COMPUTER SIMULATION OF A MULTICOMPONENT, MULTISTAGE BATCH DISTILLATION PROCESS

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ABSTRACT

The material and energy balance equations for a batch distillation column were derived and a computer simulation was developed to solve these equations. The solution follows a modified Newton-Raphson approach for inverting and solving the matrices of material and energy balance equations. The model is unique in that it has been designed to handle hypothetical hydrocarbon components. The simulation can handle columns up to 50 trays and systems of up to 100 components.

The model has been used to simulate True Boiling Point (TBP) diagrams for a variety of crude oils. This simulation is also applicable to simple laboratory batch distillations. The model was designed to accurately combine data files to simulate actual crude blending procedures. The model will combine files and calculate the results quickly and easily.

The simulation involves removing material from the column at steady-state. The removal fraction is made small enough to approach continuity. This simulation can be adapted for use on microcomputers, although it will require extensive computation time.

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NOMENCLATURE

A_i, B_i, C_i	Antoine's vapor pressure equation coefficients
d	Partial derivative
H^L_j, H^V_j	Liquid or vapor enthalpy on tray j
h^L_{ij}, h^V_{ij}	Component liquid or vapor enthalpy
i	Reference for a component
j	Reference for a tray
K_{ij}	K-value of component i on tray j
L_j	Total liquid flow leaving tray j
l_{ij}	Component liquid flow leaving tray j
m	Total number of trays in a column
n	Total number of components in system
o	Subscript referring to the previous iteration
P	System pressure
P_i	Partial pressure of component i
p_i	Vapor pressure of component i
T	Temperature
t	Time
V_j	Total vapor flow leaving tray j
v_{ij}	Component vapor flow leaving tray j
x_i	Mole fraction of liquid component i
y_i	Mole fraction of vapor component i

CHAPTER I

INTRODUCTION

Distillation is a process in which components of a mixture can be separated. Vapor and liquid streams are brought into contact with each other via trays or with packing material. A distillation column is a series of plates in a cylindrical shell or a shell filled with an inert packing material. Due to the differences in gravity, vapor travels upward to contact with liquid flowing downward.

Columns with plates have an obvious number of trays and packed columns are mathematically represented as having a certain number of equivalent theoretical trays. Each tray or stage is assumed to be in equilibrium. In other words, the vapor and liquid streams leaving a particular stage are at the same temperature and pressure and are in thermodynamic equilibrium with each other. Thermodynamic relationships can then be used to find the compositions of either stream given the other and the temperature or pressure.

Liquid that reaches or initially starts in the bottom of the column is heated and gradually vaporized by a reboiler and sent back up the column. Vapor that reaches the top of the column is cooled until it condenses and then is either sent back down the column as reflux or removed as product. Lighter components in the mixture tend to move up the column in the vapor phase. Consequently the top product stream consists of the lightest components in the mixture. Heavier components tend to concentrate in the bottom of the column.

Two types of distillation processes exist. Continuous distillation is a steady-state operation with feed and product streams. The second type, batch distillation, is a transient operation. Batch distillation generally refers to an operation in which overhead product is withdrawn continuously or semi-continuously. The mixture of interest is initially charged to the reboiler in this type of column.

Batch distillation is a typical laboratory procedure (ASTM II, 1987) used as one means of characterizing a crude oil. Atmospheric and vacuum distillation are performed and the vapor temperature in the condenser is plotted against the volume percent removed to generate a true boiling point (TBP) diagram. Additionally, volume fractions can be analyzed to determine the physical properties of the fraction. The ultimate goal of this program is to generate fractional data and TBP diagrams with blended crudes.

The need for a TBP diagram and other laboratory data has been detailed well by Lockwood et. al. (1951):

> Analytical data obtained by standardized equipment and operating procedures are required as a basis for the selection of refinery processing schemes and their evaluation, to provide data

> for design or alteration of process equipment, and as a basis for contractual relationships involving the sale or exchange of crude petroleum.

The batch distillation simulation has been developed on a VAX mainframe computer but can be run on a microcomputer. However, computational time will be greatly increased. The purpose of this research has been to develop a simulation as a crude oil analytical aid. The simulation replicates the laboratory generation of a TBP diagram. The model will also combine data files to generate TBP diagrams of blends of crude oils.

The model allows an engineer to blend several streams in varying proportions and to generate a combined stream TBP. This combined stream TBP can then be recharacterized and used for process simulation work.

This is of particular interest for at least two reasons. It provides a sound basis for the recharacterization and it greatly reduces the time and effort involved in the recharacterization. For example, production streams from several wells may be combined for transport and/or processing. A field sample from each well may have been analyzed and characterized for later use in process calculations. The several production streams may then be combined and the original characterizations could certainly be used as input to the model.

Each sample will usually have about 10 pure components and 10 to 20 hypothetical components. The total number of components for a combination of only four crude oils will approach 90 components in the mixture. This can become quite cumbersome to handle. Even with a mainframe computer, the time requirements for any process simulator will be quite extensive. To make efficient use of the currently popular and widely available personal computers and microcomputers, the number of components must be reduced to a more reasonable level of about 15 to 30.

Hand calculations and estimates of the blending and recharacterization can be extremely frustrating and time consuming. This batch distillation simulation will handle the 90 components if the volumetric percentage of each crude in the mixture is entered. The output from the model can then be used to recharacterized the combined sample with the expected 10 pure and 10 to 20 hypothetical components. A characterized system is now available to be used in generating phase diagrams for pipeline fluid flow calculations or for process simulations.

The simulation adds versatility in that it can accurately predict the TBP characteristics of blends of crude oils. In situations where the engineer has control of the relative amounts of the streams to be combined, the model can be used to quickly and easily obtain characteristic data for a process involving mixed crude feed streams. Optimization of the volume percentage of each crude in the blend will also be simple and accurate.

The simulation is an interactive and user-friendly package. It contains a large data base of component properties and also has the capability of generating properties for hypothetical components based on a few common parameters. The user is able to set the column and program parameters and default values have been provided if the user is uncertain of correct values.

CHAPTER II

LITERATURE SEARCH

Previous literature has been presented on continuous distillation, various forms of batch distillation and solution methods for both types of distillation problems. The previous works on computer solutions of batch distillation columns are few in number and generally limited in scope. The intent of this search is to provide background information on distillation in general, to look at computer simulations of distillation with an emphasis on transient problems, and to take a cursory look at matrix solution methods.

Introduction

Crude oil must be carefully analyzed to properly optimize a process design scheme. One key ingredient in this evaluation is a True Boiling Point (TBP) curve generated by a batch distillation process. A model of this process should be able to replicate the TBP using K-value and enthalpy data for the components involved or by generating this data through some characteristic parameters. To date, no computer program, possibly other than a proprietary program, has been found to adequately simulate a multicomponent, multistage batch distillation process combining both material and energy balances.

Distillation Information

Any discussion of distillation would be incomplete without mentioning Charles Holland's Fundamentals of Multicomponent Distillation (1981). This book is almost always referenced in any article on distillation. For those unfamiliar with distillation principles, this book is a logical starting point for a study of the basic information. General material and energy balance equations are given and equilibrium relationships are presented.

Batch Distillation

According to Distefano (1968) most of the work on transient distillation has been in the form of upsets from steady-state in a continuous distillation system rather than the inherently unsteady-state batch distillation processes. Unsteady-state continuous distillation is much easier to handle than batch. Continuous distillation problems are usually relatively small upsets from steady-state. Batch distillation must deal with losing components from the column completely.

Multicomponent, multistage batch distillation is also difficult to model due to the inherent problems associated with a time dependent process. This transient behavior results from removing material from the system over the entire period of operation without adding any new material. Obviously, the composition of the material in the column will be changing with time. Simulations are generally attempted with the removal of material at specific time increments after steady-state total reflux conditions have been achieved.

Much work has been completed on the modeling of continuous distillation problems and even continuous distillation with upsets from steady-state behavior. The work in the field of batch distillation has been much more limited. Guy (1983) presented a representative paper on the solution of a multistage, binary process and Rooney (1984) has published the corresponding paper on a single stage, multicomponent unit. Neither method is suitable for the generation of a TBP diagram.

One of the latest treatises on batch distillation simulation is by Roche (1987). Roche is mainly concerned with the application of this simulation to full-scale production units and has only dealt with binary systems. However, he has developed an interesting concept. Roche simulates batch distillation with a reflux splitter. At any particular time, condenser material is either all product or completely refluxed back to the column. The reflux ratio is the time of total reflux divided by the time of product removal.

"The basic assumption of a reflux splitter batch distillation column is that the column equilibrates during the period of total reflux." (Roche, 1987) Roche simplifies the time dependent differential material and energy balance equations by modeling the column as steady-state at total reflux. Although TBP diagram generation batch distillation does not involve reflux splitters and the systems of interest are not binary, the principle of steady-state modeling at total reflux is applicable.

Numerous techniques are available for the continuous solution and many authors claim that their methods would work equally well for the transient cases. A number of these articles have been reviewed. Steady-state distillation was studied to learn solution techniques and methods of handling the balance equations.

Economopoulos (1978) has developed a distillation program that characterizes a continuous distillation system based on a generalized tower model. Each tray can have a feed, vapor and liquid product streams, and heat leaks. An ′inside-out′ type technique is used by linearizing the vapor-liquid equilibria to achieve an approximate solution before the rigorous equilibria equations are incorporated to reach a final answer. Economopoulos has incorporated a dynamic solution algorithm to increase the stability of the solution. Steady-state can be approached without the necessity of good initial estimations of the column conditions. This dynamic solution algorithm is very efficient for start-up and step change simulation although the solution is not rigorous due to his use of an approximation of the differential equation involving liquid hold-up. This same approach will theoretically also work for batch distillation but has not been proven in practice. However, it would be incredibly time intensive.

Amundson and Pontinen (1958) developed one of the first solutions to a continuous distillation process. Their paper was also one of the initial works in generating the complete material and energy balance equations. Some of their simplifications include fitting the equilibrium data to a polynomial function, assuming constant molal overflow and using the Newton approximation to correct temperatures. No attempt was made to develop a method of solving the matrix generated to find the tray compositions. The authors recognized that techniques were available to do this.

Friday and Smith (1964) analyzed the solution of an equilibrium stage model equation. They discussed the techniques available and similarities and differences in distillation and absorber type problems. Their analysis noted that most equilibrium stage models differed in the choice of matrix solution method. They noted that a sum rates method would best converge a wide-boiling range of components. The sum rates method involves obtaining a new stage vapor rate from the energy balance and generating a new stage temperature using the calculated bubble points. Most distillation problems calculate a temperature and use this temperature estimate to obtain the component rates. The authors did not formulate a computer solution, although they did describe the computer program that they envisioned as the most versatile solution.

Tomich (1970) also describes a program for the solution of a generalized equilibrium stage, capable of handling either absorber or distillation problems. All of the equations are solved simultaneously using Broyden's (1965) method, a modified Newton-Raphson iteration. Tomich's method is capable of solving most continuous column as it avoids the often numerically unstable tray to tray iteration methods. Numerical stability is ensured as each iteration step moves toward the solution using a simultaneous matrix equation solution. Tomich was one of the first to apply simultaneous matrix equation solution to steady-state distillation. However, much work has been done since in reducing the computational difficulties.

Thomas (1981) has added a unique twist to his design by taking into account vapor as well as liquid holdup. Some simplifications must be made to incorporate vapor holdup. The vapor and liquid on each tray are assumed to be in equilibrium. The author also assumes that the enthalpies are a function of temperature only. However, these assumptions are already made in almost every formulation. Other assumptions include perfect mixing in each phase so that Dalton's and Raoult's Laws of partial pressures hold in the vapor and liquid phases respectively. Thomas goes on to generate the matrix of material and energy balance equations but does not develop a technique to solve them. He realizes that analytical solutions are available although they may be quite time intensive.

Kuno (1984) developed two methods to improve the convergence of Wang and Henke's (1966) tridiagonal matrix method of solution. The first method was a partial normalization technique. Kuno later improved this by linearizing the enthalpy equations to simplify the calculation of partial derivatives. His partial normalization technique improves convergence by damping the rate changes to improve vapor rates. His enthalpy method expands on his vapor rate improvements for key components. Problems would otherwise occasionally arise when the improved liquid rates do not yield an enthalpy balance.

One of the more recent works in steady-state distillation simulation is from Wei (1984). His simulation is simplified by limiting components, feed and product streams and by eliminating tray heaters/coolers. Other simplifications strictly define liquid holdup, linear liquid enthalpies and quadratic vapor enthalpies. Although they would seem to be of restricted value, his assumptions closely parallel those of the transient problems. Wei also does not propose a solution technique.

Not only does Charles Holland present a complete work in describing distillation, but he has also dealt with the solution of batch distillation problems using his θ method of convergence in Unsteady-State Processes with Applications in Multicomponent Distillation (1966). Theta (θ) becomes a multiplier in a set of multipliers based on the ratio of liquid holdups on the trays. The θ method calculates new tray temperatures by improving the mole fractions. Eventually, the temperature profile for a column will cease to change and the column conditions will be specified. Calculations of the θ's either up or down the column can result in progressively worse specifications. With relatively simple columns and good initial conditions, this method is fairly reliable and shorter than other tray to tray techniques in terms of computation time. Tray to tray iteration techniques, however, have generally been replaced by matrix solution techniques because of their tendency to diverge.

Currently, the most important works in the field of equilibrium stage modeling and specifically distillation column modeling belong to Richard A. Russell of Badger America, Inc. and Joseph F. Boston and his various co-workers. Although the work of Boston and others have originated the currently popular 'inside-out' distillation solution technique, Russell (1983) presents the most complete information in his update of Boston's material. Distillation is one of the process simulations available on The Badger Company's GMB (General Material Balance) system. (Russell, 1980) Russell claims that his technique is flexible enough to handle absorbers, all kinds of fractionators, crude and vacuum columns, and pumparounds and sidestrippers. He guarantees quick convergence even for poor initial specifications.

As with Boston et. al. (1984), the inside-out matrix solution technique is used. Enthalpies and K-values are linearized initially to approach the solution without wasting time with excess matrix inversions. The results from linearizing variables can be thought of as very accurate initial guesses for the complete matrix inversion solution.

By far the most important advances in multistage separation simulation have been developed by Joseph F. Boston in conjunction with several others. He developed an ′inside-out′ technique to greatly improve the speed of computation and to reduce the chance of non-convergence for poorly described systems. Boston has worked on multistage separations (Boston, 1970), and developed his ′inside-out′ technique for equilibrium flash calculations (Boston and Britt, 1978). He later applied it to other multistage separations (Boston, 1980), and finally to batch distillation (Boston, et. al., 1984).

In two articles in The Canadian Journal of Chemical Engineering, Boston and S.L. Sullivan, Jr. (1972 and 1974) presented their approach for the rigorous simultaneous solution of the system of material and energy balance equations. Previously, Gaussian elimination had been the method of choice for the matrix solution. Gaussian elimination can often lead to excessive propagation of errors and in any case requires too much computation time.

In the ´inside-out´ method, stage temperatures and interstage phase rates are chosen as the successive approximation variables. Either the liquid or vapor phase rates can be chosen and the other rates are calculated from the total mass balance. The component material balance and the phase equilibrium equation specify the component flow rates or mole fractions. The component material balances are solved and new temperatures and phase rates are calculated from the bubble-point and the energy balance equations. The component material balances are in tridiagonal matrix form which is a convenient form for solving simple columns and requires minimal storage.

Boston originally formulated his ´inside-out´ technique with H.I. Britt as published in Great Britain. (Boston and Britt, 1978) This article summarizes the major advantages of this method:

1) Complex variable models are used only to formulate simple iteration model parameters.

2) These new parameters are basically independent and thus accurate initiallization is not necessary.

3) A loop is generated with only one parameter embodying the temperature and phase ratio.

4) Temperatures, pressures, vapor and liquid compositions and phase fractions are used to calculate new iteration variables.

5) The converged iteration loop conditions can be used to find the actual solution easily.

A bubble point calculation is used to determine new temperatures and new K-values. The stripping and rectifying factors are based on tray vapor and liquid flows. These flows are set by the distillate rate, reflux ratio and the tray energy balances.

Boston's inside-out' solution method is outlined in detail in this American Chemical Society publication (Boston, 1980). It is recognized that methods such as the simultaneous approach of Newton-Raphson find solutions to the set of describing equations far better than the iterative tray to tray methods. Boston has attempted to find a new solution that converges as quickly as any previous solutions while avoiding the dependence of Newton-Raphson on accurate initial estimates.

In this method, the set of K-value and enthalpy correlations for each tray are replaced by single 2-parameter models which are then used as iteration variables in the 'outer-loop'. These new iteration variables are relatively independent of temperature, pressure, and composition. The inner loop is described in terms of a single variable composed of temperature and the phase ratio. The temperatures, pressures, and compositions resulting from the inner loop are used to formulate new outer loop parameters until convergence within the desired tolerance is achieved.

As with all authors, Boston claims to have achieved very rapid convergence. However, it makes sense that his method would be quicker since extensive equilibrium and enthalpy calculations have been reduced dramatically. Also, vapor and liquid composition estimates are not needed and poor initial estimates of temperatures and pressures are not automatically fatal. If fixed product rates are used, direct iteration can be used. This guarantees a fast computation as the Jacobian matrix does not have to be calculated and inverted. The 'inside-out' technique is advantageous in that it allows the user to converge solutions without any good idea of the final answer. However, the effort to simplify the calculations may not be necessary for limited boiling systems with few feeds, few withdrawals and no heater/coolers.

Boston, et. al. (1984) have developed computer routines that simulate a multistage, multicomponent batch distillation process. This simulation, called 'BATCHFRAC' is marketed through Process Simulation Associates, Inc. The system uses Boston's 'inside-out' technique and is capable of handling many different operating conditions.

Batch distillation has usually been formulated as a set of coupled, nonlinear ordinary differential equations of unsteady-state mass and enthalpy balances. The system is often very stiff due to large swings in component volatilities or liquid holdups. Stiffness is overcome by decreasing step sizes which can greatly increase the computational time. A difficult situation arises when the step size has to be made so small that the round-off and truncation errors build uncontrollably. Also, a system is not guaranteed to be in mass balance.

'BATCHFRAC' uses the 'inside-out' technique and a variable step size, implicit backward difference integration technique to solve the set of coupled, nonlinear ordinary differential equations. The ′inside-out′ technique allows the solution of the mass and energy balance equations through the use of iteration variables while accumulating few errors. The step size can be changed every iteration to reduce even further the error generation.

Two important early works in the area of batch distillation simulation were by Meadows (1963) and Distefano (1968). Both of these works were well ahead of their time although improved solution techniques have since outdated both works. Both formulated essentially the same equations and made the same standard assumptions which are listed from Meadows (1963):

1) The composition of a vapor rising from a given tray is related to the composition of the liquid on the tray by a known function.

2) The liquid composition is uniform across a given tray, and of the same composition as the liquid overflowing to the tray below.

3) Vapor holdup in the column is negligible compared to that of the liquid.

4) The operation is adiabatic, except for heat added to the kettle and removed by the condenser.

5) The volume of liquid holdup on any tray and the condenser is constant (but possibly different for each tray) throughout the distillation.

6) Perfect mixing occurs in the condenser.

7) A total condenser is used.

Meadows (1963) used a finite-difference solution technique, while Distefano (1968) used direct substitution with adaptive acceleration and damping. Both of these techniques are iterative tray to tray procedures that are prone to error propagation and divergence.

It should be noted that all of the above simulation techniques require K-value and enthalpy data. These data will have to be provided through tables, models, and equations of state. None appear to have been developed for handling hypothetical components.

Solution Methods

The material and energy balance equations form a set of nonlinear simultaneous equations. The solution of these equations will become one iteration in the batch distillation process. As Broyden (1965) notes,

> Although it may be impossible to prove by mathematics alone that a solution exists, this fact may be inferred from the physical analogy. Similarly, although the solution may be unique, it is hoped that familiarity with the physical analogue will enable a sufficiently good initial estimate to be found so that any iterative process that may be used will in fact converge to the physically significant solution.

Broyden analyzed the Newton method of solution which is given by:

$$X_{i+1} = X_i - A_i^{-1} * f_i \qquad [1]$$

which is a solution for $f(X)=0$. A_i is the Jacobian matrix (df_i/dx_i) evaluated at X_i. f is a generalized function and X is the variable of interest (Broyden, 1965). The Jacobian can be difficult to formulate. The partial derivatives may have to be obtained numerically and it is very time intensive to calculate every one. Newton's method may not always converge without some modifications, but convergence can be assured with a good initial estimate of the solution conditions. Newton's method does have its drawbacks, but it remains the method of choice for solving these systems of equations for the following reasons. It is relatively simple; it is theoretically sound; and with good initial estimates its convergence is rapid.

Gallun and Holland (1982) have developed a method to simplify the solution of unsteady-state distillation problems. Generally, the mathematical description of a column results in a large number of differential and algebraic equations that are not functions of state variables (temperature, pressure, flow rate, and composition). An attempt is usually made to reduce the number of equations and to express them in terms of state variables. This manipulation usually results in added difficulties and greater errors. Gear's method (Gear, 1969 and 1986), was chosen by the authors as the solution technique.

Generally, two methods have been used previous to Gallun and Holland (1982): Michelsen's (1976) method, a semi-implicit Runge-Kutta method, and linear multistep methods using numerical differentiation techniques. The Runge-Kutta method requires the generation of the Jacobian matrix at least every iteration. This stipulation requires the calculation of partial derivatives which is not always applicable to the thermodynamic relationships used and takes quite a bit of computation time.

Michelsen's method is, however, an improvement over explicit fourth-order Runge-Kutta methods which are not applicable for stiff systems. Stiff systems, which are systems with large differences in the magnitude of the eigen values, are common in distillation calculations. The explicit form requires that the stepsize be on the order of the inverse of the largest eigen value. This condition usually requires a prohibitively small stepsize for stiff systems. Michelsen's improvement is the adjustment of the step size at each iteration to avoid divergence in the solution of stiff systems. The solution generally follows a Newton-Raphson approach.

Gear's method involves the addition of an extra variable and algebraic equation for each stage. Therefore, derivatives can be generated without the problems associated with applying the chain rule. The equations do not have to be changed to accommodate state variables, and derivatives that are difficult to calculate do not have to be approximated by linear or low-order difference techniques. Elimination of the extra variable and equation forces partial derivatives to be calculated. This elimination may be desirable if the form of the enthalpy function is relatively straightforward because the partial derivatives will be easy to calculate.

Gentry (1970) has an interesting method of solution which is vaguely similar to Gaussian elimination (Venit and Bishop, 1981). The material and energy balances form systems of tridiagonal matrices. The tridiagonal matrix is rewritten as a matrix with the non-zero coefficients placed beginning in the first column. Therefore an mxn matrix becomes an mx3 matrix. The resulting matrix is then treated with row operations similar to Gaussian elimination. Finally, back substitution is required to achieve the results.

Gentry (August, 1970) has formulated another solution technique to describe distillation processes. He proposes to linearize all the variables by the method of quasi-linearization. The mass and energy balances can be described as systems of tridiagonal matrices of these coefficients. If it is assumed that the temperatures, flow rates and compositions can be decoupled, Gaussian elimination can be used to solve the equations. The energy and component material balances and the equilibrium relationships are all linearized by approximating these non-linear functions as linear.

Although Gaussian elimination is fast and easy to apply, it is probably not desirable for systems of coupled equations such as these. Both of Gentry's approaches are interesting and may be adequate for special systems, but they are not general enough for serious consideration.

Goldstein and Stanfield (1970) have used the standard

Newton-Raphson solution technique and worked to improve its speed and efficiency. Dependent variables for the algorithm are usually compositions, temperatures, and loadings; while the independent variables would be heat duties and feeds. However, if product purity is desired, the heat duties will become dependent.

Probably their most important discovery is that the ordering of the equations can improve the speed of computation. Material balances grouped by component are faster than those grouped by trays. Goldstein and Stanfield (1970) also found that a partial triangularization technique will result in a much smaller matrix to invert. The linearization of temperature and loading profiles near product streams is another assumption used to speed convergence. This linearization assumption will have to be removed to obtain the final solution.

Newman's method (1968) of solution is probably not the quickest of the methods studied. It is however, the most general and it is quite useful for many different operating conditions. This method is even applicable for problems other than distillation. As Newman says, "for special problems it may be possible to devise more efficient methods, but with a loss of generality and an expense of effort." (Newman, 1968)

Newman employs a linearization technique similar to that of Gentry (August, 1970). Newman notes that iterating with linearized equations will often result in convergence in the non-linear problem. Convergence does not depend on the initial estimates of the solution conditions. The initial estimate is used to generate another approximation and the process is iterated until convergence within the desired tolerance is achieved.

A distillation column model is composed of a set of non-linear, coupled material and energy balance and equilibrium equations. These equations resemble a finite difference approximation because an equation for a tray is dependent on both the tray above and the tray below.

Newman´s method requires significant storage space. However, it is also very flexible since the energy balance is included in the linearization. The computation time could be reduced if the flow rates were fixed and the tray temperatures were allowed to set the compositions. This simulation would then set the enthalpy balance.

Errors can occur when trying to achieve convergence in the non-linear equations; errors can also occur in the difference approximation; and finally round-off and truncation errors occur within the computer. Newman warns that there may be problems with convergence if some region(s) contain sharp variations in the independent variables. The temperature and flow rate linearization technique of Goldstein and Stanfield (1970) may be useful to eliminate this convergence problem.

The distillation solution assumes a temperature profile through the column and then calculates the component distributions through equilibrium calculations based on these assumed temperatures. Initially the temperature profile is assumed to be linear through the column. The tray temperatures will then have to be corrected in order for the mole fractions of both the liquid and vapor phases to sum to unity on each tray. Newman has developed a method to correct the tray temperatures that is based on a linear relationship between the component distributions and the temperatures (Newman, 1963).

The temperature correction is given as:

$$T_j - T_j^\circ = \sum_{j=1}^{m} \left[\left[\sum_{i=1}^{n} \frac{dl_{ij}}{dT_j} \right]^{-1} \left[L_j - L_j^\circ \sum_{i=1}^{n} x_{ij}^\circ \right] \right] \qquad [2]$$

The calculation of the partial derivatives of component liquid flows with respect to temperature is taken from the material balance. Effects of adjacent trays and equilibrium calculations are also accounted for in this equation.

Newman also has a method for improving the liquid flow rate estimations which involves the column energy balance. The liquid flow correction is generally the same as the temperature correction except that in the last term, the liquid flow rates have been replaced with tray temperatures. Both the temperature and liquid flow corrections will have to be damped to correct oscillations and diverging corrections. The temperature correction may produce ridiculous new estimates, but the direction of these estimates is usually correct (Newman, 1963). The correction factor is usually limited to 10°F for temperature and 40% for liquid flows to ensure the eventual convergence of the solution.

John Newman has developed a computer technique for the matrix inversion solution and the temperature and liquid flows corrections. This solution may not be the most efficient in terms of either time or storage, but is probably the most versatile and most likely to guarantee convergence. It encompasses a correction procedure to speed convergence. His computer technique has been selected for its versatility in handling many different column conditions. His program has been obtained and applied to this simulation.

CHAPTER III

TBP GENERATION PRINCIPLES

Introduction

In looking at the generation of a TBP diagram, the first step would be to examine the actual laboratory procedures. This chapter will look at the details of these procedures and then will pursue the equations which describe a distillation column in general and a batch distillation process in particular. Finally, a description of the simulation will be presented.

Laboratory Procedures

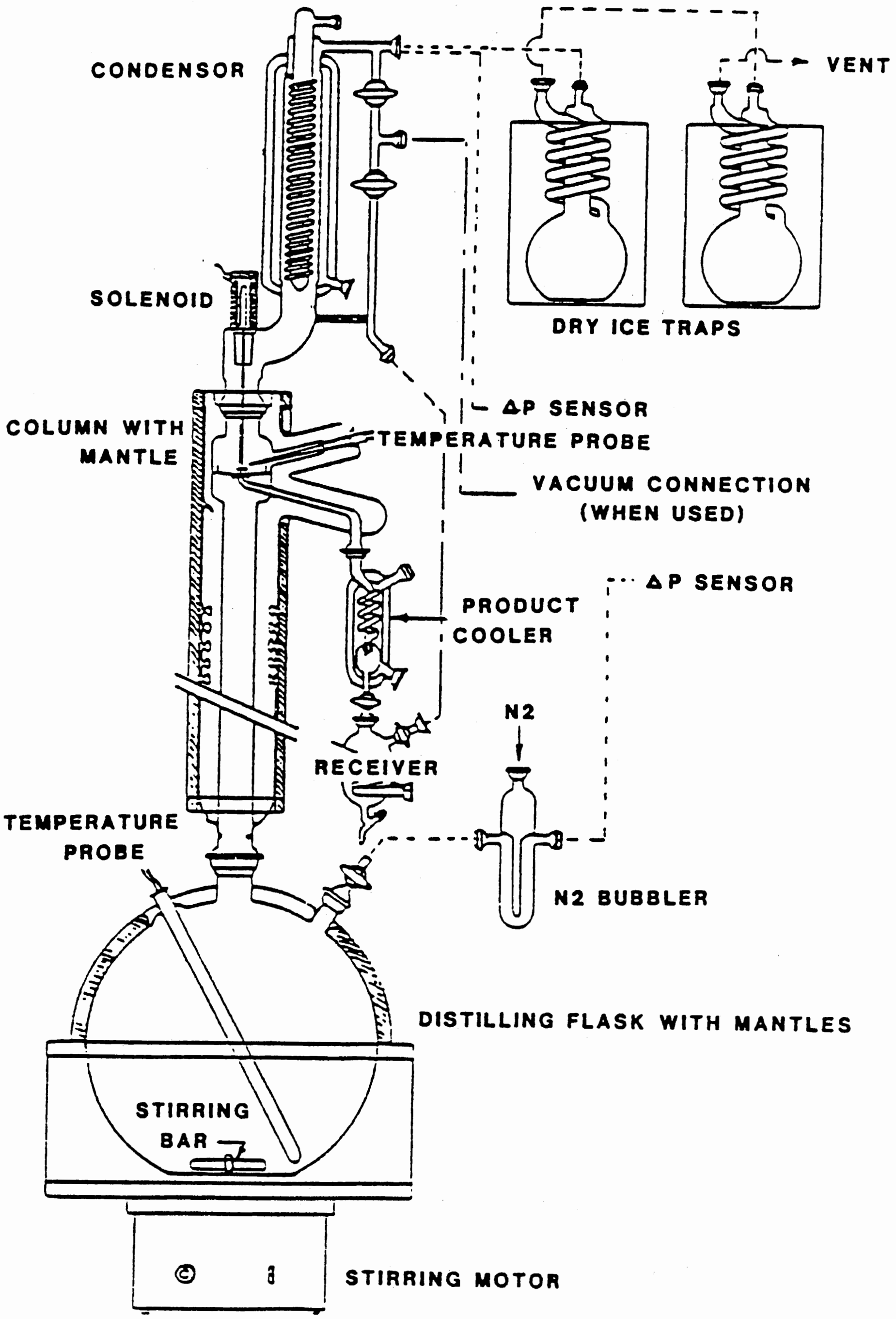
This batch distillation simulation is based on ASTM D 2892-84 (ASTM II, 1987), the standard test method for the distillation of crude petroleum in a 15 theoretical plate column. This section discusses the laboratory procedures which are duplicated in the simulation.

The procedure is detailed for the batch distillation of stabilized crude petroleum in a tower of 14 to 18 theoretical plates (preferably 15) with a reflux ratio (L/D) of 5:1. The results are in the form of TBP (true boiling point) curves of temperature versus weight and volume percent distilled. A 0.5 to 30 L sample of crude petroleum is distilled to a maximum of 750°F and temperature, pressure, and any other pertinent variables are recorded at specified intervals and after each fraction is collected.

As stated in the laboratory procedure, this experiment is just one of many tests that are performed on a crude oil. "It provides an estimate of the yields of fractions of various boiling ranges." (ASTM II, 1987) The different fractions produced can be further evaluated and studied although those analytical evaluations are not a part of this laboratory procedure nor of this simulation.

The procedures are relatively straight forward for a laboratory distillation and details of this can be found in the experimental explanation. Figure 1 is a diagram of the laboratory apparatus.

The steps in the TBP distillation are as follows. Initially, the mass of the crude should be calculated before it is added to a chilled still. The column is operated at total reflux at atmospheric pressure until equilibrium is reached. The initial step after equilibrium is reached is to debutanize the crude. The condenser is initially maintained at -20°C and anything that is not condensed at this temperature will be collected in dry ice traps. Fractions should be collected every 5-10°C in vapor temperature. For every fraction the time, volume, vapor temperature and temperature of the boiling liquid should be recorded. After the vapor temperature reaches about 65°C, refrigerant in the condenser can be replaced with water at



Source: 1987 Annual Book of ASTM Standards, Petroleum Products, Lubricants and Fossil Fuels (II), 05.02. Philadelphia: American Society for the Testing of Materials, p. 693.

Figure 1. Typical Batch Distillation Apparatus

ambient temperature.

Fractions are continually collected until the vapor temperature reaches 210°C or until the boiling liquid temperature exceeds 310°C. If either of these temperatures are reached or if cracking begins, the pressure will have to be reduced. If fractions at higher temperatures are required, the pressure should be reduced to 100 mm Hg. The still should be simultaneously cooled so the crude does not resume boiling. The distillation is run at total reflux for about 15 minutes to reheat the column and then fractions can immediately withdrawn. If more fractions are again required above a boiling temperature of 310°C. The restart procedures should be repeated, but the pressure should not be reduced below 1 mm Hg. Typical pressures are 50, 10, 5, 2, and 1 mm Hg. The reflux ratio may be set to 2:1 to increase the distillation rate. Samples can be taken until the final cut point has been reached or until the temperature in the boiling liquid is above 310°C at 2 mm Hg.

Again, all cuts should be recorded with the time, volume, vapor temperature, and the temperature of the boiling liquid. If any residuals are left, the column should be cooled to allow any static holdup to drain down into the still. The holdup should be blended with the residuals and this fraction should be weighed and its density calculated.

Another laboratory procedure commonly used is the spinning band batch distillation column (Lockwood et. al., 1951). This column employs a twisted spinning band to provide a surface for vapor-liquid contact. The band extends into the still pot to act as a stirring rod. The band is aligned closely to walls of the column so that vapor cannot travel up the sides unhindered. Enough clearance is to be provided that binding does not occur. The band is revolved at about 3000 rpm in such a direction to oppose the rising vapors.

The column is vacuum-jacketed and silvered to prevent heat loss and is operated under typical conditions: atmospheric pressure initially, usually a 5:1 reflux rate, and total reflux. The equivalent of 20 theoretical trays are achieved at normal operating conditions although a drop to about 15 theoretical trays can be expected at high boilup rates. The usual drops in pressure to sequentially 10, 2, and finally 1 mm Hg are performed. However, the temperatures are allowed to rise to as much 600°F before the pressure is reduced. The final cut can be taken at 650°F at 1 mm Hg.

Another type of laboratory batch distillation is referred to as ASTM distillation and it is described under ASTM D86-82 (ASTM I, 1987). This method is an inefficient distillation of petroleum products although it is easy to perform and the equipment involved is fairly common.

The apparatus consists entirely of a flask with a short neck opening into a product removal or condenser tube. This tube extends diagonally down from the top of the neck. No packing or trays are incorporated to provide surface area for the contact of vapor and liquid phases. Reflux is limited to condensation at ambient temperature on the sides of the neck. Removal of product is continuous until either the end point or dry point is reached. Vapor temperatures are recorded as the initial drop of product is collected, after 5 percent has been collected, and subsequently after 10 percent and each multiple of 10 percent until the dry point or end point is reached. The temperature at this point is also recorded.

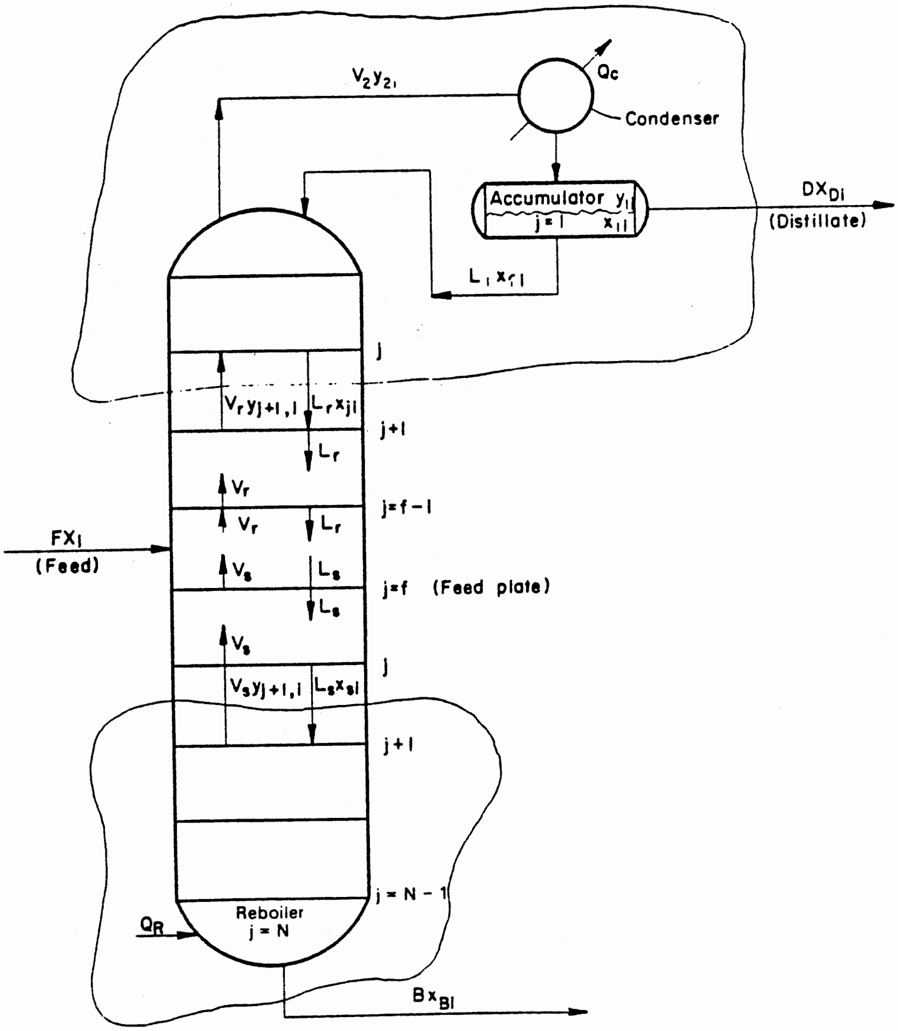
Background

Distillation is based on the principle that in heating a liquid mixture, the more volatile components will tend to vaporize quicker. Conversely, when cooling a vapor mixture, the less volatile components will tend to condense quicker. "A distillation column consists of a space for contacting vapor and liquid streams for the purpose of effecting mass transfer between the two phases." (Holland, 1981) A typical schematic of a distillation column is shown in Figure 2. To fully describe the conditions of a distillation column, four types of equations have to be satisfied:

1) Equilibrium relationships
2) Total material balance
3) Component material balances
4) Energy balances

Equilibrium Relationships

Several conditions must be met for a two-phase mixture



Source: Holland, Charles D., <u>Fundamentals of Multicomponent Distillation.</u> New York: McGraw-Hill Book Company, 1981, p. 5.

Figure 2. Sketch of a Conventional Column

to be at equilibrium. First, the temperatures of the liquid and vapor phases must be equal. Next, the pressures of both of the phases must be equal. Finally, the ability of a component to move into the vapor phase from the liquid phase must be exactly balanced by its likelihood to return to the liquid phase (Denbigh, 1955).

The last condition can be described by a combination of Raoult's and Henry's laws as:

$$Py_i = p_i x_i \qquad\qquad y_i = (p_i/P)x_i \qquad\qquad [3]$$

Since the mole fractions will always sum to unity, for any tray the following relations hold:

$$y_i = 1.0 \qquad\qquad x_i = 1.0 \qquad\qquad [4]$$

The term (p_i/P) can be represented as K_i or the K-value for component i and Equation 3 becomes:

$$y_i = K_i x_i \qquad\qquad [5]$$

K_i is a function of pressure and temperature. For a two-phase (vapor and liquid) system to be in equilibrium, the system will have to be at its bubble point temperature, its dew point temperature, or somewhere in between. The bubble point temperature is that temperature where an equilibrium mixture is all liquid. This can be described mathematically as:

$$K_i x_i = 1.0 \qquad\qquad [6]$$

A system is at its bubble point when this equation is satisfied. Similarly a system is at its dew point (when it is all vapor) at equilibrium when the following is satisfied:

$$y_i/K_i = 1.0 \qquad [7]$$

Total Material Balance

The total material balance is relatively easy to describe. The summation of streams entering the column equals the summation of streams leaving the column. For a simple continuous column, this is usually represented as:

$$F = D + B \qquad [8]$$

where the moles in the feed stream (F) equal the sum of the moles in the distillate stream (D) plus the moles in the bottoms stream (B). A batch distillation arrangement has no entering or leaving streams for each iteration so the equation reduces to the trivial solution.

A total material balance can also be performed around a single tray in the column. In this case, for a simple system, the balance becomes:

$$L_{j+1} + V_{j-1} = V_j + L_j \qquad [9]$$

This is represented in Figure 3.

Component Material Balance

The component material balance as stated by Boston

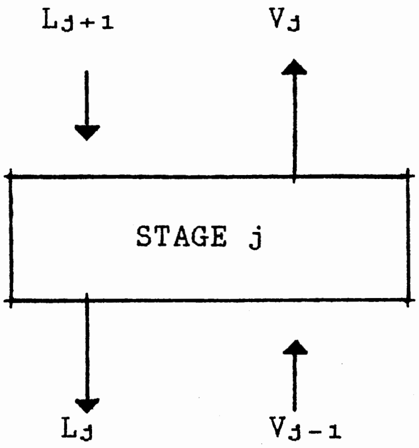


Figure 3. Schematic of a Single, Ideal Tray

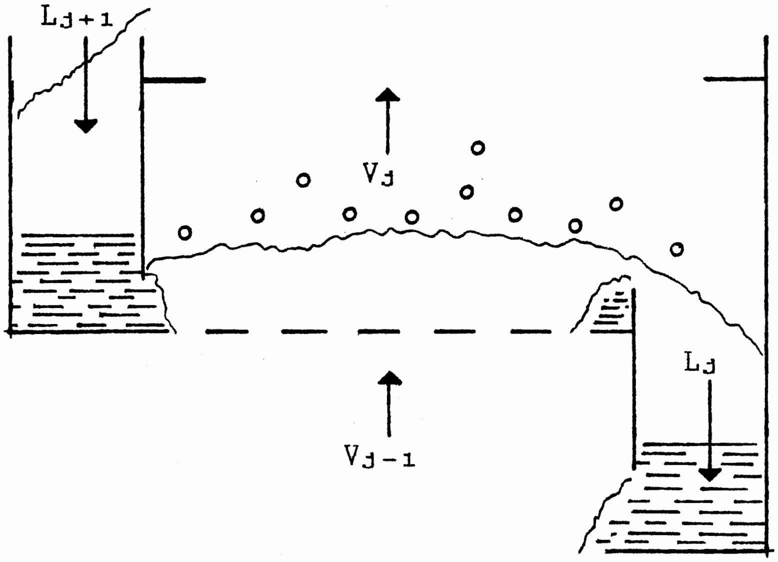


Figure 4. Schematic of a Single Tray with Liquid Holdup

(1970) for the tray in Figure 3 is:

$$y_{ij-1}V_{j-1} + x_{ij+1}L_{j+1} = y_{ij}V_j + x_{ij}L_j \qquad [10]$$

If the component liquid and vapor flows respectively are defined as:

$$l_{ij} = x_{ij}L_j \qquad v_{ij} = y_{ij}V_j \qquad [11]$$

Then the component material balance becomes:

$$v_{ij-1} + l_{ij+1} = v_{ij} + l_{ij} \qquad [12]$$

To simplify the computations, all the component vapor flows can be described in terms of the component liquid flows:

$$v_{ij} = y_{ij}V_j = K_{ij}x_{ij}V_j = K_{ij}V_jl_{ij}/L_j \qquad [13]$$

Therefore, the final statement of the component material balance is:

$$l_{ij} + (K_{ij}V_j/L_j)*l_{ij} - l_{ij+1} - (K_{ij-1}V_{j-1}/L_{j-1})*l_{ij-1} = 0 \qquad [14]$$

Russell (1983) defined two terms, B_{ij} and C_{ij}, to simplify Equation 14 even further. B_{ij} and C_{ij} can be written as:

$$B_{ij} = 1 + (K_{ij}V_j/L_j) \qquad C_{ij} = -(K_{ij-1}V_{j-1}/L_{j-1}) \qquad [15]$$

This leads to a final result for a component material balance on a tray as:

$$B_{ij}l_{ij} - l_{ij+1} + C_{ij}l_{ij-1} = 0 \qquad [16]$$

A matrix that describes the component material balances for each tray in the column can now be very easily formulated. The total number of trays is considered for this example to be equal to m and the tray numbering system begins with the reboiler. The matrix for a component is:

$$\begin{bmatrix} B_{im} & C_{im} & & & & \\ -1 & B_{im-1} & C_{im-1} & & & \\ & & \ddots & & & \\ & & & -1 & B_{i2} & C_{i2} \\ & & & & -1 & B_{i1} \end{bmatrix} \cdot \begin{bmatrix} l_{im} \\ l_{im-1} \\ \vdots \\ l_{i2} \\ l_{i1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} \qquad [17]$$

For a conventional continuous distillation system, adaptions could be made to handle side product streams and the column vector of zeroes would be replaced by a column vector that denoted the feed streams to each tray.

Energy Balances

Heat or energy balances are computed for each tray and not for each component. It is assumed no heat loss occurs from any tray. The matrix of tray energy balances will be developed using the same simplifying techniques as that of a component material balance. The total energy balance for a single tray is:

$$L_{j+1}H^{L}_{j+1} = V_{j-1}H^{V}_{j-1} = V_{j}H^{V}_{j} + L_{j}H^{L}_{j} \qquad [18]$$

and the corresponding balance accounting for individual components is:

$$V_{j-1} \; y_{ij-1}h^{V}_{ij-1} + L_{j+1} \; x_{ij+1}h^{L}_{ij+1} = V_{j} \; y_{ij}h^{V}_{ij} + L_{j} \; x_{ij}h^{L}_{ij} \qquad [19]$$

Denoting the component vapor and liquid flows as:

$$v_{ij} = y_{ij}V_{j} \qquad l_{ij} = x_{ij}L_{j} \qquad [20]$$

leads to the Equation 21:

$$v_{ij-1}h^{V}_{ij-1} + \; l_{ij+1}h^{L}_{ij+1} = \; v_{ij}h^{V}_{ij} + \; l_{ij}h^{L}_{ij} \qquad [21]$$

Eliminating the component vapor flows by defining:

$$v_{ij} = y_{ij}V_{j} = K_{ij}x_{ij}V_{j} = K_{ij}V_{j}l_{ij}/L_{j} \qquad [22]$$

will yield the following equation:

$$(V_{j-1}/L_{j-1}) \; K_{ij-1}l_{ij-1}h^{V}_{ij-1} + \; l_{ij+1}h^{L}_{ij+1} = (V_{j}/L_{j}) \; K_{ij}l_{ij}h^{V}_{ij} + \; l_{ij}h^{L}_{ij}, \qquad [23]$$

which can be rearranged to give:

$$l_{ij}(\; h^{L}_{ij} + (V_{j}/L_{j}) \; K_{ij}h^{V}_{ij}) - (V_{j-1}/L_{j-1}) \; K_{ij-1}l_{ij-1}h^{V}_{ij-1} - \; l_{ij+1}h^{L}_{ij+1} = 0. \qquad [24]$$

If the coefficients B_{j} and C_{j} are defined parallel to those in the material balance derivation:

$$B_{j} = \; h^{L}_{ij} + (V_{j}/L_{j}) \; K_{ij}h^{V}_{ij}$$
$$C_{j} = -(V_{j-1}/L_{j-1}) \; K_{ij-1}h^{V}_{ij-1}. \qquad [25]$$

The final result, a matrix equation describing the system energy balance, can be written:

$$\begin{bmatrix} B_m & C_m & & & & \\ -h^L{}_{im} & B_{m-1} & C_{m-1} & & & \\ & -h^L{}_{im-1} & B_{m-2} & C_{m-2} & & \\ & & & \ddots & & \\ & & & -h^L{}_{i3} & B_2 & C_2 \\ & & & & -h^L{}_{i2} & B_1 \end{bmatrix} \cdot \begin{bmatrix} l_{im} \\ l_{im-1} \\ l_{im-2} \\ \cdot \\ \cdot \\ \cdot \\ l_{i2} \\ l_{i1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0 \end{bmatrix} \qquad [26]$$

<u>Transient Equations</u>

The equations for batch distillation are often handled in a very similar manner, although there are some differences to account for the transient behavior. Obviously, the equilibrium relationships and the overall column material balance would remain the same. Liquid holdups and vapor holdups can be taken into account. The vapor holdup is generally so small in relation to the liquid holdup that it is neglected. A typical distillation tray is shown in Figure 4.

The equations are treated the same way as in the continuous system except that the product column vectors of zeroes in the continuous case is now replaced with a product column vector of the holdup differential. The equations become for a total material balance on a tray:

$$dH_j/dt = V_j + L_j - L_{j+1} - V_{j-1} \qquad [27]$$

and for a component material balance on a tray:

$$d(x_{ij}H_j)/dt = y_{ij}V_j + x_{ij}L_j - y_{ij-1} - x_{ij+1}L_{j+1} \qquad [28]$$

The component enthalpy balance on a tray is written as:

$$d(H_j \quad x_{ij} h^L_{ij})/dt = V_j \quad y_{ij} h^V_{ij} + L_j \quad x_{ij} h^L_{ij} -$$
$$V_{j-1} \quad y_{ij-1} h^V_{ij-1} - L_{j+1} \quad x_{ij+1} h^L_{ij+1} \qquad [29]$$

Degrees of Freedom

The degrees of freedom of a system refers to the number of intensive properties that must be specified to completely describe a system. If batch distillation can be thought of as a series of equilibrium processes, a degrees of freedom analysis can be used to set the parameters of the distillation.

For an equilibrium system that does not involve chemical reaction, the Gibbs phase rule (Van Wylen and Sonntag, 1978) states that:

$$P + V = C + 2 \qquad [30]$$

where: P = the number of phases
V = the variance of the degrees of freedom
C = the number of components

Expanding this idea to a process, a degrees of freedom analysis has been presented in Chapter II of the Phillips Fractionation Workshop (Erbar, 1983). The number of variables that must be specified in order to completely describe the process, N_s, is:

$$N_s = N_v - N_r + N_t \qquad [31]$$

where: N_v = the total number of degrees of freedom in a process
N_r = the number of variables fixed by restraints on the process
N_t = the number of recurring variables in the process

A single stream will have C+2 independent variables; C-1 independent compositions and one variable each for the stream temperature, pressure and flow rate. A single equilibrium stage is composed of 4 streams and a heat leak term. The total number of degrees of freedom for a single stage becomes 4(C+2)+1 or 4C+9. However, restraints on the stage amount to 2C+3 variables; C component balance equations, C phase distribution equations, an overall energy balance and the implied equilibrium equality of temperature and pressure of the vapor and liquid streams leaving that stage. Therefore, N_s for a single stage is 2C+6.

Similar procedures can be followed to find that C+4 variables are required for both the condenser and reboiler and C+5 variables for a reflux divider. Combining all of these elements for a single column with m stages and no feed streams:

$$\begin{array}{r} m\,(2C + 6) \\ 2\,(\;C + 4) \\ C + 5 \\ \hline 2Cm + 6m + 3C + 13 \end{array} \quad \text{degrees of freedom} \qquad [32]$$

Eliminating 2(m-1) redundant streams or 2Cm+4m-2C-4 variables leaves 5C+2m+17 as the total number of variables needed to specify this column.

For a distillation column with a total condenser and a total reboiler and no bottoms product, there are 5 independent streams; the liquid from and the vapor to the bottom tray, the vapor from the top tray, the liquid reflux, and the liquid product. This accounts for 5(C+2) variables and leaves 2m+7 variables left to specify. The heat leak on each tray is assumed to be zero and the column is assumed to have no pressure drop so that each tray will be at atmospheric pressure. These specifications account for an additional 2m variables. Finally, the pressures in the reboiler, the condenser and the reflux divider will all be set to atmospheric; the temperatures in the reboiler and condenser will be specified; and the reflux rate and the number of trays will be set.

Simulation

Before beginning a description of the simulation, one should note that a rigorous description of the procedures from startup to final cooldown has not been attempted. Rather, the model only describes the state of the system at total reflux equilibrium.

> In batch distillation one has two alternative procedures from which to chose. In one case, one can consider the initial time as that in which heat is initially applied to the reboiler. In this case, the model must account for the thermal dynamics of the column itself, the filling of the trays with liquid, etc. A more practical approach is to assume that the product drawoff is to commence from a batch column operating at total reflux steady-state . . . The initial conditions for the unsteady-state model were the results of a total reflux steady-state calculation. (Distefano, 1968)

The actual program is divided up into four sections: nomenclature, block data, the main program, and the various subroutines. The nomenclature section has been supplied to provide a convenient reference for understanding the code.

It includes the nomenclature that has been provided earlier in this paper and, in most cases, duplicates it exactly. It is however, much more comprehensive. The section also includes every variable, array, and subroutine referenced within the code of the program as well as a definition.

Block Data

The block data section is listed under BLOCK DATA DIST and it includes data for Antoine's equation coefficients, molecular weights, liquid enthalpy coefficients, heat of vaporizations, and specific gravities. The uses of the data will be explained later. Antoine's equation coefficient data comes from three sources: Jordan (1954), Lange's Handbook of Chemistry (Dean, 1985), and Felder and Rousseau (1978). The liquid enthalpy coefficients are from API (1976) and the heat of vaporization data comes from Lange's (Dean, 1985). The specific gravities are all at 60°F referenced to water at 60°F and they come from either Lange's (Dean, 1985) or GPSA (1981).

All of the above data are provided for the 61 components listed in Table I (Erbar, 1987) and space has been provided for an additional 39 hypothetical or additional components. Product options are also set in the block data section. The array INN is set for fixed bottoms and overhead product rates and array INN also sets the number of constant molal overflow iterations.

TABLE I

PURE COMPONENT LIST

NUMBER	NAME	NUMBER	NAME
1	Hydrogen	32	2-methyl-1-Butene
2	Methane	33	3-methyl-1-Butene
3	Ethane	34	2-methyl-2-Butene
4	Propane	35	1-Hexene
5	i-Butane	36	Cyclopentane
6	n-Butane	37	Methylcyclopentane
7	i-Pentane	38	Cyclohexane
8	n-Pentane	39	Methylcyclohexane
9	neo-Pentane	40	Benzene
10	n-Hexane	41	Toluene
11	n-Heptane	42	o-Xylene
12	n-Octane	43	m-Xylene
13	n-Nonane	44	p-Xylene
14	n-Decane	45	Ethylbenzene
15	n-Undecane	46	Nitrogen
16	n-Dodecane	47	Oxygen
17	n-Tridecane	48	Carbon Monoxide
18	n-Tetradecane	49	Carbon Dioxide
19	n-Pentadecane	50	Hydrogen Sulfide
20	n-Hexadecane	51	Sulfur Dioxide
21	n-Heptadecane	52	2-methyl-Pentane
22	Ethylene	53	3-methyl-Pentane
23	Propylene	54	2,2 dimethyl-Butane
24	1-Butene	55	2,3 dimethyl-Butane
25	cis-2-Butene	56	1-Heptene
26	trans-2-Butene	57	Propadiene
27	i-Butene	58	1,2-Butadiene
28	1,3 Butadiene	59	Ethylcyclopentane
29	1-Pentene	60	Ethylcyclohexane
30	cis-2-Pentene	61	Water
31	trans-2-Pentene		

The Main Program

The primary purpose of the main portion of the program is to formulate the material and energy balance equations. Its other major functions are to perform the iterations required to remove overhead product, to account for the diminishing amount of material in the column, and to read the components and data for the desired simulation.

The initial lines of code are used to clear the program of data from any previous runs. The temperature, vapor, and liquid profiles and the matrix handling arrays are all set equal to zero. The tray composition storage is also set to zero. Only the condenser and reboiler temperatures and the amount left of each component are kept as estimates for the next iteration.

The next portion of the program deals with the reading in of data and column conditions and with the setting up of a smaller data base for use in the program. Variables read in include the initial system pressure, the reboiler and condenser temperature estimates, the liquid feed temperature and the estimated reflux rate. The user is also allowed to set the number of trays, the withdrawal rate, and the cut off point to end the distillation. Also read in are the component identification numbers and the component feed rates. The feed rates should be in moles and should be for a degassed system. It is suggested that the feed be flashed at anywhere from 32°F to room temperature to remove the non-condensables.

A file is generated for each set of component input data so that changes in the column parameters can be easily made. Up to six files can be created for input data along with one file that is provided for the storage of crude blending data. More than one crude file can be combined to generate the crude blend. Crudes are blended on the basis of volume and the proportions of each crude can be set by the user. Each of the input data files and the crude blend file will have a corresponding output data file. Only the last run of a particular system can be saved by the simulator.

If hypothetical components are desired, the program will prompt the user for the normal boiling point, the molecular weight, and the specific gravity. The molecular weight can be calculated in the program if the user desires this option. The Antoine′s equation parameters will then be calculated using the formula of Dreisbach (1952). Next, some constants needed in the matrix inversion based on the number of components and stages are calculated. Finally, a loop is provided to select values from the block data set to build a data set consisting of only those data for the components of interest in the particular system.

To begin the calculations, temperature and liquid flow profiles are generated from user inputs to the program. The initial temperature profile is linear. The vapor rate profile is then generated from a material balance using the assumed liquid rate profile. The component material balance equations are developed using these profiles. On the first pass iteration, bubble point calculations are used to find new reboiler and condenser liquid temperature estimates and the program will loop back to calculate new profiles. On each subsequent pass, the reboiler and condenser temperatures will be recalculated although no further attempts will be made to linearize the temperature profile. If the input temperature estimates are good, the calculated bubble point temperatures will speed convergence dramatically. Estimates over 200°F away from the correct temperature may lead to a diverged solution.

For subsequent passes through the program following the initial one, the new condenser compositions are compared against the old compositions. If the difference is less than the allowable tolerance, the iteration is converged and the program can print the results of that run. If not, the program will continue.

After the material balance equations are calculated, the matrix storage arrays are generated and the subroutine used to invert and solve the Jacobian matrix is called. If the number of runs is within the maximum constant molal overflow passes allowed, the program will make the temperature corrections and loop back to the beginning. The temperature corrections are based on the inverted matrix of the partial derivatives of the component liquid flows with respect to temperature. The energy balance equations will be added to the matrix solution after the constant molal overflow passes.

Next, the program will take the results of the matrix inversion and calculate new tray temperatures and liquid flow rate profiles. These new profiles will be used to calculate tray component compositions at the beginning of the program. Convergence is achieved whenever the new compositions are within the allowable range around the old compositions. The temperature and liquid rate corrections are bounded to ensure against divergence. The new tray temperatures must be within 10°F of the old and the restriction on the liquid rate correction is within 40 percent of the old rate. The bounds for the temperature and liquid rate corrections are supplied as default values and may be changed by the user.

For a converged iteration, the molar withdrawal is converted to a volume percent and the temperature is calculated to completely condense the withdrawal stream. The amount of each component in the column is adjusted to reflect the moles that have been withdrawn. If the amount of a particular component goes to zero, it is noted and future calculations reflect the loss of that particular component. The iteration number, the condenser and reboiler temperatures, the volume percent of that particular iteration, and the total volume percent distilled are all printed as output. If the maximum allowed temperature or volume percent distilled is reached, that particular simulation run will end.

Band and Solver Subroutines

The matrix solution subroutines, BAND and SOLVER, are modified code from Newman (1968). There is not any intent to derive a matrix solution. Many variations are available and it is not difficult to find one applicable to almost any system or program. The technique of Newman was selected for its versatility and its expertise in avoiding diverging calculations. The credit for the application of Newman´s procedure belongs to MAXISIM (Erbar, 1987).

Equilibrium Calculations Subroutines

The K-value calculations are based on a combination of Raoult´s and Dalton´s laws and then use of the definition of Henry´s law to find the K-value. Raoult´s law:

$$P_1 = p_1 x_1 \qquad [33]$$

is valid for mixtures where the molecules are of similar size and when association and chemical combination can be neglected (Robinson and Gilliland, 1950). Raoult´s law is usually valid as x_1 approaches unity and can be valid for any value of x_1 provided that the mixture is of similar substances such as a mixture of straight-chain hydrocarbons (Felder and Rousseau, 1978).

The most common form of Dalton´s law is:

$$P_1 + P_2 + P_3 + \ . \ . \ . + P_n = P \qquad [34]$$

If the ideal gas law is applicable to both the components and the mixture (Robinson and Gilliland, 1950), then

$$P_i = y_i P \qquad [35]$$

Combining Raoult's and Dalton's laws yields:

$$y_i P = p_i x_i \qquad [36]$$

If the total system pressure is less than 2 atmospheres and the liquid phase is ideal (Green, 1984), then

$$K_i = p_i/P \quad \text{and} \quad y_i = K_i x_i \qquad [37]$$

These derivations also require both the vapor temperature and pressure to equal the liquid temperature and pressure.

Antoine's equation is used in the subroutine KVALUE to calculate the K-values. The form of the equation is

$$p_i = \log (A_i - B_i/(T + C_i)) \qquad [38]$$

with the pressure in mm Hg and the temperature in °C. The values of A_i, B_i, and C_i have been provided for the 61 pure components. If hypothetical fractions are needed, the log base 10 function becomes a natural log function with the pressure in psia and the temperature in °F. The approximation of A_i, B_i, and C_i for this formula are calculated in the main program from Dreisbach's (1952) equations. K-values are limited to the range of 10^{-10} to 10^{+10} for calculational purposes. The derivative of the K-value is also computed in this subroutine. It will be needed not only in the main program, but also in the calculation of bubble and dew point temperatures.

The bubble point is that temperature where the mixture in question has a single phase: saturated liquid. This corresponds to:

$$y_i = 1.0 \quad \text{or} \quad K_i x_i = 1.0 \qquad [39]$$

The solution of this equation will be some type of trial and error technique in which a temperature is assumed, K-values calculated, and iterations performed until the conditions of Equation 39 are reached. The solution technique of choice for systems using K-values derived from vapor pressure calculations is Newton's approximation (Holland, 1981 and Carnahan et. al., 1964). The dew point temperature is similar except that it is the saturated vapor temperature. Saturated vapor conditions hold for:

$$x_i = 1.0 \quad \text{or} \quad y_i/K_i = 1.0 \qquad [40]$$

The steps to find the dew point temperature are virtually the same as those of the bubble point temperature. These two trial and error subroutines can be found under BUBBLE and DEWPT.

Enthalpy Calculation Subroutines

The enthalpy and enthalpy derivative calculations used in the energy balance equations are relatively simple polynomial expansions of absolute temperatures. The calculations are found in VENTH, VLNTH, and VENHDT. The data for the pure components comes from Chapter 7 of the America Petroleum Institute's Project 44 (API, 1976). The hypothetical enthalpy and enthalpy derivative calculations come from the GPAK*H computer program (Erbar, 1974). These hypothetical enthalpies and derivatives are only functions of temperature, but their coefficients are functions of specific gravity and mean average boiling point.

Solution Strategy

The program details have been presented and the code is available in Appendix A, but it may not be readily apparent to the reader exactly how iteration solutions are achieved. A logic diagram has been presented in Figure 5 to aid in clarification. Borrowing liberally from Gas Conditioning and Processing, Volume 3 (Maddox and Erbar, 1982), the solution strategy is detailed.

1) Input the system of interest
    A) Column extremities temperatures
    B) Components and relative amounts
    C) Hypothetical components' parameters

2) Calculate the feed conditions

3) Estimate the temperature and liquid rate profiles

4) Calculate the vapor rate profile

5) Calculate the K-values based on the estimated temperatures

6) Estimate the component liquid and vapor rates for each tray

7) Set up material and energy balance equations and solve

8) Correct temperature and liquid and vapor

rate profiles and

9) Loop back to (4) if the solution has not converged

10) For a converged iteration, the iteration number, the condenser and reboiler temperatures, the volume percent removed for that iteration, and the total volume percent removed are printed

11) Loop back to (2) if there is still material left in the column to be distilled

12) Either rerun this system with new parameters, run a new system, or exit from the program

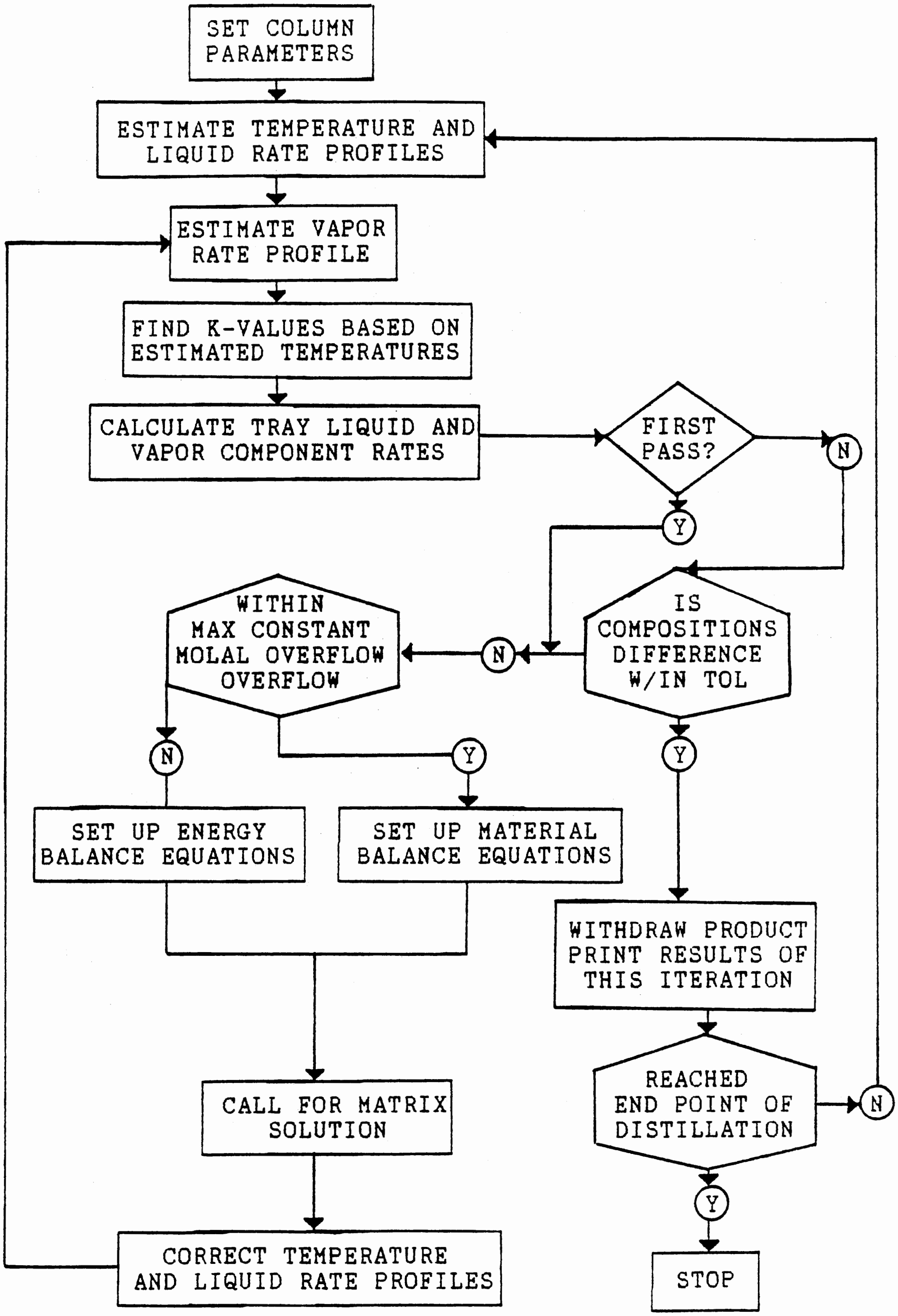


Figure 5. Simulation Logic Diagram

CHAPTER IV

RESULTS AND DISCUSSION

Introduction

This simulation was performed using data from three sources: a light North Sea crude, a medium weight Middle Eastern crude, and a heavy South American crude. This section will attempt to describe the uses of the model and the validity of its results. Any deviations from physical reality will be pursued. First however, a brief review will made of the assumptions used in developing the model and the solution techniques employed to achieve convergence.

Assumptions

Any model formulated will contain certain assumptions to allow the description of the physical scenario while still permitting a realistic problem scope. This model is no different in this respect from any of its predecessors. A typical laboratory procedure is initially run at a constant pressure, usually atmospheric (ASTM II, 1987) and the column is jacketed to prevent heat loss (Lockwood et. al., 1951). Thus, this model also assumes atmospheric pressure and no pressure drop within the column and that the column is adiabatic. In reality, the intent is that both the pressure drop and heat loss remain very small if not negligible. The other assumptions are detailed in the Batch Distillation section of the Literature Review, Chapter 2 as given by Meadows (1963).

Most batch distillation programs are developed to handle product removal beginning from a column operating at total reflux (Distefano, 1968). Equations to describe the heating of the column and the filling of the trays with liquid are difficult, at best, to develop and apply. After product removal commences, liquid is removed from the tray continuously until the distillation is stopped. A simplifying assumption of this model is that product is removed at steady-state. In actuality, product is withdrawn in such small amounts, approximately 10-20 volume percent per hour (ASTM II, 1987), that at any particular time deviations from steady-state are small. The model removes small, discrete amounts of liquid after steady-state is achieved in the equations. If the amounts removed are small enough, the removal approaches continuity.

Convergence Techniques

Convergence is achieved by improving the temperature distribution and the tray liquid flows until the compositions in the top tray become constant. The corrections are borrowed from Newman (1963) and are bounded to virtually eliminate the chance of divergence.

It is crucial in a Newton-Raphson iteration solution technique to have good initial guesses of the column conditions. In this simulation, appropriate temperature estimates are required as the tray compositions are functions of the temperature profile. A well-specified problem has an infinitely better chance of finding a solution than a poorly defined problem. Most parameters in the program will either be known or the default values will suffice. Top and bottom tray temperatures, however, can vary widely. If the simulation is run to replicate laboratory results, convergence will probably be attained easily using the temperature estimates generated in the laboratory. The program automatically adjusts temperatures for iterations after the initial removal, so only the top and bottom temperatures for the generation of the first cut of product are needed.

If the simulation is conducted to determine the properties of a liquid mixture, it is important to have accurate estimates. As a very crude estimate, the temperature used for degassing can be used for the top tray and that temperature plus an additional 300°F can be used for the bottom tray. If the sample to be tested is very heavy, these estimates will not suffice. The simulation will calculate bubble point temperatures to improve these guesses, but this subroutine will not be able to generate temperatures if the estimates are too far away (200-300°F) from the correct answers.

The basic premise of the model has been that the column is at steady-state at a constant molar percentage removal rate. This differs slightly from the physical situation, as mentioned in the Assumptions section, in that removal is not rigorously steady-state. In reality, batch distillation consists of transient, continuous removal after steady-state is initially achieved at total reflux. However, assuming steady-state between tiny removals of material eases the computational difficulties and approaches the laboratory distillation as the removal rate becomes increasingly smaller.

Input Data

Some general information on input variables was provided earlier. This section will expand on the previous work to include the default parameters. The basis for these default parameters will be detailed in a subsequent section.

The variables that can be set by the user include typical distillation parameters such as the number of stages, the initial system pressure, the condenser and reboiler temperature estimates, the liquid feed temperature, the reflux ratio, and the different components and their feed rates. Feed rates in this sense refers to the amounts added to the still pot. Parameters indigenous to transient operations include: the removal rate and the point set to end the distillation, either a volume percentage or a temperature limit. Most distillation simulations allow the condenser and reboiler type to be specified. In this batch simulation, however, it is necessary to use a total condenser and total reboiler. In general, a total condenser is usually used in TBP distillations to achieve total reflux initially.

Default variables have been provided for guidance and convenience. As much as possible, defaults follow the laboratory guidelines. Reflux is set at 5:1, atmospheric pressure is nominally 760 mm Hg, and the number of stages is specified at 10. The removal rate is set at 4 molar percent which corresponds to approximately 1-2 volume percent. The first cuts are at or near the 4 mole percent withdrawal but they contain more moles per unit volume and hence a smaller volume percentage. As the number of moles in a fraction withdrawn decreases, its relative volume increases. Generally, the total volume for a cut is fairly constant.

Defaults of 1000°F or 95 volume percent distilled have been provided to end the simulation run. Different laboratory TBPs will have a continuum of end points of temperature and volume percent distilled. These defaults have been initialized at high values to enable the program to extrapolate the TBP as far as the user wishes.

The feed to the still pot is entered as a series of components. The pure components available have been listed earlier and space is provided for an additional 89 components. Any components that are entered outside of the pure component bounds must have a normal boiling point, a specific gravity and a molecular weight attached. These data are used to prepare Antoine's equation and enthalpy coefficients. All of the hypothetical components entered must be hydrocarbons for the simulation to properly generate K-value and enthalpy data.

It is suggested that the system be degassed or flashed between room temperature and 32°F to remove the various noncondensables. The freezing point of water was chosen as the lower limit because ice is often used in the condenser. Without the degassing, the simulation will generate a large temperature difference between the top and bottom tray and convergence will be difficult. Also, the volume of the gases is usually slight and they will only act to drop the lower temperature end of the TBP dramatically. It is important to extrapolate the TBP data to 100 volume percent distilled to properly characterize the crude. Even rough estimates in these very heavy fractions will help the simulation generate a proper TBP.

The default values for the temperatures are 100, 400, and 70°F for the condenser, reboiler, and liquid feed respectively. The feed temperature is chosen as a normal room temperature. A medium crude will initially come to steady-state at about 100°F for the top tray and approximately 400°F for the bottom tray. However, very light or very heavy crudes may need to have the temperature profile modified down or up respectively.

Validation of the Model

Three wide-ranging systems were run to generate TBPs to compare to experimental data: a light weight (39.8°API) North Sea crude, a medium weight (26.8°API) Middle Eastern crude, and a heavy (10.1°API) South American crude. All of this data is proprietary industrial data and will be referenced through the rest of the paper as experimental data. An equal volume mixture of the Middle East and South American crudes was also analyzed. The TBPs generated by the simulation were compared with those generated experimentally. Deviations were noted in volume percent distilled at a certain temperature and in temperature at a specified volume percent distilled. All of these simulations were run with the following default parameters: 760 mm Hg pressure, 10 trays, 5:1 reflux ratio, and 4 molar percent withdrawal. The top tray temperature estimate was adjusted to 250°F for the heavy South American crude.

Deviations are found by taking differences from a base case. For example, a volume percent distilled is chosen. The experimental temperature at this point is recorded as a basis. The temperature calculated by the simulation is taken by linearizing between two adjacent volume percentages. Although this is not rigorously accurate, the deviation from linearity between two volume percentage points is negligible. Generally, two volume points are only 1-2 percent apart. If a specified temperature is used to find deviations in volume, the linearity assumption between adjacent points is not as accurate. The difference between two points can be as much as 60°F or 10 percent of the total temperature range in question. Usually, however, two points are no more than 5 percent or 30°F apart.

In general, the more fractions that are used to characterize the crude, the better the simulated TBP will be. If few fractions are used, the TBP will tend to stair step. Stair stepping is the tendency of the TBP to remain at or near a constant temperature for some range of distillation. The TBP will only be as accurate as the characterization of the crude. Obviously, the more fractions that are included in the characterization, the more accurate the simulation will be.

Estimates of the very heavy fractions will not be very accurate if they are extrapolated. However, these fractions affect the distillation and should be projected as carefully as possible. The simulation of the TBP into these uncertain regions should not be valued any more than that of extrapolated experimental data.

North Sea Crude

The North Sea (39.8°API) crude was unique in two respects: it was the lightest crude analyzed and it was the only crude that consisted of both hypothetical and pure components. The list of components and the simulation inputs can be found in Table II. Nine pure components including nitrogen, carbon dioxide, and methane and ten

TABLE II

NORTH SEA CRUDE INPUTS

	FEED (MOLES)				
	ORIGINAL	AFTER DEGASSING	NORMAL BOILING POINT (F)	MOLECULAR WEIGHT	SPECIFIC GRAVITY
Nitrogen	0.69				
Carbon Dioxide	0.12				
Methane	47.06	0.17			
Ethane	5.69	0.16			
Propane	4.39	0.50			
i-Butane	0.95	0.25			
n-Butane	2.42	0.87			
i-Pentane	1.11	0.69			
n-Pentane	1.46	1.02			
Fraction 1	6.88	6.38	159.7	85.09	0.7082
Fraction 2	5.73	5.71	254.5	114.21	0.7426
Fraction 3	4.91	4.91	348.6	145.12	0.7739
Fraction 4	4.23	4.23	438.6	178.86	0.8016
Fraction 5	3.67	3.67	519.8	213.83	0.8251
Fraction 6	3.18	3.18	596.5	250.97	0.8461
Fraction 7	2.67	2.67	684.3	297.96	0.8689
Fraction 8	2.19	2.19	785.8	357.39	0.8938
Fraction 9	1.56	1.56	994.3	490.92	0.9412
Fraction 10	1.08	1.08	1274.2	677.31	0.9981
Total	100.00	39.24			

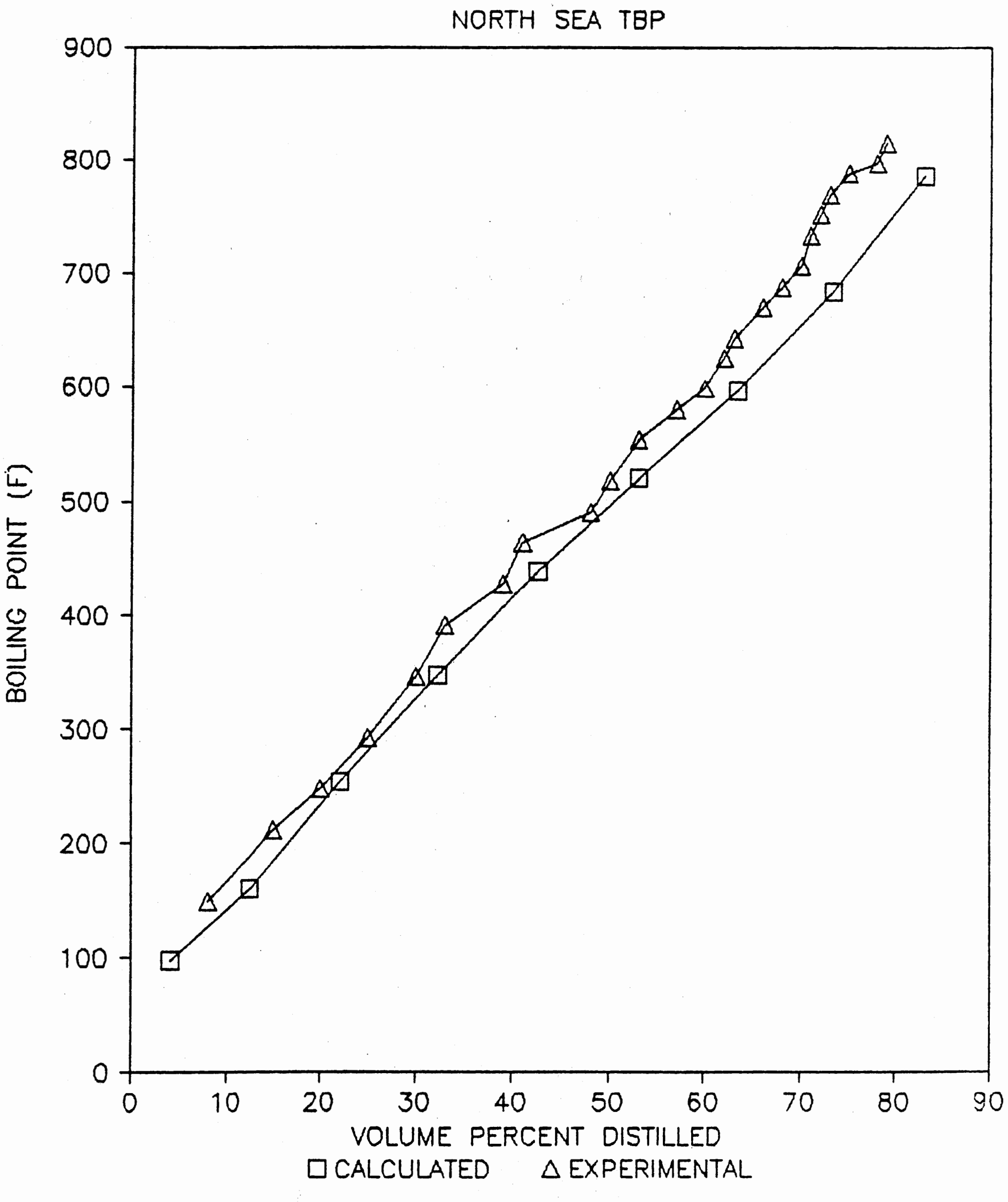


Figure 6. North Sea Crude TBP Diagram

TABLE III

NORTH SEA CRUDE DEVIATION ANALYSIS

	PERCENT VOLUME			TEMPERATURE (F)		
RUN	EXPERIMENTAL	CALCULATED	% DEVIATION	EXPERIMENTAL	CALCULATED	% DEVIATION
1	8.0	5.650	-29.375	149.0	159.7	7.181
2	15.0	13.591	-9.393	212.0	254.5	20.047
3	20.0	14.340	-28.300	248.0	254.5	2.261
4	25.0	22.928	-8.288	293.0	348.6	18.976
5	33.0	33.114	0.345	392.0	386.3	-1.444
6	41.0	43.102	5.127	464.0	438.6	-5.466
7	50.0	44.191	-11.618	518.0	519.9	0.359
8	53.0	54.842	3.475	554.0	520.9	-5.982
9	60.0	63.403	5.672	599.0	596.5	-0.412
10	63.0	63.983	1.560	644.0	596.6	-7.354
11	66.0	64.331	-2.529	671.0	684.3	1.984
12	70.0	73.604	5.149	707.0	684.3	-3.209
13	75.0	83.026	10.701	788.0	785.8	-0.278
14	79.0	83.105	5.196	815.0	785.8	-3.582

hypothetical fractions are included. This crude was experimentally flashed at 60°F to remove all of these three gases. The simulation feed was flashed at 32°F and not all of the methane was removed. The amount left was so small however, that it will have little effect on the TBP other than to drop the temperature of the first cut.

The experimental and simulated TBPs are shown in Figure 6. The deviations of the simulation from the experimental data can be easily seen and are tabulated in Table III. As can be seen, the temperature will always be lower at a certain volume than the experimental value and the volume percent distilled will always be higher at a set temperature. The magnitude of these deviations is generally about 10 percent. There is no way that errors can be estimated in the laboratory work and so all the data will be shown as deviations from the experimentally derived information. These results, which can be found in Appendix B, show that the calculation of the North Sea crude TBP tended to stair step.

Middle Eastern Crude

The results from the simulation of the Middle Eastern crude (26.8°API) are very similar to those of the North Sea crude except that the deviations in the individual datum points are much less. Deviations of less than 1 percent can be expected in temperature and less than 1 1/2 percent in volume percent distilled. Both the volume percent and

TABLE IV

MIDDLE EASTERN CRUDE INPUTS

	VOLUME PERCENT	FEED (MOLES)	NORMAL BOILING POINT (F)	MOLE WEIGHT	SPECIFIC GRAVITY
Fraction 1	2.6	5.865	89	83	0.639
Fraction 2	1.4	3.087	130	87	0.655
Fraction 3	2.0	4.304	178	91	0.668
Fraction 4	2.0	4.079	207	98	0.682
Fraction 5	2.0	3.985	242	103	0.700
Fraction 6	2.0	3.764	264	112	0.719
Fraction 7	2.0	3.665	291	117	0.732
Fraction 8	2.0	3.585	321	122	0.746
Fraction 9	2.0	3.402	345	130	0.755
Fraction 10	2.0	3.205	368	140	0.766
Fraction 11	2.0	3.068	394	148	0.775
Fraction 12	2.0	2.932	421	157	0.785
Fraction 13	2.0	2.786	463	162	0.795
Fraction 14	2.0	2.758	492	171	0.805
Fraction 15	2.0	2.646	517	180	0.813
Fraction 16	2.0	2.514	540	190	0.820
Fraction 17	2.0	2.434	567	200	0.830
Fraction 18	2.0	2.345	590	210	0.840
Fraction 19	2.0	2.241	616	221	0.845
Fraction 20	2.0	2.138	637	233	0.850
Fraction 21	2.0	2.086	667	241	0.858
Fraction 22	2.0	1.997	686	254	0.865
Fraction 23	2.0	1.841	705	266	0.881
Fraction 24	2.0	1.833	732	283	0.885
Fraction 25	2.0	1.757	767	297	0.890
Fraction 26	2.0	1.710	787	307	0.897
Fraction 27	8.0	5.653	880	385	0.928
Fraction 28	10.0	4.863	1010	475	0.963
Fraction 29	10.0	5.020	1130	580	0.993
Fraction 30	10.0	4.361	1250	675	1.004
Fraction 31	10.0	3.886	1380	790	1.048
Total		100.000			

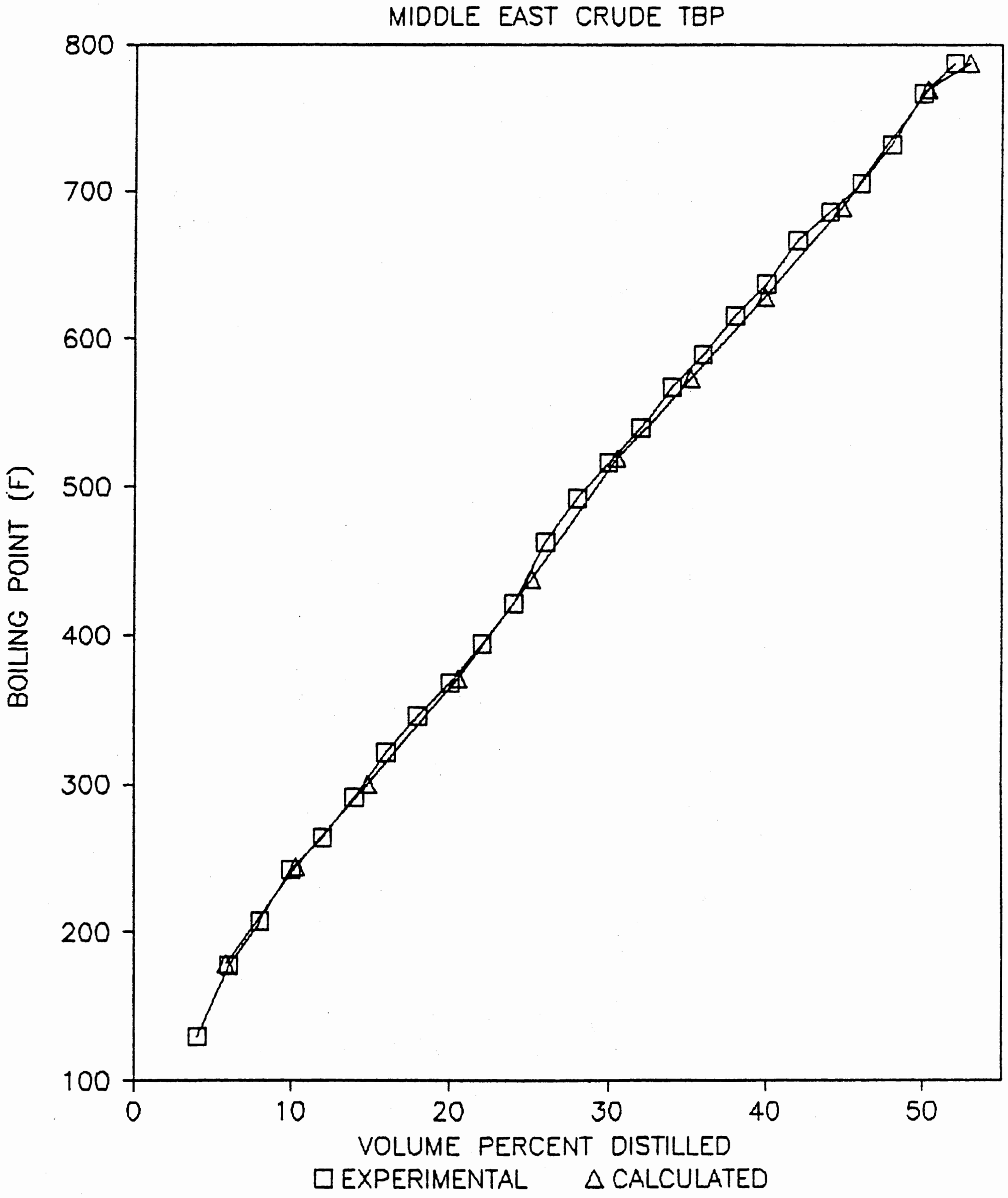


Figure 7. Middle Eastern Crude TBP Diagram

TABLE V

MIDDLE EASTERN CRUDE DEVIATION ANALYSIS

	PERCENT VOLUME			TEMPERATURE (F)		
RUN	EXPERIMENTAL	CALCULATED	% DEVIATION	EXPERIMENTAL	CALCULATED	% DEVIATION
1	4.0	4.070	1.750	89.0	89.3	0.337
2	6.0	5.772	-3.800	128.0	128.0	-1.538
3	8.0	8.049	0.612	178.0	179.6	0.899
4	10.0	10.198	1.980	207.0	206.2	-0.386
5	12.0	12.156	1.300	242.0	238.6	-1.405
6	14.0	14.084	0.600	264.0	262.6	-0.530
7	16.0	16.324	2.025	291.0	289.7	-0.447
8	18.0	18.071	0.394	321.0	316.4	-1.433
9	20.0	20.331	1.655	345.0	344.5	-0.145
10	22.0	22.033	0.150	368.0	363.9	-1.114
11	24.0	24.382	1.592	394.0	393.5	-0.127
12	26.0	26.522	2.008	421.0	415.6	-1.283
13	28.0	28.028	0.100	463.0	453.3	-2.095
14	30.0	30.353	1.177	492.0	491.5	-0.102
15	32.0	32.576	1.800	517.0	511.9	-0.986
16	34.0	34.111	0.326	540.0	533.4	-1.222
17	36.0	36.456	1.267	567.0	564.9	-0.370
18	38.0	38.620	1.632	590.0	583.9	-1.034
19	40.0	40.655	1.637	616.0	608.0	-1.299
20	42.0	42.190	0.452	637.0	630.3	-1.052
21	44.0	44.507	1.152	667.0	662.8	-0.630
22	46.0	46.749	1.628	686.0	679.9	-0.889
23	48.0	48.749	1.560	705.0	697.4	-1.078
24	50.0	50.190	0.380	732.0	725.0	-0.956
25	52.0	52.942	1.812	767.0	761.6	-0.704
26				787.0	779.1	-1.004

temperature deviations are included in Table V. The inputs to the simulation are given in Table IV. The last 5 fractions are estimated from extrapolations of the experimental TBP, molecular weight, and °API graphs which are included in Appendix C. The experimental and calculated TBPs are shown in Figure 7.

The very small deviations from the experimental data can be attributed to the greater effort in the characterization of the feed. The North Sea crude contained several pure components; however, each of the ten hypothetical fractions represented approximately 7 percent of the degassed feed. In the Middle Eastern crude, fractions represented 2 volume percent each through the range of interest in the temperatures. This more detailed characterization led to the elimination of stair stepping and allowed more accurate results.

South American Crude

The deviations in the results from the heavy South American crude (10.1°API) follow the magnitude and direction of the deviations in the Middle Eastern crude. Deviations in temperature were basically the same in magnitude, but because of the higher temperatures involved, the percent deviation dropped to less than 1/2 percent. Generally the temperatures will be within 10°F and the volumes will be within 1/2 percent in magnitude. The percent volume deviations averaged just over 1 1/2 percent for this crude.

TABLE VI

SOUTH AMERICAN CRUDE INPUTS

	VOLUME PERCENT	FEED (MOLES)	NORMAL BOILING POINT (F)	MOLE WEIGHT	SPECIFIC GRAVITY
Fraction 1	1.9	4.438	294	147	0.746
Fraction 2	1.9	4.400	396	162	0.815
Fraction 3	2.2	4.775	454	179	0.844
Fraction 4	2.0	4.089	495	195	0.866
Fraction 5	2.0	4.114	538	211	0.881
Fraction 6	2.0	3.601	572	227	0.888
Fraction 7	2.2	3.715	605	244	0.895
Fraction 8	1.9	3.018	635	262	0.904
Fraction 9	2.1	3.198	666	276	0.913
Fraction 10	1.9	2.768	695	291	0.921
Fraction 11	2.3	3.176	727	309	0.927
Fraction 12	1.6	2.141	747	321	0.933
Fraction 13	2.0	2.563	770	337	0.938
Fraction 14	2.0	2.465	793	353	0.945
Fraction 15	2.0	2.375	817	369	0.952
Fraction 16	2.0	2.286	848	385	0.956
Fraction 17	2.0	2.207	895	400	0.959
Fraction 18	13.0	11.663	1080	503	0.986
Fraction 19	13.0	9.897	1270	606	1.009
Fraction 20	20.0	12.513	1550	764	1.044
Fraction 21	20.0	10.598	1840	922	1.068
Total		100.000			

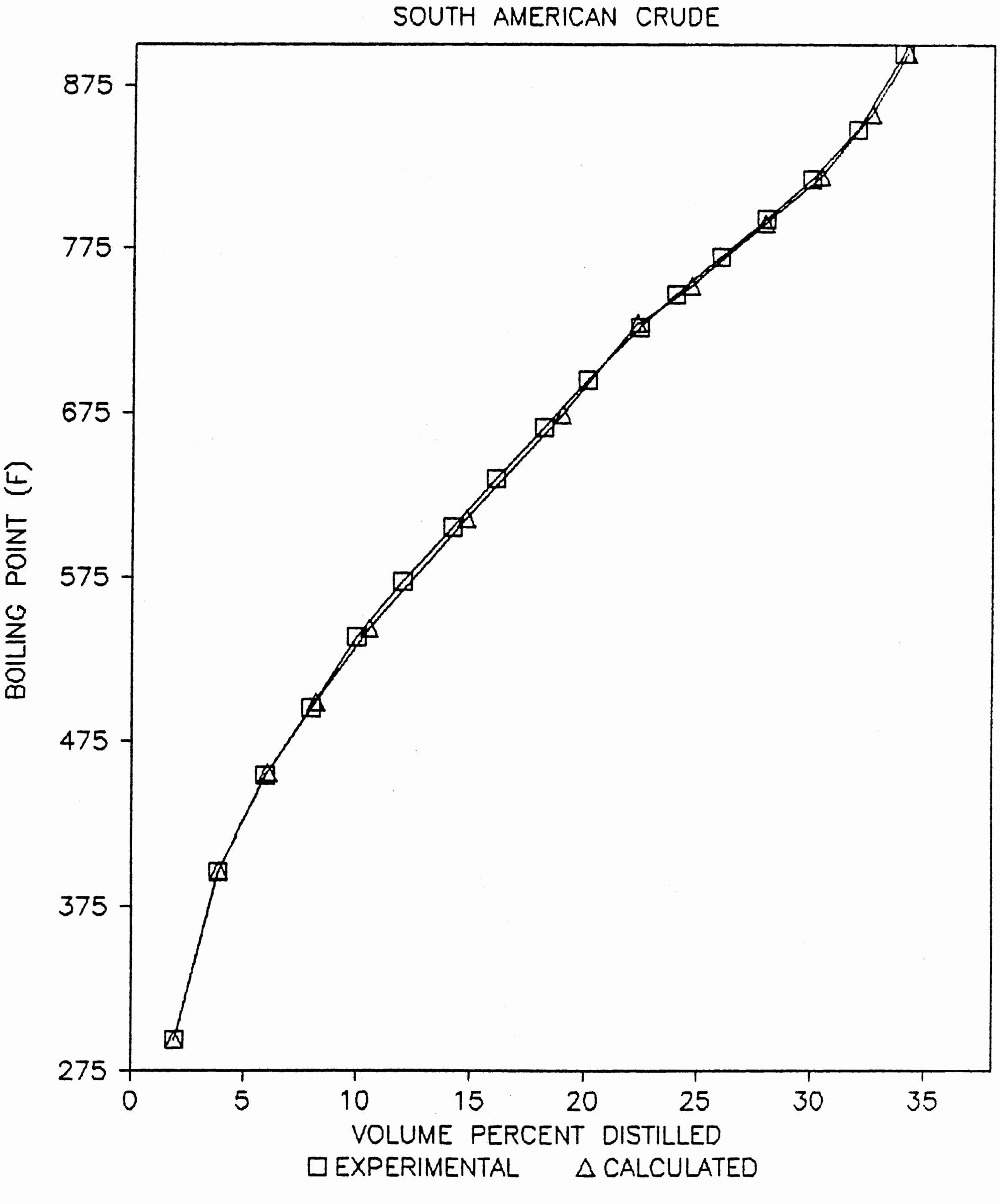


Figure 8. South American Crude TBP Diagram

TABLE VII

SOUTH AMERICAN CRUDE DEVIATION ANALYSIS

	PERCENT VOLUME			TEMPERATURE (F)		
RUN	EXPERIMENTAL	CALCULATED	% DEVIATION	EXPERIMENTAL	CALCULATED	% DEVIATION
1	1.9	1.717	-9.632	294.0	294.6	0.204
2	3.8	3.827	0.711	396.0	396.6	0.152
3	6.0	6.056	0.933	454.0	455.5	0.330
4	8.0	8.043	0.538	495.0	497.1	0.424
5	10.0	10.623	2.630	538.0	539.8	0.335
6	12.0	12.157	1.308	572.0	568.7	-0.577
7	14.2	13.949	-1.768	605.0	607.5	0.413
8	16.1	16.316	1.342	635.0	631.5	-0.551
9	18.2	18.020	-0.989	666.0	667.9	0.285
10	20.1	20.332	1.154	695.0	691.3	-0.532
11	22.4	22.108	-1.304	727.0	730.5	0.481
12	24.0	24.406	1.692	747.0	742.2	-0.643
13	26.0	26.202	0.777	770.0	767.6	-0.312
14	28.0	28.191	0.682	793.0	791.1	-0.240
15	30.0	30.235	0.783	817.0	814.0	-0.367
16	32.0	32.077	0.241	848.0	840.4	-0.896
17	34.0	34.227	0.668	895.0	889.6	-0.603

This crude was also represented by approximately one hypothetical fraction for every 2 volume percent distilled. The input data for this crude can be found in Table VI. The last four fractions have been extrapolated from data included in Appendix D. The deviations are tabulated in Table VII and both the experimental and model generated TBPs are shown in Figure 8.

Crude Blending

The crux of this work has been to develop a model that would generate a TBP for a blend of two or more crudes. This model was applied to an equal volume mixture of the South American and the Middle Eastern crudes. The crude blend TBP generated is shown in Figure 9. The results of the crude blending distillation calculation are included in Appendix E. Without any experimental data, no analysis can be made on the accuracy of these results. However, the diagram generated appears as would be expected. The lower temperature and volume end duplicated the lighter Middle Eastern crude data and the higher temperature and volume end followed the heavier South American crude as expected. The behavior in the middle portion of the distillation performed as expected graphically, although it is impossible to quantitatively describe this behavior.

Optimum Operating Parameters

Although ASTM D-2892 (ASTM II, 1987) listed the proper

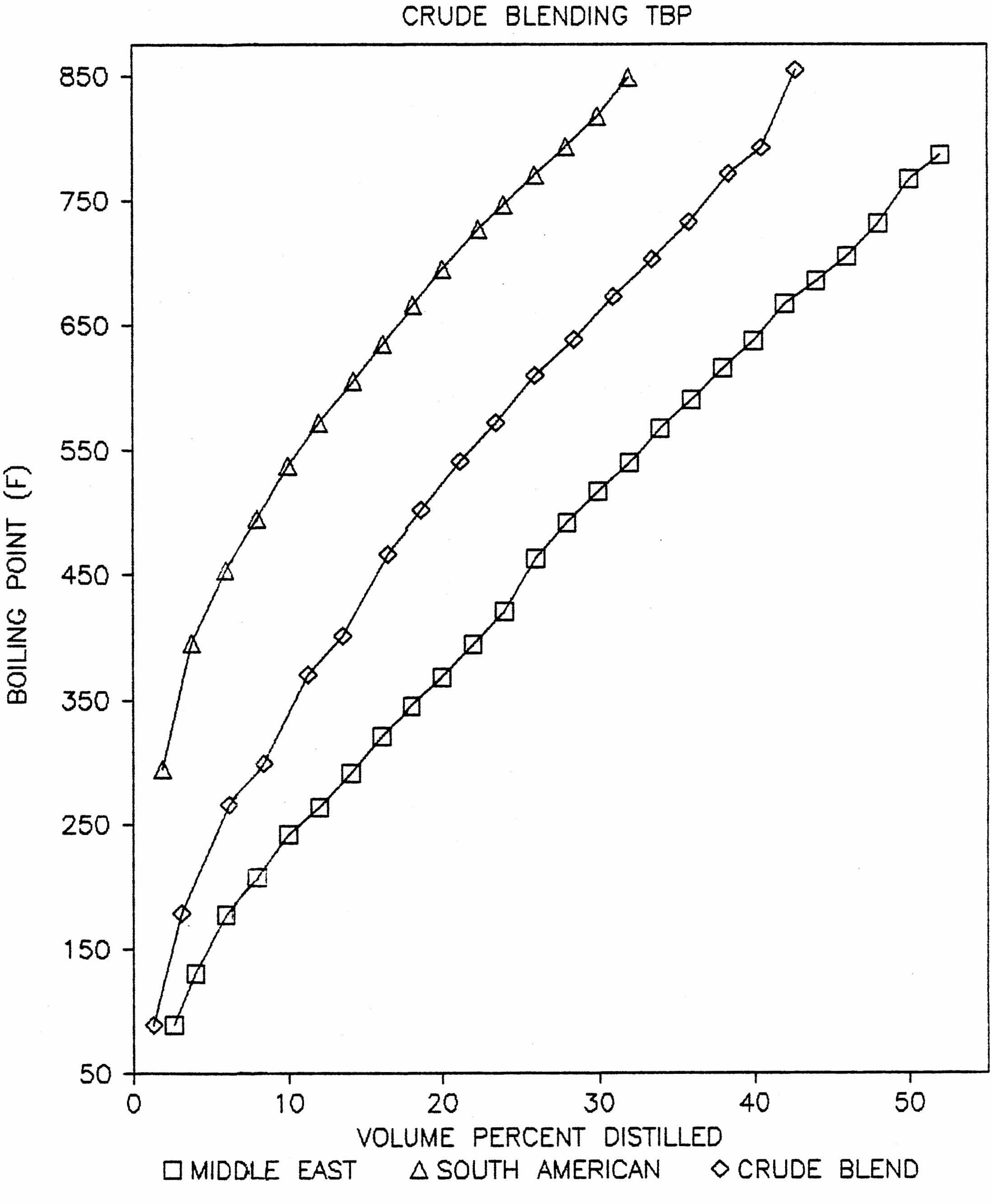


Figure 9. Blended Crude TBP Diagram

operating specifications for the generation of TBP data, it was not readily apparent that these parameters would be the most suitable for this simulation. Variables that were examined for their validity include: pressure, temperature correction, number of trays, reflux ratio, and molar percent removal. All were analyzed using the Middle Eastern crude as a sample system. All were also compared to the default values for this system and deviations were noted with respect to temperature at a constant volume percent distilled. The results from the simulation for all of these comparisons can be found in Appendix E.

Although atmospheric pressure is rarely 760 mm Hg, most experiments are referenced to this pressure. No data was collected analyzing pressure effects since the boiling point temperatures will still need to be corrected and given at 760 mm Hg. However, in an experimental distillation, the pressure is dropped whenever the still temperature reaches a certain a value, usually between 500 and 600°F depending on the apparatus. A simulation was run that dropped the pressure whenever the vapor temperature reached 400°F or the still temperature reached 550°F. Pressures were dropped sequentially to 100, 10, 2, and finally 1 mm Hg. Distillation was discontinued if either of these temperatures was exceeded at 1 mm Hg.

As can be seen in Table VIII, the magnitude of the percent deviations between this method and the procedure of not correcting the temperatures was generally less than 1

TABLE VIII

TEMPERATURE CORRECTION DEVIATION ANALYSIS

		TEMPERATURE (F)		
RUN	PERCENT VOLUME	CALCULATED	CORRECTED	PERCENT DEVIATION
1	42.6	440	438	-0.455
2	53.1	520	520	0.000
3	63.3	597	594	-0.503
4	73.4	684	692	1.170
5	83.0	786	780	-0.763

TABLE IX

VARIABLE TRAYS DEVIATION ANALYSIS

		TEMPERATURE (F)				
RUN	PERCENT VOLUME	CALCULATED	TWO TRAYS	PERCENT DEVIATION	TWENTY TRAYS	PERCENT DEVIATION
1	1.81	89.10	97.02	8.899	89.01	-0.099
2	4.08	130.18	116.41	-10.581	130.12	-0.048
3	6.37	181.13	173.17	-4.395	182.40	0.700
4	8.65	215.50	209.86	-2.616	217.45	0.905
5	11.76	260.44	251.38	-3.482	261.84	0.537
6	14.18	292.45	282.18	-3.511	291.19	-0.433
7	16.46	322.93	309.97	-4.013	324.15	0.377
8	19.01	351.62	343.68	-2.258	353.56	0.549
9	22.14	395.59	376.81	-4.748	394.14	-0.367
10	24.44	421.74	409.97	-2.791	421.04	-0.167
11	26.61	464.61	449.28	-3.300	465.44	0.177
12	29.00	497.54	491.00	-1.315	500.22	0.539
13	31.39	526.53	517.53	-1.710	529.51	0.565
14	34.26	569.84	549.82	-3.513	567.52	-0.406
15	36.62	592.24	577.37	-2.511	591.03	-0.205
16	38.86	619.09	604.39	-2.373	618.31	-0.125
17	40.96	640.08	628.71	-1.776	641.80	0.269
18	43.46	673.40	657.63	-2.342	676.12	0.403
19	45.74	694.79	668.67	-3.760	698.41	0.522
20	48.04	725.72	709.22	-2.273	729.55	0.528
21	50.30	770.04	737.12	-4.276		
22	52.62	787.10	778.50	-1.092		

percent. Since temperatures generated in vacuum distillation have to be corrected to atmospheric pressure, it was decided to discontinue the practice of duplicating the physical situation exactly for this case. The model is not limited in its generation of temperatures, so there is no need to create extra work for the user in correcting temperatures, which must be computed using tables provided in ASTM D-2892 (ASTM II, 1987).

The effect of the number of trays on the results of the distillation is more pronounced than any other variable. The deviations are given in Table IX. Using a minimum of two trays reduces the efficiency of the distillation dramatically. The very first cut removes substantially less of the first fraction and so has a much higher temperature. All of the subsequent cuts are lower in temperature as more of the lighter components are found in these cuts. Deviations run from over 5°F to almost 35°F.

The percent deviations found in Table IX are generally less than 1/2 percent. However, analyzing the results given in Appendix E shows that stair stepping occurs at twenty stages. Twenty trays improves the efficiency of the distillation so much that stair stepping will occur. Ten trays were selected to avoid stair stepping while still ensuring efficient distillation. Because deviations are less than one percent, ten trays is just as effective as twenty without the undesirable side effect. Fewer trays will also reduce the computation time.

The effect of changing the reflux is not as dramatic. A very low reflux ratio (0.01:1) leads to deviations of up to 5°F as shown in Table X. A very high reflux ratio (50:1) shows very little change from a default reflux ratio of 5:1. Deviations are generally on the order of one-tenth of a degree in magnitude or less. Because deviations are less than one-half of a percent, a reflux ratio of 5:1 is as efficient as needed.

Finally, the effect of changing the removal rate was analyzed. Although the model does not take into account literal time, the removal rate is a parallel parameter. It was felt that 4 molar (1-2 volumetric) percent removal was the minimum required to accurately simulate the physical reality which often removes samples in 2 volumetric percent increments. Any lesser amount would be too efficient and would lead to stair stepping; it would also become too time intensive. The 4 molar percent withdrawal was left as a minimum value and the effects of increasing this rate were analyzed.

A removal rate of 15 molar percent was studied and the deviations between it and a 4 percent rate are shown in Table XI. This larger removal rate shows deviations from the calculated values of up to about 10°F. Also, as is shown in Appendix E, and as should be inherently obvious, the amount of material removed in each cut is much greater. The reduction in the total number of data points leads to a less accurate TBP diagram.

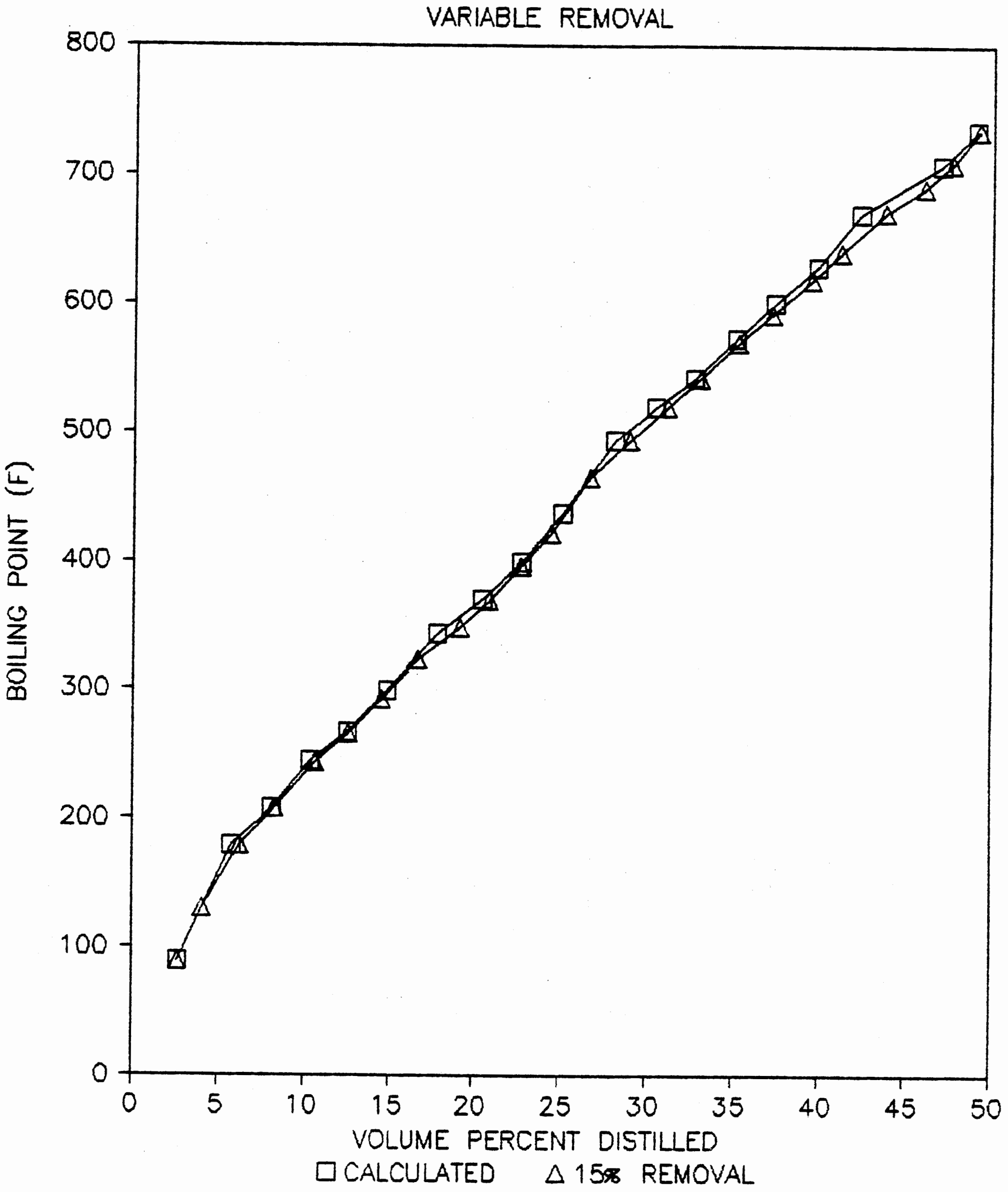


Figure 10. Variable Removal Rate TBP Analysis

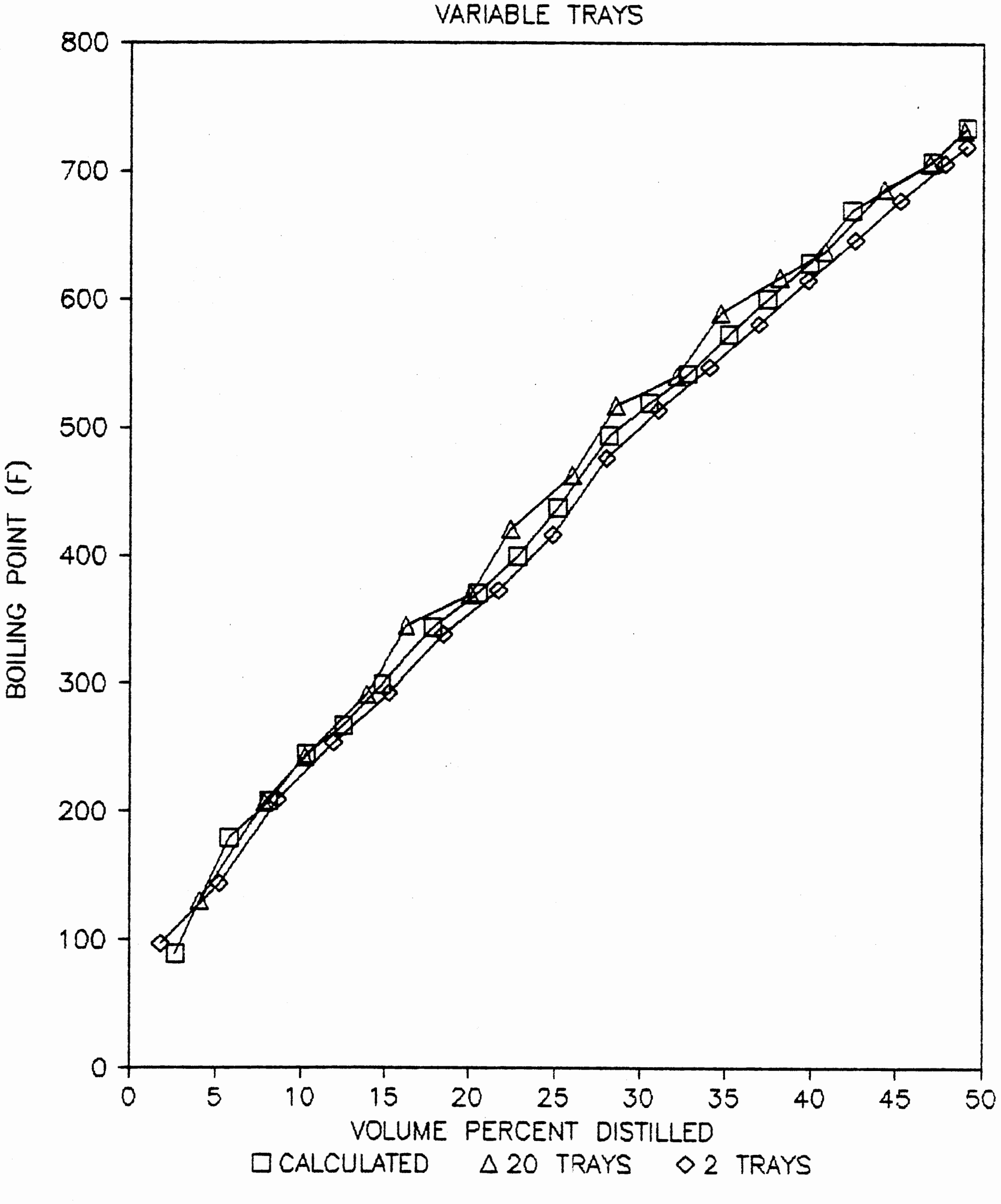


Figure 11. Variable Trays TBP Analysis

TABLE X

VARIABLE REFLUX DEVIATION ANALYSIS

		TEMPERATURE (F)				
RUN	PERCENT VOLUME	CALCULATED	0.01:1 REFLUX	PERCENT DEVIATION	50:1 REFLUX	PERCENT DEVIATION
1	1.81	89.10	89.15	0.064	89.10	0.007
2	4.08	130.18	130.22	0.028	130.18	-0.001
3	6.37	181.13	181.66	0.293	181.14	0.001
4	8.65	215.50	220.18	2.174	215.50	-0.001
5	11.76	260.44	259.74	-0.271	260.38	-0.023
6	14.18	292.45	289.84	-0.893	292.50	0.016
7	16.46	322.93	325.40	0.765	323.07	0.045
8	19.01	351.62	353.30	0.478	351.69	0.019
9	22.14	395.59	392.79	-0.708	395.61	0.006
10	24.44	421.74	421.63	-0.025	421.83	0.022
11	26.61	464.61	467.12	0.539	465.43	0.176
12	29.00	497.54	499.07	0.308	495.54	-0.401
13	31.39	526.53	527.79	0.240	526.52	-0.002
14	34.26	569.84	566.36	-0.610	569.84	0.000
15	36.62	592.24	590.53	-0.290	592.25	0.001
16	38.86	619.09	617.65	-0.232	619.10	0.002
17	40.96	640.08	643.09	0.471	640.09	0.001
18	43.46	673.40	674.93	0.227	673.40	0.000
19	45.74	694.79	695.84	0.152	694.79	0.000
20	48.04	725.72	725.32	-0.056	725.67	-0.006
21	50.30	770.04	766.40	-0.473	770.04	0.000
22	52.62	787.10	785.74	-0.172	787.10	0.000

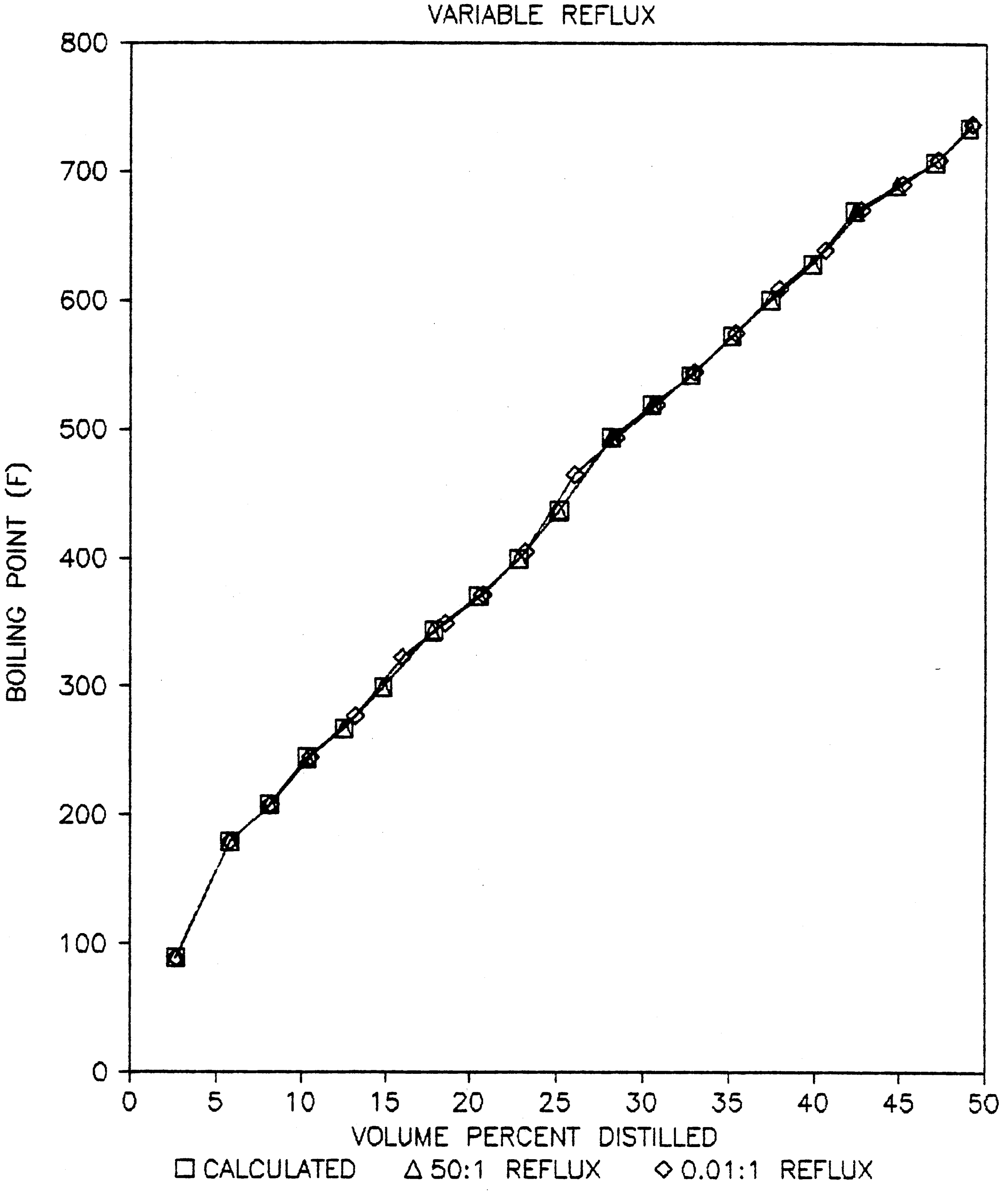


Figure 12. Variable Reflux Rate TBP Analysis

TABLE XI

VARIABLE REMOVAL RATE DEVIATION ANALYSIS

		TEMPERATURE (F)		
RUN	PERCENT VOLUME	CALCULATED	15 % REMOVAL	PERCENT DEVIATION
1	4.09	130.48	130.18	-0.235
2	8.24	209.72	207.68	-0.975
3	12.56	267.82	265.71	-0.786
4	16.76	327.35	323.31	-1.234
5	20.92	374.08	369.88	-1.122
6	24.52	423.54	421.71	-0.430
7	28.99	497.51	494.49	-0.608
8	31.19	524.89	519.21	-1.082
9	33.10	548.32	542.08	-1.138
10	37.26	598.91	592.43	-1.083
11	41.24	646.15	639.40	-1.044
12	46.03	697.66	690.04	-1.091
13	49.19	738.92	733.78	-0.695
14	52.96	787.17	787.12	-0.006

TABLE XII

MIDDLE EASTERN CRUDE ASTM DISTILLATION COMPARISON

		TEMPERATURE (F)		
RUN	PERCENT VOLUME	EXPERIMENTAL	CALCULATED	PERCENT DEVIATION
1	0	122	117.20	-3.934
2	5	178	149.78	-15.854
3	10	240	182.36	-24.017
4	20	370	230.66	-37.659
5	30	475	399.66	-15.861
6	40	545	535.88	-1.673
7	50	569	615.33	8.142

ASTM Distillation

An ASTM distillation is a very inefficient process. No cooling is provided to generate reflux and no contacting material is provided as surface area for contacting the vapor and liquid streams. The still is heated very rapidly and consequently many of the heavier components are vaporized and carried over more quickly than would normally be expected. Changing these variables in the simulation will allow an adequate representation of this type of distillation.

The simulation must be given an integer for the number of trays and this number must be greater than 1. Although this distillation probably has less than 2 theoretical stages, it will have to be modeled with 2 using the current solution procedure. Reflux cannot be set to zero and so is set to a very small number. The withdrawal rate is set to a high percentage, 10 percent or more, to duplicate the high heating rate in the laboratory process. Finally, an efficiency factor is applied to the withdrawal of each component. In this case, each component is multiplied by 0.5+I, where I is the number of the component. The amount of each component withdrawn is then normalized so that no more than was calculated will be withdrawn. The efficiency factor serves to increase the proportion of the heavier components in the distillate.

The results of this type of distillation on the Middle Eastern crude can be found in Appendix E. A temperature

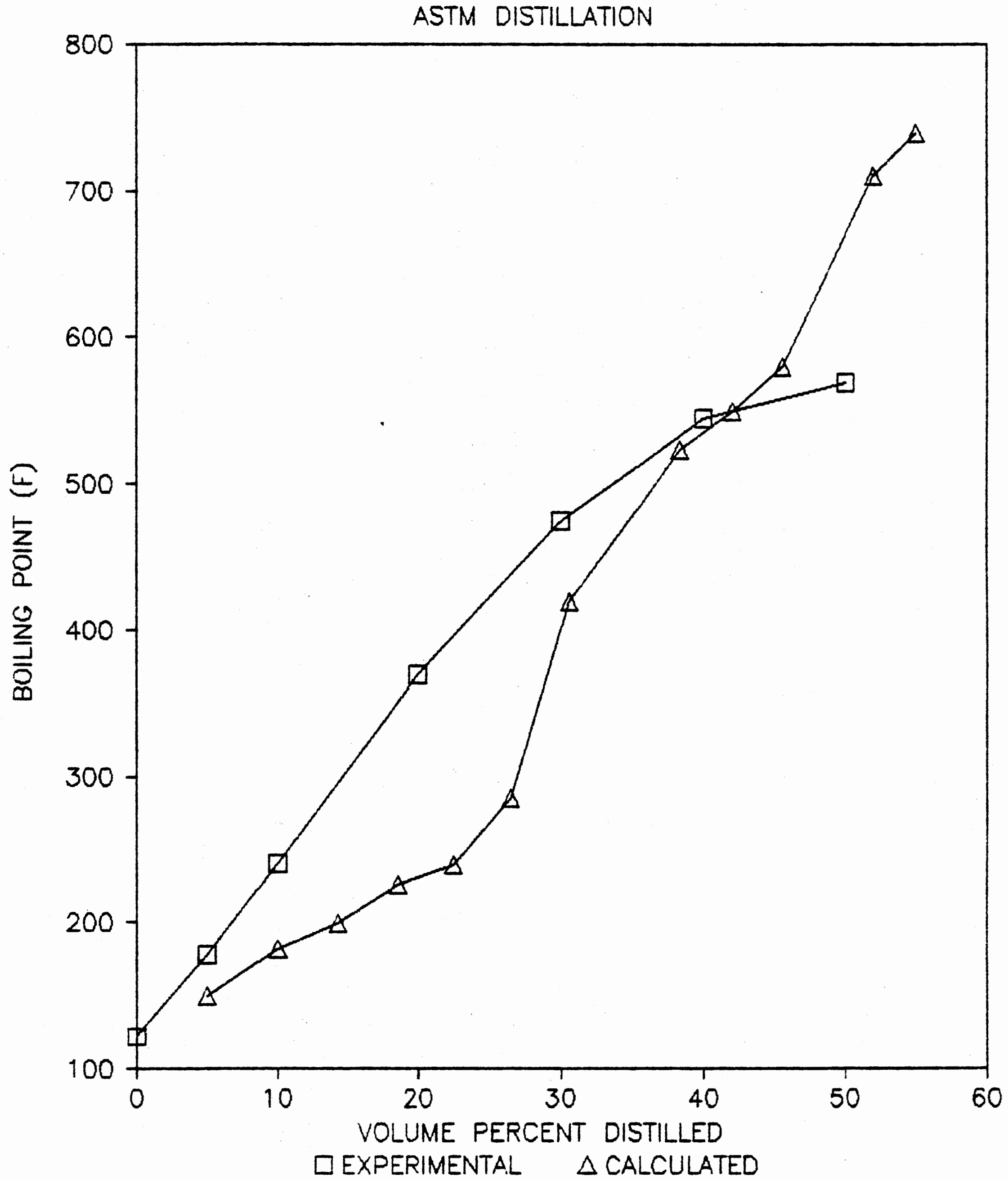


Figure 13. ASTM Distillation TBP Diagram

deviation comparison with this simulation and experimental data can be found in Table XII. As can be seen, replication is only adequate with an average deviation of 15 percent. This type of simulation generally starts with a rapid temperature rise, then a fairly level temperature follows through a certain volume percent distilled range, and finally there will be another rapid temperature rise. The results from this simulation reached the level temperature range sooner than the experimental data, which explains the large deviations in the 5-30 volume percent distilled range.

Conclusion

The simulation model analyzed in this chapter was found to be valid for the replication of batch distillation and especially for the generation of TBP diagrams. The default parameters chosen were also shown to be accurate. Comparisons with three sets of experimental data showed deviations of less than 10 percent in all cases. It was also shown that the distillation parameters can have a significant effect on the results. The default parameters should not be modified unless the actual apparatus and distillation process warrant the change.

CHAPTER V

CONCLUSION AND RECOMMENDATIONS

Conclusion

A batch distillation simulation has been developed to provide an interactive and user friendly means of simulating True Boiling Point experiments. A data base has been provided for numerous pure components, and algorithms have been included to enable the user to add other components or hypothetical fractions. The user can also specify most of the column operating conditions. The results will be furnished in the form of a table listing both the condenser and reboiler temperatures, the volume percentage of that cut and the total volume percent distilled.

The experimental requirements for operating parameters were checked to determine their validity in the model. In only one case, was one changed. The number of theoretical trays was lowered from 15 to 10. This change was made just to improve the results and to decrease the computation time.

The model was checked with three sets of experimental data. The simulation generation of data was, in all cases, within 10 percent of the experimental data. The model was found to be dependent on the characterization of the crude oil. The crude should be characterized accurately to enable a representative simulation. Also, defining as many fractions as possible increases the accuracy of the simulation.

The model was used to simulate a blending of crudes. Although there was not any experimental data to validate the TBP, a visual inspection led to the conclusion that the model is also very effective in simulating TBP data for crude blends.

Recommendations

Every model has its own peculiar liabilities and drawbacks and this simulation is no different. Several alternatives will be explored to improve the solution technique, to reduce the limitations of the model, and to increase the scope of the model.

It is recognized that Newman´s (1968) solution technique may not be the best possible technique. That solution was chosen for its generality and its ability to avoid diverging solutions. A technique such as Boston´s (1980) ´inside-out´ method may be more efficient. It may also be possible to rearrange the matrices to reduce storage and decrease computation time.

The current solution may be modified to reduce computation time by saving more of the data from a previous cut to speed convergence for the next cut. This was studied briefly, but an extensive study may produce dramatic results. It may also be more effective to describe the material and energy balances in terms of the variant, liquid holdup.

A study of the effects of startup during the preliminary total reflux phase of this process would also be interesting. The effects of gradually heating the column, filling the trays with liquid, and moving towards equilibrium could be studied. The model of this procedure would be truly transient. Even the equations containing holdup differentials would not be applicable to the startup procedures. New equations would have to be formulated to account for these new heating and tray filling effects.

Future improvements for this simulation include applying the model to other batch distillation applications. Any process that mixes two or more feed streams could use this model as a simulation tool. Optimization studies for the mixing of streams could also be conducted quickly and easily using this model.

Although this simulation has been developed and used on a VAX mainframe computer, it could also be used on a microcomputer with minimum effort. However, the computational time will be very extensive. It may be possible to improve the efficiency of the simulation so that its use on a microcomputer will be feasible.

REFERENCES

Amundson, Neal R. and Arlene J. Pontinen (1958). Multicomponent Distillation Calculations on a Large Digital Computer. Industrial and Engineering Chemistry, 50(5), 730-736.

API (1976). Technical Data Book--Petroleum Refining (Third Edition). Washington, D.C.: American Petroleum Institute.

ASTM D2892-84 (1987). Standard Test Method for Distillation of Crude Petroleum (15-Theoretical Plate Column). 1987 Annual Book of ASTM Standards, Petroleum Products, Lubricants and Fossil Fuels (II), 05.02, Philadelphia: American Society for the Testing of Materials, 679-682.

ASTM D86-82 (1987). Standard Method for Distillation of Petroleum Products. 1987 Annual Book of ASTM Standards, Petroleum Products, Lubricants and Fossil Fuels (I), 05.01, Philadelphia: American Society for the Testing of Materials, 8-13.

Boston, Joseph F. (1970). Ph.D. Dissertation. Tulane University, New Orleans, 28-40.

Boston, J.F., and S.L. Sullivan (1972). An Improved Algorithm for Solving the Mass Balance Equations in Multistage Separation Processes. The Canadian Journal of Chemical Engineering, 50, 663-668.

Boston, J.F. and S.L. Sullivan (1974). A New Class of Solution Methods for Multicomponent, Multistage Separation Processes. The Canadian Journal of Chemical Engineering, 52, 52-63.

Boston, J.F. and H.I. Britt (1978). A Radically Different Formulation and Solution of the Single-Stage Flash Problem. Computers and Chemical Engineering, 2, 109-122.

Boston, Joseph F. (1980). Inside-out Algorithms for Multicomponent Separation Process Calculations. Proceedings of Symposium on Computer Applications to Chemical Engineering Process Design and Simulation, American Chemical Society, 135-151.

Boston, J.F., H.I. Britt, S. Jirapongphan, and V.B. Shah (1984). An Advanced System for the Simulation of Batch Distillation Operations. Chemical Process Design, 203-237.

Carnahan, Brice, H.A. Luther, and J.O. Wilkes (1964). Applied Numerical Methods, New York: John Wiley and Sons.

Dean, John A., Editor (1985). Lange's Handbook of Chemistry (Thirteenth Edition). New York: McGraw Hill Book Company.

Denbigh, Kenneth (1955). The Principles of Chemical Equilibrium. New York: Cambridge University Press.

Distefano, G.P. (1968). Mathematical Modeling and Numerical Iteration of Multicomponent Batch Distillation Equations. AICHE Journal, 14(1), 190-199.

Dreisbach, Robert R. (1952). Pressure-Volume-Temperature Relationships of Organic Compounds (Third Edition). Sandusky, Ohio: Handbook Publishers, Inc.

Economopoulos, Alexander P. (1978). A Fast Computer Method for Distillation Calculations. Chemical Engineering, 85(8), 91-100.

Erbar, John H. (1974). GPA*K: Calculating Phase Equilibria for Hydrocarbon and Selected Non-hydrocarbon Systems. Tulsa, OK: Gas Processors Association.

Erbar, John H. (1983). Phillips' Fractionation Workshop. Bartlesville, OK: Phillips Petroleum Company.

Erbar, John H. (1987). MAXISIM: A Dual Purpose Complete Process Design Simulation System/Simple Equilibrium Calculation Program. Ruth C. Erbar, Editor, Stillwater, OK: SCI.

Felder, Richard M. and Ronald W. Rousseau (1978). Elementary Principles of Chemical Processes. New York: John Wiley and Sons.

Friday, John R. and Richard D. Smith (1964). An Analysis of the Equilibrium Stage Separations Problem--Formulation and Convergence. AICHE Journal, 10(5), 698-706.

Gallun, Steven E. and Charles D. Holland (1982). Gear's Procedure for the Simultaneous Solution of Differential and Algebraic Equations with Application to Unsteady-State Distillation Problems. Computers and Chemical Engineering, 6(3), 231-244.

Gear, C. William (1969). Computer Organization and Programming. New York: McGraw Hill Book Company.

Gear, C. William (1986). Computer Applications and Algorithms. Chicago: Science Research Associates, Inc.

Gentry, James W. (1970). Solution of Block-Band Matrices. Industrial Engineering Chemistry Fundamentals, 9(4), 671-673.

Gentry, James W. (August, 1970). An Improved Method for Numerical Solution of Distillation Processes. The Canadian Journal of Chemical Engineering, 48, 451-455.

Goldstein, Robert P. and Robert B. Stanfield (1970). Flexible Method for the Solution of Distillation Design Problems Using the Newton-Raphson Technique. Industrial Engineering Chemical Process Design and Development, 9(1), 78-84.

GPSA (1981). Engineering Data Book (Ninth Edition, Fifth Revision). Tulsa, OK: Gas Processors Suppliers Association.

Green, Don W. (1984). Perry's Chemical Engineers Handbook (Sixth Edition). New York: McGraw Hill Book Company.

Guy, John L. (1983). Modeling Batch Distillation in Multitray Columns. Chemical Engineering, 90(1), 99-103.

Holland, Charles D. (1966). Unsteady-State Processes with Applications in Multicomponent Distillation. Englewood Cliffs, NJ: Prentice-Hall, Inc., 229-243.

Holland, Charles D. (1981). Fundamentals of Multicomponent Distillation. New York: McGraw Hill Book Company.

Jordan, T. Earl (1954). Vapor Pressure of Organic Compounds. New York: Interscience Publishers, Inc.

Kuno, Minoru (1981). Enthalpy Method for Converging Distillation Calculations. Industrial and Engineering Chemical Process Design and Development, 23(3), 166-168.

Lockwood, J.A., R.L. LeTourneau, R. Matteson, and F. Sipos (1951). Modern Analytical Distillation of Crude Petroleum. Analytical Chemistry, 23(10), 1398-1404.

Maddox, Robert N. and John H. Erbar (1982). Gas Conditioning and Processing, Volume 3: Advanced Techniques and Applications. Norman, OK: Campbell

Petroleum Series.

Meadows, E.L. (1963). Multicomponent Batch Distillation on a Digital Computer. Chemical Engineering Progress Symposium Series Number 46, 59, Charles E. Huckaba and Gilbert Monet, Symposium Editors, New York: American Institute of Chemical Engineers, 48-55.

Michelsen, Michael L. (1976). An Efficient General Purpose Method for the Integration of Stiff Ordinary Differential Equations. AICHE Journal, 22(3), 594-597.

Newman, John (1963). Temperature Computed for Distillation. Hydrocarbon Processing and Petroleum Refiner, 42(4), 141-144.

Newman, John (1968) Numerical Solution of Coupled, Ordinary Differential Equations. Industrial and Engineering Chemistry Fundamentals, 7(13), 514-517.

Robinson, Clark S. and Edwin R. Gilliland (1950). Elements of Fractional Distillation. New York: McGraw Hill Book Company, 26-29.

Roche, E.C., Jr. (1987). Verification of the Scale-Up/Scale-down of Laboratory and Production Batch Distillation Columns. 1987 Summer Computer Simulation Conference.

Rooney, John M. (1984). Simulating Batch Distillation. Chemical Engineering, 91(10), 61-64.

Russell, R.A. (1980). Chemical Process Simulation--The GMB System. Computers and Chemical Engineering, 4, 167-190.

Russell, R.A. (1983). A Flexible and Reliable Method Solves Single-Tower and Crude Distillation Column Problems. Chemical Engineering, 90(21), 53-59.

Thomas, Philip J. (1981). Dynamic Simulation of Multicomponent Distillation Processes. Industrial Engineering Chemical Process Design and Development, 20 (1), 166-168.

Tomich, John F. (1970). A New Simulation Method for Equilibrium Stage Processes. AICHE Journal, 16(2), 229-232.

Van Wylen, Gordan J. and Richard E. Sonntag (1978). Fundamentals of Classical Thermodynamics. New York: John Wiley and Sons, 553.

Venit, Stewart and Wayne Bishop (1981). Elementary Linear

Algebra. Boston: Prindle, Weber, and Schmidt.

Wang, J.C., and G.E. Henke (1966). Tridiagonal Matrix for Distillation. *Hydrocarbon Processing*, *45*(8), 155-162.

Wei, Chiu-Han (1984). Dynamic Simulation of Multicomponent Distillation Columns: A Tool for Process Analysis, Control Design and Operator Training. *Proceedings of the 1984 Computer Simulation Conference*, The Society for Computer Simulation, 616-619.

APPENDIXES

APPENDIX A

SIMULATION CODE

```
C MAY 1, 1988
C     BATCH.FOR
C     BATCH DISTILLATION
C
C                 NOMENCLATURE
C
C  VARIABLES
C   AL1           ASSUMED LIQUID BOTTOMS RATE (AL1=0.0)
C   ALNS          ESTIMATED REFLUX RATE
C   API           DENSITY MEASUREMENT OF A COMPONENT
C   COF[A-E]      COEFFICIENTS USED IN DETERMININA A HYPO-
C                   THETICAL MOLECULAR WEIGHT
C   DETERM        MATRIX DETERMINATE
C   DLLIM         MAXIMUM CORRECTION FOR LIQUID FLOW
C   DTLIM         MAXIMUM CORRECTION FOR TRAY TEMPERATURE
C   DRAWT         TOTAL MOLES WITHDRAWN DURING DISTILLATION
C   EFF,EFFSTP    COMPONENT EFFICIENCY FACTOR,  EFF+EFFSTP*I
C   EQ            TEMPORARY STORAGE FOR K-VALUE AT TRAY JG
C   FLIQ          TOTAL LIQUID FLOW RATE OF FEED
C   FRAC          PERCENTAGE FACTOR FOR CRUDE BLENDING
C   FTOT          TOTAL FEED RATE
C   HF1           TOTAL FEED ENTHALPY
C   HL,HLU        TEMPORARY STORAGE FOR COMPONENT LIQUID ENTHALPY
C   HV,HVB        TEMPORARY STORAGE FOR COMPONENT VAPOR ENTHALPY
C   IFEZ          FEED PHASE (0,1)=(L,V)
C   ITERAT        ITERATION COUNTER
C   ITILE         STORAGE FOR TITLE OF RUN
C   JG            ITERATION COUNTER FOR STAGE NUMBER
C   NC            NUMBER OF COMPONENTS
C   NEGV          CHECK FOR NEGATIVE VAPOR FLOW
C   NMXCMP        MAXIMUM NUMBER OF COMPONENTS ALLOWED
C   NMXPRE        MAXIMUM NUMBER OF PURE COMPONENTS IN DATA BASE
C   NP1           NC+1
C   NP2           NC+2
C   NP2T          N-NOVAP IN BAND
C   NP3           NC+3
C   NP32          NC+3=NP3
C   NRUN          ITERATION COUNTER FOR WITHDRAWALS
C   NS            NUMBER OF STAGES
C   NSMAX         MAXIMUM NUMBER OF STAGES ALLOWED
C   NSM1          NS-1
C   N2P1          (2*NP3)+1
C   N2P31         (2*N)+1
C   MAXLIQ        TEMPORARY STORAGE FOR TRAY LIQUID FLOW RATE
C   PTOT          TOTAL SYSTEM PRESSURE
C   REFLUX        REFLUX RATIO TO COLUMN
C   SUMERR        MAXIMUM ALLOWABLE ERROR IN TRAY 1
C   TFEED         FEED TEMPERATURE
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C    TB             TEMPERATURE OF TRAY BELOW
C    TU             TEMPERATURE OF TRAY ABOVE
C    T1             ESTIMATED REBOILER TEMPERATURE
C    TNS            ESTIMATED CONDENSER TEMPERATURE
C    TTERM          MAXIMUM TEMPERATURE ALLOWED IN THE CONDENSER
C    VOLUME         TOTAL VOLUME PERCENTAGE WITHDRAWN
C    VTERM          MAXIMUM VOLUME PERCENTAGE WITHDRAWN ALLOWED
C    WDRAW          NUMBER OF MOLES WITHDRAWN DURING 1 ITERATION
C
C       ONE-DIMENSIONAL ARRAYS
C   VARIABLE    DIMENSION
C    AK,AA          NC        K-VALUE COMPUTATION VARIABLES
C    AH,AAH         NC        ENTHALPY COMPUTATION VARIABLES
C    AL             JG        ASSUMED LIQUID RATE
C    BK,BB          NC        K-VALUE COMPUTATION VARIABLES
C    BH,BBH         NC        ENTHALPY COMPUTATION VARIABLES
C    BP             NC        NORMAL BOILING POINT OF HYPOTHETICAL
C    CB,QQ          NC        TEMPORARY STORAGE FOR TRAY COMPOSITIONS
C    CK,CC          NC        K-VALUE COMPUTATION VARIABLES
C    CH,CCH         NC        ENTHALPY COMPUTATION VARIABLES
C    DH,DDH         NC        ENTHALPY COMPUTATION VARIABLES
C    DELTAH,DELH    NC        ENTHALPY COMPUTATION VARIABLES
C    DEQ            NC        TEMPORARY STORAGE FOR K-VALUE DERIVATIVE
C    DHB,DHJG       NC        TEMPORARY STORAGE FOR ENTHALPY
C                               DERIVATIVE
C    EH,EEH         NC        ENTHALPY COMPUTATION VARIABLES
C    EQ             NC        TEMPORARY STORAGE FOR K-VALUE
C    ERR            NSMAX     FUNCTION USED TO CALCULATE COMPOSITIONS
C    FEED           NC        STORAGE FOR MATERIAL LEFT TO BE
C                               DISTILLED
C    FH,FFH         NC        ENTHALPY COMPUTATION VARIABLES
C    FX             NC        FEED COMPONENT STORAGE
C    G              NC+3      TRAY FORCING STORAGE FUNCTION
C    GSG            NC        COMPONENT SPECIFIC GRAVITY
C    HVB            NC        TEMPORARY STORAGE FOR VAPOR ENTHALPY
C    HLU            NC        TEMPORARY STORAGE FOR LIQUID ENTHALPY
C    ID             NC        STORAGE VARIABLE FOR COMPONENT ID NUMBER
C    INN            K=1,3     PRODUCT OPTIONS
C                               INN(1)-FIXED BOTTOMS RATE
C                               INN(2)-FIXED OVERHEAD RATE
C                               INN(3)-NUMBER OF CONSTANT MOLAL
C                                        OVERFLOW ITERATIONS
C    SAVE           JG        TEMPORARY STORAGE FOR C(I,J)
C    SG,SPG         NC        SPECIFIC GRAVITY STORAGE
C    T              JG        TRAY TEMPERATURE
C    V              JG        TRAY VAPOR RATE
C    VOL            NC        COMPONENT VOLUME PERCENTAGE
C    WMOL,WMW       NC        MOLECULAR WEIGHT COMPUTATION VARIABLES
C
C       TWO-DIMENSIONAL ARRAYS
C   VARIABLE    DIMENSION
C    A           NC+3,NC+3      STORAGE FOR COMPOSITION ON TRAY
C                                 BELOW
C    B           NC+3,NC+3      STORAGE FOR COMPOSITION ON TRAY
```

```
C                                 IN QUESTION
C    C          NC+3,NC+3      TRAY MOLAR COMPOSITIONS
C    D          NC+3,(2*NC)+7  TRAY OBJECTIVE FUNCTION;MATRIX SOLN
C    EQDT       NC,NS          FUNCTION FOR K-VALUE DERIVATIVE
C    EQUIL      NC,NS          FUNCTION FOR K-VALUE
C    HHL        NC,NS          FUNCTION FOR LIQUID COMPONENT ENTHPY
C    HHV        NC,NS          FUNCTION FOR VAPOR COMPONENT ENTHLPY
C    Q          NC,NS          TEMP STORAGE FOR TRAY MOLAR COMPS
C    X          NC+3,NC+3      TRAY COMPOSTION STORAGE
C    Y          NC+3,NC+3      TRAY COMPOSTION STORAGE
C
C       THREE-DIMENSIONAL ARRAYS
C   VARIABLE    DIMENSION
C    E          NC+3,NC+4,NS   TRAY JACOBIAN STORAGE ARRAY
C
C   SUBROUTINES
C    BAND(J)                SETS UP MATRIX TO BE SOLVED
C    BUBBLE(J)              CALCULATES BUBBLE POINT
C    DEWPT(JG)              CALCULATES DEW POINT
C    KVALUE(I,T)            CALCULATES K-VALUES
C    NORM(FTOT)             NORMALIZES MOLAR COMPOSITIONS
C    SOLVER(K,L,DETERM)     SOLVES THE MATRIX
C    VENHDT(I,T)            CALCULATES VAPOR COMP ENTHALPIES
C    VENTH(I,T)             CALCULATES LIQUID COMP ENTH DERIVATIVES
C    VLNTH(I,T)             CALCULATES LIQUID COMP ENTHALPIES
C    VLNDT(I,T)             CALCULATES VAPOR COMP ENTH DERIVATIVES
C
C     COMMON DATA BLOCK
C
      BLOCK DATA DIST
      COMMON/VAR/AA(61),BB(61),CC(61),WMW(61)
      COMMON/VAR2/AAH(61),BBH(61),CCH(61)
      COMMON/VAR3/DDH(61),EEH(61),FFH(61),DELH(61),GSPG(61)
      COMMON/OPTION/INN(3)
C
C  JORDAN'S VAPOR PRESSURES OF ORGANIC COMPOUNDS
C    (LANGE'S FOR COMPONENTS 1,13-20,24-25,28-29,32,34-35,
C      46-51,56-58; AND CHEM PROCESSES FOR 61)
C          K=(LOG(A-(B/(T+C)))/PTOT
C
      DATA AA/5.82438,6.611847,6.80266,6.82973,6.74804,6.83029,
     1 6.80380,6.85221,6.73812,6.87773,6.90319,6.92374,6.93893,
     2 6.94365,6.97220,6.99795,7.00756,7.01300,7.02359,7.02867,
     3 7.0143,6.74756,6.81960,6.79290,6.88468,6.86952,6.84134,
     4 6.84999,6.84424,6.87540,6.90575,6.84637,6.82612,
     5 6.96659,6.85770,6.88673,6.86280,6.84498,6.82689,6.89745,
     6 6.95334,7.00289,7.00659,6.9909,6.95366,6.49457,7.28228,
     7 6.69422,9.81066,6.99392,6.69144,6.83907,6.84884,6.83712,
     8 6.8700,6.90187,5.7137,6.99383,6.86472,6.87041,8.10765/
C
      DATA BB/67.5078,389.93,656.40,813.20,882.80,945.90,1027.25,
     1 1064.63,950.84,1171.530,1268.586,1355.126,1431.82,1495.17,
     2 1569.57,1639.27,1690.67,1740.88,1789.95,1830.51,1865.1,
     3 585.00.785.00.908.80,967.32,960.80,923.20,930.546,1044.01,
```

```
     4 1069.466,1083.987,1039.69,1013.474,1124.33,1148.62,1124.162,
     5 1186.059,1203.526,1272.864,1206.350,1343.943,1477.519,
     6 1460.498,1453.840,1421.914,255.680,999.900,291.743,
     7 1347.786,768.130,319.013,1135.410,1152.368,1273.594,
     8 1315.503,1258.345,458.06,1014.117,1286.60,1384.036,1750.286/
C
      DATA CC/275.700,266.00,256.00,248.00,2*240.00,234.00,232.00,
     1 237.00,224.366,216.954,209.517,202.01,193.86,187.70,
     2 181.84,174.22,167.72,161.38,154.45,149.20,255.00,247.00,
     3 238.54,237.87,2*240.00,238.854,233.50,230.786,232.965,
     4 236.65,236.816,239.63,225.35,231.361,226.040,222.863,
     5 221.630,220.237,219.377,214.024,214.889,215.367,212.931,
     6 266.550,237.190,267.99,743.00,249.09,266.697,226.572,
     7 227.129,215.072,214.157,219.30,196.07,242.274,219.50,
     8 215.128,235.0/
C
C  LANGE'S HANDBOOK OF CHEMISTRY
C
      DATA WMW/2.016,16.04,30.07,44.10,58.12,58.12,3*72.15,
     1 86.18,100.21,114.23,128.26,142.29,156.31,170.34,184.37,
     2 198.40,212.42,226.45,240.41,28.05,42.08,4*56.10,54.09,
     3 6*70.14,84.16,70.13,2*84.16,98.19,78.11,92.14,4*106.17,
     4 28.01,32.00,28.01,44.01,34.08,64.07,4*86.18,98.90,
     5 40.06,54.09,98.18,112.22,18.02/
C
C  API:  TECHNICAL DATA BOOK--PETROLEUM REFINING
C            HL=A+(B*T)+(C*T**2)+(D*T**3)+(E*T**4)+(F*T**5)
C                HL[=]BTU/LB  T[=]RANKINE
C
      DATA AAH/12.32674,58.40160,163.05960,165.72380,162.08110,
     1 164.44400,169.01630,173.46090,145.60320,133.19390,
     2 134.12590,130.57280,126.71600,118.42310,156.57930,
     3 152.44400,151.999100,150.25060,148.84100,146.85880,
     4 144.59410,173.77850,193.22930,187.76640,210.45030,
     5 187.24240,179.26680,208.81850,175.27340,5*0.0,167.42860,
     6 229.11130,203.57300,209.80430,191.58840,225.05180,4*0.0,
     7 193.42630,-0.93401,-0.98176,-0.97557,4.77805,-0.61782,
     8 1.39433,152.96710,148.17180,166.76920,0.0,162.87650,
     9 229.26380,197.38100,196.95860,173.54180,-2.46342/
C    A,89*0.0/
C
      DATA BBH/3.199617,0.571700,0.264878,0.172601,0.046682,
     1 0.098571,-0.031504,-0.002795,0.004372,0.229107,0.182090,
     2 0.173084,0.169056,0.203347,-0.023843,-0.018522,-0.022933,
     3 -0.022048,-0.024114,-0.022825,-0.023563,0.144963,
     4 0.030810,-0.018519,-0.042795,0.037032,0.033009,-0.100603,
     5 -0.006874,5*0.0,-0.004262,-0.174553,-0.163500,-0.149848,
     6 -0.168390,-0.122662,4*0.0,-0.093633,0.255204,0.227486,
     7 0.256524,0.114433,0.238575,0.110263,0.041484,0.095013,
     8 -0.119500,0.0,-0.007807,0.033745,0.039560,-0.152454,
     9 -0.084958,0.457392/
C    A,89*0.0/
C
      DATA CCH/3.927862,-2.943122,-0.250140,0.940410,3.348013,
```

```
     1 2.691795,4.698836,4.400733,4.064654,-0.815691,0.347292,
     2 0.488101,0.581255,-0.349035,4.607729,4.538933,4.595173,
     3 4.580788,4.607172,4.590237,4.599069,1.710121,3.512242,
     4 4.263451,4.034318,3.551222,3.782637,5.651872,4.210531,
     5 5*0.0,4.196656,4.878999,5.315238,4.572747,5.444843,
     6 4.310824,4*0.0,4.390639,-0.177935,-0.373050,-0.229112,
     7 1.011325,-0.244571,0.330290,3.116936,1.605403,6.005360,
     8 0.0,4.259363,3.715168,3.479813,5.279018,4.278138,
     9 -0.525117/
C    A,89*0.0/
C
      DATA DDH/-2.934520,4.231568,2.923341,2.155433,0.144230,
     1 0.518202,-0.982825,-0.862875,-0.276464,4.527826,3.218786,
     2 3.054008,2.926114,4.070565,-0.998387,-0.964642,-0.997582,
     3 -0.9919639,-1.007675,-1.000209,-1.006645,0.761974,
     4 -0.494661,-0.940582,-0.684280,-0.560440,-0.733312,
     5 -2.123463,-0.908305,5*0.0,-0.882105,-0.790213,-1.239759,
     6 -0.387392,-1.126886,-1.138140,4*0.0,-1.126299,0.158913,
     7 0.483017,0.222803,-0.264936,0.410673,0.089125,0.622252,
     8 2.399189,-1.780500,0.0,-0.904956,-1.062607,-0.756071,
     9 -1.232110,-0.283095,0.645939/
C    A,89*0.0/
C
      DATA EEH/10.900690,-15.267400,-12.860530,-10.709860,
     1 -3.164196,-4.201390,1.029852,0.817644,-2.174529,
     2 -25.231790,-18.366030,-17.365470,-16.558500,-23.064410,
     3 1.084149,1.013931,1.083507,1.071259,1.104474,1.089122,
     4 1.10366,-4.503085,-0.226171,1.072240,0.134493,0.158471,
     5 0.697566,4.830541,1.003804,5*0.0,0.925317,-0.259001,
     6 1.465505,-1.791242,0.751131,1.494985,4*0.0,1.458215,
     7 -0.322032,-1.852433,-0.563256,0.347063,-1.301258,
     8 -0.773135,-6.385257,-16.146920,2.920860,0.0,0.959607,
     9 1.864623,0.840374,1.467753,-2.216911,-2.027592/
C    A,89*0.0/
C
      DATA FFH/-13.878670,19.452610,18.220570,15.927940,
     1 5.428928,6.560421,-0.294847,-0.197154,4.685030,
     2 47.480200,33.769380,31.248310,29.296090,42.968970,
     3 -0.331217,-0.296646,-0.330908,-0.325375,-0.341474,
     4 -0.333900,-0.340757,6.664928,1.125539,-0.349830,
     5 0.878860,0.444673,-0.174830,-4.738449,-0.315910,5*0.0,
     6 -0.270520,1.873384,-0.497681,3.793529,0.606023,
     7 -0.564766,4*0.0,-0.543200,0.158927,2.474881,0.455878,
     8 -0.131400,1.448520,1.292865,12.592750,32.727430,
     9 -1.344890,0.0,-0.284711,-1.435039,-0.265154,
     A -0.499779,4.555816,2.363096/
C    B,89*0.0/
C
C LANGE'S HANDBOOK OF CHEMISTRY
C     KCAL/GMOLE
C
      DATA DELH/0.216,1.953,3.517,4.487,2*5.352,3*6.160,
     1 6.896,7.575,8.225,8.820,9.388,9.920,10.430,10.910,
     2 11.380,11.820,12.240,12.640,3.237,4.400,5.238,0.0,5.580,
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     3 0.0,5.420,6.020,6.240,6.230,6.094,5.750,6.287,6.760,
     4 6.524,6.950,7.160,7.440,7.352,7.930,8.800,8.690,8.600,
     5 8.500,1.333,1.630,1.444,0.0,4.463,5.955,6.643,6.711,6.287,
     6 6.519,7.430,4.450,5.820,7.715,8.200,9.717/
C    A,89*0.0/
C
C  SPECIFIC GRAVITIES  60F/60F
C     BASE DENSITY   WATER = 62.365 lbm/ft3
C          GPSA DATABOOK FOR 1-14,23-29,36-53,55,58,61
C          LANGE'S HANDBOOK OF CHEM FOR 15-21,35,54,56
C
      DATA GSPG/0.07107,0.3,0.3583,0.5075,0.5630,0.5842,0.6244,
     10.6311,0.5966,0.6640,0.6883,0.7070,0.7219,0.7342,0.741,
     20.751,0.757,0.765,0.770,0.774,0.775,0.835,0.5217,0.6013,
     30.6271,0.6101,0.6005,0.6272,0.6457,5*0.0,0.673,0.7504,
     40.7536,0.7834,0.7740,0.8845,0.8719,0.8847,0.8688,0.8658,
     50.8717,0.8094,1.1421,0.7894,0.8176,0.7871,1.397,0.6579,
     60.6689,0.649,0.6664,0.697,0.0,0.658,2*0.0,1.000/
C
C  PRODUCT OPTIONS
C
      DATA INN/0,4,10/
      END
C
      COMMON/VAR/AA(61),BB(61),CC(61),WMW(61)
      COMMON/VAR2/AAH(61),BBH(61),CCH(61)
      COMMON/VAR3/DDH(61),EEH(61),FFH(61),DELH(61),GSPG(61)
      COMMON/OPTION/INN(3)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100),PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
      INTEGER NP1,NP2,NP3,N2P31,NP32,NSM1
      INTEGER ITERAT,ICHECK,NEGV
      INTEGER L1,LNS
      REAL HL,HV,HLU,HVB,MAXLIQ
C
      DIMENSION CB(100),EQ2(100),DEQ2(100)
      DIMENSION CB3(100),EQB3(100),DEQ3(100)
      DIMENSION HVB3(100),HLU3(100),DHB(100),DHJG(100)
      DIMENSION Q(100,50),QQ(50),VOL(50)
      DIMENSION T(50),FX(100),FEED(100)
      CHARACTER*50 ITILE
      CHARACTER*2 KSTAGE,IP,IT,KID,KRE,KFEED,KFDS,IRW,KTERM
      CHARACTER*2 KSTART,KRUN,ICOMB,KMORV,KOUT,KEFF,KLIM
C
      DATA NI,NO,NMAX,NSMAX,LIM/5,6,60,25,75/
      DATA TOL,SUMERR,FLIQ/2*0.01,0.0/
```

```
      DATA H2ODEN/62.365/
      DATA IFEZ,NMXPRE,NMXCMP,XFL/0,61,150,1/
      DATA NPROG,NDRAW,ICHECK,NEGV/4*0/
      DATA COFA,COFB/3.4660932,3.66593025E-8/
      DATA COFC,COFD/0.00000319803,0.010703069/
      DATA COFE/0.000510687/
C
      NMNHYP=NMXPRE+1
      WRITE (NO,1951)
 1951 FORMAT (10X,'*******************************************
     A*******',/,10X,'*',48X,'*',/,10X,'*         WELCOME TO
     B BATCH DISTILLATION          *',/,10X,'*   PLEASE BE SURE
     C YOU HAVE DEGASSED YOUR FEED   *',/,10X,'*     OR FLASH
     D YOUR FEED AT ROOM TEMPERATURE     *',/,10X,'*',48X,'*',
     E/,10X,'*',48X,'*',/,10X,'*******************************
     F*******************')
  502 CONTINUE
      WRITE (NO,1950)
 1950 FORMAT (///,5X,'ENTER THE TITLE : ')
      READ (NI,1070) ITILE
 1070 FORMAT (A50)
      WRITE (NO,1868)
 1868 FORMAT (/,5X,'WOULD YOU LIKE TO SEE THE RESULTS OF THE
     1 LAST RUN? (Y,N)')
      READ (NI,2868) KOUT
 2868 FORMAT (A2)
      IF(KOUT.NE.'Y') GO TO 1869
      OPEN (UNIT=11, FILE='OUTPUT2.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      READ (11,2892) NRNMAX
 2892 FORMAT (I3)
      CLOSE (UNIT=11, STATUS='KEEP')
      WRITE (NO,2080) ITILE
 2080 FORMAT (/,5X,A50)
      WRITE (NO,2985)
 2985 FORMAT (//,3X,'NRUN',5X,'TCOND',5X,'TREB',5X,'% VOL',5X
     1,'VOLUME',5X,'PTOT')
      OPEN (UNIT=10, FILE='OUTPUT1.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      DO 1870, I=1,NRNMAX
      READ (10,1871) NRUN,TCOND,T(1),PERVOL,VOLUME
 1871 FORMAT (I3,4(E12.5))
      WRITE (NO,2098) NRUN,TCOND,T(1),PERVOL,VOLUME,PTOT
 2098 FORMAT (3X,I3,2(2X,F8.3),3(1X,F9.4))
 1870 CONTINUE
 1872 CLOSE (UNIT=10, STATUS='KEEP')
 1869 HF1=0.0
      CHECK=0.0
      FRAC=100.0
      ITERAT=-1
      REFLUX=5.0
      WDRAW=0.04
      NS=10
      DRAWT=0.0
```

```
      PTOT=760.0
      T1=400.0
      TNS=100.0
      TFEED=70.0
      EFF=1.0
      EFFSTP=0.0
      KCOUNT=1
      VTERM=95.0
      TTERM=1250.0
      DTLIM=10.0
      DLLIM=0.4
      NRUN=0
      KOLD=KCOUNT
      NRUN1=0
      T1OLD=T1
      TNSOLD=TNS
      NC=0
      VOLUME=0.0
      NSTR=0
      NSTAR=0
 1111 NRUN=NRUN+1
      ITERAT=-1
      FLIQ=0.0
      DO 100, I=1,NSMAX
      T(I)=0.0
      V(I)=0.0
      AL(I)=0.0
      DO 100, J=1,NMAX
      SAVE(J,I)=0.0
      Q(J,I)=0.0
      DO 100, K=1,NMAX
      C(J,K)=0.0
      E(K,J,I)=0.0
  100 CONTINUE
C
      IF(NRUN.LE.1) GO TO 690
      FTOT=0.0
      DO 79, I=KCOUNT,NC
      FX(I)=FEED(I)
      FTOT=FTOT+FX(I)
   79 CONTINUE
      GO TO 5552
  690 OPEN (UNIT=10, FILE='OUTPUT1.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='NEW')
      IF(ICOMB.EQ.'Y') GO TO 9130
      WRITE (NO,9145)
 9145 FORMAT (/,5X,'IS THIS A RESTART')
      READ (NI,2945) KSTART
 2945 FORMAT (A2)
      FTOT=0.0
      IF(KSTART.NE.'Y') GO TO 8450
 9130 NCOLD=1
      NCNEW=0
      IF(ICOMB.NE.'Y') GO TO 9131
```

```
      WRITE (NO,9134)
 9134 FORMAT (/,5X,'HOW MANY FILES DO YOU WISH TO
     1 COMBINE?')
      READ (NI,*) NFLES
      DO 9133, J=1,NFLES
      WRITE (NO,9135) J
 9135 FORMAT (/,5X,'ENTER THE VOLUMETRIC PERCENTAGE OF
     1 FRACTION ',I1,/,5X,'IN THE TOTAL VOLUME')
      READ (NI,*) FRAC
 9131 WRITE (NO,9132)
 9132 FORMAT (/,5X,'ENTER THE FILE NUMBER (1, 2, 3, 4, 5, 6,
     A OR 7) '/,5X,'TO RETRIEVE THE DATA FILE FROM.',/,5X,
     B'FILE 7 IS ONLY FOR THE CRUDE BLEND FILE.')
      READ (NI,2132) INPUT
 2132 FORMAT (I2)
      IF(INPUT-2) 9115,9116,9117
 9115 KFL=1
      OPEN (UNIT=KFL, FILE='BATCH1.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      GO TO 9119
 9116 KFL=2
      OPEN (UNIT=KFL, FILE='BATCH2.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      GO TO 9119
 9117 IF(INPUT-4) 8000,9118,8001
 8000 KFL=3
      OPEN (UNIT=KFL, FILE='BATCH3.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      GO TO 9119
 9118 KFL=4
      OPEN (UNIT=KFL, FILE='BATCH4.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      GO TO 9119
 8001 IF(INPUT-6) 9120,8002,8005
 9120 KFL=7
      OPEN (UNIT=KFL, FILE='BATCH5.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      GO TO 9119
 8002 KFL=8
      OPEN (UNIT=KFL, FILE='BATCH6.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
      GO TO 9119
 8005 KFL=9
      OPEN (UNIT=KFL, FILE='BATCH7.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='OLD')
 9119 READ (KFL,1049) NC,NSTAR
 1049 FORMAT (2(I3))
      NCNEW=NCNEW+NC
      DO 1249, I=NCOLD,NCNEW
      READ (KFL,1149) ID(I),AK(I),BK(I),CK(I),GSG(I),WMOL(I),FX(I)
 1149 FORMAT (I3,6(E12.5))
      FX(I)=FX(I)*FRAC/100.0
 1249 CONTINUE
      NCOLD=NCOLD+NC
```

```
      CLOSE (UNIT=KFL, STATUS='KEEP')
      IF(ICOMB.NE.'Y') GO TO 8500
      NSTR=NSTR+NSTAR
 9133 CONTINUE
      NSTAR=NSTR
      OPEN (UNIT=9, FILE='BATCH7.DAT', FORM='FORMATTED',
     A ACCESS='SEQUENTIAL', STATUS='NEW')
      NC=NCNEW
      WRITE (9,9139) NC,NSTAR
 9139 FORMAT (2(I3))
      DO 9137, I=1,NC
      WRITE (9,9138) ID(I),AK(I),BK(I),CK(I),GSG(I),WMOL(I),FX(I)
 9138 FORMAT (I3,6(E12.5))
 9137 CONTINUE
      CLOSE (UNIT=9, STATUS='KEEP')
      GO TO 8500
C
C  READ IN PARAMETERS FOR PROBLEM.  IF THE PROGRAM IS STARTING
C     INITIALLY DO NOT OVERWRITE OLD FILES
C
 8450 IF(NPROG.NE.0) GO TO 8500
      WRITE (NO,8451)
 8451 FORMAT (/,5X,'ENTER THE NUMBER OF FILES YOU ARE
     1CURRENTLY SAVING'/,5X,'(ENTER A NUMBER 0-6)')
      READ (NI,*) NUMBER
      KFL=KFL+NUMBER
      IF(KFL.EQ.5) KFL=7
 8500 WRITE (NO,1)
    1 FORMAT (//,5X,'THE PROGRAM DEFAULTS TO 10 EQUILIBRIUM
     1 STAGES.',/,5X,'DO YOU WISH TO CHANGE THIS? (Y,N)')
      READ (NI,3011) KSTAGE
 3011 FORMAT (A2)
      IF(KSTAGE.NE.'Y') GO TO 3012
      WRITE (NO,2)
    2 FORMAT (/,5X,'ENTER THE NUMBER OF STAGES')
      READ (NI,*) NS
      IF(NS.LE.1.OR.NS.GT.45) NS=10
C
 3012 WRITE (NO,3)
    3 FORMAT (//,5X,'THE DEFAULT PRESSURE IS 760 mm Hg.'
     A,/,5X,'DO YOU WISH TO CHANGE THIS PRESSURE? (Y,N)')
      READ (NI,1014) IP
 1014 FORMAT (A2)
      IF(IP.NE.'Y') GO TO 1012
      WRITE (NO,1013)
 1013 FORMAT (5X,'ENTER THE SYSTEM PRESSURE')
      READ (NI,*) PTOT
C
 1012 WRITE (NO,2300)
 2300 FORMAT (//,5X,'THE PROGRAM DEFAULTS TO 400 F FOR THE
     1 REBOILER,',/,5X,'100 F FOR THE CONDENSER, AND 70 F FOR
     2 THE',/,5X,'FEED TEMPERATURE.',/,5X,'DO
     2 YOU WISH TO CHANGE THESE? (Y,N)')
      READ (NI,1015) IT
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```
 1015 FORMAT (A2)
      IF(IT.NE.'Y') GO TO 1016
      WRITE (NO,2333)
 2333 FORMAT (/,5X,'ENTER REBOILER TEMPERATURE ESTIMATE (F)')
      READ (NI,*) T1
      WRITE (NO,2330)
 2330 FORMAT (/,5X,'ENTER CONDENSER TEMPERATURE ESTIMATE (F)')
      READ (NI,*) TNS
      IF(T1.LT.0.0.OR.T1.GT.550.0) T1=400.0
      IF(TNS.LT.32.0.OR.TNS.GT.400.0) TNS=100.0
      WRITE (NO,2400)
 2400 FORMAT (/,5X,'ENTER LIQUID FEED TEMPERATURE (F): ')
      READ (NI,*) TFEED
C
 1016 IF(ICOMB.EQ.'Y'.OR.KSTART.EQ.'Y') GO TO 1175
      NSTAR=0
      NB=0
      WRITE (NO,611)
  611 FORMAT (///,5X,'ID NUMBERS 62-150 ARE RESERVED FOR HYPO
     1THETICALS')
 1036 DO 5, J=1,NMAX
      NB=NB+1
      WRITE (NO,6) J
    6 FORMAT (/,5X,'ENTER ID NUMBER FOR COMP ',I2)
      READ (NI,7) ID(J)
    7 FORMAT (I3)
      IF(ID(J).GT.NMXPRE.AND.ID(J).LE.NMXCMP) NSTAR=NSTAR+1
      IF(ID(J).LT.1.OR.ID(J).GT.NMXCMP) GO TO 88
    5 CONTINUE
   88 NC=NB-1
      WRITE (NO,1031)
 1031 FORMAT (5X,'YOU HAVE ENTERED THE FOLLOWING COMPONENTS')
      DO 1032, I=1,NC
      WRITE (NO,1033) I,ID(I)
 1033 FORMAT (5X,I3,3X,I3)
 1032 CONTINUE
      WRITE (NO,1034)
 1034 FORMAT (/,5X,'DO YOU WISH TO CHANGE ANY? (Y,N)')
      READ (NI,1035) KID
 1035 FORMAT (A2)
      IF(KID.EQ.'Y') GO TO 1036
      IF(NSTAR.EQ.0) GO TO 1045
      WRITE (NO,1046)
 1046 FORMAT (/,5X,'FOR THE FOLLOWING HYPOTHETICALS YOU WILL
     1 NEED TO ENTER',/,5X,'THE NORMAL BOILING POINT, THE MOL
     2ECULAR WEIGHT,',/,5X,'AND THE SPECIFIC GRAVITY',/,
     35X,'IF YOU DO NOT KNOW THE VALUE OF THE MOLECULAR
     4 WEIGHT,'/,5X,'ENTER A -9 AND THE PROGRAM WILL
     5 CALCULATE IT'/)
      KBOP=NC-NSTAR
      DO 1045, J=1,NSTAR
      KCAN=KBOP+J
 1166 WRITE (NO,704) J
  704 FORMAT (5X,'ENTER THE NORMAL BOILING POINT, THE MOLECU
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```
     1LAR WEIGHT,',/,5X,'AND THE SPECIFIC GRAVITY FOR FRACTION '
     2,I2)
      READ (NI,*) BP(KCAN),WMOL(KCAN),GSG(KCAN)
C   ANTOINE'S COEFFICIENTS AND CALCULATIONS ARE FROM R. R.
C      DREISBACH, 'PVT RELATIONSHIPS OF ORGANIC COMPOUNDS'
C        (1952)
      IF(BP(KCAN).GT.356.0) GO TO 702
      BK(KCAN)=2.3025851*(1313.01+4.27937*BP(KCAN)+0.002649*
     1BP(KCAN)**2.0)
      GO TO 703
  702 BK(KCAN)=2.3025851*(1653.16+3.1744*BP(KCAN)+0.0042493*
     1BP(KCAN)**2.0)
  703 CK(KCAN)=382.0
      AK(KCAN)=2.687572+BK(KCAN)/(CK(KCAN)+BP(KCAN))
      API=141.5/GSG(KCAN)-131.5
      IF(WMOL(KCAN).LE.0.0) WMOL(KCAN)=EXP(COFA+COFB*BP(KCAN)
     1**2.0+COFC*API*BP(KCAN)+COFD*API+COFE*API**2.0)
      WRITE (NO,777) BP(KCAN),WMOL(KCAN),GSG(KCAN),
     1AK(KCAN),BK(KCAN),CK(KCAN)
  777 FORMAT (/,5X,'YOU HAVE ENTERED THE FOLLOWING PARAMETERS:',
     1/,7X,'NORMAL BOILING POINT = ',F12.4,/,7X,'MOLECULAR
     2 WEIGHT     = ',F12.4,/,7X,'SPECIFIC GRAVITY     = ',F12.4,/
     3,5X,'AND YOU HAVE CALCULATED THESE ANTIONE COEFFICIENTS A,
     4 B, & C:'/,4X,3(2X,F16.4))
      WRITE (NO,1164)
 1164 FORMAT (/,5X,'DO YOU WANT TO RE-ENTER THE DATA'/5X,'FOR
     1 THIS FRACTION ? (Y,N)')
      READ (NI,1165) KRE
 1165 FORMAT (A2)
      IF(KRE.EQ.'Y') GO TO 1166
 1045 CONTINUE
 1063 WRITE (NO,1051)
 1051 FORMAT (/,5X,'WOULD YOU LIKE TO ENTER THE FEED IN MOLES
     1 (M)'/5X,'OR AS A VOLUME PERCENT (V)')
      READ (NI,2051) KMORV
 2051 FORMAT (A2)
      FTOT=0.0
      DO 1054, I=1,NC
      WRITE (NO,1052) I
 1052 FORMAT (/,5X,'ENTER THE FEED FOR COMP ',I2)
      READ (NI,*) FX(I)
 1054 CONTINUE
 1175 IF(KMORV.NE.'V') GO TO 1275
      WRITE (NO,1155)
 1155 FORMAT (/,5X,'YOU HAVE ENTERED THE FOLLOWING FEEDS',
     1/,13X,'ID',8X,'VOL %')
      GO TO 1156
 1275 WRITE (NO,1055)
 1055 FORMAT (/,5X,'YOU HAVE ENTERED THE FOLLOWING FEEDS',
     1/,13X,'ID',8X,'MOLES')
 1156 FTOT=0.0
      DO 1056, I=1,NC
      WRITE (NO,1057) I,ID(I),FX(I)
 1057 FORMAT (5X,I2,5X,I3,5X,F10.4)
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      FTOT=FTOT+FX(I)
 1056 CONTINUE
      IF(KMORV.NE.'V') GO TO 1157
      WRITE (NO,1158) FTOT
 1158 FORMAT (/,5X,'THE TOTAL FEED IS ',F10.4,1X,'VOL %')
      GO TO 1159
 1157 WRITE (NO,1064) FTOT
 1064 FORMAT (/,5X,'THE TOTAL FEED IS ',F10.4,1X,'MOLES')
 1159 WRITE (NO,1058)
 1058 FORMAT (/,5X,'DO YOU WISH TO CHANGE THESE? (Y,N)')
      READ (NI,1059) KFEED
 1059 FORMAT (A2)
      IF (KFEED.NE.'Y') GO TO 1167
      WRITE (NO,1168)
 1168 FORMAT (/,5X,'DO YOU WANT TO CHANGE ALL FEEDS? (Y,N)')
      READ (NI,1169) KFDS
 1169 FORMAT (A2)
      IF(KFDS.EQ.'Y') GO TO 1063
      WRITE (NO,1170)
 1170 FORMAT (/,5X,'HOW MANY FEEDS DO YOU WANT TO CHANGE?')
      READ (NI,*) KFI
      DO 1172, I=1,KFI
      WRITE (NO,1173)
 1173 FORMAT (5X'ENTER THE ID NUMBER OF THE COMPONENT YOU
     1 WISH TO CHANGE.')
      READ (NI,*) KCFD
      WRITE (NO,1183)
 1183 FORMAT (5X,'ENTER THE NEW FEED RATE')
      READ (NI,*) CFEED
      DO 1176, J=1,NC
      IF(KCFD.EQ.(ID(J))) FX(J)=CFEED
 1176 CONTINUE
 1172 CONTINUE
      GO TO 1175
C
 1167 WRITE (NO,1017)
 1017 FORMAT (//,5X,'THE DEFAULT FOR REFLUX IS 5:1 AND 4%
     1 FOR WITHDRAWAL.',/,5X,'DO YOU WISH TO CHANGE THESE
     2 (Y,N)')
      READ (NI,1018) IRW
 1018 FORMAT (A2)
      IF(IRW.NE.'Y') GO TO 1021
      WRITE(NO,2200)
 2200 FORMAT (/,5X,'ENTER ESTIMATED REFLUX RATE')
      READ (NI,*) REFLUX
      IF(REFLUX.LE.(0.0).OR.REFLUX.GT.(20.0)) REFLUX=5.0
      WRITE (NO,2222)
 2222 FORMAT (/,5X,'ENTER THE WITHDRAWAL RATE')
      READ (NI,*) WDRAW
 1021 WRITE (NO,3031)
 3031 FORMAT (/,5X,'THE PROGRAM DEFAULTS TO AN EFFICIENCY FAC
     1TOR'/,5X,'APPLIED TO EACH COMPONENT OF A+B*I',/,5X,'WHERE
     2 A AND B ARE 1.0 AND 0.0 AND I IS',/,5X,'THE NUMBER OF THE
     3 COMPONENT'/,5X,'DO YOU WANT TO CHANGE A AND B? (Y,N)')
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```
      READ (NI,3032) IEFF
 3032 FORMAT (A3)
      IF(IEFF.NE.'Y') GO TO 3033
      WRITE (NO,3034)
 3034 FORMAT (/,5X,'ENTER THE NEW VALUES FOR A AND B')
      READ (NI,*) EFF,EFFSTP
 3033 WRITE (NO,3036)
 3036 FORMAT (/,5X,'THE PROGRAM LIMITS THE TEMPERATURE AND
     1 LIQUID FLOW RATE'/,5X,'CORRECTIONS TO 10 F AND 40
     2 PERCENT RESPECTIVELY'/,5X,'DO YOU WANT TO CHANGE
     3 THESE?  (Y,N)')
      READ (NI,3037) KLIM
 3037 FORMAT (A3)
      IF(KLIM.NE.'Y') GO TO 3038
      WRITE (NO,3039)
 3039 FORMAT (/,5X,'ENTER THE TEMPERATURE CORRECTION IN F.')
      READ (NI,*) DTLIM
      WRITE (NO,3042)
 3042 FORMAT (/,5X,'ENTER THE LIQUID FLOW CORRECTION AS A
     1 PERCENTAGE.')
      READ (NI,*) DLLIM
 3038 WRITE (NO,1022)
 1022 FORMAT (5X,'THE PROGRAM WILL TERMINATE AT 95 VOL%
     1 DISTILLED',/,5X,'OR AT A CONDENSER TEMPERATURE OF
     2 1250 F.',/,5X,'DO YOU WANT TO CHANGE THESE? (Y,N)')
      READ (NI,1023) KTERM
 1023 FORMAT (A2)
      IF(KTERM.NE.'Y') GO TO 9851
      WRITE (NO,1024)
 1024 FORMAT (5X,'ENTER THE VOL% TERMINATION')
      READ (NI,*) VTERM
      WRITE (NO,1026)
 1026 FORMAT (5X,'ENTER THE TEMPERATURE TERMINATION')
      READ (NI,*) TTERM
 9851 WRITE (NO,1080) ITILE
 1080 FORMAT (/,5X,A50)
      WRITE (NO,985)
  985 FORMAT (///,3X,'NRUN',5X,'TCOND',5X,'TREB',5X,'% VOL',5X
     1,'VOLUME',5X,'PTOT')
C
      JSTAR=NC-NSTAR
      NP1=NC+1
      NP2=NP1+1
      NP3=NP2+1
      N2P31=2*NP3+1
      NP32=NP3
      NSM1=NS-1
C
C  SET UP DATA ARRAY TO BE ACCESSED FOR THIS PROBLEM
C
 1019 TVOL=0.0
      DO 112, I=KCOUNT,NC
      K=0
      K=ID(I)
```

```
      IF(K.GT.NMXPRE) GO TO 1129
      AK(I)=AA(K)
      BK(I)=BB(K)
      CK(I)=CC(K)
      WMOL(I)=WMW(K)
      AH(I)=AAH(K)
      BH(I)=BBH(K)
      CH(I)=CCH(K)
      DH(I)=DDH(K)
      EH(I)=EEH(K)
      FH(I)=FFH(K)
      DLTH(I)=DELH(K)
      GSG(I)=GSPG(K)
 1129 IF(KMORV.EQ.'V') FX(I)=FX(I)*GSG(I)*H2ODEN/WMOL(I)
      TVOL=TVOL+FX(I)*WMOL(I)/(GSG(I)*H2ODEN)
  112 CONTINUE
      IF(KFL.EQ.1) OPEN (UNIT=KFL, FILE='BATCH1.DAT', FORM=
     1'FORMATTED', ACCESS='SEQUENTIAL', STATUS='NEW')
      IF(KFL.EQ.2) OPEN (UNIT=KFL, FILE='BATCH2.DAT', FORM=
     1'FORMATTED', ACCESS='SEQUENTIAL', STATUS='NEW')
      IF(KFL.EQ.3) OPEN (UNIT=KFL, FILE='BATCH3.DAT', FORM=
     1'FORMATTED', ACCESS='SEQUENTIAL', STATUS='NEW')
      IF(KFL.EQ.4) OPEN (UNIT=KFL, FILE='BATCH4.DAT', FORM=
     1'FORMATTED', ACCESS='SEQUENTIAL', STATUS='NEW')
      IF(KFL.EQ.7) OPEN (UNIT=KFL, FILE='BATCH5.DAT', FORM=
     1'FORMATTED', ACCESS='SEQUENTIAL', STATUS='NEW')
      IF(KFL.EQ.8) OPEN (UNIT=KFL, FILE='BATCH6.DAT', FORM=
     1'FORMATTED', ACCESS='SEQUENTIAL', STATUS='NEW')
      WRITE (KFL,1567) NC,NSTAR
 1567 FORMAT (2(I3))
      DO 1767, I=1,NC
      WRITE (KFL,1667) ID(I),AK(I),BK(I),CK(I),GSG(I),WMOL(I),FX(I)
 1667 FORMAT (I3,6(E12.5))
 1767 CONTINUE
      CLOSE (UNIT=KFL, STATUS='KEEP')
C
      LAST=NS+1
      DO 555, I=1,NC
      CALL VLNTH(I,TFEED)
      HF1=HF1+FX(I)*HHL(I,TFEED)
  555 CONTINUE
 5552 FLIQ=FLIQ+FTOT
C
C  PRINT INITIAL CONDITIONS
C
C
C GENERATE INITIAL PROFILES
C
  344 ENS=FLOAT(NS*(NS+1))/2.0
      TBMTD=(TNS-T1)/FLOAT(NS-1)
      ELBMR=FLIQ/ENS
      ALNS=REFLUX*WDRAW*FTOT
      AL1=WDRAW*FTOT
      DO 444, JA=1,NS
```

```
      IF(JA.EQ.1) GO TO 445
      IF(JA.EQ.NS) GO TO 446
      T(JA)=T1+TBMTD*FLOAT(JA-1)
      AL(JA)=ALNS+ELBMR*FLOAT(NS-JA)
      GO TO 444
  445 T(JA)=T1
      AL(JA)=AL1
      GO TO 444
  446 T(JA)=TNS
      AL(JA)=ALNS
  444 CONTINUE
      IF(ITERAT.GE.1) GO TO 3440
C
C BEGIN ITERATIONS
C
      IF(ICHECK.GE.1000) GO TO 1111
 9999 CONTINUE
   12 ITERAT=ITERAT+1
      VNS=WDRAW*FTOT
      DO 1280, J=1,NS
      V(J)=0.0
 1280 CONTINUE
C
C CALCULATE ASSUMED VAPOR RATES
C
      NEGV=0
      V(1)=AL(2)-AL(1)
      IF(V(1).GT.0.0) GO TO 11
      V(1)=1.0
      NEGV=1
   11 DO 10, JB=2,NSM1
      V(JB)=AL(JB+1)+V(JB-1)-AL(JB)
      IF((V(JB)).LE.CHECK) V(JB)=V(JB-1)
   10 CONTINUE
      V(NS)=VNS
      IF(NEGV.EQ.1) V(1)=V(2)
C
C CALCULATE ASSUMED LIQUID COMPOSITIONS
C
      DO 170, J=1,NS
      ERR(J)=0.0
      DO 175, I=KCOUNT,NC
      EQUIL(I,T(J))=0.0
      EQDT(I,T(J))=0.0
      Q(I,J)=0.0
  175 CONTINUE
  170 CONTINUE
      DO 17, IA=KCOUNT,NC
      PCE2=0.0
      PIECE1=0.0
      PIECE3=0.0
      DENOM=0.0
      EQB=0.0
      ERB=0.0
```

```
      PCE1B=0.0
      CALL KVALUE(IA,T(1))
      PCE1B=V(1)*EQUIL(IA,T(1))
      DENOM=AL(1)+PCE1B
      ERR(1)=1.0/DENOM
      Q(IA,1)=FX(IA)*ERR(1)
      EQB=EQUIL(IA,T(1))
      ERB=ERR(1)
      DO 16, JC=2,NS
      CALL KVALUE(IA,T(JC))
      PIECE1=V(JC)*EQUIL(IA,T(JC))
      PCE2=PCE1B*AL(JC)
      DENOM=AL(JC)+PIECE1-(ERB*PCE2)
      ERR(JC)=1.0/DENOM
      Q(IA,JC)=V(JC-1)*EQB*Q(IA,JC-1)*ERR(JC)
      EQB=EQUIL(IA,T(JC))
      ERB=ERR(JC)
      PCE1B=PIECE1
   16 CONTINUE
C
      DO 15, JD=1,NSM1
      JE=NS-JD
      PIECE3=ERR(JE)*Q(IA,JE+1)*AL(JE+1)
      Q(IA,JE)=Q(IA,JE)+PIECE3
   15 CONTINUE
      DO 1511, JE=1,NS
      IF((Q(IA,JE)).LT.CHECK) Q(IA,JE)=ABS(Q(IA,JE))
 1511 CONTINUE
   17 CONTINUE
C
C NORMALIZE THE ASSUMED COMPOSITIONS
C
      DO 1964, I=1,NC
      DO 1965, J=1,NP3
      C(I,J)=0.0
 1965 CONTINUE
 1964 CONTINUE
      DO 19, JF=1,NS
      SUMX=0.0
      DO 18, IB=KCOUNT,NC
      SUMX=SUMX+Q(IB,JF)
   18 CONTINUE
      IF(SUMX.EQ.CHECK) GO TO 19
      DO 13, IC=KCOUNT,NC
      C(IC,JF)=Q(IC,JF)/SUMX
   13 CONTINUE
   19 CONTINUE
      IF(ITERAT.GT.LIM) GO TO 220
      L1=1
      CALL BUBBLE(L1,T(1))
      T1=1.15*T(1)
      LNS=NS
      CALL BUBBLE(LNS,T(NS))
      TNS=T(NS)
```

```
 3441 IF(ITERAT.LE.1) GO TO 344
C
C CHECK FOR NON-CONVERGENCE
C
 3440 DO 21, IC=KCOUNT,NC
C     DO 21, JCC=1,NS
      IF(ABS(C(IC,NS)-SAVE(IC,NS)).GT.SUMERR) GO TO 27
C     IF(ABS(C(IC,JCC)-SAVE(IC,JCC)).GT.SUMERR) GO TO 27
   21 CONTINUE
      NEGV=1
C
C MESSAGES CONCERNING CONVERGENCE
C
  220 IF(NEGV.GT.0) GO TO 221
      WRITE (NO,3500)
 3500 FORMAT (/,2X,'THIS IS NOT A CONVERGED SOLUTION')
      GO TO 1201
C 221 WRITE (NO,3600)
C3600 FORMAT (/,2X,'THIS IS A CONVERGED SOLUTION')
  221 CTOT=0.0
      VOLT=0.0
      DO 99, I=KCOUNT,NC
      EQUIL(I,T(NS))=0.0
      QQ(I)=0.0
      CALL KVALUE(I,T(NS))
      EQUIL(I,T(NS))=(EFF+EFFSTP*I)*EQUIL(I,T(NS))
      QQ(I)=C(I,NS)
      C(I,NS)=C(I,NS)*EQUIL(I,T(NS))
      CTOT=CTOT+C(I,NS)
   99 CONTINUE
      IF(CTOT.LE.0.0) GO TO 970
      DO 970, I=KCOUNT,NC
      C(I,NS)=C(I,NS)/CTOT
  970 CONTINUE
      DO 97, I=KCOUNT,NC
      VOL(I)=0.0
      DRAW=V(NS)*C(I,NS)
      IF((FX(I)).LT.DRAW) DRAW=FX(I)
      VOL(I)=DRAW*WMOL(I)/(GSG(I)*H2ODEN)
      VOLT=VOLT+VOL(I)
      FEED(I)=FX(I)-DRAW
      IF((FEED(I)).LE.0.0) KCOUNT=KCOUNT+1
      IF(KCOUNT.GT.NC) GO TO 1201
      DRAWT=DRAWT+DRAW
   97 CONTINUE
      PERVOL=(VOLT/TVOL)*100.0
      VOLUME=VOLUME+PERVOL
      IF(VOLUME.GT.VTERM) GO TO 1201
      TCOND=T(NS)
      LLNS=NS
      CALL BUBBLE(LLNS,TCOND)
      IF(TCOND.LE.40.0) GO TO 9751
      IF(TCOND.GT.TTERM) GO TO 1201
 9751 DO 975, I=KCOUNT,NC
```

```
      IF((FEED(I)).GT.0.0) GO TO 9750
      C(I,NS)=0.0
      GO TO 975
 9750 C(I,NS)=0.0
      C(I,NS)=QQ(I)
  975 CONTINUE
      WRITE (NO,98) NRUN,TCOND,T(1),PERVOL,VOLUME,PTOT
   98 FORMAT (3X,I3,2(2X,F8.3),3(1X,F9.4))
      WRITE (10,1867) NRUN,TCOND,T(1),PERVOL,VOLUME
 1867 FORMAT (I3,4(E12.5))
      GO TO 1202
C
   27 DO 28, IF=KCOUNT,NC
      DO 28, JIF=1,NS
      SAVE(IF,JIF)=C(IF,JIF)
   28 CONTINUE
      JG=0
C
C START TRAY CALCULATIONS
C
      VB2=0.0
   30 JG=JG+1
      DO 311, IH=1,NP3
      G(IH)=0.0
      DO 31, KA=1,NP3
      A(IH,KA)=0.0
      B(IH,KA)=0.0
      D(IH,KA)=0.0
      X(IH,KA)=0.0
      Y(IH,KA)=0.0
      DO 29, L=1,NS
      E(IH,KA,L)=0.0
      EQUIL(IH,L)=0.0
      EQDT(IH,L)=0.0
   29 CONTINUE
      IF(KA.LT.NS) GO TO 31
      C(IH,KA)=0.0
   31 CONTINUE
  311 CONTINUE
C
C START WITH CONSTANT MOLAL OVERFLOW
C
      G(NP1)=1.0
      DO 38, II=KCOUNT,NC
      B(NP1,II)=1.0
      CALL KVALUE(II,T(JG))
      B(II,NP1)=EQDT(II,T(JG))*C(II,JG)*V(JG)
      IF(JG.GE.NS) GO TO 33
      D(II,II)=-AL(JG+1)
      D(II,NP2)=-C(II,JG+1)
      GO TO 35
   33 B(II,NP1)=0.0
      B(NP1,II)=EQUIL(II,T(JG))
      B(NP1,NP1)=B(NP1,NP1)+C(II,JG)*EQDT(II,T(JG))
```

```
   35 IF(JG.LE.1) GO TO 37
      A(II,II)=-EQ2(II)*VB2
      A(II,NP1)=-DEQ2(II)*CB(II)*VB2
      A(II,NP3)=-EQ2(II)*CB(II)
   37 B(II,II)=AL(JG)+EQUIL(II,T(JG))*V(JG)
      B(II,NP2)=C(II,JG)
      B(II,NP3)=EQUIL(II,T(JG))*C(II,JG)
      IF(JG.EQ.1) G(II)=FX(II)
 6791 CB(II)=0.0
      CB(II)=C(II,JG)
      EQ2(II)=0.0
      EQ2(II)=EQUIL(II,T(JG))
      DEQ2(II)=0.0
      DEQ2(II)=EQDT(II,T(JG))
   38 CONTINUE
      VB2=V(JG)
C  CONSTANT MOLAL OVERFLOW ITERATIONS
      IF(ITERAT.GT.INN(3)) GO TO 40
      NP3=NP3-2
C
C  CALL BAND FOR CONSTANT MOLAL ITERATIONS
C
C     WRITE (NO,3000) ITERAT,JG
C3000 FORMAT (/,2X,'THE FIRST CALL TO BAND',/,2X,'ITERAT = ',
C    1 I3,5X,'TRAY = ',I2)
      CALL BAND(JG,NP3,NS)
      NP3=NP3+2
      IF(JG.GE.NS) GO TO 65
      GO TO 30
C
C INCLUDE ITERMEDIATE TRAY EFFECTS AND ENTHALPY EFFECTS
C
C    BOTTOM TRAY HAS NO VAPOR COMING FROM BELOW
   40 DO 9150, I=1,NC
      DO 9150, J=1,NS
      EQUIL(I,J)=0.0
      EQDT(I,J)=0.0
      HHV(I,J)=0.0
      HHL(I,J)=0.0
      DHVDT(I,J)=0.0
 9150 CONTINUE
      B(NP3,NP2)=1.0
      B(NP3,NP3)=1.0
      IF(JG.GT.1) GO TO 405
      G(NP3)=FTOT-AL(JG)-V(JG)
      GO TO 406
  405 G(NP3)=-AL(JG)-V(JG)
  406 D(NP3,NP2)=-1.0
      A(NP3,NP3)=-1.0
      IF(JG.GT.1) GO TO 49
      DO 8951, IJ=KCOUNT,NC
      EQB3(IJ)=0.0
      DEQ3(IJ)=0.0
      HVB3(IJ)=0.0
```

```
      HLU3(IJ)=0.0
C  THE VAPOR ENTHALPY DERIVATIVE EQUALS THE LIQUID
C     ENTHALPY DERIVATIVE
      CB3(IJ)=0.0
      CALL KVALUE(IJ,T(1))
      EQB3(IJ)=EQUIL(IJ,T(1))
      DEQ3(IJ)=EQDT(IJ,T(1))
      CALL VENTH(IJ,T(1))
      HVB3(IJ)=HHL(IJ,T(1))
      CALL VENHDT(IJ,T(1))
      DHB(IJ)=DHVDT(IJ,T(1))
      CALL VLNTH(IJ,T(2))
      HLU3(IJ)=HHL(IJ,T(2))
      CB3(IJ)=C(IJ,JG)
 8951 CONTINUE
      VB3=V(JG)
C
C HANDLE BOTTOMS SPECIFICATIONS (FIXED BOTTOMS RATE)
C
      B(NP2,NP2)=1.0
      G(NP3)=G(NP3)+AL(JG+1)
C
C CALL BAND FOR BOTTOM TRAY
C
C     WRITE (NO,3001) ITERAT,JG
C3001 FORMAT (/,2X,'THE SECOND CALL TO BAND',/,2X,'ITERAT = ',
C    1 I3,5X,'STAGE = ',I2)
      CALL BAND(JG,NP3,NS)
      GO TO 30
   49 IF(JG.GE.NS) GO TO 52
C
C TOP TRAY HAS NO LIQUID COMING DOWN FROM ABOVE
C INCLUDE ALL EFFECTS DUE TO COMPOSITION AND ENTHALPY
C
      G(NP3)=G(NP3)+AL(JG+1)+V(JG-1)
      NU=JG+1
      DO 51, IJ=KCOUNT,NC
      CALL KVALUE(IJ,T(JG))
      CALL VENTH(IJ,T(JG))
      CALL VLNTH(IJ,T(NU))
      IF(NU.EQ.NSM1) GO TO 9505
 9505 B(NP2,NP2)=B(NP2,NP2)+HLU3(IJ)*C(IJ,JG)
      B(NP2,NP3)=B(NP2,NP3)+HHV(IJ,T(JG))*EQUIL(IJ,T(JG))
     1*C(IJ,JG)
      D(NP2,NP2)=D(NP2,NP2)-HHL(IJ,T(NU))*C(IJ,NU)
      A(NP2,NP3)=A(NP2,NP3)-HVB3(IJ)*EQB3(IJ)*CB3(IJ)
      A(NP2,IJ)=-HVB3(IJ)*EQB3(IJ)*VB3
      B(NP2,IJ)=HLU3(IJ)*AL(JG)+HHV(IJ,T(JG))*V(JG)*EQUIL(IJ,
     1T(JG))
      D(NP2,IJ)=-HHL(IJ,T(NU))*AL(NU)
      A(NP2,NP1)=A(NP2,NP1)-VB3*CB3(IJ)*(HVB3(IJ)*DEQ3(IJ))
      B(NP2,NP1)=B(NP2,NP1)+C(IJ,JG)*V(JG)*HHV(IJ,T(JG))*EQDT
     1(IJ,T(JG))
      IF(NU.EQ.NSM1) GO TO 51
```

```
      EQB3(IJ)=0.0
      EQB3(IJ)=EQUIL(IJ,T(JG))
      DEQ3(IJ)=0.0
      DEQ3(IJ)=EQDT(IJ,T(JG))
      HVB3(IJ)=0.0
      HVB3(IJ)=HHV(IJ,T(JG))
      HLU3(IJ)=0.0
      HLU3(IJ)=HHL(IJ,T(NU))
      DHB(IJ)=0.0
      DHB(IJ)=DHJG(IJ)
      DHJG(IJ)=0.0
      DHJG(IJ)=DHVDT(IJ,T(NU))
      CB3(IJ)=0.0
      CB3(IJ)=C(IJ,JG)
   51 CONTINUE
      VB3=V(JG)
      G(NP2)=HF1
C     WRITE (NO,3002) ITERAT,JG
C3002 FORMAT (/,2X,'THE THIRD CALL TO BAND',/,2X,'ITERATION = ',
C    1 I3,5X,'STAGE = ',I2)
C
C INTERMEDIATE TRAY CALL TO BAND WITH EVERYTHING
C
      CALL BAND(JG,NP3,NS)
      GO TO 30
C
C INCLUDE OVERHEAD SPECIFICATIONS
C    FIXED OVERHEAD PRODUCT RATE
C
   52 B(NP2,NP3)=1.0
   62 G(NP3)=G(NP3)+VB3
C     WRITE (NO,3003) ITERAT,JG
C3003 FORMAT (/,2X,'THE FOURTH CALL TO BAND',/,2X,'ITERATION = ',
C    1 I3,5X,'STAGE = ',I2)
      CALL BAND(JG,NP3,NS)
C
C LAST CALL TO BAND AND CALCULATE NEW CHANGES IN PROFILES
C  MAX LIQUID RATE CHANGE PER TRAY IS 40%, MAX TEMP CHANGE IS 2.5F
C
      ALPRE=0.0
      DO 640, JH=1,NS
      MAXLIQ=ABS(C(NP2,JH))-DLLIM*AL(JH)
      IF(MAXLIQ.LE.0.0) GO TO 64
      C(NP2,JH)=AL(JH)*0.4*C(NP2,JH)/ABS(C(NP2,JH))
   64 AL(JH)=AL(JH)+C(NP2,JH)
      IF(JH-2) 640,6411,6410
 6411 ALPRE=AL(JH)
      GO TO 640
 6410 IF(AL(JH).GT.ALPRE) AL(JH)=ALPRE
      ALPRE=AL(JH)
  640 CONTINUE
      TPRE=0.0
   65 DO 67, JI=1,NS
      IF((ABS(C(NP1,JI))-DTLIM).LE.0.0) GO TO 670
```

```
      C(NP1,JI)=DTLIM*C(NP1,JI)/ABS(C(NP1,JI))
  670 T(JI)=T(JI)+C(NP1,JI)
      IF(JI.GT.1) GO TO 6710
      TPRE=T(JI)
      GO TO 67
 6710 IF(T(JI).GT.TPRE) T(JI)=TPRE
      TPRE=T(JI)
   67 CONTINUE
      IF(ITERAT.EQ.15) GO TO 221
      GO TO 12
C
C RETURN TO CALCULATIONS
C
 1202 IF(NRUN.LT.100) GO TO 1111
 1201 NRNMAX=NRUN-1
      OPEN (UNIT=11, FILE='OUTPUT2.DAT', FORM='FORMATTED',
     1 ACCESS='SEQUENTIAL', STATUS='NEW')
      WRITE (11,2052) NRNMAX
 2052 FORMAT (I3)
      CLOSE (UNIT=11, STATUS='KEEP')
      CLOSE (UNIT=10, STATUS='KEEP')
      WRITE (NO,9010)
 9010 FORMAT (/,5X,'WOULD YOU LIKE ANOTHER RUN? (Y,N)')
      READ (NI,2010) KRUN
 2010 FORMAT (A2)
      IF(KRUN.NE.'Y') GO TO 9012
      NPROG=1
      WRITE (NO,9020)
 9020 FORMAT (/,5X,'WOULD YOU LIKE TO COMBINE FILES? (Y,N)')
      READ (NI,2020) ICOMB
 2020 FORMAT (A2)
      IF(ICOMB.NE.'Y') GO TO 9022
      KFL=9
      GO TO 502
 9022 KFL=KFL+1
      IF(KFL.EQ.8) KFL=1
      IF(KFL.EQ.5) KFL=7
      GO TO 502
 9012 WRITE (NO,1200)
 1200 FORMAT (/,2X,'PROGRAM COMPLETED--THANK YOU')
      STOP
      END
C
C SUBROUTINE BAND
C
      SUBROUTINE BAND(J,N,NJ)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100),FK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
```

```
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
      DATA DETERM,NVAP,NF2T,NBAND,N2P1/0.0,4*0/
  101 FORMAT(/,2X,'THE DETERMINATE IS ZERO AT STAGE ',I3)
      NBAND=N+1
      N2P1=2*N+1
      IF((J-2).GT.0) GO TO 11
      IF((J-2).EQ.0) GO TO 6
C
C THE FIRST CALCULATION IS DIFFERENT BECAUSE IT LACKS AN IMAGE
C    POINT FOR CENTRAL DIFFERENCE
C EQUATION 6 IN ARTICLE:  STORE X AND G IN D
C
      DO 1, I=1,N
      D(I,N2P1)=G(I)
      DO 2, L=1,N
      LPN=L+N
      D(I,LPN)=X(I,L)
    2 CONTINUE
    1 CONTINUE
      CALL SOLVER(N,N2P1,DETERM)
      DETERM=ABS(DETERM)-0.00001
      IF (DETERM.GT.0.0) GO TO 4
      WRITE (NO,101) J
C
C  CREATE THE BEGINNINGS OF THE E ARRAY
C
    4 DO 5, K=1,N
      E(K,NBAND,J-1)=D(K,N2P1)
      DO 51, L=1,N
      E(K,L,J-1)=-D(K,L)
      LPN=L+N
      X(K,L)=-D(K,LPN)
   51 CONTINUE
    5 CONTINUE
      RETURN
C
C THE SECOND TRAY IS DIFFERENT BECAUSE OF THE EFFECT ON THE
C   FIRST TRAY
C
    6 DO 7, I=1,N
      DO 7, K=1,N
      DO 7, L=1,N
      D(I,K)=D(I,K)+A(I,L)*X(L,K)
    7 CONTINUE
   11 CONTINUE
      IF((J-NJ).LT.0) GO TO 260
      DO 111, I=1,N
      DO 111, L=1,N
      DO 111, M=1,N
      G(I)=G(I)+Y(I,L)*E(L,N,J-2)
      A(I,L)=A(I,L)+Y(I,M)*E(M,L,J-2)
  111 CONTINUE
  260 CONTINUE
```

```
    DO 12, I=1,N
    D(I,NBAND)=-G(I)
C
C EQUATION 8 IN ARTICLE
C
    DO 12, L=1,N
    D(I,NBAND)=D(I,NBAND)+A(I,L)*E(L,NBAND,J-1)
    DO 12, K=1,N
C
C EQUATION 10 IN ARTICLE
C
    B(I,K)=B(I,K)+A(I,L)*E(L,K,J-1)
  12 CONTINUE
    CALL SOLVER(N,NBAND,DETERM)
    DETERM=ABS(DETERM)-1.0E-5
    IF(DETERM.GT.0.0) GO TO 14
    WRITE (NO,101) J
  14 DO 15, K=1,N
    DO 15, M=1,NBAND
    E(K,M,J)=-D(K,M)
  15 CONTINUE
    IF(J.LT.NJ) GO TO 20
    DO 17, K=1,N
    C(K,J)=E(K,NBAND,J)
  17 CONTINUE
    DO 18, JJ=2,NJ
    M=NJ-JJ+1
    NP2T=N-NVAP
    DO 18, K=1,NP2T
    C(K,M)=E(K,NBAND,M)
    DO 18, L=1,N
C
C EQUATION 7 IN ARTICLE
C
    C(K,M)=C(K,M)+E(K,L,M)*C(L,M+1)
  18 CONTINUE
    DO 19, LL=1,NP2T
    DO 19, KK=1,NP2T
C
C EQUATION 5 IN ARTICLE
C
    C(KK,1)=C(KK,1)+X(KK,LL)*C(LL,3)
  19 CONTINUE
  20 CONTINUE
    RETURN
    END
C
C   THIS SUBROUTINE (SOLVER) SOLVES THE MATRICES USING A
C     A VERY SIMPLE FORM OF PIVOTING WHEN APPLIED TO THE
C     GAUSS-JORDAN TECHNIQUE
C
    SUBROUTINE SOLVER(N,M,DETERM)
    COMMON/BATCH/ID(100),WMOL(100)
    COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
```

```
      COMMON/KVAL/AK(100),BK(100),CK(100),PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
      DATA CHECK1,CHECK2/1.0E-8,0.0/
C
C LOOK FOR ZEROES IN THE MAIN DIAGONAL. IF THEY EXIST, LOOK
C    DOWN THE COLUMN FOR A NON-ZERO ENTRY AND SWAP ROWS.  THIS
C    IS REQUIRED BY THE STORAGE TECHNIQUE.
C
      DO 3000, J=1,N
      AMULT=0.0
      ABJJ=ABS(B(J,J))
      QUIRK=ABJJ-CHECK1
      IF (QUIRK.LT.CHECK2) GO TO 2101
      IF(ABJJ) 2101,2101,2000
 2101 IF(J.EQ.N) GO TO 4000
      JP1=J+1
      KK=0
      DO 1995, IK=JP1,N
      KK=KK+1
      QUIRK=ABS(B(IK,J))-1.0E-8
      IF(QUIRK.GT.0.0) GO TO 1990
 1995 CONTINUE
      GO TO 4000
 1990 DO 1999, I=J,N
      QUIRK=B(J,I)
      B(J,I)=B(KK,I)
      B(KK,I)=QUIRK
 1999 CONTINUE
      DO 1998, I=1,M
      QUIRK=D(KK,I)
      D(J,I)=D(KK,I)
      D(KK,I)=QUIRK
 1998 CONTINUE
 2000 IF((B(J,J)).EQ.CHECK2) GO TO 4000
      AMULT=1.0/B(J,J)
C
C THE SOLUTION OF THE MATRIX NOW FOLLOWS THE TYPICAL GAUSS-
C    JORDAN MANNER WITH THE MODIFICATION OF THIS FORM OF
C    PIVOTING.
C
      DO 2001, I=J,N
      B(J,I)=B(J,I)*AMULT
 2001 CONTINUE
      DO 2010, I=1,M
      D(J,I)=D(J,I)*AMULT
 2010 CONTINUE
      DO 2200, K=1,N
      AMLT=0.0
```

```
      AMLT=B(K,J)
      IF(K.EQ.J) GO TO 2200
      DO 2100, LIA=J,N
      B(K,LIA)=B(K,LIA)-AMLT*B(J,LIA)
 2100 CONTINUE
      DO 2200, MI=1,M
      D(K,MI)=D(K,MI)-AMLT*D(J,MI)
 2200 CONTINUE
 3000 CONTINUE
      RETURN
 4000 DETERM=0.0
      RETURN
      END
C
C     SUBROUTINE CALCULATES BUBBLE POINT TEMPERATURE
C
      SUBROUTINE BUBBLE(J,TBUB)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100),PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
      DIMENSION YK(99),YKDT(99),PKK(99),EKK(99),EKD(99)
      INTEGER NCOND
      EOF=LOG(10.0)
      NCOND=J
      PSI=(PTOT/760.0)*14.696
   32 SUMB=0.0
      SUMBDT=0.0
      DO 320, I=1,NC
      PKK(I)=0.0
      EKK(I)=0.0
      EKD(I)=0.0
      YK(I)=0.0
      YKDT(I)=0.0
  320 CONTINUE
      TBF=(TBUB-32.0)/1.8
      DO 33, II=1,NC
      IF((C(II,NCOND)).LE.0.0) GO TO 33
      IF(ID(II).GT.NMXPRE) GO TO 3700
      DENOM=TBF+CK(II)
      IF(DENOM.LE.(0.0)) GO TO 33
      PKK(II)=AK(II)-BK(II)/DENOM
      CALC=PKK(II)-LOG10(PTOT)
      IF(CALC.GE.(-7.0)) GO TO 350
      GO TO 33
  350 IF(CALC.GE.(7.0)) GO TO 360
      EKK(II)=10.0**CALC
      GO TO 370
```

```
  360 EKK(II)=10000000.0
  370 EKD(II)=EOP*EKK(II)*BK(II)/(DENOM**2)
      GO TO 3750
C  DREISBACH
 3700 DINO=TBUB+CK(II)
      IF(DINO.LE.0.0) GO TO 33
      PK(II)=AK(II)-BK(II)/DINO
      IF((PK(II)).LE.(-20.0)) GO TO 33
      EKK(II)=EXP(PK(II))/PSI
      EKD(II)=EKK(II)*BK(II)/(DINO**2.0)
 3750 YK(II)=C(II,NCOND)*EKK(II)
      YKDT(II)=C(II,NCOND)*EKD(II)
      SUMB=SUMB+YK(II)
      SUMBDT=SUMBDT+YKDT(II)
   33 CONTINUE
      FCALC=SUMB-1.0
      IF(ABS(FCALC).LT.TOL) GO TO 34
      IF(SUMBDT.EQ.0.0) GO TO 34
      TBUB=TBUB-FCALC/SUMBDT
      GO TO 32
   34 RETURN
      END
C
C     SUBROUTINE CALCULATES DEW POINT TEMPERATURE
C
      SUBROUTINE DEWPT(J,TDEW)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100),PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
      DIMENSION XK(100),XKDT(100)
      INTEGER NREB
      EOP=LOG(10.0)
      NREB=J
      PSI=(PTOT/760.0)*14.696
   32 SUMD=0.0
      SUMDDT=0.0
      TDF=(TDEW-32.0)/1.8
      DO 33, II=1,NC
      IF((C(II,NREB)).LE.0.0) GO TO 33
      IF(ID(II).GT.NMXPRE) GO TO 2300
      DENOM1=TDF+CK(II)
      IF (DENOM1.LE.0.0) GO TO 33
      PK(II)=AK(II)-BK(II)/DENOM1
      CLC=PK(II)-LOG10(PTOT)
      IF(CLC.GE.10.0) CLC=10.0
      IF(CLC.LE.(-10.0)) CLC=-10.0
      EQKK=10.0**CLC
```

```
      EQKD=EOP*EQKK*BK(II)/(DENOM1**2.0)
      GO TO 5
C  DREISBACH
 2300 DENOM2=TDEW+CK(II)
      IF(DENOM2.LE.0.0) GO TO 33
      PK(II)=AK(II)-BK(II)/DENOM2
      CLC=PK(II)-LOG(PTOT)
      IF(CLC.GT.20.0) CLC=20.0
      IF(CLC.LE.(-20.0)) CLC=-20.0
      EQKK=EXP(CLC)/PSI
      EQKD=EQKK*BK(II)/(DENOM2**2)
    5 XK(II)=C(II,NREB)/EQKK
      XKDT(II)=C(II,NREB)*EQKD/(EQKK**2.0)
      SUMD=SUMD+XK(II)
      SUMDDT=SUMDDT+XKDT(II)
   33 CONTINUE
      FCALC=SUMD-1.0
      IF(ABS(FCALC).LT.TOL) GO TO 34
      IF(SUMDDT.EQ.0.0) GO TO 34
      TDEW=TDEW+FCALC/SUMDDT
      GO TO 32
   34 RETURN
      END
C
C     VAPOR PRESSURE SUBROUTINE - CALCULATES K-VALUES
C                                 AND K-VALUE DERIVATIVES
C       LOG VP IN MM OF HG
C       TEMPERATURE IN DEGREES CELCIUS
C                RADULT'S LAW
C
      SUBROUTINE KVALUE(I,T)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61).CH(61).DH(61).EH(61).FH(61).DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100).PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105).A(105,105).B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50).HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC.JSTAR.NMXPRE
      EPO=LOG(10.0)
      PSI=(PTOT/760.0)*14.696
      IF(ID(I).GT.JSTAR) GO TO 10
      IF(I.GT.JSTAR) GO TO 10
      TF=(T-32.0)/1.8
      DENOM=TF+CK(I)
      IF(DENOM.GE.(0.0)) GO TO 15
      EQUIL(I,T)=0.0
      EQDT(I,T)=0.0
      RETURN
   15 PK(I)=AK(I)-BK(I)/DENOM
      CALC=PK(I)-LOG10(PTOT)
      IF(CALC.GE.(-10.0)) GO TO 25
```

```
      EQUIL(I,T)=1.0E-10
      GO TO 27
   25 IF(CALC.LE.(10.0)) GO TO 26
      EQUIL(I,T)=1.0E+10
      GO TO 27
   26 EQUIL(I,T)=10.0**CALC
   27 EQDT(I,T)=EPO*EQUIL(I,T)*BK(I)/((TT+CK(I))**2)
      RETURN
C  DREISBACH
   10 DINO=T+CK(I)
      IF(DINO.LE.0.0) GO TO 3750
      PK(I)=AK(I)-BK(I)/(T+CK(I))
      EQUIL(I,T)=EXP(PK(I))/PTOT
      EQDT(I,T)=EQUIL(I,T)*BK(I)/((T+CK(I))**2)
      RETURN
 3750 EQUIL(I,T)=0.0
      EQDT(I,T)=0.0
      RETURN
      END
C
C     SUBROUTINE CALCULATES VAPOR ENTHALPIES
C
      SUBROUTINE VENTH(I,T)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100),PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
C     DIMENSION DLBTU(25)
C
C  BASE OF HHV = 0.0, AT T = -200.0 FAHRENHEIT
C
C  ENTHALPY CALCULATIONS FOR THE HYPOTHETICAL FRACTIONS ARE
C     FROM JOHN ERBAR'S AND THE GPSA GPA*K COMPUTER PROGRAM
C       (AUGUST, 1974)
C
      DATA C0,C1,C2,C3,C4,C5,C6/311.30335,3.542502,-.0052716
     A1944,3.5353777,43.401618,-8.9530784,.35118581/
      DATA C7,C8,C9,C10,C11,C12/-.81862040,-2.8568658,
     A1.7024654,-1.4886832,.08395563,.0042934703/
      DATA C13,C14,C15,C16,C17,C18/-3.0836492,3.1073165
     1,-5.8323815,-5.6334748,9.1745019,-5.9563889/
      TABS=T+459.6
      IF(ID(I).GT.NMXPRE) GO TO 100
      HHV(I,T)=AH(I)+TABS*(BH(I)+TABS*(CH(I)*1.0E-4+TABS*(DH(I)
     1*1.0E-7+TABS*(EH(I)*1.0E-11+TABS*(FH(I)*1.0E-15)))))
      HHV(I,T)=HHV(I,T)*WMOL(I)
      RETURN
C  GPA*K
```

```
  100 UOPK=((BP(I)+459.6)**(1.0/3.0))/GSG(I)
      API=141.5/GSG(I)-131.5
      HA=C0+C1*API+C2*(API**2.0)+C3*1.0E-4*(API**3.0)+C4*UOPK
     1+C5*(UOPK**2.0)+C6*(UOPK**3.0)+C18*1.0E-3*API*UOPK
      HB=C7+C8*1.0E-5*API+C9*1.0E-6*(API**2.0)+C10*1.0E-8*(API
     1**3.0)+C11*UOPK+C12*1.0E-4*(UOPK**2.0)+C13*1.0E-4*(UOPK**3.0)
      HC=C14*1.0E-4+C15*1.0E-8*API
      HD=C16*1.0E-8+C17*1.0E-11*API
      HHV(I,T)=WMOL(I)*(HA+HB*TABS+HC*(TABS**2.0)+HD*
     1(TABS**3.0))
      RETURN
      END
C
C     SUBROUTINE CALCULATES VAPOR ENTHALPY TEMPERATURE
C          DERIVATIVES
C
      SUBROUTINE VENHDT(I,T)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100),PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
C
C  BASE OF HHV = 0.0, AT T = -200.0 FAHRENHEIT
C
C  GPA*K
      DATA C0,C1,C2,C3,C4,C5,C6/311.30335,3.542502,-.0052716
     A1944,3.5353777,43.401618,-8.9530784,.35118581/
      DATA C7,C8,C9,C10,C11,C12/-.81862040,-2.8568658,
     A1.7024654,-1.4886832,.08395563,.0042934703/
      DATA C13,C14,C15,C16,C17,C18/-3.0836492,3.1073165
     1,-5.8323815,-5.6334748,9.1745019,-5.9563889/
      TABS=T+459.6
      IF(ID(I).GT.NMXPRE) GO TO 100
      DHVDT(I,T)=BH(I)+TABS*(2.0*CH(I)*1.0E-4+TABS*(3.0*DH(I)
     A*1.0E-7+TABS*(4.0*EH(I)*1.0E-11+TABS*(5.0*FH(I)*1.0E-15))))
      DHVDT(I,T)=DHVDT(I,T)*WMOL(I)
      RETURN
C  GPA*K
  100 UOPK=((BP(I)+459.6)**(1.0/3.0))/GSG(I)
      API=141.5/GSG(I)-131.5
      HB=C7+C8*1.0E-5*API+C9*1.0E-6*(API**2.0)+C10*1.0E-8*(API
     1**3.0)+C11*UOPK+C12*1.0E-4*(UOPK**2.0)+C13*1.0E-4*(UOPK**3.0)
      HC=C14*1.0E-4+C15*1.0E-8*API
      HD=C16*1.0E-8+C17*1.0E-11*API
      DHVDT(I,T)=WMOL(I)*(HB+HC*TABS+HD*
     1(TABS**2.0))
      RETURN
      END
```

```
C
C     SUBROUTINE CALCULATES LIQUID ENTHALPIES
C
      SUBROUTINE VLNTH(I,T)
      COMMON/BATCH/ID(100),WMOL(100)
      COMMON/ENH/AH(61),BH(61),CH(61),DH(61),EH(61),FH(61),DLTH(61)
      COMMON/KVAL/AK(100),BK(100),CK(100),PK(100),EQK(100)
      COMMON/GRAVIT/GSG(100),BP(100)
      COMMON/FEED/C(105,105),E(105,105,50),D(105,225)
      COMMON/MTRX/X(105,105),Y(105,105),A(105,105),B(105,105)
      COMMON/RATE/AL(50),V(50),G(105),SAVE(100,50)
      COMMON/EQB/EQUIL(100,50),EQDT(100,50),ERR(50)
      COMMON/DENTH/DHVDT(100,50),HHL(100,50),HHV(100,50)
      COMMON/RUN/TOL,PTOT,NS,NC,JSTAR,NMXPRE
      DIMENSION DLBTU(25)
C
C  BASE OF HHV = 0.0, AT T = -200.0 FAHRENHEIT
C
C  ENTHALPY CALCULATIONS FOR THE HYPOTHETICAL FRACTIONS ARE
C     FROM JOHN ERBAR'S AND THE GPSA GPA*K COMPUTER PROGRAM
C       (AUGUST, 1974)
C
      DATA C0,C1,C2,C3,C4,C5,C6/311.30335,3.542502,-.0052716
     A1944,3.5353777,43.401618,-8.9530784,.35118581/
      DATA C7,C8,C9,C10,C11,C12/-.81862040,-2.8568658,
     A1.7024654,-1.4886832,.08395563,.0042934703/
      DATA C13,C14,C15,C16,C17,C18/-3.0836492,3.1073165
     1,-5.8323815,-5.6334748,9.1745019,-5.9563889/
      TABS=T+459.6
      IF(ID(I).GT.NMXPRE) GO TO 100
      HHL(I,T)=AH(I)+TABS*(BH(I)+TABS*(CH(I)*1.0E-4+TABS*(DH(I)
     1*1.0E-7+TABS*(EH(I)*1.0E-11+TABS*(FH(I)*1.0E-15)))))
      HHL(I,T)=HHL(I,T)*WMOL(I)
      DLBTU(I)=DLTH(I)*1000.0*3.968321/2.20462
      HHL(I,T)=HHL(I,T)-DLBTU(I)
      RETURN
C  GPA*K
  100 UOPK=((BP(I)+459.6)**(1.0/3.0))/GSG(I)
      API=141.5/GSG(I)-131.5
      HA=C0+C1*API+C2*(API**2.0)+C3*1.0E-4*(API**3.0)+C4*UOPK
     1+C5*(UOPK**2.0)+C6*(UOPK**3.0)+C18*1.0E-3*API*UOPK
      HB=C7+C8*1.0E-5*API+C9*1.0E-6*(API**2.0)+C10*1.0E-8*(API
     1**3.0)+C11*UOPK+C12*1.0E-4*(UOPK**2.0)+C13*1.0E-4*(UOPK**3.0)
      HC=C14*1.0E-4+C15*1.0E-8*API
      HD=C16*1.0E-8+C17*1.0E-11*API
      HHL(I,T)=WMOL(I)*(HA+HB*TABS+HC*(TABS**2.0)+HD*
     1(TABS**3.0))
      DLBTU(I)=DLTH(I)*1000.0*3.968321/2.20462
      HHL(I,T)=HHL(I,T)-DLBTU(I)
      RETURN
      END
*
```

APPENDIX B

NORTH SEA CRUDE RESULTS

APPENDIX B

NORTH SEA CRUDE RESULTS

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	1.736	1.736	-138.43	246.33
2	1.080	2.816	-168.30	246.65
3	1.279	4.096	97.22	246.88
4	1.876	5.971	159.71	266.76
5	1.801	7.772	159.71	278.77
6	1.729	9.501	159.71	293.46
7	1.660	11.160	159.71	311.86
8	1.344	12.504	159.71	335.57
9	1.970	14.475	254.51	361.35
10	1.892	16.366	254.51	372.10
11	1.816	18.183	254.51	384.86
12	1.743	19.926	254.51	400.29
13	1.674	21.600	254.51	419.31
14	0.538	22.138	254.54	442.22
15	1.933	24.071	348.61	451.42
16	1.855	25.926	348.61	460.60
17	1.781	27.707	348.61	471.20
18	1.710	29.417	348.62	483.56
19	1.642	31.059	348.62	498.15
20	1.179	32.238	348.66	515.57
21	1.819	34.057	438.61	530.83
22	1.746	35.804	438.62	538.42
23	1.676	37.480	438.62	547.05
24	1.609	39.089	438.63	556.97
25	1.545	40.635	438.64	568.49
26	1.483	42.118	438.67	582.05
27	0.478	42.596	438.91	598.22
28	1.632	44.228	519.83	604.25
29	1.566	45.794	519.83	610.60
30	1.504	47.298	519.83	617.71
31	1.444	48.741	519.84	625.73
32	1.386	50.127	519.86	634.85
33	1.330	51.458	519.89	645.32
34	1.277	52.735	519.98	657.45
35	0.306	53.041	520.86	671.67
36	1.389	54.430	596.52	675.44
37	1.334	55.764	596.52	681.04
38	1.280	57.044	596.52	687.26
39	1.229	58.273	596.52	694.20

APPENDIX B (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
40	1.180	59.453	596.53	702.00
41	1.133	60.586	596.53	710.83
42	1.088	61.674	596.55	720.92
43	1.044	62.718	596.58	732.54
44	0.656	63.374	596.72	746.09
45	1.128	64.503	685.31	756.15
46	1.083	65.586	685.31	760.96
47	1.040	66.626	685.31	766.24
48	0.998	67.624	685.31	772.09
49	0.958	68.582	685.31	778.58
50	0.920	69.502	685.31	785.84
51	0.883	70.386	685.31	794.02
52	0.848	71.234	685.32	803.30
53	0.814	72.048	685.33	813.92
54	0.784	72.829	685.34	826.23
55	0.586	73.415	685.40	840.64
56	0.847	74.263	785.81	853.70
57	0.814	75.076	785.81	858.12
58	0.781	75.857	785.81	862.96
59	0.750	76.607	785.81	868.29
60	0.720	77.327	785.81	874.20
61	0.691	78.018	785.81	880.77
62	0.663	78.681	785.81	888.15
63	0.637	79.318	785.81	896.47
64	0.611	79.929	785.81	905.97
65	0.587	80.516	785.81	916.91
66	0.563	81.079	785.81	929.68
67	0.541	81.620	785.81	944.82
68	0.519	82.139	785.81	963.08
69	0.498	82.638	785.81	985.61
70	0.383	83.020	785.81	1014.10
71	0.604	83.625	994.31	1042.70

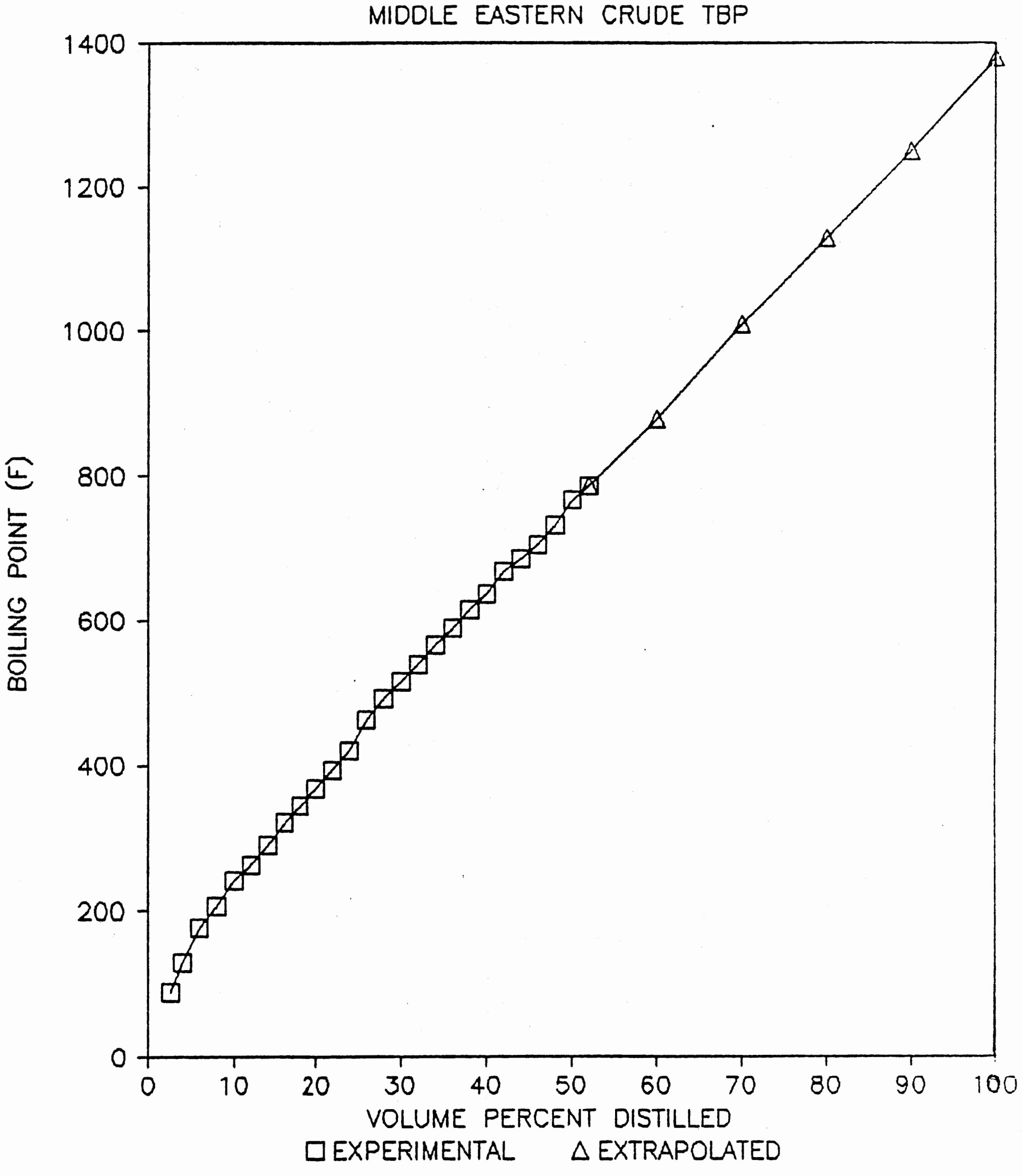
APPENDIX C

MIDDLE EASTERN CRUDE INPUTS AND RESULTS

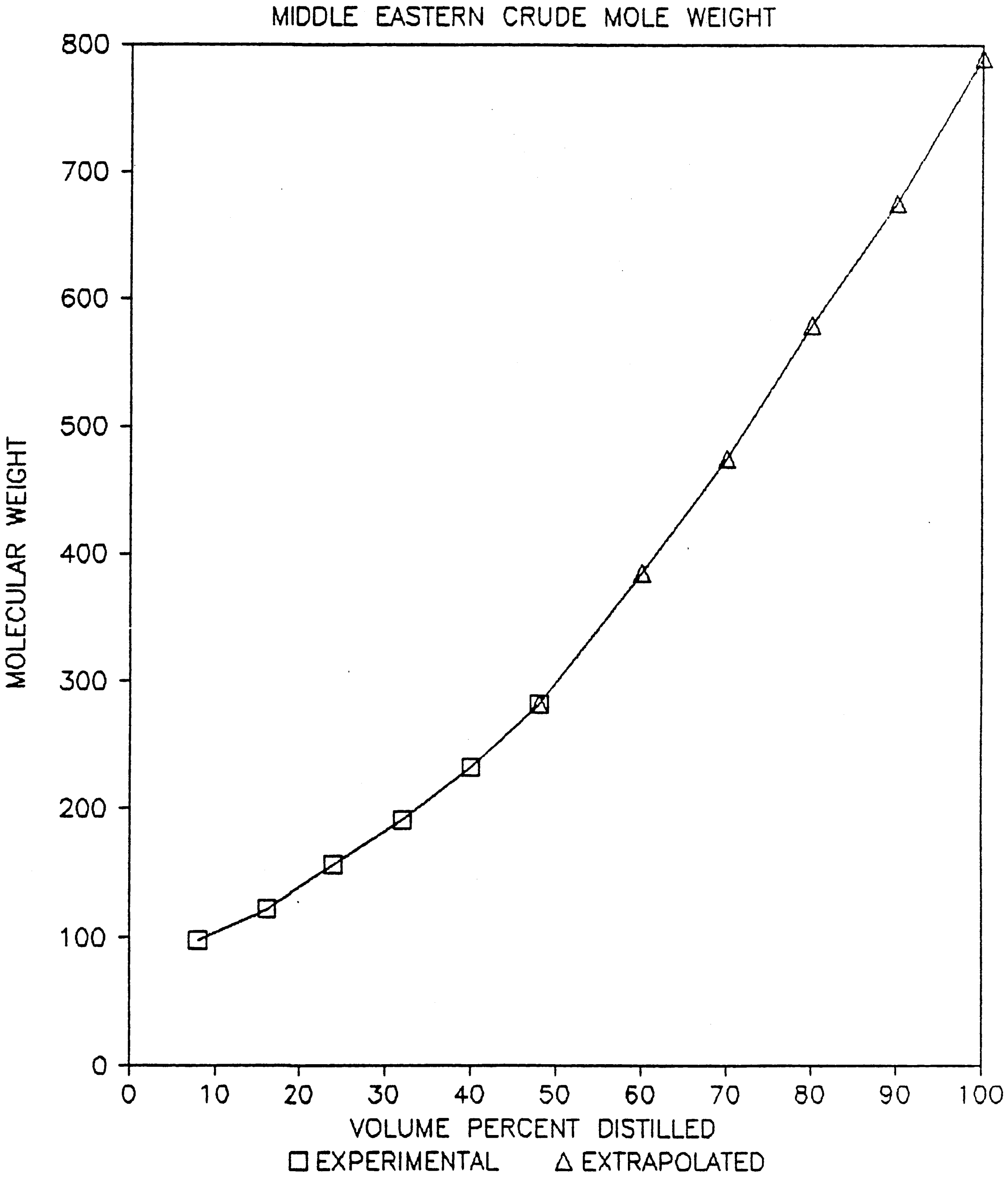
APPENDIX C

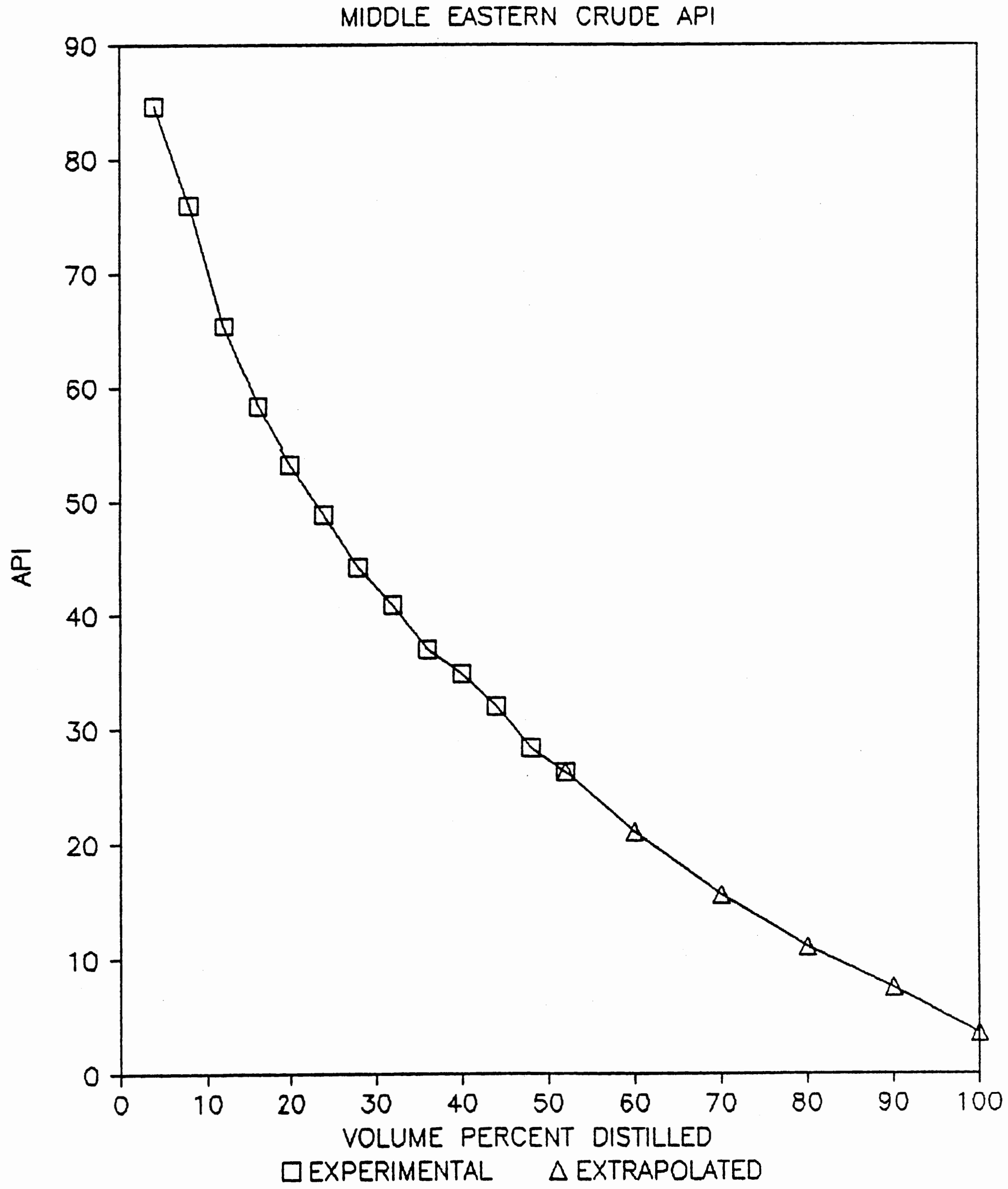
MIDDLE EASTERN CRUDE INPUTS

	VOLUME PERCENT	NORMAL BOILING POINT (F)	MOLECULAR WEIGHT	SPECIFIC GRAVITY
Fraction 1	2.6	89		
Fraction 2	1.4	130		0.655
Fraction 3	2.0	178		
Fraction 4	2.0	207	98	0.682
Fraction 5	2.0	242		
Fraction 6	2.0	264		0.719
Fraction 7	2.0	291		
Fraction 8	2.0	321	122	0.746
Fraction 9	2.0	345		
Fraction 10	2.0	368		0.766
Fraction 11	2.0	394		
Fraction 12	2.0	421	157	0.785
Fraction 13	2.0	463		
Fraction 14	2.0	492		0.805
Fraction 15	2.0	517		
Fraction 16	2.0	540	191	0.820
Fraction 17	2.0	567		
Fraction 18	2.0	590		0.840
Fraction 19	2.0	616		
Fraction 20	2.0	637	233	0.850
Fraction 21	2.0	667		
Fraction 22	2.0	686		0.865
Fraction 23	2.0	705		
Fraction 24	2.0	732	283	0.885
Fraction 25	2.0	767		
Fraction 26	2.0	787		0.897



MIDDLE EASTERN CRUDE TBP
BOILING POINT (F)
1400
1200
1000
800
600
400
200
0
0
10
20
30
40
50
60
70
80
90
100
VOLUME PERCENT DISTILLED
□ EXPERIMENTAL
△ EXTRAPOLATED


MIDDLE EASTERN CRUDE MOLE WEIGHT
MOLECULAR WEIGHT
800
700
600
500
400
300
200
100
0
0
10
20
30
40
50
60
70
80
90
100
VOLUME PERCENT DISTILLED
□ EXPERIMENTAL
△ EXTRAPOLATED


MIDDLE EASTERN CRUDE API
API
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
VOLUME PERCENT DISTILLED
□ EXPERIMENTAL
△ EXTRAPOLATED

APPENDIX C

MIDDLE EASTERN CRUDE RESULTS

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	1.806	1.806	89.096	252.443
2	0.855	2.660	89.366	285.503
3	1.416	4.076	130.180	306.693
4	1.726	5.802	178.847	334.210
5	0.570	6.373	181.134	358.934
6	1.723	8.096	207.726	367.766
7	0.555	8.650	215.500	392.889
8	1.679	10.329	244.429	399.629
9	1.434	11.763	260.444	422.266
10	0.762	12.526	267.345	440.885
11	1.654	14.180	292.452	450.784
12	0.674	14.854	299.900	472.885
13	1.604	16.458	322.930	481.079
14	1.448	17.906	343.843	502.154
15	1.107	19.013	351.625	519.648
16	1.503	20.516	370.290	534.798
17	1.619	22.135	395.591	557.222
18	0.705	22.839	399.160	580.015
19	1.595	24.435	421.740	590.538
20	0.719	25.153	437.467	614.637
21	1.455	26.608	464.614	622.789
22	1.541	28.149	494.330	641.827
23	0.847	28.996	497.538	659.374
24	1.510	30.506	519.202	669.762
25	0.886	31.392	526.529	687.595
26	1.391	32.783	542.351	697.923
27	1.481	34.264	569.840	715.284
28	0.922	35.186	573.043	731.765
29	1.438	36.624	592.245	742.987
30	0.820	37.443	600.785	760.297
31	1.415	38.858	619.086	769.658
32	1.000	39.859	628.893	786.791
33	1.100	40.958	640.079	798.731
34	1.373	42.331	670.067	813.193
35	1.133	43.464	673.401	828.592
36	1.328	44.792	689.439	843.335
37	0.952	45.744	694.787	860.942
38	1.273	47.017	707.722	874.853
39	1.026	48.044	725.721	895.395

APPENDIX C (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
40	0.993	49.036	734.556	910.619
41	1.262	50.299	770.043	927.844
42	1.312	51.431	771.749	945.964
43	1.193	52.523	787.097	965.942
44	0.335	52.959	787.166	988.702
45	1.371	54.330	880.002	996.245
46	1.317	55.647	880.002	1006.321
47	1.264	56.910	880.003	1017.964
48	1.213	58.124	880.003	1031.598
49	1.165	59.289	880.004	1047.822
50	1.118	60.407	880.006	1067.504
51	0.697	61.104	880.016	1090.816
52	1.243	62.347	1010.008	1109.784
53	1.193	63.541	1010.008	1117.418
54	1.146	64.687	1010.009	1126.010
55	1.100	65.786	1010.010	1135.759
56	1.056	66.842	1010.011	1146.929
57	1.014	67.856	1010.015	1159.869
58	0.973	68.829	1010.022	1175.054
59	0.612	69.441	1010.053	1193.146
60	1.077	70.518	1130.004	1206.895

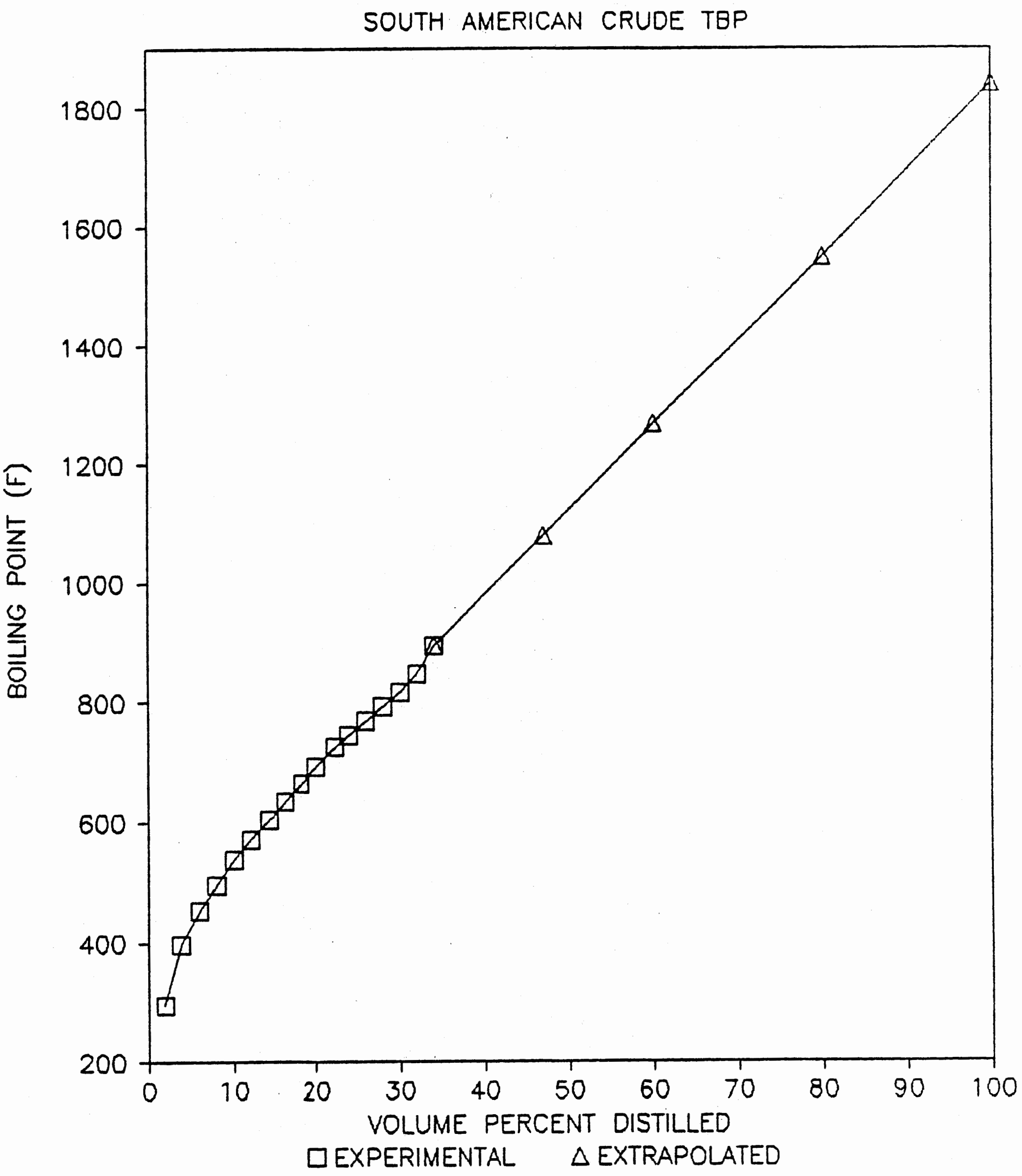
APPENDIX D

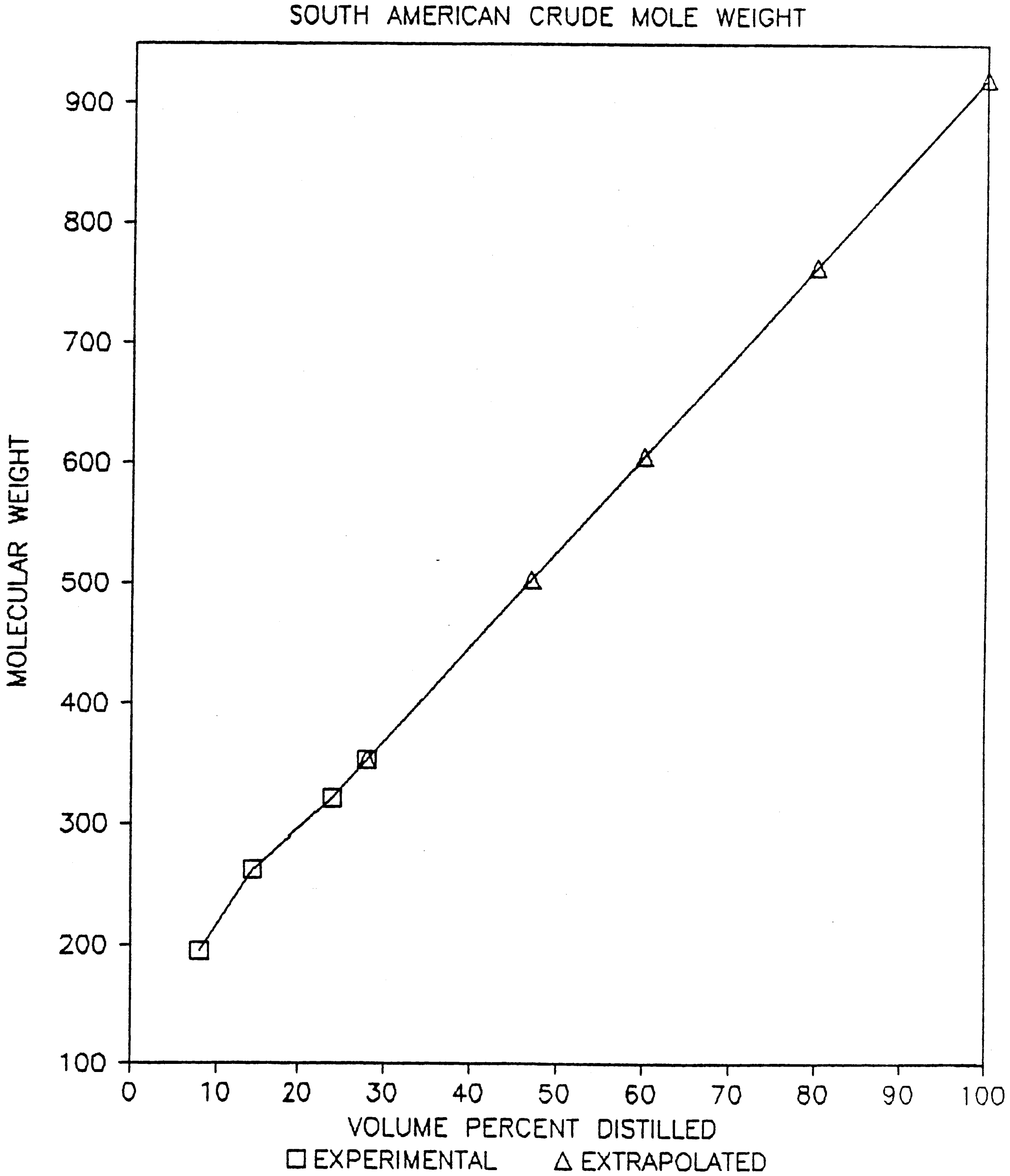
SOUTH AMERICAN CRUDE INPUTS AND RESULTS

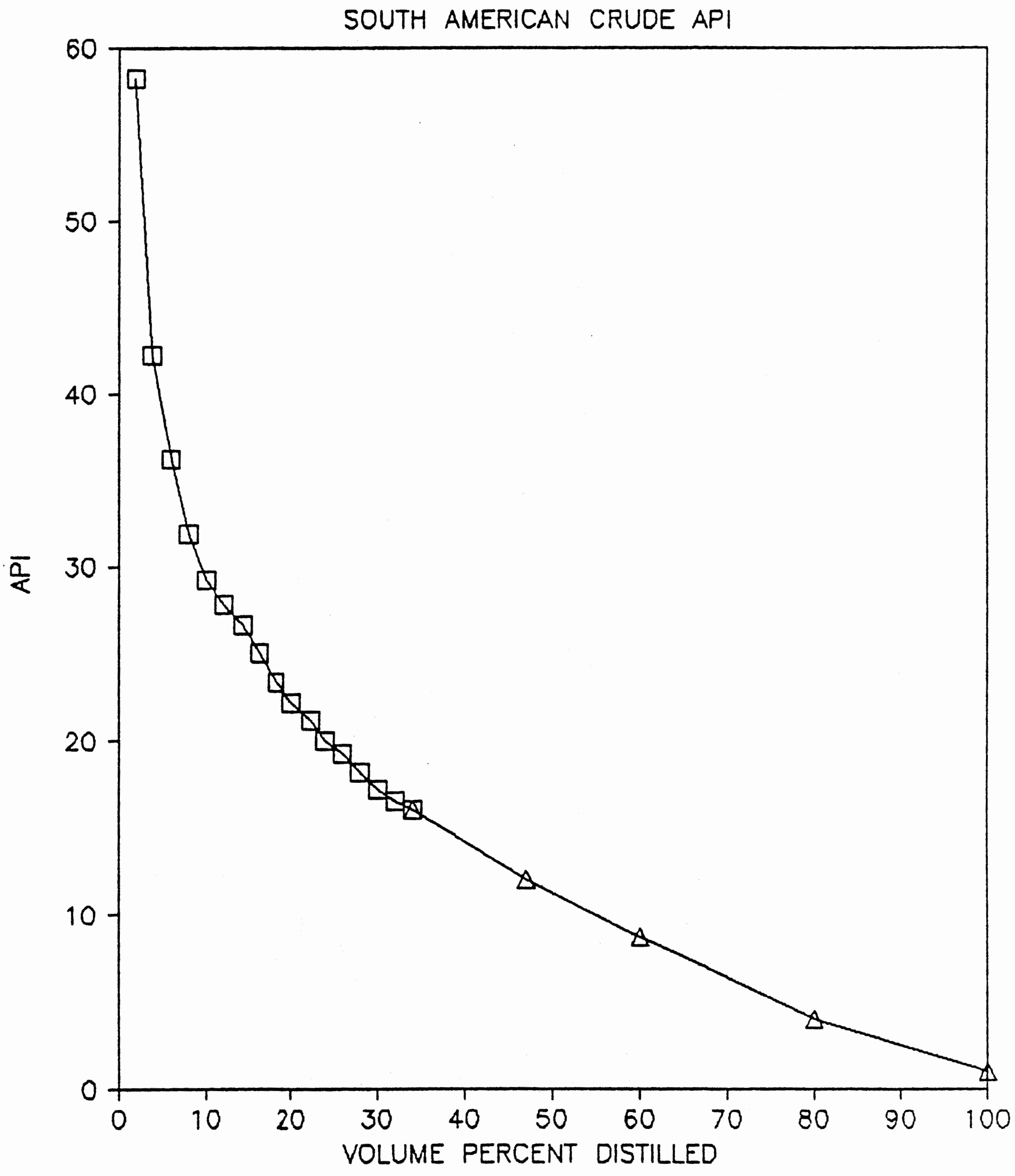
APPENDIX D

SOUTH AMERICAN CRUDE INPUTS

	VOLUME PERCENT	NORMAL BOILING POINT (F)	MOLECULAR WEIGHT	SPECIFIC GRAVITY
Fraction 1	1.9	294		0.746
Fraction 2	1.9	396		0.815
Fraction 3	2.2	454		0.844
Fraction 4	2.0	495	195	0.866
Fraction 5	2.0	538		0.881
Fraction 6	2.0	572		0.888
Fraction 7	2.2	605		0.895
Fraction 8	1.9	635	262	0.904
Fraction 9	2.1	666		0.913
Fraction 10	1.9	695		0.921
Fraction 11	2.3	727		0.927
Fraction 12	1.6	747	321	0.933
Fraction 13	2.0	770		0.938
Fraction 14	2.0	793	353	0.945
Fraction 15	2.0	817		0.952
Fraction 16	2.0	848		0.956
Fraction 17	2.0	895		0.959


SOUTH AMERICAN CRUDE TBP
BOILING POINT (F)
200
400
600
800
1000
1200
1400
1600
1800
0
10
20
30
40
50
60
70
80
90
100
VOLUME PERCENT DISTILLED
□ EXPERIMENTAL
△ EXTRAPOLATED


SOUTH AMERICAN CRUDE MOLE WEIGHT
MOLECULAR WEIGHT
900
800
700
600
500
400
300
200
100
0
10
20
30
40
50
60
70
80
90
100
VOLUME PERCENT DISTILLED
□ EXPERIMENTAL
△ EXTRAPOLATED


SOUTH AMERICAN CRUDE API
API
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100
VOLUME PERCENT DISTILLED
□ EXPERIMENTAL
△ EXTRAPOLATED

APPENDIX D

SOUTH AMERICAN CRUDE RESULTS

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	1.717	1.717	294.591	529.385
2	0.188	1.905	294.603	587.066
3	1.655	3.560	396.174	595.178
4	0.280	3.840	396.681	632.843
5	1.684	5.524	454.624	640.492
6	0.596	6.121	455.660	670.897
7	1.692	7.812	495.752	683.832
8	0.409	8.222	498.645	713.928
9	1.713	9.934	539.380	721.337
10	0.614	10.548	543.505	748.623
11	1.722	12.271	574.018	758.609
12	1.772	14.043	606.735	786.094
13	0.770	14.813	610.323	811.758
14	1.611	16.425	636.792	823.782
15	1.786	18.211	668.129	848.289
16	0.817	19.027	674.076	873.761
17	1.452	20.479	697.355	885.617
18	1.797	22.276	730.058	907.561
19	1.114	23.391	733.828	932.174
20	1.309	24.699	751.856	949.848
21	1.761	26.461	773.125	971.520
22	1.495	27.956	790.710	1002.686
23	1.040	28.996	800.844	1031.396
24	1.423	30.419	819.401	1054.456
25	1.718	32.137	849.030	1090.981
26	0.508	32.645	857.060	1139.892
27	1.582	34.227	895.007	1153.881
28	1.985	36.213	1080.006	1203.033
29	1.906	38.118	1080.006	1214.245
30	1.830	39.948	1080.006	1227.386
31	1.756	41.704	1080.006	1243.073
32	1.686	43.391	1080.006	1262.239
33	1.619	45.009	1080.006	1286.385
34	1.554	46.563	1080.006	1318.076
35	0.622	47.185	1080.006	1362.039
36	1.727	48.912	1270.007	1385.630
37	1.658	50.570	1270.007	1395.534
38	1.592	52.162	1270.007	1406.985
39	1.528	53.690	1270.007	1420.424

APPENDIX D (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
40	1.467	55.157	1270.007	1436.495
41	1.408	56.565	1270.007	1456.189
42	1.352	57.917	1270.007	1481.109
43	1.298	59.214	1270.007	1514.048
44	0.916	60.131	1270.007	1560.289
45	1.473	61.604	1550.007	1608.115

APPENDIX E

RESULTS FROM THE OPTIMUM PARAMETER, CRUDE BLENDING, AND ASTM DISTILLATION RUNS

APPENDIX E

RESULTS FROM THE 20 TRAY COMPARISON

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	1.806	1.806	89.008	252.443
2	0.842	2.648	89.010	285.828
3	1.425	4.072	130.008	306.480
4	1.724	5.797	178.026	334.162
5	0.322	6.118	178.162	359.064
6	1.732	7.851	207.013	364.656
7	0.299	8.149	207.063	388.959
8	1.691	9.841	242.133	393.984
9	0.401	10.242	243.133	415.506
10	1.702	11.944	264.059	421.420
11	0.304	12.247	264.299	443.874
12	1.664	13.911	291.041	448.533
13	0.359	14.270	321.127	469.143
14	1.620	15.890	322.127	474.598
15	0.449	16.338	345.428	494.568
16	1.619	17.958	346.758	500.978
17	0.537	18.495	368.091	520.890
18	1.626	20.121	369.091	528.335
19	0.286	20.407	394.082	551.277
20	1.620	22.027	394.304	555.914
21	0.402	22.428	421.010	578.668
22	1.611	24.040	421.035	585.343
23	0.402	24.442	463.077	608.121
24	1.560	26.002	463.301	614.933
25	0.492	26.494	492.149	633.714
26	1.541	28.035	493.149	640.686
27	0.519	28.554	517.216	658.347
28	1.520	30.074	518.216	665.263
29	0.539	30.613	540.125	682.575
30	1.512	32.125	541.125	689.652
31	0.491	32.616	567.242	707.085
32	1.482	34.098	568.242	713.646
33	0.588	34.686	590.160	730.204
34	1.452	36.138	591.160	737.817
35	0.560	36.697	616.348	754.498
36	1.435	38.132	617.348	761.982
37	0.657	38.789	637.105	778.110
38	1.412	40.205	637.269	786.668
39	0.547	40.752	637.269	803.518

APPENDIX E (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
40	1.372	42.124	667.511	811.155
41	0.772	42.896	668.476	826.690
42	1.344	44.240	686.546	836.927
43	0.709	44.948	687.669	853.812
44	1.297	46.245	705.185	864.239
45	0.632	46.877	706.185	882.937
46	1.292	48.169	732.056	893.833
47	0.720	48.889	732.164	912.974
48	1.265	50.153	767.505	925.980

APPENDIX E

RESULTS FROM THE 2 TRAY COMPARISON

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	1.821	1.821	97.025	252.717
2	1.762	3.584	104.574	281.530
3	1.633	5.217	143.793	317.961
4	1.671	6.888	186.259	344.256
5	1.721	8.609	209.346	365.957
6	1.672	10.281	230.179	389.208
7	1.681	11.962	254.223	411.337
8	1.672	13.634	276.726	433.128
9	1.640	15.274	293.135	454.434
10	1.634	16.908	316.375	475.315
11	1.623	18.532	338.335	496.413
12	1.599	20.130	356.089	517.231
13	1.591	21.721	372.535	538.537
14	1.581	23.302	392.464	561.407
15	1.560	24.862	416.575	584.954
16	1.574	26.436	445.970	607.460
17	1.565	28.001	475.975	628.158
18	1.538	29.539	499.195	646.297
19	1.519	31.058	513.995	662.970
20	1.498	32.556	529.852	680.141
21	1.481	34.038	547.292	697.414
22	1.460	35.498	563.643	714.551
23	1.445	36.944	581.274	731.637
24	1.425	38.369	598.685	748.569
25	1.405	39.774	615.060	765.256
26	1.385	41.159	631.028	781.966
27	1.363	42.522	646.732	798.812
28	1.342	43.864	662.254	815.799
29	1.319	45.183	677.341	833.122
30	1.296	46.479	691.652	850.888
31	1.275	47.754	705.964	869.375
32	1.256	49.010	720.104	888.789
33	1.242	50.252	736.331	909.284
34	1.237	51.499	757.331	930.516
35	1.237	52.726	780.430	951.469
36	1.242	53.968	803.678	971.585
37	1.253	55.221	829.934	990.782
38	1.258	56.479	859.120	1008.298
39	1.250	57.729	882.556	1023.314

APPENDIX E (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
40	1.216	58.945	890.358	1037.160
41	1.178	60.124	894.232	1052.230
42	1.148	61.272	901.194	1069.409
43	1.132	62.404	913.921	1088.470
44	1.141	63.545	944.784	1107.050
45	1.155	64.700	1007.724	1123.520
46	1.132	65.832	1020.537	1132.556
47	1.092	66.924	1022.746	1141.672
48	1.055	67.979	1025.810	1151.713
49	1.023	69.001	1030.220	1162.728
50	0.995	69.996	1036.838	1174.683
51	0.973	70.969	1047.159	1187.374
52	0.958	71.927	1063.405	1200.275
53	0.949	72.876	1087.729	1212.417
54	0.936	73.812	1115.544	1222.652
55	0.911	74.724	1132.283	1230.732
56	0.878	75.602	1136.410	1237.953
57	0.846	76.448	1137.770	1245.563
58	0.814	77.262	1139.560	1253.909
59	0.785	78.047	1142.111	1263.062
60	0.759	78.806	1145.922	1273.053
61	0.735	79.541	1150.982	1283.841
62	0.716	80.257	1160.509	1295.206
63	0.703	80.960	1177.709	1306.565
64	0.697	81.657	1209.443	1316.734
65	0.692	82.349	1258.496	1324.016
66	0.675	83.024	1293.850	1327.618
67	0.650	83.675	1301.467	1329.263
68	0.625	84.300	1302.318	1330.640
69	0.601	94.901	1303.054	1332.049
70	0.578	85.479	1303.845	1333.498
71	0.555	86.034	1303.711	1334.987
72	0.534	86.568	1304.557	1336.516
73	0.513	87.081	1305.469	1338.083
74	0.494	87.575	1306.454	1339.687
75	0.475	88.049	1307.518	1341.325
76	0.456	88.506	1308.667	1342.995
77	0.439	88.945	1309.909	1344.695
78	0.422	89.368	1311.251	1342.421
79	0.406	89.774	1312.702	1348.167
80	0.391	90.165	1314.269	1349.929
81	0.376	90.542	1315.959	1351.702
82	0.362	90.904	1317.779	1353.477
83	0.349	91.253	1321.736	1357.005
84	0.336	91.589	1321.833	1357.005
85	0.324	91.924	1324.073	1358.741
86	0.312	92.224	1326.456	1360.445

APPENDIX E (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
87	0.300	92.524	1328.978	1362.108
88	0.289	92.813	1331.631	1363.720
89	0.278	93.092	1334.401	1365.271
90	0.268	93.360	1337.270	1366.752
91	0.258	93.618	1340.215	1368.154
92	0.249	93.867	1343.207	1369.472
93	0.240	94.107	1346.214	1370.698
94	0.231	94.338	1349.198	1371.831
95	0.222	94.560	1352.998	1372.867
96	0.214	94.774	1355.698	1373.806
97	0.206	94.980	1358.281	1374.651

APPENDIX E

RESULTS FROM THE 50:1 REFLUX COMPARISON

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	1.806	1.806	89.102	252.443
2	0.855	2.660	89.366	285.503
3	1.416	4.076	130.179	306.692
4	1.726	5.802	178.846	334.210
5	0.570	6.373	181.130	358.934
6	1.723	8.096	207.725	367.762
7	0.553	8.648	215.466	392.884
8	1.679	10.328	244.245	399.607
9	1.424	11.752	260.278	422.239
10	0.769	12.521	267.279	440.719
11	1.654	14.175	292.446	450.725
12	0.667	14.842	299.695	472.812
13	1.604	16.447	322.914	480.943
14	1.382	17.829	342.448	501.987
15	1.139	18.968	351.127	518.617
16	1.542	20.510	370.222	534.205
17	1.619	22.129	395.585	557.151
18	0.706	22.835	399.095	579.926
19	1.595	24.430	421.736	590.476
20	0.668	25.098	436.019	614.558
21	1.504	26.602	465.316	622.146
22	1.541	28.143	494.321	641.766
23	0.849	28.992	497.487	659.300
24	1.510	30.503	519.196	669.722
25	0.884	31.386	526.453	687.547
26	1.395	32.782	542.339	697.861
27	1.481	34.263	569.836	715.273
28	0.922	35.185	573.032	731.752
29	1.438	36.623	592.241	742.976
30	0.819	37.442	600.756	760.285
31	1.415	38.857	619.081	769.639
32	0.999	39.855	628.848	786.769
33	1.102	40.957	640.067	798.691
34	1.373	42.399	670.064	813.184
35	1.133	43.463	673.393	828.582
36	1.328	44.791	689.435	843.326
37	0.952	45.743	694.777	860.931
38	1.273	47.016	707.718	874.839
39	1.024	48.040	725.644	895.379

APPENDIX E (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
40	0.996	49.036	734.543	910.563
41	1.262	50.298	770.041	927.835
42	1.132	51.430	771.745	945.954
43	1.193	52.623	787.096	965.934
44	0.336	52.959	787.165	988.691
45	1.371	54.330	880.002	996.245
46	1.317	55.647	880.002	1006.320
47	1.264	56.911	880.003	1017.964
48	1.213	58.124	880.003	1031.598
49	1.165	59.289	880.004	1047.822
50	1.118	60.407	880.006	1067.504
51	0.698	61.104	880.016	1090.816
52	1.243	62.348	1010.008	1109.784

APPENDIX E

RESULTS FROM THE 0.01:1 REFLUX COMPARISON

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	1.806	1.806	89.153	252.443
2	0.862	2.668	89.560	285.489
3	1.411	4.079	130.288	306.310
4	1.727	5.806	179.132	334.240
5	0.638	6.444	181.982	358.907
6	1.720	8.164	208.070	368.652
7	1.146	9.311	229.101	393.981
8	1.231	10.542	245.071	407.732
9	1.692	12.234	265.394	424.872
10	0.978	13.213	277.421	447.861
11	1.210	14.422	292.954	459.200
12	1.622	16.044	322.941	476.227
13	0.913	16.957	328.358	496.099
14	1.612	18.569	348.955	507.783
15	1.268	19.836	361.360	528.688
16	0.918	20.755	372.083	546.266
17	1.611	22.365	396.256	560.181
18	0.855	23.220	404.532	583.667
19	1.269	24.489	422.396	595.662
20	1.562	26.051	465.151	615.421
21	0.813	26.863	468.020	633.962
22	1.533	28.396	494.323	644.439
23	0.884	29.280	501.316	662.417
24	1.502	30.782	520.100	672.769
25	1.219	32.001	535.483	691.070
26	0.991	32.992	544.863	705.020
27	1.474	34.466	569.792	717.375
28	0.940	35.407	575.672	734.148
29	1.432	36.839	593.154	745.356
30	1.095	37.933	609.333	762.978
31	1.278	39.211	620.816	775.105
32	1.403	40.614	639.469	791.153
33	0.773	41.386	647.598	808.428
34	1.359	42.746	671.241	817.603
35	1.060	43.805	676.689	833.658
36	1.317	45.122	690.599	847.422
37	1.017	46.139	699.182	865.666
38	1.068	47.207	709.440	880.617
39	1.282	48.489	733.781	898.210

APPENDIX E (Continued)

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
40	0.716	49.205	737.807	917.935
41	1.256	50.462	770.661	930.018
42	1.093	51.555	772.748	948.498
43	1.188	52.743	787.192	968.046
44	0.224	52.967	787.489	991.323
45	1.371	54.338	880.003	996.300
46	1.316	55.654	880.003	1006.385
47	1.264	56.918	880.004	1018.038
48	1.213	58.131	880.005	1031.685
49	1.164	59.295	880.007	1047.927
50	1.118	60.413	880.011	1067.633
51	0.691	61.104	880.032	1090.976
52	1.243	62.348	1010.010	1109.785

APPENDIX E

RESULTS FROM THE 15% REMOVAL COMPARISON

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	2.658	2.658	89.102	252.443
2	1.430	4.087	130.179	306.647
3	2.175	6.262	178.852	334.342
4	1.976	8.238	207.681	366.395
5	2.395	10.633	243.839	394.956
6	1.924	12.557	265.714	425.976
7	1.941	14.498	292.478	451.153
8	2.266	16.764	323.306	477.070
9	2.479	19.243	347.976	505.633
10	1.674	20.917	369.884	537.882
11	1.880	22.797	395.978	562.294
12	1.720	24.517	421.720	589.985
13	2.231	26.748	464.690	615.720
14	2.241	28.989	494.486	643.257
15	2.205	31.194	519.209	669.693
16	1.911	33.105	542.082	695.739
17	2.202	35.306	569.451	718.565
18	1.957	37.264	592.427	744.312
19	2.276	39.540	618.835	767.741
20	1.696	41.236	639.401	794.940
21	2.536	43.772	670.440	816.061
22	2.254	46.026	690.044	847.122
23	1.596	47.622	708.452	879.064
24	1.570	49.192	733.782	904.140
25	2.458	51.649	770.222	929.856
26	1.308	52.957	787.115	969.685
27	5.143	58.100	880.002	996.236
28	3.004	61.104	880.004	1047.472
29	4.662	65.766	1010.008	1109.784
30	3.674	69.441	1010.011	1146.703
31	4.040	73.480	1130.007	1206.894

APPENDIX E

RESULTS FROM THE CRUDE BLENDING

	PERCENT VOLUME		
RUN	FRACTION	CUMULATIVE	CONDENSER TEMPERATURE (F)
1	1.314	1.314	89.132
2	0.707	2.201	130.241
3	1.045	3.066	179.007
4	0.994	4.059	207.800
5	1.101	5.160	244.111
6	1.021	6.182	265.734
7	1.630	7.812	293.029
8	0.565	8.377	299.282
9	0.837	9.214	323.371
10	1.091	10.305	348.457
11	0.941	11.246	370.561
12	1.624	12.870	395.918
13	0.601	13.472	401.672
14	0.679	14.150	422.991
15	1.482	15.632	457.681
16	0.753	16.385	466.436
17	1.599	17.984	495.059
18	0.753	18.738	501.935
19	0.981	19.718	522.772
20	1.515	21.234	541.294
21	1.045	22.279	557.375
22	1.230	23.509	572.515
23	1.248	24.757	595.063
24	1.287	26.044	610.318
25	1.036	27.080	623.200
26	1.384	28.464	638.260
27	1.575	30.039	669.579
28	0.981	31.020	673.307
29	1.313	32.333	692.078
30	1.140	33.473	702.865
31	1.106	34.579	720.557
32	1.268	35.846	732.687
33	1.074	36.921	753.302
34	1.488	38.409	771.422
35	1.048	39.456	780.511
36	1.065	40.522	791.948
37	0.962	41.483	819.309
38	1.220	42.703	853.771
39	1.542	44.245	881.048

APPENDIX E (Continued)

RUN	PERCENT VOLUME FRACTION	PERCENT VOLUME CUMULATIVE	CONDENSER TEMPERATURE (F)
40	1.480	45.724	882.048
41	1.223	46.948	883.048
42	0.512	47.460	895.061
43	1.587	49.047	1010.249
44	1.524	50.571	1010.195
45	1.043	51.613	1011.118
46	1.471	53.084	1080.444
47	1.412	54.496	1080.342
48	1.356	55.853	1080.842
49	1.304	57.156	1080.786
50	1.123	58.280	1081.795
51	1.378	59.657	1130.014

APPENDIX E

RESULTS FROM THE MIDDLE EASTERN CRUDE ASTM DISTILLATION

	PERCENT VOLUME		TEMPERATURE (F)	
RUN	FRACTION	CUMULATIVE	CONDENSER	REBOILER
1	4.999	4.999	149.78	260.91
2	4.781	9.780	181.46	300.88
3	4.469	14.250	198.76	337.31
4	4.271	18.520	225.95	383.37
5	3.996	22.517	238.68	425.53
6	3.920	26.436	284.99	498.13
7	4.175	30.612	419.33	583.61
8	3.788	34.399	403.37	612.13
9	3.886	38.285	523.80	679.79
10	3.669	41.954	549.65	715.35
11	3.493	45.446	579.42	754.49
12	3.145	48.592	547.70	782.86
13	3.372	51.963	709.64	868.77
14	3.244	55.207	739.75	911.44

VITA

Bruce Earl Baugher

Candidate for the Degree of

Master of Science

Thesis: COMPUTER SIMULATION OF A MULTICOMPONENT, MULTISTAGE BATCH DISTILLATION PROCESS

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Salem, Illinois, September 1, 1962, the son of Earl and Jarilyn Baugher.

Education: Graduated as Valedictorian from Yukon High School, Yukon, Oklahoma, in May 1981; received Bachelor of Science Degree in Chemical Engineering from Oklahoma State University in May 1985; completed requirements for the Master of Science Degree in Chemical Engineering at Oklahoma State University in July 1988.

Professional Experience: Project Engineer, U.S. Department of Energy, Albuquerque, New Mexico, June 1985 through August 1986; Research Assistant, School of Chemical Engineering, Oklahoma State University, June 1987 through May 1988.