0.66821E+03
0.67634E+03	0.68409E+03	0.69289E+03	0.70435E+03	0.71905E+03
0.73099E+03	0.74230E+03	0.75345E+03	0.76732E+03	0.79142E+03
0.59554E+03	0.60083E+03	0.60921E+03	0.62009E+03	0.63428E+03
0.64677E+03	0.65688E+03	0.66508E+03	0.67299E+03	0.68217E+03
0.68986E+03	0.69628E+03	0.70145E+03	0.70544E+03	0.70841E+03
0.71059E+03	0.71223E+03	0.71352E+03	0.71471E+03	0.71618E+03

## VAPOUR FLOW RATE

0.22064E+04	0.77225E+04	0.76734E+04	0.76041E+04	0.75174E+04
0.51144E+04	0.50529E+04	0.50079E+04	0.49755E+04	0.49511E+04
0.49300E+04	0.49075E+04	0.48773E+04	0.48269E+04	0.47099E+04
0.48899E+04	0.48438E+04	0.48011E+04	0.47856E+04	0.48081E+04
0.48544E+04	0.48929E+04	0.48931E+04	0.48468E+04	0.47799E+04
0.77013E+04	0.76554E+04	0.75923E+04	0.73996E+04	0.68500E+04
0.23035E+04	0.22662E+04	0.22105E+04	0.21471E+04	0.20991E+04
0.20823E+04	0.20882E+04	0.20937E+04	0.20809E+04	0.20460E+04
0.31998E+04	0.31554E+04	0.31245E+04	0.31043E+04	0.30913E+04
0.30819E+04	0.30737E+04	0.30655E+04	0.30550E+04	0.30383E+04

6. SUM OF SQUARES OF RESIDUALS: 0.52906E-04  
 (MAT. BAL.: 0.37485E-06 HEAT BAL.: 0.52771E-04)

TEMPERATURE (R)						
0.58141E+03	0.58366E+03	0.58617E+03	0.58933E+03	0.59325E+03		
0.59823E+03	0.60243E+03	0.60570E+03	0.60937E+03	0.61042E+03		
0.61366E+03	0.61722E+03	0.61515E+03	0.61815E+03	0.62481E+03		
0.63145E+03	0.63495E+03	0.64063E+03	0.65798E+03	0.66681E+03		
0.67499E+03	0.68306E+03	0.69224E+03	0.70404E+03	0.71893E+03		
0.73090E+03	0.74220E+03	0.75330E+03	0.76699E+03	0.79109E+03		
0.59699E+03	0.60265E+03	0.61086E+03	0.62144E+03	0.63325E+03		
0.64468E+03	0.65472E+03	0.66338E+03	0.67174E+03	0.68135E+03		
0.68914E+03	0.69562E+03	0.70087E+03	0.70494E+03	0.70801E+03		
0.71020E+03	0.71356E+03	0.71873E+03	0.72796E+03	0.74493E+03		

VAPOUR FLOW RATE						
0.22014E+04	0.24051E+04	0.26573E+04	0.25908E+04	0.25079E+04		
-0.51174E+04	0.50597E+04	0.50172E+04	0.49854E+04	0.49607E+04		
0.49384E+04	0.49148E+04	0.48833E+04	0.48316E+04	0.47136E+04		
0.49057E+04	0.48776E+04	0.48539E+04	0.48491E+04	0.48678E+04		
0.48976E+04	0.49179E+04	0.49055E+04	0.48504E+04	0.47788E+04		
0.76977E+04	0.76687E+04	0.75846E+04	0.73938E+04	0.68500E+04		
0.22963E+04	0.22627E+04	0.22140E+04	0.21572E+04	0.21074E+04		
0.26796E+04	0.26731E+04	0.20736E+04	0.20639E+04	0.20351E+04		
0.31949E+04	0.31522E+04	0.31207E+04	0.30992E+04	0.30847E+04		
0.30784E+04	0.30679E+04	0.30601E+04	0.30511E+04	0.303365E+04		

7. SUM OF SQUARES OF RESIDUALS: 0.55142E-05  
 (MAT. BAL.: 0.53997E-07 HEAT BAL.: 0.54602E-05)

TEMPERATURE (R)						
0.58138E+03	0.58360E+03	0.58608E+03	0.58919E+03	0.59304E+03		
0.59787E+03	0.60198E+03	0.60521E+03	0.60766E+03	0.60957E+03		
0.61118E+03	0.61276E+03	0.61471E+03	0.61773E+03	0.62444E+03		
0.63082E+03	0.63866E+03	0.64762E+03	0.65696E+03	0.66592E+03		
0.67424E+03	0.68242E+03	0.69167E+03	0.70352E+03	0.71847E+03		
0.73052E+03	0.74390E+03	0.75307E+03	0.76681E+03	0.79096E+03		
0.59692E+03	0.60266E+03	0.61117E+03	0.62196E+03	0.63386E+03		
0.64523E+03	0.65110E+03	0.66362E+03	0.67183E+03	0.68129E+03		
0.68899E+03	0.69509E+03	0.70057E+03	0.70460E+03	0.70763E+03		
0.70988E+03	0.71355E+03	0.71288E+03	0.71410E+03	0.71558E+03		

VAPOUR FLOW RATE						
0.22006E+04	0.23022E+04	0.26523E+04	0.25832E+04	0.24978E+04		
0.50957E+04	0.50374E+04	0.49952E+04	0.49644E+04	0.49403E+04		
0.49191E+04	0.48960E+04	0.48651E+04	0.48140E+04	0.46963E+04		
0.48841E+04	0.48544E+04	0.48354E+04	0.48389E+04	0.48645E+04		
0.48976E+04	0.49160E+04	0.48995E+04	0.48399E+04	0.47652E+04		
0.76825E+04	0.76350E+04	0.75744E+04	0.73889E+04	0.68500E+04		
0.23058E+04	0.22744E+04	0.22319E+04	0.21863E+04	0.21487E+04		
0.21259E+04	0.21145E+04	0.21048E+04	0.20867E+04	0.20520E+04		
0.32079E+04	0.31635E+04	0.31300E+04	0.31064E+04	0.30903E+04		
0.30787E+04	0.30699E+04	0.30616E+04	0.30521E+04	0.30369E+04		

203

\*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 7

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

1 235.00 PSIA 150.00 P 0.63100E+07 BTU 1.000

\*\*\* STREAM CONNECTIONS \*\*\*

LEAVING STREAM NO.	LEAVING STAGE NO	STREAM FLUID	ENTERING FRACTION	ENTERING STREAM NO	ENTERING STAGE NO
1	5	1	1.00	3	31
2	25	2	1.00	4	50
3	31	4	1.00	1	5
4	50	3	1.00	2	25

STREAM FLUID 1=LIQUID SIDE STREAM 2=VAPOUR SIDE STREAM  
3=LIQUID PRODUCT 4=VAPOUR PRODUCT

15:25:17 .03 RC=0

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO	PRESSURE PSIA	TEMP F	LIQUID FLOW LB/MOL/TIME	VAPOUR FLOW LB/MOL/TIME	HEAT DUTY BTU/TIME
1	235.00	121.78	0.55016E+04	0.22006E+04	-0.33053E+08
2	235.00	124.00	0.54517E+04	0.77022E+04	0.0
3	235.00	126.48	0.53826E+04	0.76523E+04	0.0
4	235.00	129.54	0.52972E+04	0.75832E+04	0.0
5	235.00	133.44	0.27009E+04	0.74978E+04	0.0
6	235.00	138.27	0.26426E+04	0.50957E+04	0.0
7	235.00	142.38	0.26004E+04	0.50374E+04	0.0
8	235.00	145.61	0.25695E+04	0.49952E+04	0.0
9	235.00	148.06	0.25455E+04	0.49644E+04	0.0
10	235.00	149.97	0.25243E+04	0.49403E+04	0.0
11	235.00	151.58	0.25012E+04	0.49191E+04	0.0
12	235.00	153.16	0.24792E+04	0.48969E+04	0.0
13	235.00	155.11	0.24197E+04	0.48651E+04	0.0
14	235.00	158.13	0.23015E+04	0.48140E+04	0.0
15	235.00	164.84	0.65692E+04	0.46963E+04	0.0
16	235.00	171.22	0.65396E+04	0.48841E+04	0.0
17	235.00	179.06	0.65205E+04	0.48544E+04	0.0
18	235.00	188.02	0.65240E+04	0.48354E+04	0.0
19	235.00	197.36	0.65497E+04	0.48389E+04	0.0
20	235.00	206.32	0.65828E+04	0.48645E+04	0.0
21	235.00	214.64	0.66012E+04	0.48976E+04	0.0
22	235.00	222.82	0.65846E+04	0.49160E+04	0.0
23	235.00	232.07	0.65250E+04	0.48995E+04	0.0
24	235.00	243.92	0.64503E+04	0.48399E+04	0.0
25	235.00	258.87	0.63523E+04	0.47652E+04	0.0
26	235.00	270.92	0.62047E+04	0.76825E+04	0.0
27	235.00	282.30	0.24628E+04	0.76350E+04	0.0
28	235.00	293.47	0.80567E+04	0.75744E+04	0.0
29	235.00	307.21	0.75198E+04	0.73889E+04	0.0
30	235.00	331.36	0.466977E+03	0.68500E+04	0.61639E+08
31	235.00	137.32	0.24686E+04	0.23058E+04	0.0
32	235.00	143.16	0.24261E+04	0.22744E+04	0.0
33	235.00	151.57	0.23805E+04	0.22319E+04	0.0
34	235.00	162.36	0.23429E+04	0.21863E+04	0.0
35	235.00	174.26	0.23201E+04	0.21487E+04	0.0
36	235.00	185.63	0.23057E+04	0.21259E+04	0.0
37	235.00	195.50	0.22990E+04	0.21145E+04	0.0
38	235.00	204.02	0.22809E+04	0.21048E+04	0.0
39	235.00	212.23	0.22462E+04	0.20867E+04	0.0
40	235.00	221.69	0.21925E+04	0.20520E+04	0.0
41	235.00	229.39	0.21481E+04	0.32079E+04	0.0
42	235.00	235.79	0.21146E+04	0.31635E+04	0.0
43	235.00	240.97	0.20910E+04	0.31300E+04	0.0
44	235.00	245.00	0.20749E+04	0.31064E+04	0.0
45	235.00	248.03	0.20633E+04	0.30903E+04	0.0
46	235.00	250.28	0.20545E+04	0.30787E+04	0.0
47	235.00	251.95	0.20462E+04	0.30699E+04	0.0
48	235.00	253.28	0.20367E+04	0.30616E+04	0.0
49	235.00	254.50	0.20215E+04	0.30521E+04	0.0
50	235.00	255.98	0.19846E+04	0.30369E+04	0.0

## \*\*\* MATERIAL BALANCES \*\*\*

REEDS

	PLATE NO.	15
	LB MOL/TIRE	MOE FRAC
ETHANE	0.37700E+02	0.92402E-02
PROPANE	0.21861E+04	0.52846E+00
1-BUTANE	0.46050E+03	0.98162E-01
2-BUTANE	0.71530E+03	0.17532E+00
1-PENTANE	0.39120E+03	0.61869E-01
2-PENTANE	0.26710E+03	0.65666E-01
HEXANE	0.14180E+03	0.34755E-01
OCTANE	0.11030E+03	0.27034E-01
TOTAL	0.40800E+04	

## CONNECTED STREAMS

	PLATE NO. 5	FROM 31
	LB MOLE/TIME	NOL FRACTION
ETHANE	0.59456E+01	0.25785E-02
PROPANE	0.19513E+04	0.84624E+00
IBUTANE	0.25561E+03	0.11085E+00
IBUTANE	0.92887E+02	0.40284E-01
IPENTANE	0.73460E-01	0.31859E-04
NPENTANE	0.97349E-02	0.42219E-05
HEXANE	0.79791E-06	0.36604E-09
OCTANE	0.55187E-13	0.23934E-16
TOTAL	0.23058E+04	

	PLATE NO. 25	FROM 50
	LB MOLE/TIME	NOL FRACTION
ETHANE	0.17335E-04	0.87348E-08
PROPANE	0.10793E+02	0.54382E-02
IBUTANE	0.19609E+03	0.98808E-01
IBUTANE	0.64466E+03	0.32483E+00
IPENTANE	0.55735E+03	0.28084E+00
NPENTANE	0.52583E+03	0.26496E+00
HEXANE	0.44001E+02	0.22172E-01
OCTANE	0.58530E+01	0.29492E-02
TOTAL	0.19846E+04	

	PLATE NO. 31	FROM 5
	LB MOLE/TIME	NOL FRACTION
ETHANE	0.59507E+01	0.23803E-02
PROPANE	0.19605E+04	0.78419E+00
IBUTANE	0.36248E+03	0.14499E+00
IBUTANE	0.17081E+03	0.68322E-03
IPENTANE	0.25505E+00	0.10202E-03
NPENTANE	0.42796E-01	0.17119E-04
HEXANE	0.88358E-05	0.35343E-08
OCTANE	0.27696E-11	0.11078E-14
TOTAL	0.25000E+04	

	PLATE NO. 50	FROM 25
	LB MOLE/TIME	NOL FRACTION
ETHANE	0.14775E-03	0.49249E-07
PROPANE	0.41388E+02	0.13796E-01
IBUTANE	0.44574E+03	0.14858E+00
IBUTANE	0.12523E+04	0.41742E+00
IPENTANE	0.64633E+03	0.21544E+00
NPENTANE	0.56440E+03	0.18813E+00
HEXANE	0.44009E+02	0.14670E-01
OCTANE	0.58526E+01	0.19509E-02
TOTAL	0.30000E+04	

**PRODUCTS**

	TOP PRODUCT (1)		BOTTOM PRODUCT (30)	
	LB MOLE/TIME	MOL FRAC	LB MOLE/TIME	MOL FRAC
ETHANE	0.37695E+02	0.17129E-01	0.65303E-09	0.97501E-12
PROPANE	0.21164E+04	0.96174E+00	0.19924E-01	0.29748E-04
I-BUTANE	0.40011E+02	0.18182E-01	0.38486E+01	0.57462E-02
N-BUTANE	0.64387E+01	0.29258E-02	0.23299E+02	0.34786E-01
1-PENTANE	0.51366E-03	0.23342E-06	0.16202E+03	0.24191E+00
2-PENTANE	0.31892E-04	0.14692E-07	0.22848E+03	0.34114E+00
HEXANE	0.11616E-09	0.52784E-13	0.14179E+03	0.21170E+00
OCTANE	0.17576E-19	0.79808E-23	0.11030E+03	0.16468E+00
TOTAL	0.22006E+04		0.66977E+03	

	TOP PRODUCT (31)		BOTTOM PRODUCT (50)	
	LB MOLE/TIME	MOL FRAC	LB MOLE/TIME	MOL FRAC
ETHANE	0.59456E+01	0.25785E-02	0.17335E-04	0.87348E-08
PROPANE	0.19513E+04	0.84624E+00	0.10793E+02	0.54382E-02
I-BUTANE	0.25561E+03	0.11085E+00	0.19609E+03	0.98808E-01
N-BUTANE	0.92887E+02	0.40284E-01	0.64466E+03	0.32483E+00
1-PENTANE	0.73460E-01	0.31859E-04	0.55735E+03	0.28084E+00
2-PENTANE	0.97349E-02	0.42219E-05	0.52583E+03	0.26496E+00
HEXANE	0.79791E-06	0.34600E-09	0.480012E+02	0.22172E-01
OCTANE	0.55187E-13	0.23934E-16	0.58530E+01	0.29492E-02
TOTAL	0.23058E+04		0.19846E+04	

## LIQUID SIDE STREAMS

	LIQUID (5)
	LB MOL/TIME      MOL FRAC
ETHANE	0.59507E+01
PROPANE	0.19605E+04
IBUTANE	0.36248E+03
NBUTANE	0.17081E+03
IPENTANE	0.25505E+03
NPENTANE	0.42796E+01
HEXANE	0.88358E-05
OCTANE	0.27696E-11
TOTAL	0.25000E+04

## VAPOUR SIDE STREAMS

	VAPOUR (25)
	LB MOL/TIME      MOL FRAC
ETHANE	0.14775E-03
PROPANE	0.41388E+02
IBUTANE	0.44574E+03
NBUTANE	0.12523E+04
IPENTANE	0.64633E+03
NPENTANE	0.56440E+03
HEXANE	0.44009E+02
OCTANE	0.58526E+01
TOTAL	0.30000E+04

	VAPOUR (40)
	LB MOL/TIME      MOL FRAC
ETHANE	0.91745E-04
PROPANE	0.39612E+02
IBUTANE	0.35667E+03
NBUTANE	0.68555E+03
IPENTANE	0.89136E+02
NPENTANE	0.38597E+02
HEXANE	0.93357E-02
OCTANE	0.36103E-08
TOTAL	0.12096E+04

## APPENDIX 6.2 -- EXTRACTIVE DISTILLATION SYSTEM

## \*\* PROBLEM STATEMENT \*\*

COLUMN NC 1 IS DISTILLATION COL.

NO OF PLATES= 17  
 COL PRESSURE 14.70 PSIA  
 PRESSURE DROP 0.0 PER PLATE  
 REBOILER VAPOUR 185.00 MOLES  
 REFLUX RATIO 2. 3.000

COLUMN NC 2 IS DISTILLATION COL.

NO OF PLATES= 20  
 COL PRESSURE 14.70 PSIA  
 PRESSURE DROP 0.0 PER PLATE  
 REBOILER VAPOUR 135.00 MOLES  
 REFLUX RATIO 2.000

COLUMN NC 3 IS DISTILLATION COL.

NO OF PLATES= 5  
 COL PRESSURE 14.70 PSIA  
 PRESSURE DROP 0.0 PER PLATE  
 REBOILER VAPOUR 95.00 MOLES  
 REFLUX RATIO 10.000

NO. OF FEEDS 1

FEED 1 IS IN TO PLATE 11  
 QUANTITY 0.10000E+03  
 PRESSURE 14.70  
 TEMP (F) 136.47  
 ENTHALPY 0.31804E+06

NO. OF INTERCOOLERS OR HEATERS 3

INTERCOOLER OR HEATER 1 IS ON PLATE 17  
 HEAT LOAD IS A VARIABLE

INTERCOOLER OR HEATER 2 IS ON PLATE 37  
 HEAT LOAD IS A VARIABLE

INTERCOOLER OR HEATER 3 IS ON PLATE 42  
 HEAT LOAD IS A VARIABLE

## \*\*\* STREAM CONNECTIONS \*\*\*

LEAVING STREAM NO	LEAVING STAGE NO	STREAM FLUID	ENTERING FRACTION	ENTERING STREAM NO	ENTERING STAGE NO
1	17	3	1.00	2	24
2	37	3	1.00	3	40
3	42	3	1.00	1	4

STREAM FLUID 1=LIQUID SIDE STREAM 2=VAPOUR SIDE STREAM  
 3=LIQUID PRODUCT 4=VAPOUR PRODUCT

## \*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

0 SUM OF SQUARES OF RESIDUALS 0.14636E+02  
 (MAT. BAL. 0.14605E+02 HEAT BAL. 0.31148E-01)

## TEMPERATURE (R)

0.59360E+03 0.59460E+03 0.59560E+03 0.59660E+03 0.59760E+03  
 0.59860E+03 0.59960E+03 0.60060E+03 0.60160E+03 0.60260E+03  
 0.60360E+03 0.60460E+03 0.60560E+03 0.60660E+03 0.60760E+03  
 0.60860E+03 0.60960E+03 0.60960E+03 0.60860E+03 0.60760E+03  
 0.61260E+03 0.61760E+03 0.62260E+03 0.62560E+03 0.62760E+03  
 0.62960E+03 0.63160E+03 0.63960E+03 0.63960E+03 0.63960E+03  
 0.63960E+03 0.63960E+03 0.63960E+03 0.64460E+03 0.64960E+03  
 0.65460E+03 0.65960E+03 0.66960E+03 0.63960E+03 0.65960E+03  
 0.66460E+03 0.66960E+03

## VAPOUR FLOW RATE

0.0 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03  
 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03  
 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03 0.20000E+03  
 0.20000E+03 0.18500E+03 0.0 0.16500E+03 0.16500E+03  
 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03  
 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03  
 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03 0.16500E+03  
 0.16500E+03 0.13500E+03 0.0 0.11000E+03 0.11000E+03  
 0.11000E+03 0.95000E+02

1 SUM OF SQUARES OF RESIDUALS 0.26888E+02

(MAT. BAL. 0.26868E+02 HEAT BAL. 0.20756E-01)

## TEMPERATURE (R)

0.58860E+03 0.57241E+03 0.56798E+03 0.56905E+03 0.59540E+03  
 0.59934E+03 0.60220E+03 0.60410E+03 0.60546E+03 0.60606E+03  
 0.60504E+03 0.60591E+03 0.60678E+03 0.60760E+03 0.60872E+03  
 0.61038E+03 0.61492E+03 0.59942E+03 0.60331E+03 0.60836E+03  
 0.61393E+03 0.62014E+03 0.62685E+03 0.63234E+03 0.63719E+03  
 0.64321E+03 0.65064E+03 0.66172E+03 0.66547E+03 0.66833E+03  
 0.66960E+03 0.66883E+03 0.66602E+03 0.66367E+03 0.66040E+03  
 0.65949E+03 0.66182E+03 0.61883E+03 0.64555E+03 0.66191E+03  
 0.66575E+03 0.66976E+03

## VAPOUR FLOW RATE

0.0 0.20898E+03 0.20448E+03 0.19320E+03 0.19110E+03  
 0.19305E+03 0.19446E+03 0.19545E+03 0.19634E+03 0.19736E+03  
 0.19885E+03 0.19845E+03 0.19849E+03 0.19850E+03 0.19844E+03  
 0.19817E+03 0.18500E+03 0.0 0.16256E+03 0.16196E+03  
 0.16126E+03 0.16027E+03 0.15927E+03 0.15828E+03 0.15973E+03  
 0.16040E+03 0.16126E+03 0.16322E+03 0.16441E+03 0.16332E+03  
 0.16617E+03 0.16673E+03 0.16679E+03 0.16674E+03 0.16495E+03  
 0.16196E+03 0.13500E+03 0.0 0.10848E+03 0.10784E+03  
 0.10761E+03 0.95000E+02

2 SUM OF SQUARES OF RESIDUALS : 0.12652E+02  
 (MAT. BAL. 0.12640E+02 HEAT BAL. 0.11620E-01)

## TEMPERATURE (R)

0.58681E+03	0.56812E+03	0.50798E+03	0.53224E+03	0.55262E+03
0.57342E+03	0.55770E+03	0.59704E+03	0.60290E+03	0.60578E+03
0.60442E+03	0.60955E+03	0.60565E+03	0.60628E+03	0.60715E+03
0.60924E+03	0.61767E+03	0.60194E+03	0.60591E+03	0.61171E+03
0.61708E+03	0.62159E+03	0.62547E+03	0.63072E+03	0.63367E+03
0.63696E+03	0.64167E+03	0.64903E+03	0.65100E+03	0.65209E+03
0.65384E+03	0.65347E+03	0.65155E+03	0.65075E+03	0.65090E+03
0.65513E+03	0.66144E+03	0.62463E+03	0.64486E+03	0.66216E+03
0.66624E+03	0.66968E+03			

## VAPOUR FLOW RATE

0.0	0.21603E+03	0.23357E+03	0.19962E+03	0.17356E+03
0.17630E+03	0.18142E+03	0.18952E+03	0.18685E+03	0.19200E+03
0.19598E+03	0.19599E+03	0.19607E+03	0.19609E+03	0.19595E+03
0.19533E+03	0.18500E+03	0.0	0.15899E+03	0.15809E+03
0.15739E+03	0.15633E+03	0.15502E+03	0.15270E+03	0.15483E+03
0.15533E+03	0.15524E+03	0.15671E+03	0.15781E+03	0.15819E+03
0.15877E+03	0.15892E+03	0.15935E+03	0.15985E+03	0.15641E+03
0.15241E+03	0.13500E+03	0.0	0.10649E+03	0.10324E+03
0.10329E+03	0.95000E+02			

3 SUM OF SQUARES OF RESIDUALS : 0.12652E+01  
 (MAT. BAL. 0.1263004E+01 HEAT BAL. 0.49314E-02)

## TEMPERATURE (R)

0.58688E+03	0.57961E+03	0.56798E+03	0.58133E+03	0.58019E+03
0.57967E+03	0.58540E+03	0.59394E+03	0.59970E+03	0.60388E+03
0.60316E+03	0.60361E+03	0.60462E+03	0.60444E+03	0.60506E+03
0.60694E+03	0.61686E+03	0.60220E+03	0.60543E+03	0.61092E+03
0.61563E+03	0.61940E+03	0.62270E+03	0.62878E+03	0.63301E+03
0.63728E+03	0.64181E+03	0.64716E+03	0.64791E+03	0.64833E+03
0.64784E+03	0.64616E+03	0.64329E+03	0.64148E+03	0.64221E+03
0.65001E+03	0.66038E+03	0.62706E+03	0.64156E+03	0.66127E+03
0.66629E+03	0.66970E+03			

## VAPOUR FLOW RATE

0.0	0.21743E+03	0.21095E+03	0.20217E+03	0.18761E+03
0.18644E+03	0.18416E+03	0.18488E+03	0.18681E+03	0.18986E+03
0.19434E+03	0.19481E+03	0.19489E+03	0.19492E+03	0.19479E+03
0.19406E+03	0.18500E+03	0.0	0.15867E+03	0.15815E+03
0.15795E+03	0.15676E+03	0.15467E+03	0.15107E+03	0.15368E+03
0.15481E+03	0.15326E+03	0.15719E+03	0.15854E+03	0.15887E+03
0.15920E+03	0.15934E+03	0.15912E+03	0.15801E+03	0.15449E+03
0.14847E+03	0.13500E+03	0.0	0.10705E+03	0.10102E+03
0.10094E+03	0.95000E+02			

4. SUM OF SQUARES OF RESIDUALS  $0.49263E+00$   
 (MAT. BAL.  $0.48590E+00$  HEAT BAL.  $0.67322E-02$ )

## TEMPERATURE (R)

$0.58723E+03$	$0.59757E+03$	$0.60600E+03$	$0.60172E+03$	$0.59847E+03$
$0.59641E+03$	$0.59377E+03$	$0.59352E+03$	$0.59663E+03$	$0.60077E+03$
$0.60084E+03$	$0.60091E+03$	$0.60096E+03$	$0.60094E+03$	$0.60092E+03$
$0.60188E+03$	$0.61354E+03$	$0.60213E+03$	$0.60364E+03$	$0.60356E+03$
$0.61201E+03$	$0.61366E+03$	$0.61441E+03$	$0.62062E+03$	$0.62631E+03$
$0.63213E+03$	$0.63733E+03$	$0.64029E+03$	$0.64079E+03$	$0.64036E+03$
$0.63910E+03$	$0.63717E+03$	$0.63462E+03$	$0.63200E+03$	$0.63400E+03$
$0.64539E+03$	$0.66131E+03$	$0.63946E+03$	$0.64513E+03$	$0.66386E+03$
$0.66893E+03$	$0.67088E+03$			

## VAPOUR FLOW RATE

$0.0$	$0.22009E+03$	$0.21300E+03$	$0.21307E+03$	$0.19134E+03$
$0.18906E+03$	$0.18895E+03$	$0.18720E+03$	$0.18866E+03$	$0.18806E+03$
$0.19006E+03$	$0.19197E+03$	$0.19204E+03$	$0.19213E+03$	$0.19217E+03$
$0.19156E+03$	$0.18800E+03$	$0.0$	$0.18664E+03$	$0.18702E+03$
$0.15793E+03$	$0.15696E+03$	$0.15384E+03$	$0.14780E+03$	$0.15003E+03$
$0.15183E+03$	$0.15244E+03$	$0.15450E+03$	$0.15656E+03$	$0.15774E+03$
$0.15886E+03$	$0.15983E+03$	$0.16053E+03$	$0.15997E+03$	$0.15536E+03$
$0.14473E+03$	$0.13800E+03$	$0.0$	$0.11204E+03$	$0.98779E+02$
$0.97134E+02$	$0.95000E+02$			

5. SUM OF SQUARES OF RESIDUALS  $0.45953E+00$ (MAT. BAL.  $0.43940E+00$  HEAT BAL.  $0.20125E-01$ )

## TEMPERATURE (R)

$0.58749E+03$	$0.59529E+03$	$0.59773E+03$	$0.60494E+03$	$0.60496E+03$
$0.60491E+03$	$0.60460E+03$	$0.60378E+03$	$0.60279E+03$	$0.60281E+03$
$0.60165E+03$	$0.60168E+03$	$0.60175E+03$	$0.60187E+03$	$0.60194E+03$
$0.60201E+03$	$0.60984E+03$	$0.60199E+03$	$0.60357E+03$	$0.60807E+03$
$0.61153E+03$	$0.61356E+03$	$0.61265E+03$	$0.61176E+03$	$0.61163E+03$
$0.60947E+03$	$0.60960E+03$	$0.61290E+03$	$0.61713E+03$	$0.62106E+03$
$0.62615E+03$	$0.62934E+03$	$0.63207E+03$	$0.63437E+03$	$0.63942E+03$
$0.65202E+03$	$0.66539E+03$	$0.65044E+03$	$0.66263E+03$	$0.67036E+03$
$0.67187E+03$	$0.67165E+03$			

## VAPOUR FLOW RATE

$0.0$	$0.21256E+03$	$0.21134E+03$	$0.20404E+03$	$0.18901E+03$
$0.18921E+03$	$0.18952E+03$	$0.18955E+03$	$0.18896E+03$	$0.18795E+03$
$0.18946E+03$	$0.19002E+03$	$0.19003E+03$	$0.19014E+03$	$0.19043E+03$
$0.19072E+03$	$0.18800E+03$	$0.0$	$0.16324E+03$	$0.16392E+03$
$0.16321E+03$	$0.16404E+03$	$0.16214E+03$	$0.15869E+03$	$0.15902E+03$
$0.16032E+03$	$0.15872E+03$	$0.15666E+03$	$0.15710E+03$	$0.15621E+03$
$0.15630E+03$	$0.16132E+03$	$0.16659E+03$	$0.16679E+03$	$0.16633E+03$
$0.15330E+03$	$0.13800E+03$	$0.0$	$0.12414E+03$	$0.10168E+03$
$0.97202E+02$	$0.98000E+02$			

6 SUM OF SQUARES OF RESIDUALS  $0.34480E+00$   
 (MAT. BAL.  $0.33790E+00$  HEAT BAL.  $0.69780E-02$ )

## TEMPERATURE (R)

$0.58670E+03$	$0.59391E+03$	$0.59645E+03$	$0.60132E+03$	$0.60180E+03$
$0.60234E+03$	$0.60271E+03$	$0.60283E+03$	$0.60282E+03$	$0.60304E+03$
$0.60180E+03$	$0.60182E+03$	$0.60189E+03$	$0.60212E+03$	$0.60261E+03$
$0.60357E+03$	$0.61107E+03$	$0.60294E+03$	$0.60427E+03$	$0.60817E+03$
$0.61106E+03$	$0.61330E+03$	$0.61658E+03$	$0.62314E+03$	$0.63048E+03$
$0.63653E+03$	$0.63967E+03$	$0.63994E+03$	$0.63632E+03$	$0.63272E+03$
$0.62913E+03$	$0.62610E+03$	$0.62366E+03$	$0.62219E+03$	$0.62461E+03$
$0.63985E+03$	$0.66132E+03$	$0.62568E+03$	$0.63006E+03$	$0.66786E+03$
$0.67071E+03$	$0.67144E+03$			

## VAPOUR FLOW RATE

$0.0$	$0.20961E+03$	$0.20902E+03$	$0.20225E+03$	$0.18933E+03$
$0.18846E+03$	$0.18576E+03$	$0.18610E+03$	$0.18632E+03$	$0.18637E+03$
$0.18813E+03$	$0.18872E+03$	$0.18870E+03$	$0.18870E+03$	$0.18803E+03$
$0.18922E+03$	$0.18590E+03$	$0.0$	$0.17648E+03$	$0.17600E+03$
$0.18648E+03$	$0.18178E+03$	$0.17894E+03$	$0.17134E+03$	$0.18024E+03$
$0.18734E+03$	$0.19197E+03$	$0.19332E+03$	$0.19227E+03$	$0.19012E+03$
$0.18799E+03$	$0.18627E+03$	$0.18918E+03$	$0.18366E+03$	$0.17592E+03$
$0.15338E+03$	$0.13890E+03$	$0.0$	$0.95207E+02$	$0.92399E+02$
$0.94294E+02$	$0.91400E+02$			

7 SUM OF SQUARES OF RESIDUALS  $0.11764E+00$

(MAT. BAL.  $0.11673E+00$  HEAT BAL.  $0.51062E-03$ )

## TEMPERATURE (R)

$0.58684E+03$	$0.59427E+03$	$0.59354E+03$	$0.60051E+03$	$0.60037E+03$
$0.60041E+03$	$0.60063E+03$	$0.60095E+03$	$0.60132E+03$	$0.60184E+03$
$0.60121E+03$	$0.60120E+03$	$0.60120E+03$	$0.60130E+03$	$0.60169E+03$
$0.60280E+03$	$0.61026E+03$	$0.60967E+03$	$0.60268E+03$	$0.60232E+03$
$0.61267E+03$	$0.61540E+03$	$0.61730E+03$	$0.62152E+03$	$0.62754E+03$
$0.63204E+03$	$0.63443E+03$	$0.63565E+03$	$0.63413E+03$	$0.63660E+03$
$0.63713E+03$	$0.63759E+03$	$0.63793E+03$	$0.63832E+03$	$0.64150E+03$
$0.65171E+03$	$0.66803E+03$	$0.63368E+03$	$0.65852E+03$	$0.66879E+03$
$0.67008E+03$	$0.67147E+03$			

## VAPOUR FLOW RATE

$0.0$	$0.21193E+03$	$0.21008E+03$	$0.20302E+03$	$0.18633E+03$
$0.18616E+03$	$0.18637E+03$	$0.18613E+03$	$0.18627E+03$	$0.18648E+03$
$0.18622E+03$	$0.18944E+03$	$0.18933E+03$	$0.18870E+03$	$0.18894E+03$
$0.18908E+03$	$0.18890E+03$	$0.0$	$0.18631E+03$	$0.15773E+03$
$0.18924E+03$	$0.18108E+03$	$0.16122E+03$	$0.18670E+03$	$0.16215E+03$
$0.16596E+03$	$0.16966E+03$	$0.17344E+03$	$0.17671E+03$	$0.17896E+03$
$0.17994E+03$	$0.18897E+03$	$0.18102E+03$	$0.18190E+03$	$0.17792E+03$
$0.18904E+03$	$0.13890E+03$	$0.0$	$0.16690E+03$	$0.96471E+02$
$0.95200E+02$	$0.96000E+02$			

## 8 SUM OF SQUARES OF RESIDUALS 0.76123E-01

(MAT. BAL. 0.67220E-01 HEAT BAL. 0.39620E-02)

## TEMPERATURE (R)

0.58693E+03	0.59443E+03	0.59587E+03	0.60134E+03	0.60153E+03
0.60130E+03	0.60153E+03	0.60165E+03	0.60166E+03	0.60220E+03
0.60142E+03	0.60144E+03	0.60147E+03	0.60155E+03	0.60185E+03
0.60205E+03	0.60990E+03	0.60145E+03	0.60477E+03	0.60993E+03
0.61212E+03	0.61438E+03	0.61579E+03	0.61710E+03	0.62204E+03
0.62348E+03	0.62494E+03	0.62582E+03	0.62660E+03	0.62755E+03
0.62927E+03	0.63203E+03	0.63333E+03	0.63919E+03	0.64000E+03
0.66169E+03	0.66944E+03	0.65122E+03	0.66890E+03	0.67112E+03
0.67153E+03	0.67168E+03			

## VAPOUR FLOW RATE

0.0	0.21149E+03	0.21062E+03	0.20337E+03	0.19544E+03
0.18644E+03	0.18643E+03	0.18630E+03	0.18641E+03	0.18600E+03
0.18813E+03	0.18894E+03	0.18896E+03	0.18850E+03	0.18900E+03
0.18902E+03	0.18900E+03	0.0	0.18200E+03	0.18202E+03
0.18389E+03	0.18307E+03	0.18320E+03	0.18600E+03	0.18610E+03
0.18765E+03	0.17012E+03	0.17200E+03	0.17317E+03	0.17367E+03
0.17395E+03	0.17424E+03	0.17493E+03	0.17502E+03	0.17623E+03
0.18225E+03	0.13860E+03	0.0	0.18700E+03	0.18717E+03
0.98500E+02	0.98000E+02			

## 9 SUM OF SQUARES OF RESIDUALS 0.61316E-01

(MAT. BAL. 0.60327E-01 HEAT BAL. 0.78009E-03)

## TEMPERATURE (R)

0.58697E+03	0.59432E+03	0.59572E+03	0.60129E+03	0.60131E+03
0.60130E+03	0.60148E+03	0.60164E+03	0.60192E+03	0.60225E+03
0.60144E+03	0.60148E+03	0.60150E+03	0.60151E+03	0.60196E+03
0.60304E+03	0.61024E+03	0.60234E+03	0.60242E+03	0.61036E+03
0.61377E+03	0.61619E+03	0.61770E+03	0.62000E+03	0.62647E+03
0.62991E+03	0.63162E+03	0.63201E+03	0.63202E+03	0.62956E+03
0.62706E+03	0.62447E+03	0.62363E+03	0.62700E+03	0.64033E+03
0.65056E+03	0.66840E+03	0.66903E+03	0.66872E+03	0.67000E+03
0.67135E+03	0.67150E+03			

## VAPOUR FLOW RATE

0.0	0.21162E+03	0.21094E+03	0.20313E+03	0.18604E+03
0.18602E+03	0.18611E+03	0.18610E+03	0.18620E+03	0.18600E+03
0.18604E+03	0.18674E+03	0.18600E+03	0.18690E+03	0.18687E+03
0.18603E+03	0.18600E+03	0.0	0.17000E+03	0.18607E+03
0.18640E+03	0.17724E+03	0.17724E+03	0.17172E+03	0.17200E+03
0.18622E+03	0.18765E+03	0.18640E+03	0.19007E+03	0.19061E+03
0.18636E+03	0.18739E+03	0.18640E+03	0.17400E+03	0.18300E+03
0.14140E+03	0.13860E+03	0.0	0.94737E+02	0.94600E+02
0.94600E+02	0.93000E+02			

10 SUM OF SQUARES OF RESIDUALS: 0.29567E-01  
 (MAT. BAL.: 0.29573E-01 HEAT BAL.: 0.29567E-01)

## TEMPERATURE (R)

0.58667E+03	0.59433E+03	0.59571E+03	0.60123E+03	0.60137E+03
0.60122E+03	0.60131E+03	0.60142E+03	0.60170E+03	0.60214E+03
0.60130E+03	0.60139E+03	0.60143E+03	0.60163E+03	0.60182E+03
0.60206E+03	0.61026E+03	0.60144E+03	0.60169E+03	0.61066E+03
0.61397E+03	0.61607E+03	0.61704E+03	0.62030E+03	0.62341E+03
0.62296E+03	0.63187E+03	0.63223E+03	0.63446E+03	0.63546E+03
0.63594E+03	0.63666E+03	0.63694E+03	0.63766E+03	0.64233E+03
0.66034E+03	0.66092E+03	0.66071E+03	0.66536E+03	0.67036E+03
0.67137E+03	0.67150E+03			

## VAPOUR FLOW RATE

0.0	0.58667E+03	0.59433E+03	0.59571E+03	0.60123E+03
0.10051E+03	0.10051E+03	0.10051E+03	0.10051E+03	0.10051E+03
0.18869E+03	0.18867E+03	0.18866E+03	0.18866E+03	0.18866E+03
0.18893E+03	0.18890E+03	0.0	0.17107E+03	0.17203E+03
0.17464E+03	0.17522E+03	0.17466E+03	0.16913E+03	0.17546E+03
0.18012E+03	0.18346E+03	0.18680E+03	0.15756E+03	0.18910E+03
0.19031E+03	0.19158E+03	0.19143E+03	0.18719E+03	0.18993E+03
0.14451E+03	0.13900E+03	0.0	0.97957E+02	0.95006E+02
0.95006E+02	0.95006E+02			

11 SUM OF SQUARES OF RESIDUALS: 0.18720E-01  
 (MAT. BAL.: 0.17724E-01 HEAT BAL.: 0.18960E-01)

## TEMPERATURE (R)

0.58666E+03	0.59433E+03	0.59574E+03	0.60123E+03	0.60126E+03
0.60131E+03	0.60139E+03	0.60153E+03	0.60183E+03	0.60217E+03
0.60140E+03	0.60141E+03	0.60145E+03	0.60155E+03	0.60157E+03
0.60238E+03	0.61016E+03	0.60147E+03	0.60606E+03	0.61047E+03
0.61395E+03	0.61899E+03	0.61738E+03	0.61966E+03	0.62373E+03
0.62613E+03	0.62731E+03	0.62799E+03	0.62877E+03	0.62996E+03
0.63151E+03	0.63316E+03	0.63496E+03	0.63666E+03	0.64952E+03
0.66344E+03	0.66906E+03	0.66069E+03	0.66612E+03	0.67101E+03
0.67146E+03	0.67161E+03			

## VAPOUR FLOW RATE

0.0	0.21120E+03	0.21440E+03	0.20330E+03	0.18620E+03
0.18621E+03	0.18622E+03	0.18623E+03	0.18627E+03	0.18647E+03
0.18866E+03	0.18868E+03	0.18868E+03	0.18868E+03	0.18868E+03
0.18892E+03	0.18890E+03	0.0	0.17057E+03	0.17143E+03
0.17363E+03	0.17310E+03	0.17210E+03	0.16747E+03	0.17396E+03
0.17827E+03	0.18070E+03	0.18100E+03	0.18220E+03	0.18244E+03
0.18246E+03	0.18346E+03	0.18410E+03	0.18150E+03	0.18576E+03
0.14446E+03	0.13600E+03	0.0	0.99200E+02	0.95499E+02
0.95102E+02	0.95006E+02			

12 SUM OF SQUARES OF RESIDUALS 0.11350E-01  
 (MAT. BAL. 0.31254E-01 MEAT BAL. 0.71254E-04).

## TEMPERATURE (K)

0.36667E+03	0.39434E+03	0.39373E+03	0.39122E+03	0.39122E+03
0.60130E+03	0.60130E+03	0.60130E+03	0.60130E+03	0.60130E+03
0.69140E+03	0.69140E+03	0.69140E+03	0.69140E+03	0.69140E+03
0.68297E+03	0.68297E+03	0.68297E+03	0.68297E+03	0.68297E+03
0.61410E+03	0.61410E+03	0.61410E+03	0.61410E+03	0.61410E+03
0.62934E+03	0.63120E+03	0.63280E+03	0.62934E+03	0.62622E+03
0.62934E+03	0.62934E+03	0.62934E+03	0.62934E+03	0.62934E+03
0.66295E+03	0.66295E+03	0.66295E+03	0.66295E+03	0.66295E+03
0.67106E+03	0.67106E+03	0.67106E+03	0.67106E+03	0.67106E+03

## VAPOUR FLOW RATE

0.0	0.21679E+03	0.21679E+03	0.21679E+03	0.21679E+03
0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03
0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03
0.17637E+03	0.17637E+03	0.17637E+03	0.17637E+03	0.17637E+03
0.12277E+03	0.12277E+03	0.12277E+03	0.12277E+03	0.12277E+03
0.18793E+03	0.18793E+03	0.18793E+03	0.18793E+03	0.18793E+03
0.13931E+03	0.13931E+03	0.13931E+03	0.13931E+03	0.13931E+03
0.94994E+02	0.94994E+02	0.94994E+02	0.94994E+02	0.94994E+02

13 SUM OF SQUARES OF RESIDUALS 0.22596E-02

(MAT. BAL. 0.21679E-02 MEAT BAL. 0.66734E-04).

## TEMPERATURE (K)

0.36667E+03	0.39434E+03	0.39373E+03	0.39121E+03	0.39121E+03
0.60129E+03	0.60129E+03	0.60129E+03	0.60129E+03	0.60129E+03
0.69140E+03	0.69140E+03	0.69140E+03	0.69140E+03	0.69140E+03
0.68296E+03	0.68296E+03	0.68296E+03	0.68296E+03	0.68296E+03
0.61400E+03	0.61400E+03	0.61400E+03	0.61400E+03	0.61400E+03
0.62930E+03	0.63110E+03	0.63280E+03	0.63280E+03	0.63280E+03
0.63179E+03	0.63164E+03	0.63254E+03	0.63254E+03	0.63254E+03
0.66391E+03	0.66391E+03	0.66391E+03	0.66391E+03	0.66391E+03
0.67106E+03	0.67106E+03	0.67106E+03	0.67106E+03	0.67106E+03

## VAPOUR FLOW RATE

0.0	0.21679E+03	0.21679E+03	0.21679E+03	0.21679E+03
0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03
0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03
0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03	0.13666E+03
0.17637E+03	0.17637E+03	0.17637E+03	0.17637E+03	0.17637E+03
0.12277E+03	0.12277E+03	0.12277E+03	0.12277E+03	0.12277E+03
0.18793E+03	0.18793E+03	0.18793E+03	0.18793E+03	0.18793E+03
0.13931E+03	0.13931E+03	0.13931E+03	0.13931E+03	0.13931E+03
0.94994E+02	0.94994E+02	0.94994E+02	0.94994E+02	0.94994E+02

14 SUM OF SQUARES OF RESIDUALS 0.21157E-02

(CAT. BAL. 0.19336E-03 MEAT BAL. 0.18207E-03)

## TEMPERATURE (K)

0.50057E+03	0.50134E+03	0.50073E+03	0.50121E+03	0.50130E+03
0.60120E+03	0.60130E+03	0.60150E+03	0.60162E+03	0.60217E+03
0.60140E+03	0.60145E+03	0.60149E+03	0.60160E+03	0.60160E+03
0.60290E+03	0.60160E+03	0.60160E+03	0.60097E+03	0.61070E+03
0.61090E+03	0.61010E+03	0.61777E+03	0.60090E+03	0.62617E+03
0.62230E+03	0.63030E+03	0.63150E+03	0.63140E+03	0.63210E+03
0.63200E+03	0.63030E+03	0.63307E+03	0.63040E+03	0.63140E+03
0.64610E+03	0.67010E+03	0.66371E+03	0.66570E+03	0.67114E+03
0.67150E+03	0.67160E+03			

## VAPOUR FLOW RATE

0.0	0.21157E+03	0.21042E+03	0.20320E+03	0.19610E+03
0.16050E+03	0.16077E+03	0.16037E+03	0.16040E+03	0.16030E+03
0.16090E+03	0.16090E+03	0.0	0.17300E+03	0.17400E+03
0.17513E+03	0.17530E+03	0.17494E+03	0.17494E+03	0.17504E+03
0.18050E+03	0.18370E+03	0.18572E+03	0.18570E+03	0.18744E+03
0.18772E+03	0.18784E+03	0.18618E+03	0.17800E+03	0.18600E+03
0.14637E+03	0.13900E+03	0.0	0.37000E+02	0.36168E+02
0.95032E+02	0.95000E+02			

15 SUM OF SQUARES OF RESIDUALS -0.78567E-03

(CAT. BAL. 0.74466E-03 MEAT BAL. 0.46500E-04)

## TEMPERATURE (K)

0.50057E+03	0.59430E+03	0.50073E+03	0.60121E+03	0.60124E+03
0.60120E+03	0.60130E+03	0.60150E+03	0.60132E+03	0.60217E+03
0.60140E+03	0.60145E+03	0.60149E+03	0.60150E+03	0.60160E+03
0.60290E+03	0.61010E+03	0.60170E+03	0.60090E+03	0.61090E+03
0.61410E+03	0.61621E+03	0.61750E+03	0.62000E+03	0.62400E+03
0.62777E+03	0.62797E+03	0.63030E+03	0.63091E+03	0.63121E+03
0.63130E+03	0.63150E+03	0.63207E+03	0.63770E+03	0.64500E+03
0.66837E+03	0.67031E+03	0.66622E+03	0.66993E+03	0.67110E+03
0.67150E+03	0.67160E+03			

## VAPOUR FLOW RATE

0.0	0.21157E+03	-0.21042E+03	0.20320E+03	0.19610E+03
0.16010E+03	0.16030E+03	0.16021E+03	0.16000E+03	0.16040E+03
0.16090E+03	0.16090E+03	0.16037E+03	0.15000E+03	0.16070E+03
0.16990E+03	0.16990E+03	0.0	0.17300E+03	0.17400E+03
0.17500E+03	0.17511E+03	0.17477E+03	0.16900E+03	0.17500E+03
0.18110E+03	0.18413E+03	0.18600E+03	0.18470E+03	0.18500E+03
0.18750E+03	0.18733E+03	0.18670E+03	0.17700E+03	0.18600E+03
0.13600E+03	0.13200E+03	0.0	0.96400E+02	0.96400E+02
0.95010E+02	0.95000E+02			

16 SUM OF SQUARES OF RESIDUALS 0.46230E-03  
 (MAT. BAL. 0.45865E-03 MEAT BAL. 0.36872E-03)

## TEMPERATURE (R)

0.58667E+03	0.59434E+03	0.59573E+03	0.60121E+03	0.60124E+03
0.60129E+03	0.60130E+03	0.60154E+03	0.60162E+03	0.60217E+03
0.60140E+03	0.60141E+03	0.60146E+03	0.60166E+03	0.60169E+03
0.60296E+03	0.61010E+03	0.60176E+03	0.60610E+03	0.61087E+03
0.61412E+03	0.61620E+03	0.61762E+03	0.62030E+03	0.62207E+03
0.62813E+03	0.63004E+03	0.63072E+03	0.63310E+03	0.63132E+03
0.63134E+03	0.63126E+03	0.63177E+03	0.63631E+03	0.63693E+03
0.66400E+03	0.67022E+03	0.66415E+03	0.66850E+03	0.67116E+03
0.67150E+03	0.67162E+03			

## VAPOUR FLOW RATE

0.0		0.10000E+03	0.10000E+03	0.10000E+03
0.15614E+03	0.15614E+03	0.17007E+03	0.17007E+03	0.17007E+03
0.15600E+03	0.15607E+03	0.15607E+03	0.15607E+03	0.15607E+03
0.15603E+03	0.15600E+03	0.0	0.17507E+03	0.17507E+03
0.17624E+03	0.17646E+03	0.17713E+03	0.17800E+03	0.17678E+03
0.18154E+03	0.18475E+03	0.18475E+03	0.18737E+03	0.18705E+03
0.18867E+03	0.18791E+03	0.18630E+03	0.17782E+03	0.18567E+03
0.18839E+03	0.18500E+03	0.0	0.96275E+02	0.95030E+02
0.99999E+02	0.99999E+02			

17 SUM OF SQUARES OF RESIDUALS 0.28302E-03  
 (MAT. BAL. 0.25201E-03 MEAT BAL. 0.10123E-03)

## TEMPERATURE (R)

0.58667E+03	0.59434E+03	0.59573E+03	0.60121E+03	0.60124E+03
0.60129E+03	0.60130E+03	0.60154E+03	0.60162E+03	0.60217E+03
0.60140E+03	0.60141E+03	0.60146E+03	0.60166E+03	0.60169E+03
0.60296E+03	0.61010E+03	0.60176E+03	0.60610E+03	0.61087E+03
0.61412E+03	0.61620E+03	0.61762E+03	0.62030E+03	0.62207E+03
0.62813E+03	0.63004E+03	0.63072E+03	0.63121E+03	0.63174E+03
0.63217E+03	0.63219E+03	0.63267E+03	0.63643E+03	0.63693E+03
0.66400E+03	0.67022E+03	0.66415E+03	0.66850E+03	0.67116E+03
0.67150E+03	0.67162E+03			

## VAPOUR FLOW RATE

0.0	0.21125E+03	0.21062E+03	0.20329E+03	0.19615E+03
0.15614E+03	0.15600E+03	0.15641E+03	0.15636E+03	0.15644E+03
0.15600E+03	0.15607E+03	0.15607E+03	0.15600E+03	0.15603E+03
0.15603E+03	0.15600E+03	0.0	0.17370E+03	0.17370E+03
0.17624E+03	0.17630E+03	0.17697E+03	0.17684E+03	0.17694E+03
0.18154E+03	0.18446E+03	0.18446E+03	0.18740E+03	0.18615E+03
0.18867E+03	0.18843E+03	0.18780E+03	0.17900E+03	0.18607E+03
0.18839E+03	0.18500E+03	0.0	0.96303E+02	0.95030E+02
0.99999E+02	0.99999E+02			

18 SUM OF SQUARES OF RESIDUALS : 0.30840E-03  
 (MAT. BAL. 0.20450E-03 MEAT BAL. 0.10040E-04)

## TEMPERATURE (K)

0.50067E+03	0.59434E+03	0.50573E+03	0.60181E+03	0.60124E+03
0.60120E+03	0.60130E+03	0.60150E+03	0.60100E+03	0.60217E+03
0.60140E+03	0.60141E+03	0.60145E+03	0.60150E+03	0.60100E+03
0.60290E+03	0.61017E+03	0.60173E+03	0.60007E+03	0.61000E+03
0.61410E+03	0.61620E+03	0.61760E+03	0.62030E+03	0.62514E+03
0.62620E+03	0.63004E+03	0.63077E+03	0.63180E+03	0.63100E+03
0.63210E+03	0.63230E+03	0.63300E+03	0.63793E+03	0.63100E+03
0.66630E+03	0.67030E+03	0.66807E+03	0.66991E+03	0.67110E+03
0.67153E+03	0.67162E+03			

## VAPOUR FLOW RATE

0.0	0.21120E+03	0.21042E+03	0.20329E+03	0.18610E+03
0.18600E+03	0.18610E+03	0.18620E+03	0.18640E+03	0.18600E+03
0.18600E+03	0.18607E+03	0.18607E+03	0.18600E+03	0.18600E+03
0.18693E+03	0.18693E+03	0.0	0.17364E+03	0.17400E+03
0.17587E+03	0.17613E+03	0.17607E+03	0.17607E+03	0.17672E+03
0.18146E+03	0.18494E+03	0.18632E+03	0.18720E+03	0.18774E+03
0.18603E+03	0.18600E+03	0.18600E+03	0.17672E+03	0.18607E+03
0.13866E+03	0.13866E+03	0.0	0.96402E+02	0.96064E+02
0.95011E+02	0.95000E+02			

19 SUM OF SQUARES OF RESIDUALS 0.20242E-03  
 (MAT. BAL. 0.18517E-03 MEAT BAL. 0.17249E-04)

## TEMPERATURE (K)

0.50067E+03	0.59434E+03	0.50573E+03	0.60181E+03	0.60124E+03
0.60120E+03	0.60130E+03	0.60150E+03	0.60100E+03	0.60217E+03
0.60140E+03	0.60141E+03	0.60145E+03	0.60150E+03	0.60100E+03
0.60290E+03	0.61017E+03	0.60173E+03	0.60610E+03	0.61007E+03
0.61410E+03	0.61620E+03	0.61760E+03	0.62027E+03	0.62500E+03
0.62817E+03	0.62999E+03	0.63077E+03	0.63117E+03	0.63142E+03
0.63161E+03	0.63193E+03	0.63293E+03	0.63793E+03	0.63280E+03
0.66630E+03	0.67030E+03	0.66614E+03	0.66910E+03	0.67121E+03
0.67153E+03	0.67162E+03			

## VAPOUR FLOW RATE

0.0	0.21120E+03	0.21042E+03	0.20329E+03	0.18610E+03
0.18619E+03	0.18619E+03	0.18620E+03	0.18620E+03	0.18640E+03
0.18600E+03	0.18607E+03	0.18607E+03	0.18600E+03	0.18600E+03
0.18693E+03	0.18693E+03	0.0	0.17364E+03	0.17400E+03
0.17587E+03	0.17614E+03	0.17607E+03	0.17600E+03	0.17672E+03
0.18146E+03	0.18488E+03	0.18620E+03	0.18717E+03	0.18737E+03
0.18771E+03	0.18780E+03	0.18620E+03	0.17774E+03	0.18670E+03
0.13864E+03	0.13866E+03	0.0	0.96300E+02	0.96064E+02
0.95011E+02	0.95000E+02			

20 SUM OF SQUARES OF RESIDUALS 0.89671E-04  
 (MAT. BAL. 0.68960E-04 MEAT BAL. 0.76733E-06)  
 TEMPERATURE (R)

0.58687E+03	0.59434E+03	0.59573E+03	0.60121E+03	0.60124E+03
0.60129E+03	0.60138E+03	0.60154E+03	0.60152E+03	0.60217E+03
0.60140E+03	0.60141E+03	0.60149E+03	0.60150E+03	0.60150E+03
0.60229E+03	0.61017E+03	0.60177E+03	0.60612E+03	0.61090E+03
0.61428E+03	0.61628E+03	0.61760E+03	0.62038E+03	0.62519E+03
0.62633E+03	0.63010E+03	0.63105E+03	0.63143E+03	0.63187E+03
0.63188E+03	0.63189E+03	0.63237E+03	0.63720E+03	0.63836E+03
0.64600E+03	0.67030E+03	0.68614E+03	0.68915E+03	0.67121E+03
0.67463E+03	0.67103E+03			

VAPOUR FLOW RATE

0.0	0.21123E+03	0.20321E+03	0.19321E+03	0.18610E+03
0.16619E+03	0.16619E+03	0.16619E+03	0.16619E+03	0.16619E+03
0.16600E+03	0.16600E+03	0.16600E+03	0.16600E+03	0.16600E+03
0.16601E+03	0.16601E+03	0.16601E+03	0.16601E+03	0.16601E+03
0.17617E+03	0.17630E+03	0.17699E+03	0.17697E+03	0.17675E+03
0.18173E+03	0.18200E+03	0.18644E+03	0.18700E+03	0.18800E+03
0.18620E+03	0.18620E+03	0.18632E+03	0.17710E+03	0.18384E+03
0.13794E+03	0.13794E+03	0.0	0.96160E+02	0.96036E+02
0.95600E+02	0.95600E+02			

21 SUM OF SQUARES OF RESIDUALS 0.18170E-04  
 (MAT. BAL. 0.68960E-04 MEAT BAL. 0.90881E-06)  
 TEMPERATURE (R)

0.58687E+03	0.59434E+03	0.59572E+03	0.60121E+03	0.60124E+03
0.60129E+03	0.60138E+03	0.60154E+03	0.60152E+03	0.60217E+03
0.60140E+03	0.60141E+03	0.60149E+03	0.60150E+03	0.60150E+03
0.60229E+03	0.61017E+03	0.60177E+03	0.60612E+03	0.61090E+03
0.61428E+03	0.61628E+03	0.61760E+03	0.62038E+03	0.62519E+03
0.62633E+03	0.63010E+03	0.63105E+03	0.63143E+03	0.63187E+03
0.63188E+03	0.63189E+03	0.63237E+03	0.63720E+03	0.63836E+03
0.64600E+03	0.67030E+03	0.68614E+03	0.68915E+03	0.67121E+03
0.67463E+03	0.67103E+03			

VAPOUR FLOW RATE

0.0	0.21123E+03	0.20321E+03	0.19321E+03	0.18610E+03
0.16619E+03	0.16619E+03	0.16619E+03	0.16619E+03	0.16619E+03
0.16600E+03	0.16600E+03	0.16600E+03	0.16600E+03	0.16600E+03
0.16601E+03	0.16601E+03	0.0	0.17610E+03	0.17610E+03
0.17617E+03	0.17630E+03	0.17699E+03	0.17697E+03	0.17675E+03
0.18173E+03	0.18200E+03	0.18644E+03	0.18700E+03	0.18800E+03
0.18620E+03	0.18620E+03	0.18632E+03	0.17710E+03	0.18384E+03
0.13794E+03	0.13794E+03	0.0	0.96160E+02	0.96036E+02
0.95600E+02	0.95600E+02			

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS 21

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

1 14.70 PSIA 136.47 F 0.31804E+06 BTU 1.000

## \*\*\* STREAM CONNECTIONS \*\*\*

LEAVING STREAM NO	LEAVING STAGE NO	STREAM FLUID	ENTERING STREAM NO	ENTERING STAGE NO	ENTERING STREAM NO	ENTERING STAGE NO
1	17	3	1.00	2	28	
2	37	3	1.00	3	40	
3	42	3	1.00	1	4	

STREAM FLUID 1=LIQUID SIDE STREAM 2=VAPOUR SIDE STREAM  
3=LIQUID PRODUCT 4=VAPOUR PRODUCT

ES 006

PLATE NO	PRESSURE PSIA	TEMP F	LIQUID FLOW LB MOLE/TIME	VAPOUR FLOW LB MOLE/TIME	HEAT DUTY BTU/TIME
1	14.70	127.27	0.15844E+03	0.0	-0.27822E+07
2	14.70	134.74	0.15761E+03	0.21122E+03	0.0
3	14.70	136.13	0.15047E+03	0.21042E+03	0.0
4	14.70	141.61	0.3333.0E+03	0.20322E+03	0.0
5	14.70	141.64	0.3333.0E+03	0.15612E+03	0.0
6	14.70	141.69	0.3333.0E+03	0.15612E+03	0.0
7	14.70	141.73	0.3333.0E+03	0.15612E+03	0.0
8	14.70	141.94	0.3334.0E+03	0.15621E+03	0.0
9	14.70	142.22	0.3334.0E+03	0.15621E+03	0.0
10	14.70	142.57	0.3362.0E+03	0.1564.0E+03	0.0
11	14.70	141.80	0.4360.0E+03	0.1560.0E+03	0.0
12	14.70	141.81	0.4360.0E+03	0.1560.0E+03	0.0
13	14.70	140.95	0.4360.0E+03	0.1560.0E+03	0.0
14	14.70	141.93	0.4361.0E+03	0.1560.0E+03	0.0
15	14.70	142.20	0.4361.0E+03	0.1560.0E+03	0.0
16	14.70	143.36	0.4322.0E+03	0.1569.0E+03	0.0
17	14.70	150.57	0.2472.0E+03	0.1556.0E+03	0.23664E+07
18	14.70	142.16	0.11587E+03	0.0	-0.22112E+07
19	14.70	146.52	0.11702E+03	0.1730.0E+03	0.0
20	14.70	151.29	0.11819E+03	0.1749.0E+03	0.0
21	14.70	154.60	0.11841E+03	0.1761.0E+03	0.0
22	14.70	156.68	0.11712E+03	0.17634E+03	0.0
23	14.70	158.07	0.11230E+03	0.1750.0E+03	0.0
24	14.70	160.70	0.35661.0E+03	0.17024E+03	0.0
25	14.70	163.85	0.3709.0E+03	0.1769.0E+03	0.0
26	14.70	166.68	0.3740.1E+03	0.1816.4E+03	0.0
27	14.70	170.47	0.3788.0E+03	0.1847.0E+03	0.0
28	14.70	171.42	0.3767.7E+03	0.1865.4E+03	0.0
29	14.70	171.90	0.3772.7E+03	0.1873.1E+03	0.0
30	14.70	172.12	0.3774.0E+03	0.1889.1E+03	0.0
31	14.70	172.19	0.3772.5E+03	0.1882.2E+03	0.0
32	14.70	172.29	0.3787.7E+03	0.1860.0E+03	0.0
33	14.70	173.03	0.3665.1E+03	0.1865.0E+03	0.0
34	14.70	178.06	0.3420.0E+03	0.1772.0E+03	0.0
35	14.70	192.99	0.3272.0E+03	0.1534.0E+03	0.0
36	14.70	206.14	0.3242.0E+03	0.1360.0E+03	0.0
37	14.70	210.00	0.1592.0E+03	0.1350.0E+03	0.2482.0E+07
38	14.70	196.77	0.8749.0E+02	0.0	-0.1693.0E+07
39	14.70	209.61	0.9007.0E+02	0.9016.7E+02	0.0
40	14.70	211.62	0.2755.0E+03	0.9504.1E+02	0.0
41	14.70	211.94	0.2755.0E+03	0.9500.7E+02	0.0
42	14.70	212.02	0.1905.0E+03	0.9500.0E+02	0.1694.7E+07

## \*\*\* MATERIAL BALANCES \*\*\*

## FEEDS

	PLATE NO. 11	
	LB MOL/TIME	MOL FRAC
ACETONE	0.90000E+02	0.90000E+00
ANITRILE	0.10000E+02	0.10000E+00
WATER	0.0	0.0
TOTAL	0.10000E+03	

## CONNECTED STREAMS

	PLATE NO. 4	FROM 42	
	LB MOL/TIME	MOL FRAC	
ACETONE	0.18317E-07	0.91580E-10	
ANITRILE	0.81576E-02	0.40786E-04	
WATER	0.20000E+03	0.99996E+00	
TOTAL	0.20001E+03		

MAKEUP OF WATER 0.19491E+02

	PLATE NO. 24	FROM 17	
	LB MOL/TIME	MOL FRAC	
ACETONE	0.41165E+02	0.16653E+00	
ANITRILE	0.10003E+02	0.40468E-01	
WATER	0.19603E+03	0.79300E+00	
TOTAL	0.24720E+03		

	PLATE NO. 40	FROM 37	
	LB MOL/TIME	MOL FRAC	
ACETONE	0.18396E-04	0.81350E-07	
ANITRILE	0.46188E+00	0.24403E-02	
WATER	0.18800E+03	0.99756E+00	
TOTAL	0.18926E+03		

## PRODUCTS

	TOP PRODUCT (1)		BOTTOM PRODUCT (17)	
	LB MOL/TIME	MOL FRAC	LB MOL/TIME	MOL FRAC
ACETONE	0.48835E+02	0.92467E+00	0.41165E+02	0.16653E+00
ANITRILE	0.47907E-02	0.90710E-04	0.10003E+02	0.40468E-01
WATER	0.39737E+01	0.75241E-01	0.19603E+03	0.79300E+00
TOTAL	0.52813E+02		0.24720E+03	
O	TOP PRODUCT (18)		BOTTOM PRODUCT (37)	
	LB MOL/TIME	MOL FRAC	LB MOL/TIME	MOL FRAC
ACETONE	0.41165E+02	0.71056E+00	0.15396E-04	0.81380E-07
ANITRILE	0.95416E+01	0.16470E+00	0.46185E+02	0.24403E-02
WATER	0.72265E+01	0.12474E+00	0.18880E+03	0.99756E+00
TOTAL	0.57933E+02		0.18920E+03	
	TOP PRODUCT (38)		BOTTOM PRODUCT (42)	
	LB MOL/TIME	MOL FRAC	LB MOL/TIME	MOL FRAC
ACETONE	0.15378E-04	0.17586E-05	0.18315E-07	0.10146E-09
ANITRILE	0.45369E+00	0.51884E-01	0.81568E-02	0.43186E-04
WATER	0.82903E+01	0.94811E+00	0.18051E+03	0.99995E+00
TOTAL	0.87442E+01		0.18052E+03	

## APPENDIX E.3 -- AMINE TREATING SYSTEM

## \*\* PROBLEM STATEMENT \*\*

COLUMN NO. 1 IS CONTACTOR  
 NO OF PLATES = 10  
 COL PRESSURE 250.00 PSIA  
 PRESSURE DROP 0.0 PER PLATE

COLUMN NO. 2 IS REGENERATOR  
 NO OF PLATES = 14  
 CONDENSER TEMPERATURE 120.00 (F)  
 PRESSURE 27.00 PSIA  
 COL PRESSURE 28.00 PSIA  
 PRESSURE DROP 0.33 PER PLATE

NO. OF FEEDS 1

FEED 1 IS ON TO PLATE 10  
 QUANTITY 0.13158E+05  
 PRESSURE 250.00  
 TEMP (F) 90.00  
 ENTHALPY 0.84300E+08

NO. OF LIQUID SIDE STREAMS 1

STREAM 1 LEAVES PLATE 17  
 QUANTITY 0.25500E+04

NO. OF INTERCOOLERS OR HEATERS 2

INTERCOOLER OR HEATER 1 IS ON PLATE 11  
 HEAT LOAD IS A VARIABLE.

INTERCOOLER OR HEATER 2 IS ON PLATE 24  
 HEAT LOAD (BTU/TIME) 0.13800E+08

## \*\*\* STREAM CONNECTIONS \*\*\*

LEAVING STREAM NO.	LEAVING STAGE NO.	STREAM FLUID	ENTERING STREAM NO.	ENTERING STAGE NO.
1	10	3	3	12
2	17	1	2	5
3	24	3	1	1

ENTERING TEMPS (F) - SEMILEAN 100.00  
 RICH 190.00  
 LEAN 110.00

AMINE IN LEAN AMINE STREAM 127.350 MOLES/TIME  
 SOLUTION STRENGTH (WT PCT) 15.30

## \*\*\* RATE OF CONVERGENCE WITH ITERATION NO. \*\*\*

0 SUM OF SQUARES OF RESIDUALS 0.16212E+00  
 (MAT. BAL. 0.15918E+00 HEAT BAL. 0.29369E-02)

## TEMPERATURE (K)

0.55960E+03 0.55960E+03 0.55960E+03 0.55960E+03 0.55960E+03  
 0.55960E+03 0.55960E+03 0.55960E+03 0.55960E+03 0.56960E+03  
 0.57960E+03 0.68960E+03 0.69160E+03 0.69360E+03 0.69560E+03  
 0.69760E+03 0.69960E+03 0.70160E+03 0.70360E+03 0.70560E+03  
 0.70760E+03 0.70960E+03 0.71160E+03 0.71360E+03

## VAPOUR FLOW RATE

0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05  
 0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05 0.13090E+05  
 0.80000E+02 0.24000E+03 0.30000E+03 0.60000E+03 0.61500E+03  
 0.63000E+03 0.64500E+03 0.66000E+03 0.67500E+03 0.69000E+03  
 0.70500E+03 0.72000E+03 0.73500E+03 0.75000E+03

1 SUM OF SQUARES OF RESIDUALS 0.18974E-01

(MAT. BAL. 0.18321E-01 HEAT BAL. 0.65241E-03)

## TEMPERATURE (K)

0.56069E+03 0.55928E+03 0.55877E+03 0.55859E+03 0.55853E+03  
 0.55807E+03 0.55775E+03 0.55752E+03 0.55734E+03 0.56129E+03  
 0.57960E+03 0.69281E+03 0.69858E+03 0.70159E+03 0.70388E+03  
 0.70547E+03 0.70672E+03 0.70784E+03 0.70901E+03 0.71004E+03  
 0.71109E+03 0.71220E+03 0.71338E+03 0.71496E+03

## VAPOUR FLOW RATE

0.13109E+05 0.13107E+05 0.13106E+05 0.13106E+05 0.13106E+05  
 0.13106E+05 0.13105E+05 0.13105E+05 0.13105E+05 0.13105E+05  
 0.81395E+02 0.29302E+03 0.60380E+03 0.68485E+03 0.70365E+03  
 0.71762E+03 0.72700E+03 0.73457E+03 0.75207E+03 0.75385E+03  
 0.75673E+03 0.76124E+03 0.76759E+03 0.77405E+03

2 SUM OF SQUARES OF RESIDUALS 0.48659E-02

(MAT. BAL. 0.42469E-02 HEAT BAL. 0.61894E-03)

## TEMPERATURE (K)

0.56243E+03 0.55989E+03 0.55912E+03 0.55889E+03 0.55881E+03  
 0.55858E+03 0.55851E+03 0.55853E+03 0.55851E+03 0.55744E+03  
 0.57960E+03 0.69551E+03 0.69846E+03 0.70700E+03 0.70836E+03  
 0.70939E+03 0.71043E+03 0.71163E+03 0.71231E+03 0.71300E+03  
 0.71366E+03 0.71430E+03 0.71493E+03 0.71621E+03

## VAPOUR FLOW RATE

0.13128E+05 0.13125E+05 0.13124E+05 0.13124E+05 0.13124E+05  
 0.13124E+05 0.13124E+05 0.13124E+05 0.13125E+05 0.13132E+05  
 0.82190E+02 0.36893E+03 0.67243E+03 0.73334E+03 0.75346E+03  
 0.76524E+03 0.79608E+03 0.79948E+03 0.79847E+03 0.79489E+03  
 0.79545E+03 0.99681E+03 0.79927E+03 0.80175E+03

3 SUM OF SQUARES OF RESIDUALS 0.41652E-02  
 (MAT. BAL. 0.36962E-02 HEAT BAL. 0.46896E-03)

## TEMPERATURE (K)

0.56362E+03 0.56168E+03 0.56112E+03 0.56096E+03 0.56087E+03  
 0.56130E+03 0.56166E+03 0.56180E+03 0.56183E+03 0.56094E+03  
 0.57960E+03 0.69196E+03 0.70130E+03 0.70491E+03 0.70783E+03  
 0.70938E+03 0.71051E+03 0.71145E+03 0.71221E+03 0.71292E+03  
 0.71360E+03 0.71426E+03 0.71492E+03 0.71619E+03

## VAPOUR FLOW RATE

0.13130E+05 0.13128E+05 0.13127E+05 0.13127E+05 0.13127E+05  
 0.13129E+05 0.13129E+05 0.13129E+05 0.13129E+05 0.13138E+05  
 0.80818E+02 0.28280E+03 0.59897E+03 0.70839E+03 0.73649E+03  
 0.76015E+03 0.76232E+03 0.78054E+03 0.78753E+03 0.79182E+03  
 0.79563E+03 0.79928E+03 0.80290E+03 0.80628E+03

4 SUM OF SQUARES OF RESIDUALS 0.16528E-02  
 (MAT. BAL. 0.74852E-02 HEAT BAL. 0.16760E-03)

## TEMPERATURE (K)

0.56350E+03 0.56189E+03 0.56139E+03 0.56123E+03 0.56112E+03  
 0.56156E+03 0.56183E+03 0.56200E+03 0.56204E+03 0.56039E+03  
 0.57960E+03 0.69373E+03 0.70275E+03 0.70588E+03 0.70824E+03  
 0.70959E+03 0.71058E+03 0.71146E+03 0.71221E+03 0.71290E+03  
 0.71357E+03 0.71422E+03 0.71488E+03 0.71617E+03

## VAPOUR FLOW RATE

0.13130E+05 0.13128E+05 0.13128E+05 0.13127E+05 0.13127E+05  
 0.13129E+05 0.13129E+05 0.13130E+05 0.13130E+05 0.13138E+05  
 0.80739E+02 0.32932E+03 0.62176E+03 0.68741E+03 0.72657E+03  
 0.75480E+03 0.77300E+03 0.78439E+03 0.78986E+03 0.79408E+03  
 0.79775E+03 0.80112E+03 0.80436E+03 0.80665E+03

5 SUM OF SQUARES OF RESIDUALS 0.43916E-04  
 (MAT. BAL. 0.33733E-04 HEAT BAL. 0.10183E-04)

## TEMPERATURE (K)

0.56350E+03 0.56186E+03 0.56136E+03 0.56120E+03 0.56111E+03  
 0.56153E+03 0.56179E+03 0.56194E+03 0.56196E+03 0.56035E+03  
 0.57960E+03 0.68271E+03 0.70197E+03 0.70542E+03 0.70800E+03  
 0.70942E+03 0.71047E+03 0.71139E+03 0.71215E+03 0.71285E+03  
 0.71353E+03 0.71419E+03 0.71486E+03 0.71616E+03

## VAPOUR FLOW RATE

0.13130E+05 0.13128E+05 0.13127E+05 0.13127E+05 0.13127E+05  
 0.13129E+05 0.13129E+05 0.13129E+05 0.13130E+05 0.13138E+05  
 0.81278E+02 0.31311E+03 0.60975E+03 0.68465E+03 0.72837E+03  
 0.75686E+03 0.77352E+03 0.78477E+03 0.79017E+03 0.79428E+03  
 0.79782E+03 0.80108E+03 0.80609E+03 0.80639E+03

6 SUM OF SQUARES OF RESIDUALS 0.20399E-04  
(HEAT. BAL. 0.15996E-04 HEAT BAL. 0.44027E-05)

TEMPERATURE (K)

0.56363E+03	0.56187E+03	0.56133E+03	0.56117E+03	0.56108E+03
0.56148E+03	0.56172E+03	0.56186E+03	0.56185E+03	0.56026E+03
0.57960E+03	0.69218E+03	0.70159E+03	0.70527E+03	0.70793E+03
0.70938E+03	0.71045E+03	0.71137E+03	0.71216E+03	0.71285E+03
0.71353E+03	0.71420E+03	0.71487E+03	0.71617E+03	
0.13130E+05	0.13128E+05	0.13127E+05	0.13127E+05	0.13127E+05
0.13129E+05	0.13129E+05	0.13129E+05	0.13130E+05	0.13130E+05
0.82221E+02	0.31078E+03	0.60553E+03	0.69001E+03	0.73152E+03
0.75864E+03	0.77355E+03	0.78451E+03	0.78976E+03	0.79371E+03
0.79711E+03	0.80023E+03	0.80322E+03	0.80580E+03	

## \*\*\*\*\* COMPUTED RESULTS \*\*\*\*\*

NUMBER OF ITERATIONS: 6

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

0.25000E+03 PSIA 0.90000E+02 F 0.00300E+00 B.T.U. 0.0

## \*\*\* STREAM CONNECTIONS \*\*\*

LEAVING STREAM NO.	LEAVING STAGE NO.	STREAM FLUID	ENTERING STREAM NO.	ENTERING STAGE NO.
-----------------------	----------------------	-----------------	------------------------	-----------------------

1	10	3	3	12
2	17	1	2	5
3	24	3	1	1

STREAM FLUID: 1=LIQUID SIDE STREAM 3=LIQUID PRODUCT

## \*\*\* STAGE VARIABLES \*\*\*

PLATE NO.	PRESSURE PSIA	TEMP F	LIQUID FLOW LB MOL/TIME	VAPOR FLOW LB MOL/TIME	HEAT DUTY BTU/TIME
1	250.00	104.03	0.25214E+04	0.13130E+05	0.0
2	250.00	102.27	0.25206E+04	0.13128E+05	0.0
3	250.00	101.73	0.25204E+04	0.13127E+05	0.0
4	250.00	101.57	0.25206E+04	0.13127E+05	0.0
5	250.00	101.48	0.50719E+04	0.13127E+05	0.0
6	250.00	101.00	0.50722E+04	0.13129E+05	0.0
7	250.00	102.12	0.50725E+04	0.13129E+05	0.0
8	250.00	102.26	0.50730E+04	0.13129E+05	0.0
9	250.00	102.25	0.50613E+04	0.13130E+05	0.0
10	250.00	100.66	0.51013E+04	0.13130E+05	0.0
11	27.00	120.00	0.22856E+03	0.82221E+02	-0.45829E+07
12	28.00	232.58	0.36247E+04	0.31978E+03	0.0
13	28.33	241.99	0.57997E+04	0.60555E+03	0.0
14	28.67	245.67	0.57506E+04	0.69001E+03	0.0
15	29.00	248.33	0.57777E+04	0.73152E+03	0.0
16	29.33	249.78	0.57927E+04	0.75864E+03	0.0
17	29.67	250.85	0.32536E+04	0.77355E+03	0.0
18	30.00	251.77	0.32589E+04	0.78451E+03	0.0
19	30.33	252.54	0.32628E+04	0.78976E+03	0.0
20	30.67	253.25	0.32662E+04	0.79371E+03	0.0
21	31.00	253.93	0.32693E+04	0.79711E+03	0.0
22	31.33	254.60	0.32723E+04	0.80023E+03	0.0
23	31.67	255.27	0.32753E+04	0.80322E+03	0.0
24	32.00	256.57	0.24691E+04	0.80580E+03	0.13800E+06

REFLUX RATIO FOR REGENERATOR = 2.780

## \*\*\* MATERIAL BALANCES \*\*\*

SOUR GAS FEED.

	PLATE #Q.	10
	LB MOLE/TIME	MOLE FRACTION
H2S	0.35700E+02	0.27134E-02
CO2	0.39500E+02	0.30039E-02
N2A	0.0	0.0
METHANE	0.50000E+03	0.37999E-01
NITROGEN	0.50000E+04	0.37999E+00
BUTANE	0.80000E+04	0.19399E+00
ETHANE	0.25000E+04	0.10000E+00
PROPANE	0.30000E+03	0.66398E-01
N-BUTANE	0.80000E+02	0.67638E-02
I-BUTANE	0.80000E+02	0.67638E-02
TOTAL	0.13158E+05	

## CONNECTED STREAMS

	PLATE NO.	FROM
N2S	LB POL/TIRE	HOL PRAC
CO2	0.29913E+01	0.86430E-03
HEA	0.43963E+01	0.17223E-02
WATER	0.12739E+03	0.38464E-01
HYDROGEN	0.23897E+02	0.96026E+00
ETHANE	0.47752E-25	0.16144E-29
TOTAL	0.29917E-25	0.19853E-28

PROPANE	0.21637E-26	0.36311E-29
N-BUTANE	0.65766E-35	0.24060E-31
I-BUTANE	0.50766E-28	0.24060E-31
TOTAL	0.25235E+04	

MAKEUP OF AMINE= 0.95816E-01  
WATER= 0.34338E+02

	PLATE NO.	FROM
N2S	LB POL/TIRE	HOL PRAC
CO2	0.37795E+01	0.14822E-02
HEA	0.66498E+01	0.26078E-02
WATER	0.10103E+03	0.39937E-01
HYDROGEN	0.29377E+04	0.95397E+00
ETHANE	0.29690E-17	0.10073E-20
HYDROGEN	0.26894E-19	0.10547E-22
ETHANE	0.28453E-16	0.11159E-19
ETHANE	0.13162E-16	0.31638E-20
PROPANE	0.55046E-17	0.21592E-20
N-BUTANE	0.30236E-19	0.11853E-22
I-BUTANE	0.30226E-19	0.11853E-22
TOTAL	0.25500E+04	

	PLATE NO.	FROM
N2S	LB POL/TIRE	HOL PRAC
CO2	0.41702E+02	0.81903E-02
HEA	0.50933E+02	0.39842E-02
WATER	0.22910E+02	0.94903E-01
HYDROGEN	0.47782E+00	0.23194E-03
ETHANE	0.46484E-03	0.91724E-03
ETHANE	0.38485E+00	0.67504E-03
ETHANE	0.54499E+00	0.10482E-03
ETHANE	0.24713E+00	0.49349E-04
PROPANE	0.13422E+00	0.32466E-04
N-BUTANE	0.47854E-03	0.93807E-07
I-BUTANE	0.47854E-03	0.93807E-07
TOTAL	0.51013E+04	

## PRODUCTS

	TOP PRODUCT (1)	BOTTOM PRODUCT (10)
	LB MOLE/TIME	MOLE FRACTION
H2S	0.11069E+00	0.84290E-05
CO2	0.39921E-02	0.33450E-06
HEA	0.63161E-01	0.48103E-05
WATER	0.53522E+02	0.59752E-02
HYDROGEN	0.49999E+03	0.39977E-01
ETHANE	0.20880E+04	0.79023E-06
PROPANE	0.99755E+03	0.61340E-01
N-BUTANE	0.89007E+02	0.67787E-02
I-BUTANE	0.89007E+02	0.67787E-02
TOTAL	0.13130E+05	0.51013E+04

	TOP PRODUCT (11)	BOTTOM PRODUCT (24)
	LB MOLE/TIME	MOLE FRACTION
H2S	0.35623E+02	0.43549E+00
CO2	0.39946E+02	0.48564E+00
HEA	0.45405E-03	0.55223E-05
WATER	0.51964E+01	0.62715E-01
HYDROGEN	0.46493E-01	0.36335E-03
NITROGEN	0.34463E+00	0.41942E-02
ETHANE	0.54499E+00	0.66204E-02
ETHANE	0.24715E+00	0.30060E-02
PROPANE	0.11629E+00	0.13901E-02
N-BUTANE	0.47853E-03	0.58201E-05
I-BUTANE	0.47853E-03	0.58201E-05
TOTAL	0.82271E+02	0.24691E+04

## LIQUID SIDE STREAMS

	LIQUID (17)	
	LB MOLE/TIME	MOLE FRACTION
H2S	0.37795E+01	0.14621E-02
CO2	0.66498E+01	0.26074E-02
HEA	0.10104E+03	0.39937E-01
WATER	0.24337E+04	0.95597E+00
HYDROGEN	0.25686E-17	0.10073E-20
NITROGEN	0.26894E-19	0.10547E-22
ETHANE	0.28455E-16	0.11159E-19
ETHANE	0.13368E-16	0.51638E-20
PROPANE	0.55068E-17	0.21595E-20
N-BUTANE	0.30226E-19	0.11853E-22
I-BUTANE	0.30226E-19	0.11853E-22
TOTAL	0.25500E+04	