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Distillation Simulation Using
Physical Homotopies

by

Ronald William Bondy

A THESIS

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

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Ron W. Bondy

(Student's Signature)

326 E Francis Ave.
La Habra, California
U.S.A.
90631
(Student's Permanent Address)

Date: October 6 / 1988

THE UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled Distillation Simulation Using Physical Homotopies submitted by Ronald William Boudy in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

A E Mather
....
(Supervisor)
Dr. A.E. Mather

....
(Supervisor)
Dr. K. Nandakumar

Loren Hepler
....
Dr. L. Hepler

....
Dr. D.B. Robinson

Date: October 6, 1988

ABSTRACT

One of the problems with using Newton's method to solve systems of non-linear equations is that when the algorithm fails the reason why it failed is not known. In distillation simulation, the reason is either that the starting point was poor or that the column was given physically infeasible specifications. This work investigated homotopy continuation methods to determine how they would perform when physically infeasible specifications were made on the column. It was found that continuation methods did not "blow up" as Newton's method does, and that continuation methods failed in such a way that the limiting value of the specifications could be determined.

Two new physical homotopies were developed. The first path follows in artificial heater/coolers. These were used to eliminate the residuals in the enthalpy balance equations at the start of the homotopy path. The second homotopy applied to interlinked columns. The columns were decoupled at the start of the path and the interaction between the columns was introduced as the path was followed.

Problems were studied which had physically infeasible specifications. It was found that the paths resulting from the continuation methods were smooth, and gave physical insight into what was happening in the problems. When the paths stopped, approached a limiting value asymptotically or turned around the limiting values of the specifications were indicated. While these results are encouraging, there is no guarantee that this is always true in the general case.

Multiple steady state solutions were observed for a system of interlinked columns.

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I would also like to thank Simulation Sciences for allowing me to use their computer equipment for producing my thesis.

Finally I would like to thank my wife Cathy for her patience and understanding throughout these first three years of our married life.

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Nomenclature

D	Molar Distillate Rate, kmol/h
E	General Tray Enthalpy Balance Equation
ER	Summation of Equilibrium Ratios Equation
F	Molar Flowrate, kmol/h
H	Molar Enthalpy, kJ/kmol
K	Equilibrium Ratio
L	Liquid Molar Rate, kmol/h
LF	Liquid Feed Molar Rate, kmol/h
LS	Liquid Sidedraw Molar Rate, kmol/h
m	General Tray Mass Balance Equation
p	Path Length
NS	Non Standard Equation
R	Reflux Ratio, L_1/D
S	Summation of Liquid Mole Fractions
T	Absolute Temperature, K
t	Homotopy Parameter
Q	Heat Duty, kJ/h
V	Vapour Molar Rate, kmol/h
VF	Vapour Feed Molar Rate, kmol/h
VS	Vapour Sidedraw Molar Rate, kmol/h
w	Scaling Factor
x	Liquid Mole Fraction
y	Vapour Mole Fraction

Subscripts

ar	artificial heater/cooler
c	Calculated Values from the solution of the matrix Equations 5.16
DR	Pumparound Draw Tray
i	Component Number
j	Tray Number, equation 3.1, figure 3.1
k	Tray Number for liquid draw, equation 3.1, figure 3.1
l	Tray Number for vapour draw, equation 3.1, figure 3.1
PU	Pumparound
RE	Pumparound Return Tray

Superscripts

L	Liquid
S	Specified Value
V	Vapour

Greek Letters

Δ	Difference
Σ	Summation
∂	Partial Derivative Operator

4.2 Path Following in Artificial Heater/Coolers

The two main sources of nonlinearity in distillation problems are the equilibrium relationships and the enthalpy balances. To the best of our knowledge no physical homotopy has addressed the enthalpy balance effects, and this led to the development of path following in artificial heater/coolers. The heater/coolers are 'artificial' because they are not physically present; they are just a tool used to facilitate solutions.

This method was developed to address the nonlinearity introduced into the distillation equations by the enthalpy balance. While this nonlinearity is most significant for wide boiling mixtures, it has also been found useful when solving narrow boiling mixtures. The method also has potential to be used in heat integration, heat exchanger networks, and highly exothermic or endothermic chemical reactors. Any physical models which have nonlinear enthalpy balances are candidates to be solved with this approach.

The basic idea behind path following in artificial heater/coolers is simple. The solution to a *simple problem*, for example assuming constant molar overflow (and thus neglecting enthalpy effects) is obtained first. The resulting solution for the composition and temperature clearly do not satisfy the enthalpy balance equations. The imbalance of the enthalpy equations is made up by the addition of artificial heater/coolers. The heat duties of the artificial heater/coolers are calculated such that the error in the enthalpy balance on each tray is zero. When any actual heaters or coolers are present then their duties are taken into account if they are known. In this way, if an estimate of the condenser or reboiler duty is known, then the value of the artificial heater cooler will be small. Figure 4.5 shows a schematic diagram of a 'tray' with an artificial heater/cooler.

The homotopy equation is constructed from the enthalpy balance equation in such a way that when t=0 the solution corresponds to one including the artificial heater/coolers and when t=1 the desired solution is obtained. This results from the modified heat balance which is written to include the artificial heater/cooler:

$$E_j = H^L_{j-1} L_{j-1} + H^L_k LF_k + H^V_{j+1} V_{j+1} + H^L_l VF_l -$$

$$H^L_j(L_j+LS_j) - H^V_j(V_j+VS_j) + Q_j + (1 - t)Q_{ar} = 0 \qquad (4.26)$$

This equation is the same as the normal enthalpy balance except for the addition of the $(1 - t)Q_{ar}$ term, where Q_{ar} is the value of the artificial heater/cooler.

The value of the artificial heater cooler at t=0 is a good indicator of how close the initial profile is to the true solution. If the artificial heater/coolers are small relative to the enthalpies of the streams entering and leaving the stage, then the initial temperature and vapour/liquid traffic profiles are probably very good.

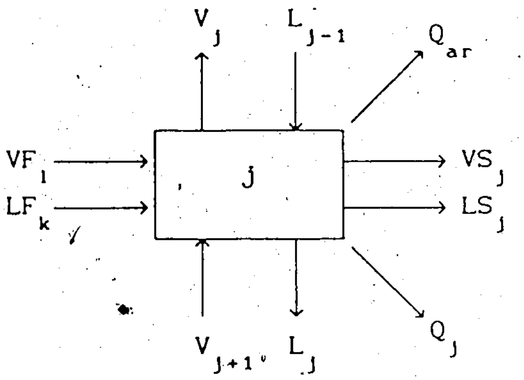


Figure 4.5

Schematic Diagram of a General Tray Showing the Addition of the Artificial Heater/Cooler

4.3 Path Following in Structure

One of the most difficult hydrocarbon distillation columns to solve is the crude column with attached sidestrippers. Browne, Ishii and Otto showed that this is done most robustly if all the equations are solved simultaneously. However, Newton's method will still fail if the initial estimate is poor. In order to address the problems associated with this type of system, path following in structure was developed.

Path following in structure is a general idea which can be used in any system which has heat and/or mass recycle streams. In a crude column, the vapour return from the sidestrippers to the main column can be considered a recycle. This is a general idea which can be applied in a large number of places.

The basic idea behind path following in structure is simple. At the start of the homotopy path the recycle stream is torn (it is not recycled). In the case of a column with sidestrippers, when the vapour return to the main column is torn, it becomes a vapour product from the sidestripper. As the homotopy path is followed, the fraction recyled is gradually increased. At the end of the homotopy path, all of the stream is recycled, and the solution to the desired problem has been reached.

Path following in structure in a column with sidestrippers is implemented as follows. Consider figure 4.6, which is a portion of a distillation column with a sidestripper attached. Tray m is the top of the sidestripper, and V_m is the tearing stream. At the start of the homotopy path (t=0) none of the stream is returned to the main column, it is all a product. While actual columns are not built this way, it is physically meaningful. This type of system will be easier to solve because there is now no interaction between the main column and the sidestripper(s).

Path following in structure usually requires modification of the original specifications in order to solve the initial problem. Suppose that a 5% true boiling point (or a purity) was specified in the distillate stream. If there was stripping steam introduced in the bottom of the reboiler, then the purity specification may be impossible to meet because at the start of the path stripping steam is not being introduced to the main column.

In this work, the original specifications were replaced by rate and reflux ratio specifications. The reflux ratio was arbitrarily set at 3, and the feed was evenly distributed between the products requiring new specifications. Initial estimates of the product rates were not implemented because if good initial estimates were available then Newton's method would probably converge anyway, and continuation would not be necessary. Section 4.4 (Path Following in Non Standard Specifications) explains how the specification equations are included in the homotopy equations as the homotopy path is followed.

Once the initial problem is solved, then path following begins. As the homotopy path is followed, the vapour stream is introduced to the main column according to tV_m and the vapour product is decreased according to $(1-t)V_m$. This strategy is very easy to implement because there is no modification to the equations for tray m. The only stage that requires modification is the general balance for tray j. This equation becomes

$$m_j = x_{j-1}L_{j-1} + x_kLF_k + x_{j+1}K_{j+1}V_{j+1} + x_mK_mtVF_m -$$

$$x_j(L_j+LS_j)-x_jK_j(V_j+VS_j)=0 \qquad (4.27)$$

The only difference between equation 5.23 and the original mass balance equation (3.1) is the introduction of the factor t into the term for the vapour feed from tray m. Note that the component subscript has been omitted for clarity.

The new enthalpy balance becomes

$$E_j = H^L_{j-1}L_{j-1} + H^L_k LF_k + H^V_{j+1}V_{j+1} + H^L_m tVF_m -$$

$$H^L_j(L_j+LS_j) - H^V_j(V_j+VS_j) + Q_j + (1-t)Q_{ar} = 0 \qquad (4.28)$$

As in the mass balance equation, the only difference in equation 4.28 from the original enthalpy balance equation (3.2) is the introduction of the factor t into the term for the enthalpy of the vapour feed from tray m and the duty of the artificial heater/cooler.

Note that the homotopy parameter t appears twice in equation 4.28. Different homotopy parameters could be used, however this would require another constraint equation in order to keep the number of variables and equations the same. Although there are no literature examples of using multiple homotopy parameters in distillation calculations, this appears to be a reasonable approach to implementing continuation methods. Using the same homotopy parameter in heat and mass balance equations couples the equations. This forces the mass and the heat to be introduced into the equation set at the same rate. Since mass and heat are fundamentally different quantities, it may be better to use different homotopy parameters for different physical quantities.

When multiple solutions occur along the same homotopy path, the homotopy path will pass through t=1.0, go through a turning point, and pass through t=1.0 again. In order for the calculations not to fail, the system of equations must be defined for t > 1.0. When path following in structure, what does $t > 1.0$ mean?

Consider figure 4.6, the diagram for path following in structure. When $t > 1.0$, more of stream V_m is returned to stage j than is drawn from stage m. This means that the stream which was a product stream is now a feed stream. As the value of t changes when $t > 1$, the physical interpretation of this is that the composition of the external feed stream of rate $|1-t| V_m$ is always the same as the composition of stream V_m.

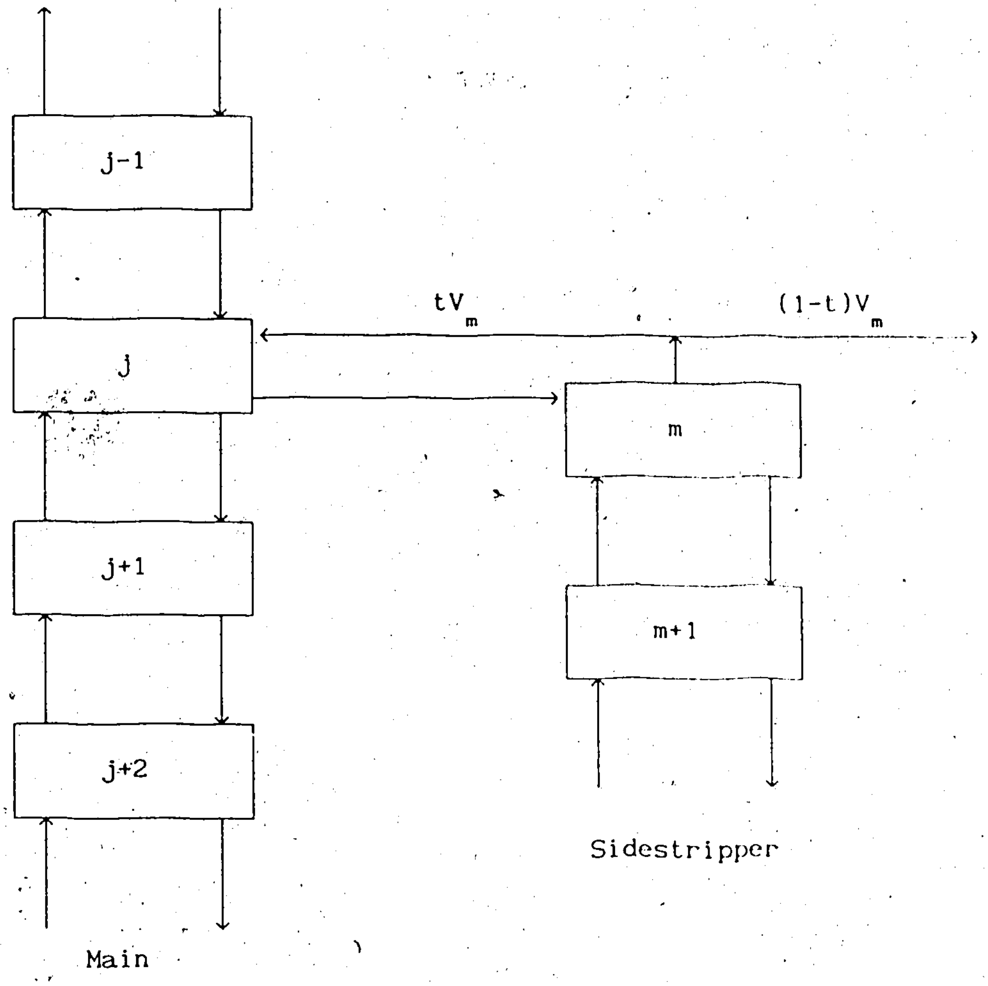


Figure 4.6
Schematic Diagram of a Distillation Column
With Sidestripper for Path Following in
Structure

4.4 Path Following in Non Standard Equations

One of the advantages of Newton's method is the great flexibility allowed for specifications. Essentially anything that can be expressed in equation form can be used as a specification, subject to mathematical and physical constraints. Ferraris (1981) shows how this can be done in distillation calculations and how to solve the resulting matrix efficiently.

Mathematically, specifications must preserve linear independence. Physically, specifications must not violate mass and energy conservation or thermodynamic limitations. For example, it is possible to specify a distillate product purity which cannot be obtained with the specified reflux ratio and number of trays.

One benefit of continuation methods using physical homotopies is the ability to detect physically infeasible specifications. Divergence due to poor initial estimates is avoided by choosing initial problems which are sufficiently easy that accurate initial estimates are not necessary. This is a strong point of this work and the efficient homotopy of Vickery and Taylor (1987). However, mathematical homotopies overcome the starting point problem the best by being able to start from any vector of initial estimates.

In order to detect when physically infeasible specifications are present using physical homotopies, the initial problem must contain specifications that are easy to solve. They can be different types of specifications (reflux ratio and product rates are good choices) or relaxed values of the desired specifications. For example, suppose it is desired to solve a column with one of the distillate products specified to a purity of 99.99%. The initial problem could be to solve an easier problem with a purity of 95%, and then path following could be used to obtain the desired solution with the 99.99% purity. This type of approach could be used to simulate the manufacture of high purity gases (oxygen, nitrogen, carbon dioxide) where cryogenic conditions are needed.

When path following, the path may stop before t=1. This usually occurs because one of the independent variables reaches a physical limit (zero flow rate, zero mole fraction). The reason that the path stops before t=1 is either that one of the specifications is infeasible for the column configuration, or that the homotopy path naturally goes through this non physical region. Unfortunately there appears to be no method to distinguish between the causes for a homotopy path going into a non physical region.

Although in this work none of the latter cases were encountered, they cannot be ruled out. If the reason that the path stops is because of a physically infeasible specification, the point where the path stops indicates the limiting value of the specification.

For example, consider a distillate purity specification. The mole fraction of the light component in the distillate (x_{11}) is desired to be 0.9999. The initial problem has been solved such that x_{11} = 0.95. The homotopy equation for this specification is

$$NS = x_{11} - 0.95 - 0.0499\ t = 0. \tag{4.29}$$

Suppose that the homotopy path stops at t = 0.1. This would indicate that the value x_{11} = 0.95499 is the maximum purity that can be achieved given the other parameters (i.e. number of trays and reflux ratio, condenser and reboiler duties) specified for the column.

To the best of our knowledge this is the first implementation of non standard specifications in physical homotopies. This approach should be compatible with other physical homotopies such as those of Taylor and Vickery. , The ability to detect non physical specifications is a great aid to solving simulation problems.

The other result of path following in non standard equations is that they may force a turning point. For example, when path following in component purity, the mole fraction of any component is constrained to be less than 1.0 because of the equation which constrains the mole fractions to sum to 1.0. Note that values of t greater than 1.0 still have physical meaning for these types of specifications. For example, consider the mole fraction constraint equation

$$NS = x_{11} - 0.80 - 0.10t = 0 \tag{4.30}$$

At the start of the path the value of x_{11} will be 0.80, and at the solution (t=1.0) x_{11} will be 0.90. However, when t=1.5, x_{11} must be 0.95, which is still physically possible. The maximum value that t can reach is t=2.0, when x_{11} would be equal to 1.0. Therefore a turning point would have to occur at or before a value of 2.0. The reason that the turning point may occur before 2.0 is that there may be something else that is physically limiting in the problem.

It is important to note that since the equations do not contain constraints on individual liquid or vapour flows, these liquid or vapour flows may become negative. These constraints could be added to the equation set as,

$$L_n - \lambda^2 = 0 \tag{4.31}$$

$$V_n - \lambda^2 = 0 \tag{4.32}$$

These constraints could also be added with the square mapping function, which has already been mentioned.

4.5 Solving the Initial Problem

The solution of the initial problem is crucial in solving problems by homotopy continuation. While for the mathematical homotopies this is trivial, for physical homotopies it usually will require some iterative calculation. An iterative calculation is undesirable because it provides an opportunity for the method to fail. However, by choosing a homotopy with a good physical basis the initial problem should almost always converge. In this work the initial problem never failed to converge for the hydrocarbon systems studied.

The first step in solving the initial problem is to initialize the liquid and vapour traffic in the column. This is done such that there are no errors in the overall mass balance. The mass balance around the condenser is done first, then the remaining trays are done in a stagewise fashion from tray 2 to the condenser.

If the distillate rate is not specified, then the specifications are checked to see if the distillate rate can be obtained by mass balance. For example, if the bottoms product rate is specified and there are only two products from the column, then the distillate product rate is the feed rate minus the specification for the bottoms rate. If the distillate rate cannot be obtained in this manner, it is not specified and there is no user estimate given, then a value of 50% of the feed is used.

Next, if the reflux ratio is not known, then a value of three is assumed. Using the distillate rate and reflux ratio the amount of liquid reflux leaving the condenser can be calculated. Then using the estimates for the distillate and liquid reflux the amount of vapour entering the condenser can be calculated.

Starting at the second tray, the vapour leaving and the liquid entering are known from the condenser calculation. Assuming constant molar overflow, the liquid leaving and vapour entering tray 2 are calculated. This procedure is repeated for each tray until the reboiler is reached. At the reboiler, the bottoms product is given by the liquid rate entering minus the vapour rate leaving the reboiler.

There are two other cases which require special attention. The first is how to treat sidestrippers. Sidestrippers are initialized before the main column liquid and vapour traffic. This is so the sidestripper draw and return rates are known when the main column is done. If the product rate from the sidestripper is not known, and it cannot be estimated from the given specifications (including a specification on the liquid draw rate from the main column), then the draw rate is estimated at 10% of the feed to the column. If the draw rate from the main column is not known, then it is assumed to be 50% greater than the sidestripper product rate. The sidestripper liquid and vapour traffic are initialized assuming constant molar overflow.

The second special case is a pumparound. If a pumparound rate was not known then it was assumed to be 50% of the liquid entering the tray from which the pumparound was drawn from. This allows the pumparound return tray traffic to be calculated before the pumparound draw tray. While these heuristics were not based on any data, they were adequate to generate good starting points for the homotopy path.

Once the liquid and vapour traffic are initialized, then the temperature profile must be calculated. One of the strengths of the proposed method is that the starting estimates for this temperature profile need not be very accurate. The temperature profile is calculated to satisfy only the equilibrium relationships. The enthalpy balances are ignored here and the path following in artificial heater/coolers remove the enthalpy balance residuals which remain after the initial problem is solved. The removal of the enthalpy balances from the initial problem makes this a very stable procedure. Another benefit of this approach is that the more accurate the initial liquid and vapour traffic the more accurate the temperature profile will be and the smaller the enthalpy balance residuals will be.

At this point the iterative procedure begins. Component liquid mole fractions are solved for using the Wang and Henke method as outlined by Henley and Seader (1981). After this, the liquid mole fractions on [illegible]re normalized. Now the temperature on each tray is found using [illegible] method such that the sum of the vapour mole fractions is [illegible]s procedure is repeated until the temperature on each tray is stable and the liquid and vapour mole fractions sum to one. When these conditions are met the initial problem has been solved.

This procedure hinges on the fact that iterating on the composition is a stable procedure. While this is true for hydrocarbon systems, this may not be true for chemical systems. Chemical systems were not studied here, and this would be a good topic for future research.

1.0 Introduction

In the modern refinery, distillation accounts for a large percentage of the energy usage. It is therefore important to be able to model the distillation process for purposes of process control and optimization. Currently there are many algorithms available to solve the model equations governing distillation processes; however there are still some difficult problems for which better algorithms are needed.

To model distillation processes requires the solution of a complex set of non-linear equations. Unfortunately, these non-linear equations require iterative solution techniques which work best when some *a priori* estimate of the solution is known. The problem with these iterative methods is that when the solution diverges, it is not known if it is because of a poor initial estimate, if it is because the specifications violate the thermodynamic constraints of the physical system or if the intermediate solution enters a non physical domain (i.e. negative mole fractions) causing the thermodynamic calculations to fail. This has always been the main problem with using Newton's method.

Recently, researchers have been investigating a new method for solving a system of non-linear equations, the homotopy continuation method. This method has two main uses. The first use is in finding a *family of solutions* to a given problem as a *physical parameter* is varied. For example it may be used to investigate how the solution to a distillation column changes as the reflux ratio is varied.

The second use of continuation methods is in finding a solution to a set of non-linear equations starting from any arbitrary starting point. This is important because there are some problems where Newton's method will only converge with an initial estimate which is very close the the initial solution, which is certainly not always possible.

2.0 Literature Review

Recently, there has been much work done using homotopy continuation methods. It is important to note that when reading the literature homotopy continuation methods are also known as homotopy methods, continuation methods, parameterized continuation methods or one parameter imbedding techniques. In this work they will be referred to as homotopy continuation or continuation methods. A history of distillation will not be given here. For excellent historical reviews, see Wang and Wang, 1981, and Seader, 1985.

Before beginning the literature review it is necessary to introduce some of the concepts and terms used when discussing continuation methods. Homotopy continuation is a general mathematical technique for solving a system of non-linear equations. Since the early 1980's it has been used in chemical engineering research to solve a wide variety of difficult distillation problems. The method consists of introducing a new parameter into the set of distillation equations (the homotopy parameter) which makes the equations easy to solve for the initial value of the parameter. The parameter value is incremented and the resulting locus of solutions (homotopy path) is tracked until the terminal value of the parameter is reached. At the terminal value the equation set reduces to the original set of equations that was to be solved.

There are two general classes of homotopy problems. The first class uses continuation to find a solution to a set of non-linear equations. The second class uses continuation to trace the value of some physical parameter in the problem, such as reflux ratio. So far most work in distillation has focused on the first class of applications, trying to get solutions to distillation problems that are difficult to converge using Newton's or other methods. This work is also concerned with applying continuation to the first class of problems.

The simplest method of path following is known as the classical continuation method or continuation by iteration. In this method, the homotopy equations are solved first at the initial value of the homotopy parameter. Then the homotopy parameter is incremented and the previous solution is used as a starting point to solve the homotopy equations at the new value of the homotopy parameter. This process is repeated until the terminal value of the homotopy parameter is reached. This approach has been shown to work satisfactorily in physical homotopies, but not in mathematical homotopies.

A more sophisticated way to solve the homotopy equations is to actually predict where the next point will be along the homotopy path. Once the prediction is made, a few steps are taken to get back onto the path. This process is repeated until the terminal value of the homotopy parameter is reached. These are known as the differential arclength continuation or predictor corrector methods. The advantage of this method is that it can follow the homotopy path around turning points.

It is possible that while path following the path will turn back on itself, that is for the homotopy parameter to begin decreasing, and going back towards the initial value of t. The point at which the homotopy path turns back on itself is called a turning point or limit point. When multiple solutions exist there will be turning points along the path.

Salgovic et al. (1981) showed that continuation methods could be used to expand the region of convergence over Newton's method. They used a linear mathematical homotopy and compared three different methods for solving the homotopy equations. Their first method integrated the homotopy equations once using an Euler integrator, then invoked Newton's method at the end of the path. Using different initial guesses, they showed where this approach converged when Newton's method diverged. They also showed that the smaller the step size in the Euler predictor, the poorer the initial estimate could be for the column to solve. The second way that they solved the homotopy equations was using a restart method with a simple Euler integrator. This was found to be very slow to converge. The third way they solved the homotopy equations was using a fifth order Runge Kutta integrator. While this gave reliable solutions, the computation time was about an order of magnitude greater than their first approach.

Bhargava and Hlavacek (1984) investigated a linear and a non linear mathematical homotopy. They applied continuation to distillation of chemical systems (systems requiring liquid phase activity coefficients). Their primary interest was to see if continuation methods were more robust than Newton's method. They found several problems (including dehydration of ethanol with benzene) which solved with continuation and diverged with Newton's method. They used continuation by iteration and the restart homotopy using Euler's method. They found that from a very poor starting point it was best to integrate the homotopy equations two or three times and then use Newton's method. From a good starting point they found it was best to use continuation by iteration.

Byrne and Baird (1985) used a proprietary homotopy to solve difficult distillation problems. Their interest was to see if continuation methods were more robust than Newton's method for highly non ideal systems such as sour water strippers and azeotropic distillation towers. Unfortunately, the homotopy they used was proprietary. They used a predictor corrector method to follow the homotopy path. They were able to solve distillation problems using continuation that did not solve with Newton's method starting from the same starting point.

Chavez et al. (1981) found multiple steady state solutions to a system of interlinked columns. They used the Newton homotopy with a predictor corrector algorithm. They also employed a sophisticated step size adjustment algorithm (Georg, 1980) which determined what the size of the next predictor step should be. In the original work the multiple solutions were found by trying different arbitrary starting guesses.

Requiring different starting guesses to find multiple solutions is unsatisfactory because an infinite number of starting points would be required to ensure that all solutions had been found. The most desirable situation is to have all of the solutions along the same homotopy path. Chavez et al. followed the homotopy paths past the endpoints (t-1.0) to see if the paths would turn around and return to a different solution. When this was done the liquid and vapour traffic and some mole fractions became negative. To get around this problem, Lin et al.(1987) used a square mapping function that allowed them to find all of the solutions of Chavez et al. along a single path. The square mapping function constrains the values of the mole fractions, liquid and vapour flows and temperature to be positive, and allows the independent (mapped) variables to be negative. The drawback to the method is that 2^n (where n is the dimension of the problem) new solutions are introduced. While the method of Lin et al. cannot guarantee that all the solutions will indeed be on a single path, the results are encouraging because for their problem they were successful.

Vickery and Taylor (1986) used physical homotopies to show that continuation has a wider region of convergence than Newton's method. They solved the difficult problems of extractive and azeotropic distillation. They have used path following in thermodynamics and in tray efficiency. The driving force behind their approach to solving problems by continuation is to develop a physical homotopy which deals with the main source of non linearity in the physical problem. For the problems of extractive and azeotropic distillation the main source of non linearity is in the liquid phase activity coefficients. Hence they chose first to path follow in K values. At the start of the homotopy path they solve the system with ideal K values. As they follow the path they introduce the non linearity from the activity coefficients into the K value. They have also used path following in stage efficiency. The idea here is that at low stage efficiency there is very little separation and so this problem is easy to solve. As the stage efficiency is increased, the problem becomes more non linear, and because the non linearity is being introduced incrementally it is easy to solve each point along the homotopy path.

Vickery and Taylor were able to solve problems that failed using continuation alone. It is interesting to note that they reported very little benefit using predictor corrector methods instead of classical continuation by iteration. This implies that physical homotopies result in paths which are smoother, which is the desired case. Also, they did not encounter any turning points, whereas Chavez et al. (1986) did. The only drawback to the work of Vickery and Taylor is that they only used distillate and reflux ratio specifications. It would appear that they can also use general specifications, as developed in this thesis.

Ellis et al. (1986) used continuation to path follow in physical parameters, bottoms rate and liquid sidedraw rate. They compared Euler's method, the semi-implicit Runge-Kutta and Gear's method to integrate the homotopy equations. They reported that Gear's method performed the best. Unfortunately they did not consider any sort of step size predictor for Euler's method as others had done to provide an additional basis for comparison.

Kovach and Seider (1987) solved an extractive distillation column using a mathematical homotopy. They model the equation set the same as Wayburn and Seader and use the Newton homotopy. In their model two liquid phases were allowed to form on any stage. In order to determine when two liquid phases were present, they did a liquid liquid equilibrium (LLE) flash calculation. They also employed a physical homotopy in their LLE flash calcluations.

They also report good success; however they indicate that each problem initially requires manual tuning of the parameters involved in the predictor step of following the homotopy path. This is disconcerting because it restricts the use of their methods to only those people who are knowledgeable with the details of predictor corrector algorithms.

These papers have concentrated on applying different types of homotopies to solve complex hydrocarbon and chemical distillation systems. They have shown that path following can increase the region of convergence over Newton's method. However, none have considered the question of whether or not path following algorithms can offer a reliable method of determining when physically impossible specifications have been made. This work seeks to answer this question.

3.0 Mathematical Model

In this chapter the equations used to model distillation are presented, as well as the structure of the Jacobian matrix and a degree of freedom analysis. The distillation model uses ideal stages, and allows for pumparounds, sidestrippers and side heaters and coolers. The model does not include entrainment or chemical reaction.

3.1 Distillation Equations

The equations solved are the mass and energy balance equations, equilibrium relationships and mole fraction constraint equations. These are written for the general tray shown in Figure 3.1. The sign conventions adopted here are that heat and mass flows in are positive and heat and mass flows out are negative. Here LF_k denotes a liquid feed from stage k and VF_l denotes a vapour feed from stage l. Liquid and vapour draws from stage j are denoted by LS_j and VS_j respectively. F_j is an external fixed feed.

3.1.1 Component Mass Balance Equation

Equation (3.1) is for a given component on stage j. For clarity the component subscript has been omitted.

$$m_j = F_j z_j + x_{j-1} L_{j-1} + x_k LF_k + x_{j+1} K_{j+1} V_{j+1} + x_l K_l VF_l - x_j(L_j + LS_j) - x_j K_j (V_j + VS_j) = 0 \qquad (3.1)$$

This formulation allows for liquid and vapour traffic between non adjacent stages. LF_k is the rate of liquid from stage k that feeds stage j (i.e. a liquid pumparound return stream), and VF_l is the rate of vapour from stage l that feeds stage j (i.e. the vapour return to the main column from the top of a sidestripper). F_j is the rate of an external (fixed) feed, and z_j the concentration of component i in the external feed. LS_j and VS_j are the rates of liquid and vapour product streams from stage j.

The substitution $y_j=K_jx_j$ has already been made in equation 3.1 to remove the vapour mole fraction y_j from the equation set. If the Murphree vapour phase efficiency were used, then the vapour mole fractions could not be removed from the equation set. Also note that because there are no chemical reactions, the material balance can be written either in terms of mass or moles. Mole balances are used here because mole fractions are required in the equation of state calculations.

3.1.2 Enthalpy Balance Equations

The enthalpy balance for a general tray is given by

$$E_j = F_jH_j^F + H_{j-1}^L L_{j-1} + H_k^L LF_k + H_{j+1}^V V_{j+1} + H_i^V VF_i -$$

$$H_j^L(L_j+LS_j) - H_j^V(V_j+VS_j) + Q_j = 0 \qquad (3.2)$$

For heat addition $Q_j>0$ and for heat removal $Q_j<0$.

3.1.3 Sum of Liquid Mole Fractions

$$S_j = \sum_i x_{ij} - 1 = 0 \qquad (3.3)$$

3.1.4 Sum of Equilibrium Ratios

$$ER_j = \sum_i K_{ij}x_{ij} - 1 = 0 \qquad (3.4)$$

3.15 Specification Equations

For any given distillation problem, the number of specifications is equal to the number of degrees of freedom. The degrees of freedom analysis will be presented in section 3.3. Specification equations are implemented as described by Ferraris (1981). A discussion of incorporating specification equations in the homotopy equations is found in section 5.4. Following are the five types of specification equations used in this work. Note that due to the flexibility of Newton's method many other types of specifications are possible.

a) Flow Rate Specification

$$NS_1 = F - F^S = 0 \qquad (3.5)$$

Here F denotes any molar flowrate, and F^S is the desired (specified) flowrate. In this work the flowrates available for specification are the distillate, bottoms, and sidestripper product rates, the pumparound rate, and the rate of the liquid draw from the main column to feed the sidestripper.

b) Mole Fraction Purity Specification

$$NS_2 = x_{ij} - x^S_{ij} = 0 \qquad (3.6)$$

Here x_{ij} denotes the liquid mole fraction for the i^{th} component on the j^{th} stage, and x^S_{ij} is the specified value. In this work the purity specification was implemented for product streams.

c) Reflux Ratio

$$NS_3 = L_1 - R^S D = 0 \qquad (3.7)$$

Here L_1 is the molar rate of liquid from the condenser which enters the second tray, R^S is the specified reflux ratio, and D is the molar distillate rate.

d) Pumparound Energy Balance

$$NS_4 = F_{PU} (H^L_{RE} - H^L_{DR}) - Q_{PU} = 0 \qquad (3.8)$$

Here F_{PU} is the pumparound flowrate, H^L_{RE} and H^L_{DR} are the pumparound liquid return and draw enthalpies, and Q^S_{PU} is the specified pumparound heat duty.

e) Pumparound Flow Rate

$$NS_5 = F_{PU} - F^S_{PU} = 0 \qquad (3.9)$$

Here F_{PU} is the pumparound flowrate and F^S_{PU} is the specified (desired) pumparound flow rate.

f) Pumparound Duty

$$NS_6 = Q_{PU} - Q^S_{PU} = 0 \tag{3.10}$$

Here Q_{PU} is the pumparound duty and Q^S_{PU} is the specified (desired) pumparound duty.

g) Pumparound Temperature Difference

$$NS_7 = T_{RE} - T_{DR} - \Delta T^S = 0 \tag{3.11}$$

Here T_{RE} and T_{DR} are the pumparound return and draw temperatures, and ΔT^S is the specified temperature difference. Note that $\Delta T^S > 0$ to cool the liquid.

It is important to note that for pumparounds only two specifications are allowed, since specifying two of pumparound rate, duty and return thermal condition (i.e., pumparound return temperature) fixes the third unspecified quantity. Non standard specification equation 4 (equation 3.8) is an enthalpy balance for the pumparound, and does not contain any specified values. Therefore a pumparound with two specifications contains equation 3.8 and two of equations 3.9, 3.10 or 3.11.

3.2 Jacobian Elements and Structure

Solving all equations in a non linear system simultaneously using Newton's method has long been recognized as the preferred method for solving a system of non linear equations. However only in the last 10 years has the computing power been available to make Newton's method a viable choice for solving distillation problems. This is due to the large number of equations that result in a distillation problem. When solving a problem using Newton's method, the calculation of the Jacobian matrix (the matrix of first partial derivatives) is where most of the calculation time is spent.

To get around the problem of solving all of the equations simultaneously, a number of tearing procedures have been proposed. The method of Wang and Henke (1966) solved the component material balance for each component individually. They showed that this could be done using a simple tridiagonal matrix structure, which gave the method low solution times. However, it was found that the method worked best for narrow boiling mixtures, and was unstable for wide boiling mixtures.

The method of Boston and Sullivan (1974, later extended by Russell, 1983) used an Inside/Out loop structure. In the inner loop, simple thermodynamic models were used to model enthalpy and K values. In the outer loop the simple thermodynamic models were updated using rigorous models, and a convergence check was made. The independent variables chosen were the stripping factors, and a tridiagonal system of equations was solved for component mole rates. By solving for component mole rates the solution was always in mass balance, and this helped to accelerate the solution. This method has been found to very robust and is used by at least five commercial simulators today. However, due to the approximations used in the K value model (K values are modelled in the inner loop as functions of temperature only) the algorithm does not work well for chemical systems which require liquid phase activity coefficients.

Naphtali and Sandholm (1971) were the first to solve all of the distillation equations simultaneously using Newton's method. This is also known as the Global Newton Raphson method. They showed that if the equations were grouped by stage that a block tridiagonal Jacobian resulted. Their method worked well for both wide and narrow boiling mixtures, and for columns with or without condensers or reboilers.

However, to solve the resulting Jacobian matrix it had to be partially stored on disk because computer random access memories were not as large as they are today. Their block tridiagonal structure forms opened the way for the simultaneous solution of the distillation equations using Newton's method.

Ishii and Otto (1973) also solved all equations simultaneously, but partitioned the equations into submatrices for the component material balances and energy balances. This also required that the tridiagonal matrix be inverted and Ishii developed a fast algorithm to do this. Later, Browne, Ishii and Otto(1977) showed that for systems of distillation columns, simultaneous solutions were faster than solving each column separately and iterating between the tear streams.

With faster CPU's and larger memory, the Global Newton Raphson is becoming the standard way to solve large sparse problems. Questions concerning scaling and conditioning of the Jacobian to enlarge the region of convergence and thus produce reliable and flexible algorithms are the subjects of current research. Global Newton Raphson was chosen in this work because of the flexiblity in specifications and the ease of use in continuation schemes. As will be shown, the Jacobian matrix for use in continuation methods is the same as that used in the Global Newton Raphson method, except that an extra row and column are added to the borders of the matrix.

3.2.1 Jacobian Structure

The Jacobian structure will be illustrated for a distillation column with sidestripper and a distillation column with two pumparounds. These distillation columns are shown in figures 3.2 and 3.3. Since the simulator is developed in a modular form, it can handle any number of trays and components, with no restrictions on pumparound return and draw trays. First the non-zero structure of the Jacobian for the column with attached sidestripper will be considered.

Figure 3.4 shows the block tridiagonal bordered structure which results for the distillation column with sidestripper. Based on the recommendations of Wayburn(1983) the sidestripper trays are inserted in the Jacobian after the tray where the liquid draw from the main column is taken. This results in the submatrices for the liquid from tray 3 to tray 4 and the vapour from tray 4 to tray 3 being away from the block tridiagonal submatrices. There are 7 different types of submatrices in figures 3.4 and 3.5. Each one represents the different internal and external streams in a distillation column. Figures 3.6 through 3.12 show the non-zero structure for each of the submatrices. The example presented has 4 components. Note that the equations are arranged such that as many diagonal entries are non-zero as possible. This results in less rearrangement for the sparse matrix package. Also note that the important derivative of enthalpy with respect to temperature is found on the diagonal. This will be one of the larger elements in the matrix, thus helping to form a diagonally dominant structure.

Note that there is no enthalpy balance equation for the condenser or reboiler. This is possible because the duty is not a specification. The duties are calculated from the converged solution (the temperatures of the condenser and reboiler are calculated to meet the bubble point condition). Figures 3.9 and 3.10 show how the non-standard specification equation replaces the enthalpy balance in the condenser and reboiler. NS_1, NS_2, and NS_3 correspond to equations 3.5, 3.6 and 3.7 respectively.

Figure 3.11 shows the non-zero structure for the Jacobian for the liquid feed to the top of a sidestripper. This is the same as submatrix type A, except that the coefficients for the liquid rate are zero. This is because only the compositions and enthalpy from the draw tray influence the top tray of the sidestripper. The liquid draw rate is another variable which appears on the border of the Jacobian.

By introducing the liquid draw rate as another variable into the system of equations, it is necessary to introduce another equation to keep the system well posed. This is shown as the row which is appended to the Jacobian as shown in figure 3.4. While the simplest equation to introduce is one which fixes the rate of the liquid draw rate, any specification which does not violate mathematical or thermodynamic constraints can be used. Specifications are discussed in greater detail in section 5.4.

Figures 3.5 and 3.5a show the Jacobian structure for a column with two pumparounds. Each pumparound introduces an additional three equations and three unknowns into the Jacobian matrix. The unknowns for each pumparound are the pumparound flowrate, duty, and return temperature. Two specification equations are allowed, and an enthalpy balance for the pumparound is required. In the example in figure 3.5, the first pumparound has the flowrate and duty specified, and the second pumparound has the flowrate and temperature difference specified.

In this work the specifications introduced for the additional pumparound variables relate to the pumparounds. However, Newton's method does not restrict the additional specification ~~equat~~ions to the pumparounds, any valid specification is acceptable. Suppose it was desired to find the pumparound flow and duty which would meet two additional purity specifications beside the usual distillate rate and reflux ratio specifications. Although any arbitrary values could be specified for the purities, they may not be possible with the reflux and distillate rates specified. There will most likely be a small range over which additional feasible specifications could be made.

3.2.2 Component Mass Balance Derivatives

The derivatives for the component mass balance equations follow. Note that the component subscript has been omitted for clarity. The partial derivatives of K values with respect to composition have been assumed to be zero. The small error which is introduced into the Jacobian matrix will at worst slow convergence. It does not affect the final solution because the K values are calculated rigorously from the equation of state, and are always used in the evaluation of the model equations 3.1 through 3.9. For hydrocarbon systems, the composition effect on the K values is minimal and so setting them to zero does not have any noticeable effect on convergence.

$$\frac{\partial m_j}{\partial x_{j-1}} = L_{j-1} \tag{3.12}$$

$$\frac{\partial m_j}{\partial L_{j-1}} = x_{j-1} \tag{3.13}$$

$$\frac{\partial m_j}{\partial x_k} = LF_k \tag{3.14}$$

$$\frac{\partial m_j}{\partial LF_k} = x_k \tag{3.15}$$

$$\frac{\partial m_j}{\partial x_{j+1}} = K_{j+1} V_{j+1} \tag{3.16}$$

$$\frac{\partial m_j}{\partial V_{j+1}} = x_{j+1}K_{j+1} \qquad (3.17)$$

$$\frac{\partial m_j}{\partial T_{j+1}} = x_{j+1}V_{j+1}\frac{\partial K_{j+1}}{\partial T_{j+1}} \qquad (3.18)$$

$$\frac{\partial m_j}{\partial x_i} = K_i VF_i \qquad (3.19)$$

$$\frac{\partial m_j}{\partial VF_i} = x_i K_i \qquad (3.20)$$

$$\frac{\partial m_j}{\partial T_i} = x_i VF_i \frac{\partial K_i}{\partial T_i} \qquad (3.21)$$

$$\frac{\partial m_j}{\partial x_j} = -(L_j + LS_j + K_j(V_j + VS_j)) \qquad (3.22)$$

$$\frac{\partial m_j}{\partial L_j} = -x_j \qquad (3.23)$$

$$\frac{\partial m_j}{\partial LS_j} = -x_j \qquad (3.24)$$

$$\frac{\partial m_j}{\partial V_j} = -x_j K_j \qquad (3.25)$$

$$\frac{\partial m_j}{\partial VS_j} = -x_j K_j \qquad (3.26)$$

$$\frac{\partial m_j}{\partial T_j} = -x_j(V_j + VS_j)\frac{\partial K_j}{\partial T_j} \qquad (3.27)$$

Note that equations 3.24 and 3.26 are necessary when sidedraws are variables. This occurs for pumparounds when the rate is not specified, and for the liquid draw from the main column to a sidestripper when the sidestripper rate is a variable.

3.2.3 Enthalpy Balance Derivatives

The following are the partial derivatives for the enthalpy balance equations. The component subscript has been omitted for clarity.

$$\frac{\partial E_j}{\partial L_{j-1}} = H^L_{j-1} \tag{3.28}$$

$$\frac{\partial E_j}{\partial x_{j-1}} = L_{j-1} \frac{\partial H^L_{j-1}}{\partial x_{j-1}} \tag{3.29}$$

$$\frac{\partial E_j}{\partial T_{j-1}} = L_{j-1} \frac{\partial H^L_{j-1}}{\partial T_{j-1}} \tag{3.30}$$

$$\frac{\partial E_j}{\partial LF_k} = H^L_k \tag{3.31}$$

$$\frac{\partial E_j}{\partial x_k} = LF_k \frac{\partial H^L_k}{\partial x_k} \tag{3.32}$$

$$\frac{\partial E_j}{\partial T_k} = LF_k \frac{\partial H^L_k}{\partial T_k} \tag{3.33}$$

$$\frac{\partial E_j}{\partial V_{j+1}} = H^V_{j+1} \tag{3.34}$$

$$\frac{\partial E_j}{\partial x_{j+1}} = V_{j+1} \frac{\partial H^V_{j+1}}{\partial x_{j+1}} \tag{3.35}$$

$$\frac{\partial E_j}{\partial T_{j+1}} = V_{j+1} \frac{\partial H^V_{j+1}}{\partial T_{j+1}} \tag{3.36}$$

$$\frac{\partial E_j}{\partial VF_l} = H^V_l \tag{3.37}$$

$$\frac{\partial E_j}{\partial x_l} = VF_l \frac{\partial H^V_l}{\partial x_l} \tag{3.38}$$

$$\frac{\partial E_1}{\partial T_1} = LF_1 \frac{\partial H^L_1}{\partial T_1} \qquad (3.39)$$

$$\frac{\partial E_j}{\partial L_j} = -H^L_j \qquad (3.40)$$

$$\frac{\partial E_j}{\partial LS_j} = -H^L_j \qquad (3.41)$$

$$\frac{\partial E_j}{\partial V_j} = -H^V_j \qquad (3.42)$$

$$\frac{\partial E_j}{\partial VS_j} = -H^V_j \qquad (3.43)$$

$$\frac{\partial E_j}{\partial x_j} = -(L_j + LS_j) \frac{\partial H^L_j}{\partial x_j} - (V_j + VS_j) \frac{\partial H^V_j}{\partial x_j} \qquad (3.44)$$

$$\frac{\partial E_j}{\partial T_j} = -(L_j + LS_j) \frac{\partial H^L_j}{\partial T_j} - (V_j + VS_j) \frac{\partial H^V_j}{\partial T_j} \qquad (3.45)$$

3.2.4 Sum of Liquid Mole Fractions

$$\frac{\partial S_j}{\partial x_j} = 1 \qquad (3.46)$$

3.2.5 Sum of Equilibrium Ratios

$$\frac{\partial ER_j}{\partial x_j} = K_j \qquad (3.47)$$

$$\frac{\partial ER_j}{\partial T_j} = \sum x_j \frac{\partial K_j}{\partial T_j} \qquad (3.48)$$

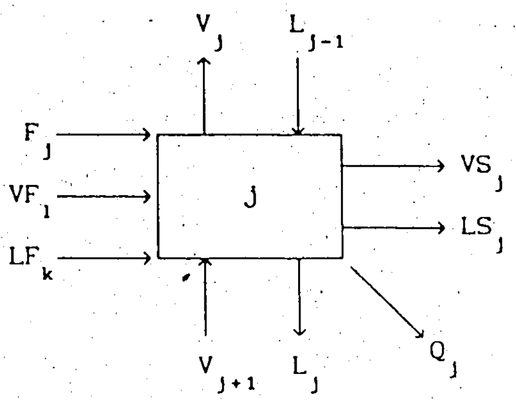


Figure 3.1
Schematic Diagram of a General Tray

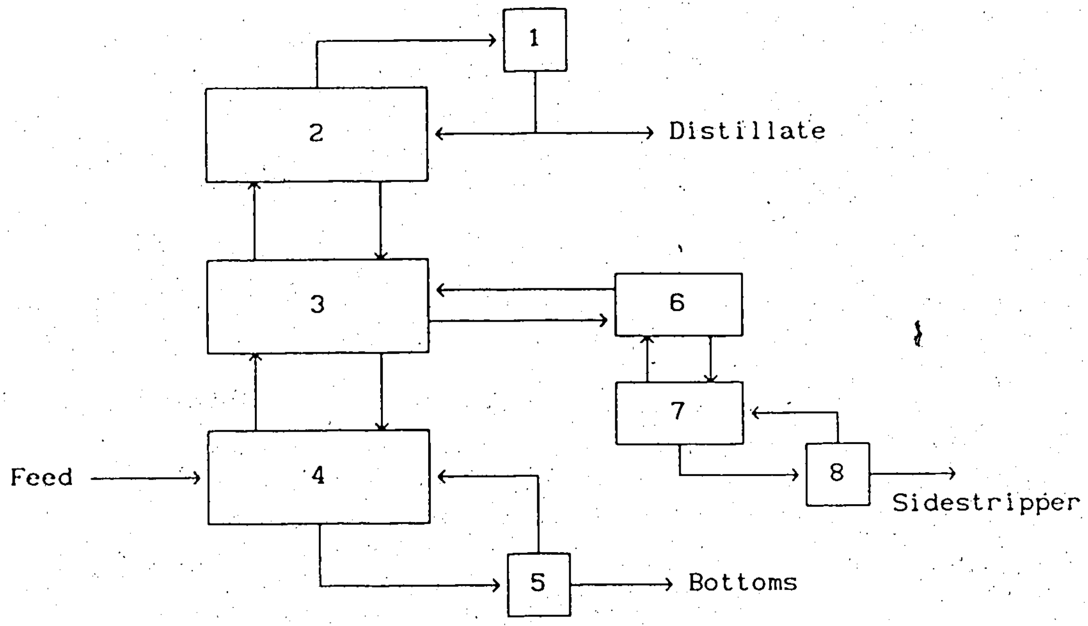


Figure 3.2

Schematic Diagram of Distillation Column
With Sidestripper

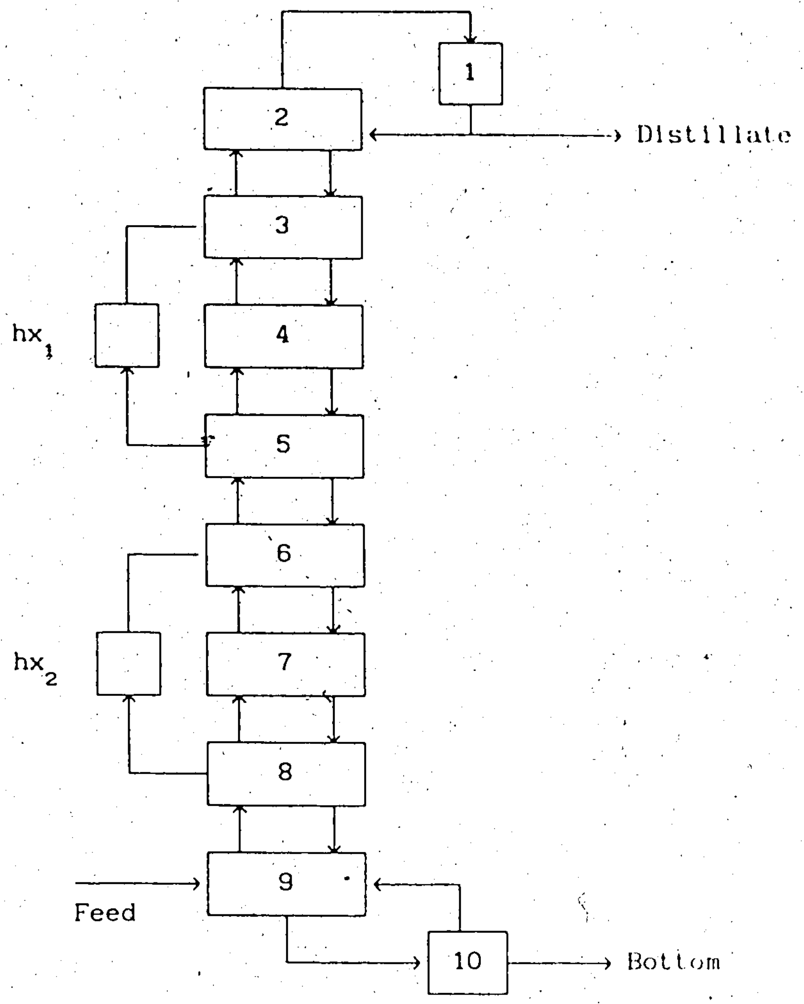
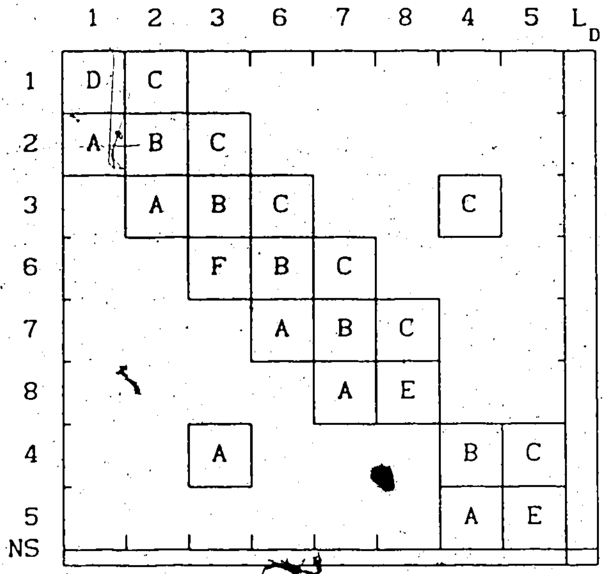


Figure 3.3

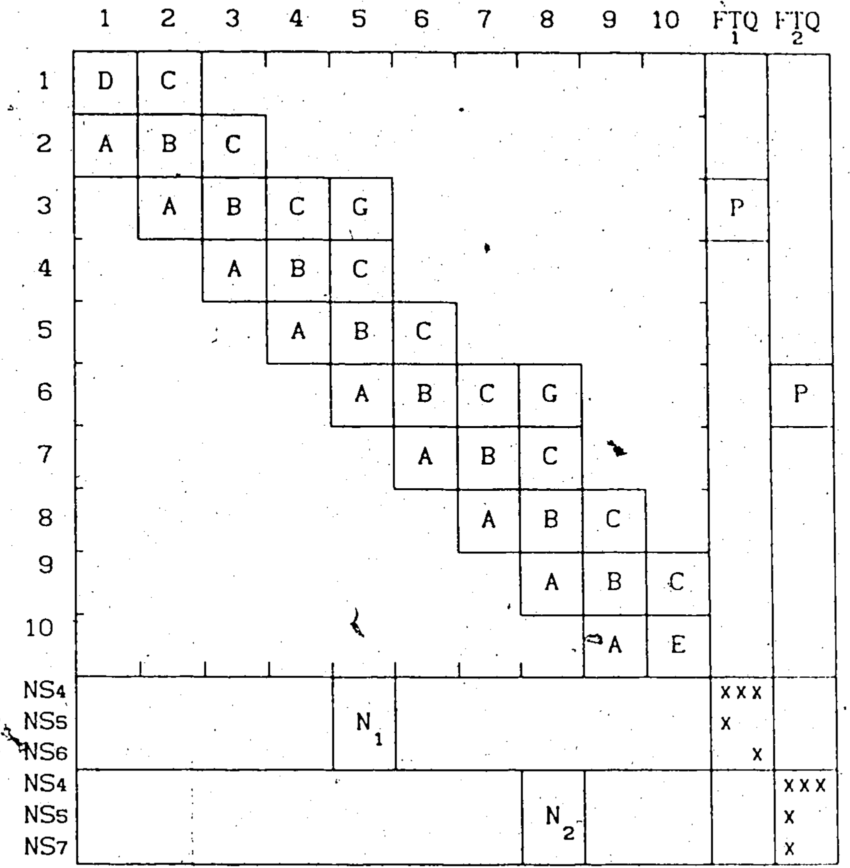
Schematic Diagram of Distillation Column
With Two Pumparounds



	1	2	3	6	7	8	4	5	L_D
1	D	C							
2	A	B	C						
3		A	B	C			C		
6			F	B	C				
7				A	B	C			
8					A	E			
4			A				B	C	
5							A	E	
NS									

Figure 3.4

Jacobian Submatrix Structure
For Column With Sidestripper



	1	2	3	4	5	6	7	8	9	10	FTQ 1	FTQ 2
1	D	C										
2	A	B	C									
3		A	B	C	G						P	
4			A	B	C							
5				A	B	C						
6					A	B	C	G				P
7						A	B	C				
8							A	B	C			
9								A	B	C		
10									A	E		
NS4					N_1						x x x	
NS5											x	
NS6											x	
NS4								N_2				x x x
NS5												x
NS7												x

Figure 3.5

Jacobian Submatrix Structure
For Column With Two Pumparounds

	x_{15}	x_{25}	x_{35}	x_{45}	L_5	V_5	T_5
NS_4							X
NS_5							
NS_6							

Submatrix N_1

	x_{15}	x_{25}	x_{35}	x_{45}	L_5	V_5	T_5
NS_4							X
NS_5							
NS_7							X

Submatrix N_2

	F	T	Q
m_1	X		
m_2	X		
m_3	X		
m_4	X		
SF			
ER			
E	X	X	

Submatrix P

Figure 3.5a

Submatrices for Pumparounds from Figure 3.5

	x_1	x_2	x_3	x_4	L	V	T
m_1	X				X		
m_2		X			X		
m_3			X		X		
m_4				X	X		
SF							
ER							
E	X	X	X	X	X		X

Figure 3.6

Non-Zero Jacobian Elements for Liquid Feed
(Submatrix Type A)

	x_1	x_2	x_3	x_4	L	V	T
m_1	X				X	X	X
m_2		X			X	X	X
m_3			X		X	X	X
m_4				X	X	X	X
SF	X	X	X	X			
ER	X	X	X	X			X
E	X	X	X	X	X	X	X

Figure 3.7

Non-Zero Jacobian Elements For Liquid
And Vapour Leaving a Tray
(Submatrix Type B)

	x_1	x_2	x_3	x_4	L	V	T
m_1	X					X	X
m_2		X				X	X
m_3			X			X	X
m_4				X		X	X
SF							
ER							
E	X	X	X	X		X	X

Figure 3.8

Non-Zero Jacobian Elements for Vapour Feed
(Submatrix Type C)

	x_1	x_2	x_3	x_4	L	D	T
m_1	X				X	X	
m_2		X			X	X	
m_3			X		X	X	
m_4				X	X	X	
SF	X	X	X	X			
ER	X	X	X	X			X
NS_1						X	
NS_2	X						
NS_3					X	X	

Figure 3.9

Non-Zero Jacobian Elements For Condenser
(Submatrix Type D)

	x_1	x_2	x_3	x_4	B	V	T
m_1	X				X	X	X
m_2		X			X	X	X
m_3			X		X	X	X
m_4				X	X	X	X
SF	X	X	X	X			
ER	X	X	X	X			X
NS_1					X		
NS_2	X						
NS_3					X	X	

Figure 3.10

Non-Zero Jacobian Elements For Reboiler
(Submatrix Type E)

	x_1	x_2	x_3	x_4	L	V	T
m_1	X						
m_2		X					
m_3			X				
m_4				X			
SF							
ER							
E	X	X	X	X			X

Figure 3.11

Non-Zero Jacobian Elements for Liquid Feed
to Top of Sidestripper
(Submatrix Type F)

	x_1	x_2	x_3	x_4	L	V	T
m_1	X						
m_2		X					
m_3			X				
m_4				X			
SF							
ER							
E	X	X	X	X			

Figure 3.12

Non-Zero Jacobian Elements for Pumparound Feed Composition Effects (Submatrix Type G)

3.3 Degrees of Freedom Analysis

The difference between the number of independent equations and variables in a given system of equations is called the degrees of freedom. The number of variables specified must equal the degrees of freedom so that a solution to the system of equations can be found, if a solution does indeed exist. In this work only solutions in the real domain are considered.

A degrees of freedom analysis is performed here as outlined by Henley and Seader(1980). The basic idea is that every system can be broken down into a number of smaller subsystems. This process is repeated until the subsystems correspond to systems for which the degrees of freedom are already known. Then the degrees of freedom for each subsystem are summed, taking into account interlinking streams. Table 3.1 lists all the subsystems used here and the number of degrees of freedom for each system. Appendix I has a sample calculation showing that the number of degrees of freedom for a total condenser is C+4 (where C is the number of components).

Table 3.1
Degrees of Freedom for Subsystems

Subsystem	Degrees of Freedom
Total Condenser	C+4
Reflux Divider	C+5
N Stage Cascade	2N+2C+5
Interlink Stage	3C+9
Feed Stage	3C+8
Partial Reboiler	C+4
Tray with Sidedraw	2C+7

Note: C= number of components
N= number of stages

Figure 3.12 shows how the distillation column with sidestripper is simplified to do the degrees of freedom analysis. The degrees of freedom are calculated as follows:

Main Column	Degrees of Freedom
Total Condenser	$C + 4$
Reflux Divider	$C + 5$
N_1 Stage Cascade	$2N_1 + 2C + 5$
Interlinking Stage	$3C + 9$
N_2 Stage Cascade	$2N_2 + 2C + 5$
Feed Stage	$3C + 8$
N_3 Stage Cascade	$2N_3 + 2C + 5$
Partial Reboiler	$C + 4$
Sub Total	$2(N_1+N_2+N_3) + 15C + 45$
13 Repeated Streams	$- 13(C + 2)$
Total	$2(N_1+N_2+N_3) + 2C + 19$

To simplify matters, let $N = N_1+N_2+N_3+4$, which is equal to the total number of equilibrium stages in the distillation column (note that the reflux divider is not counted as an equilibrium stage).

Total degrees of freedom = $2N + 2C + 11$ for the main column.

Sidestripper	Degrees of Freedom
M_1 Stage Cascade	$2N_1 + 2C + 5$
Partial Reboiler	$C + 4$
Sub Total	$2M_1 + 3C + 9$
2 Repeated Streams	$- 2(C + 2)$
Total	$2M_1 + C + 5$

Substitute $M = M_1 + 1$ so that M is the total number of equilibrium stages in the sidestripper.

Total degrees of freedom = 2M + C + 3 for the sidestripper.

Now the total degrees of freedom for the system can be found.

COMPLETE SYSTEM:

Main Column	2N + 2C + 11
Sidestripper	2M + C + 3
Sub Total	2(N + M) + 3C + 14
2 Repeated Streams	− 2(C + 2)
Total Degrees of Freedom for the system	2(N + M) + C + 10

The next step is to sum the degrees of freedom used up in assumptions regarding the known quantities of the distillation column. These assumptions are:

1) Pressure of all stages including condenser, reboilers and the reflux divider.	M+N+1
2) Heat transfer to/from all stages including the reflux divider, but excluding the condenser and reboiler.	M+N−2
3) Degrees of subcooling in condenser	1
4) Number of stages in each column	1
5) Interlinking stage location	1
6) Feed stage location	1
7) Feed component flowrates, temperature and pressure	C + 2
Total Specifications	2(M+N) + C + 6

The number of additional specifications is given by

Total Degrees of Freedom	2(N + M) + C + 10
− Total Specifications	2(N + M) + C + 6
Additional Specifications	4

Therefore there are four more specifications which can be made. In this work they were chosen from product molar rate specifications, product purity specifications, reflux ratio, or by specifying the molar rate of the liquid sidedraw from the main column to the sidestripper.

The second example for a degrees of freedom analysis is a distillation column with two pumparounds. Figure 3.12 shows the subsystem breakdown for this system. Note that in this system each tray is a subsystem. As for Case 1 the degrees of freedom are calculated by summing the degrees of freedom for the subsystems and correcting for the redundant streams.

Column with Two Pumparounds	Degrees of Freedom
Condenser	C + 4
Reflux Divider	C + 5
Stage 2	2C + 7
Pumparound Return	3C + 8
Stage 4	2C + 7
Pumparound Draw	2C + 7
Pumparound Return	3C + 8
Stage 7	2C + 7
Pumparound Draw	2C + 7
Feed Stage	3C + 8
Partial Reboiler	C + 4
Pumparound Cooler	C + 4
Pumparound Cooler	C + 4
Subtotal	24C + 80
23 Repeated Streams	-23(C + 2)
Degrees of Freedom	C + 34

The next step now is to sum up the degrees of freedom used up in the assumed known quantities:

1) Heat transfer to/from all stages including reflux divider and excluding the condenser, reboiler, and pumparound cooler duties.	9
2) Pressure of all stages, reflux divider, and pumparound coolers	13
3) Subcooling in the total condenser and pumparound coolers.	3
4) Feed temperature, pressure and composition	C + 2
5) Feed stage location	1
Total	C + 28

The number of remaining specifications is given by

Total degrees of freedom of the system	C + 34
- Assumptions	C + 28
Total Degrees of Freedom of System	6

For this system there are six remaining degrees of freedom. This is intuitive as follows. A distillation column with condenser and reboiler alone has two additional specifications. Each pumparound has two degrees of freedom (specify two of pumparound rate, heat duty and temperature difference and the third quantity may be calculated). Since there are two pumparounds this gives a total of six additional specifications. In this work the remaining six specifications may be selected from pumparound rate, duty, temperature difference, product molar rate, reflux ratio or a product purity.

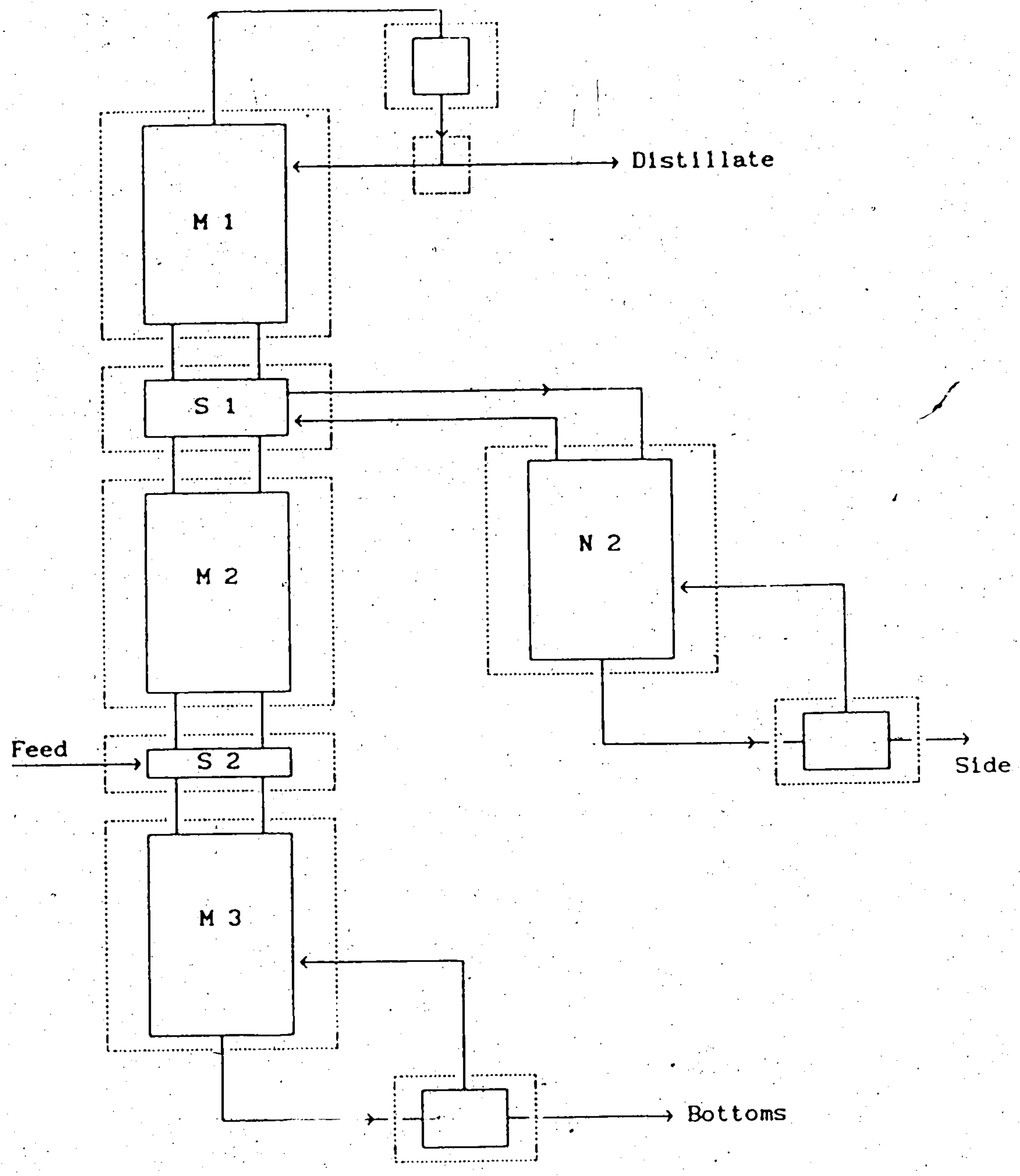


Figure 3.13
Subsystem Breakdown for Degrees of
Freedom Analysis for Distillation Column
with Sidestripper

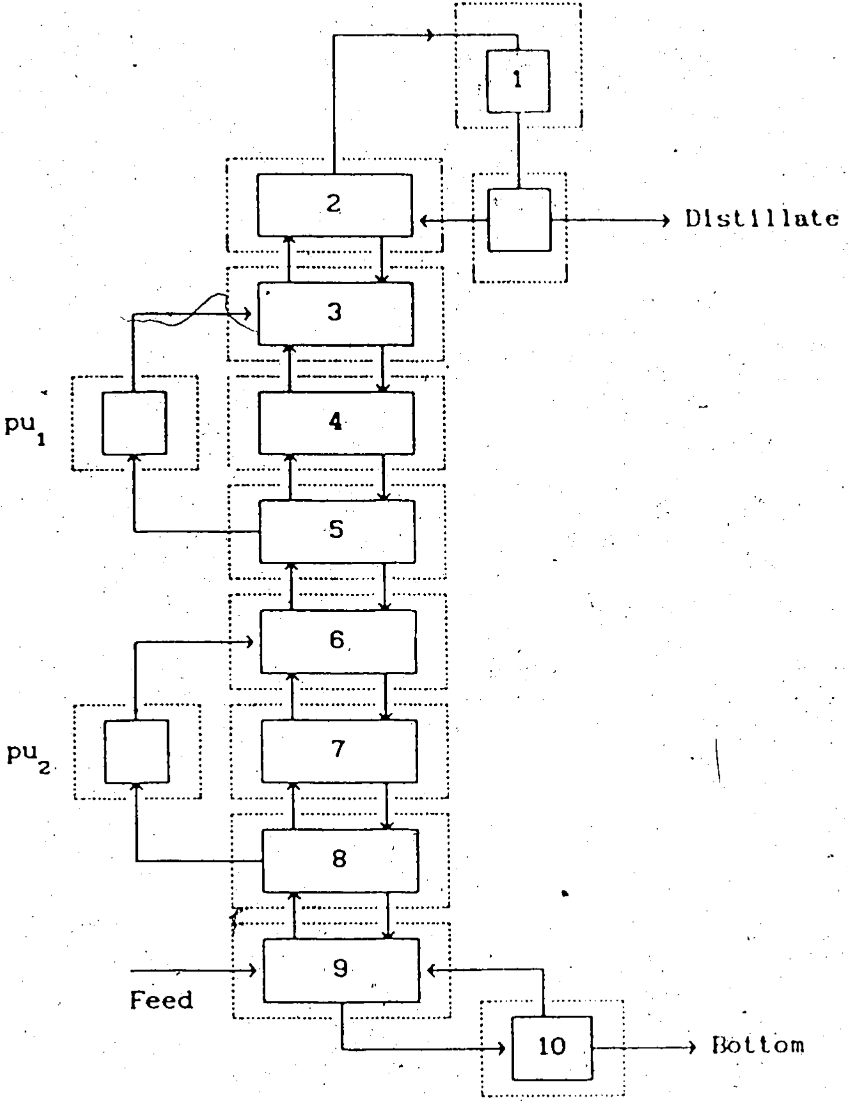


Figure 3.14

Subsystem Breakdown for Degrees of Freedom Analysis for Distillation Column with Two Pumparounds

4.0 Solution Algorithm

In this work the distillation equations are cast as a set of homotopy equations. These homotopy equations are then solved using differential arclength homotopy continuation. This chapter introduces the reader to the principles of homotopy continuation and provides details of the new homotopies developed in this work.

Two new physical homotopies are introduced here and their behaviour with a hydrocarbon mixture is explored. The first homotopy uses artificial heater/coolers to deal with the nonlinearity introduced into the distillation equations by the enthalpy balance. The second homotopy uses the structure of the problem to deal with the interactions between a main distillation column and a sidestripper.

Another new aspect of this work is the ability to include a wide range of nonstandard specification equations. This has not been done previously for physical homotopies. The concepts developed here can easily be applied to other physical homotopies such as in the work of Vickery and Taylor. First however the mathematics of homotopy continuation will be explained.

4.1 Solving a General System of Equations Using Continuation

Suppose it is desired to find the solution X^* to the system of equations

$$F(X) = 0 \tag{4.1}$$

$F(X) = 0$ is a vector valued function which can be expanded to

$$\begin{aligned} f_1(x_1, x_2, x_3, \ldots, x_n) &= 0 \\ f_2(x_1, x_2, x_3, \ldots, x_n) &= 0 \\ f_3(x_1, x_2, x_3, \ldots, x_n) &= 0 \\ &\vdots \\ f_n(x_1, x_2, x_3, \ldots, x_n) &= 0 \end{aligned} \tag{4.2}$$

Suppose that there exists another system $G(X) = 0$ for which the solution X^* is known or is easily found. The homotopy equations are created by blending $F(X)$ and $G(X)$ together. This is done using the homotopy parameter t (where t is a scalar). One possible (and popular) form of the homotopy equations is given by the general linear convex homotopy

$$H(X,t) = tF(X) + (1-t)G(X) = 0 \tag{4.3}$$

The homotopy equations have the following characteristics:

$$H(X,t=0) = G(X) = 0 \tag{4.4}$$

$$H(X,t=1) = F(X) = 0 \tag{4.5}$$

At t=0 the homotopy equations reduce to $G(X) = 0$, which is the simple system of equations. At t=1 the homotopy equations reduce to $F(X) = 0$, which is the desired set of equations. The locus of points at the solution to the homotopy equations for the different values of t is the homotopy path. Note that other forms of the homotopy equations are possible:

$$H(X,t) = (1-e^{-at})F(X) + e^{-at}G(X) = 0 \tag{4.6}$$

In the discussion which follows only the linear homotopy (4.3) will be considered.

There are many different choices for the function $G(X)$. The simplest is the fixed point homotopy,

$$G(X) = (X - X_0) = 0 \tag{4.7}$$

where X_0 is an arbitrary starting point. While this homotopy has flexibility with respect to the choice of an intial starting point, it suffers from poor scaling (Wayburn, 1983).

Another popular homotopy is the Newton homotopy,

$$G(X) = F(X) - F(X_0) = 0 \tag{4.8}$$

The homotopy equations reduce to

$$H(X,t) = F(X) - F(X_0) + tF(X_0) = 0 \qquad (4.9)$$

This is the homotopy used by Wayburn(1983) and Kovach(1986) to solve distillation problems.

The homotopies presented so far have been mathematical homotopies. These homotopies are general mathematical formulae which can be applied to any system of nonlinear equations. Another class of homotopy is the custom or physical homotopy. These homotopies exploit some aspect of the equation set or physical system. As their names imply e form of the homotopy equation will differ from problem to problem. Vickery and Taylor(1986) have used a physical homotopy in the solution of azeotropic distillation problems. Whether mathematical or physical homotopies are best for solving distillation problems is currently the subject of much debate.

There are also two different applications for homotopy continuation. The first one (which has already been presented) is to solve a system of nonlinear equations by introducing an artificial parameter t into the formulation. The second application is to trace out the locus of solutions as some physical parameter appearing naturally in the problem is varied. For example, reflux ratio could be chosen as the homotopy parameter. First a solution to the problem at a given reflux ratio must be found. Then the homotopy path could be followed and the solutions at different reflux ratios generated.

Another potentially important application is in the field of optimization. First the optimization problem must be cast as a set of equations (this can be done using Lagrange multipliers) and solved. Then the optimum can be traced as the homotopy path is followed with respect to some physical parameter. Multiple solutions can also be found using continuation methods(Lin et al., 1987). In this work continuation methods are used to find the solution to the distillation equations. For examples of path following with respect to a physical parameter in distillation see Ellis et al., 1986.

Up to this point it has been assumed that it is possible to follow the homotopy path that is formed by solving the equations as the homotopy parameter is varied from zero to one. The methods for following the homotopy path can be put into two groups. The first method is continuation by iteration, or the classical method. This is very easy to implement but is not capable of solving a system with a turning point along the homotopy path. However, Vickery and Taylor(1986) report good results using this method with physical homotopies. The second is the differential arclength method which is the method used in this study. This method is more robust than the previous method because it makes use of the information of how the variables change as the path is followed. First the classical method and then the differential arclength method will be presented.

4.1.1 Classical Homotopy Continuation

The classical continuation method can be easily incorporated into any existing method of solving a system of equations independent of the method used to solve the equations. The idea is very simple. First the equations are solved for some value of the homotopy parameter for which a solution is easily found. Then the homotopy parameter is incremented and the previous solution is used as the starting point for the solution at the current value of the homotopy parameter. This process is repeated until the desired value of the homotopy parameter has been reached.

Following is an algorithm to implement the classical continuation method.

```
1. Solve $H(X,t_0) = 0$.
If the solution fails, then stop.  Another value of $t_0$ should
be tried.
2. Let $t_k = t_{k-1} + \Delta t_k$.
If $t > t_f$ then $t = t_f$.
3. Solve $H(X,t_k) = 0$.
If $t_k = t_f$ and the solution was successful
    THEN
        stop
    ELSE if the solution was successful
        THEN
            go to step 2
        ELSE $\Delta t_{k+1} = \Delta t_k / 2$.
If $\Delta t_{k+1} > \Delta t_{min}$
    THEN
        go to step 2
    ELSE
        stop, classical continuation failed.
```

Figure 4.1 shows the solution space of the functions from example 2 of Vasquez et al., 1987. This was chosen as an example of a very difficult system to illustrate their new functional transformation method. The neighbourhood around the solution to this system of equations is seen to be such that the lines are nearly parallel, and it is difficult to determine the solution from the graph. It is well known that in linear syste this would result in a nearly singular system, so it is not suprising that this is difficult to solve by Newton's method alone.

Figures 4.2 and 4.3 show the homotopy paths which result from solving the system using the Newton homotopy from starting points of (20,20) and (1,1) respectively. The path starting from (20,20) can be solved very easily by classical continuation. However, the path starting at (1,1) turns back on itself, and so classical continuation will fail for this starting point. The point where the path turns back on itself is called a turning point.

One of the drawbacks to Newton's method is that different starting points can produce very different homotopy paths. Unfortunately it cannot be determined *a priori* which starting point will produce the simplest (straightest) homotopy path.

Figure 4.4 shows the homotopy path which results when this system is solved using a custom homotopy. This homotopy is developed in Appendix II. In this instance the custom homotopy does not seem to offer any advantages over Newton's method.

4.1.2 Differential Arclength Homotopy Continuation

Arclength continuation takes the ideas of classical continuation one step farther. Arclength continuation makes use of the information "How do the independent variables change as the path is followed?" That is, the values of $\frac{\partial x_1}{\partial p}$ and $\frac{\partial t}{\partial p}$ are used, where p is the path or arc length. Once these values are obtained a predictor step is taken as to where the next point is along the path. Then corrector steps are taken to get close to or on the path again. First the method used to obtain the derivatives with respect to the path length will be explained.

Consider the general set of homotopy equations;

$$\begin{aligned} h_1(x_1, x_2, x_3, \ldots, x_n, t) &= 0 \\ h_2(x_1, x_2, x_3, \ldots, x_n, t) &= 0 \\ h_3(x_1, x_2, x_3, \ldots, x_n, t) &= 0 \\ &\vdots \\ h_n(x_1, x_2, x_3, \ldots, x_n, t) &= 0 \end{aligned} \tag{4.10}$$

Now differentiate these equations with respect to path length using the chain rule. (4.11)

$$\begin{aligned} \frac{\partial h_1}{\partial p} &= \frac{\partial h_1}{\partial x_1}\frac{\partial x_1}{\partial p} + \frac{\partial h_1}{\partial x_2}\frac{\partial x_2}{\partial p} + \frac{\partial h_1}{\partial x_3}\frac{\partial x_3}{\partial p} + \ldots + \frac{\partial h_1}{\partial x_n}\frac{\partial x_n}{\partial p} + \frac{\partial h_1}{\partial t}\frac{\partial t}{\partial p} = 0 \\ \frac{\partial h_2}{\partial p} &= \frac{\partial h_2}{\partial x_1}\frac{\partial x_1}{\partial p} + \frac{\partial h_2}{\partial x_2}\frac{\partial x_2}{\partial p} + \frac{\partial h_2}{\partial x_3}\frac{\partial x_3}{\partial p} + \ldots + \frac{\partial h_2}{\partial x_n}\frac{\partial x_n}{\partial p} + \frac{\partial h_2}{\partial t}\frac{\partial t}{\partial p} = 0 \\ \frac{\partial h_3}{\partial p} &= \frac{\partial h_3}{\partial x_1}\frac{\partial x_1}{\partial p} + \frac{\partial h_3}{\partial x_2}\frac{\partial x_2}{\partial p} + \frac{\partial h_3}{\partial x_3}\frac{\partial x_3}{\partial p} + \ldots + \frac{\partial h_3}{\partial x_n}\frac{\partial x_n}{\partial p} + \frac{\partial h_3}{\partial t}\frac{\partial t}{\partial p} = 0 \\ &\;\;\vdots \\ \frac{\partial h_n}{\partial p} &= \frac{\partial h_n}{\partial x_1}\frac{\partial x_1}{\partial p} + \frac{\partial h_n}{\partial x_2}\frac{\partial x_2}{\partial p} + \frac{\partial h_n}{\partial x_3}\frac{\partial x_3}{\partial p} + \ldots + \frac{\partial h_n}{\partial x_n}\frac{\partial x_n}{\partial p} + \frac{\partial h_n}{\partial t}\frac{\partial t}{\partial p} = 0 \end{aligned}$$

At this point the system is not square. There are n+1 unknowns ($\frac{\partial x_1}{\partial p}$ through $\frac{\partial x_n}{\partial p}$ and $\frac{\partial t}{\partial p}$) and there are only n homotopy equations that can be differentiated. To get around this the n dimensional Pythagorean theorem is added as a constraint equation to facilitate the solution. This equation is

$$\left[\frac{\partial x_1}{\partial p}\right]^2 + \left[\frac{\partial x_2}{\partial p}\right]^2 + \left[\frac{\partial x_3}{\partial p}\right]^2 + \ldots + \left[\frac{\partial x_n}{\partial p}\right]^2 + \left[\frac{\partial t}{\partial p}\right]^2 = 1 \tag{4.12}$$

This equation can also be written in discrete form as

$$(\Delta x_1)^2 + (\Delta x_2)^2 + (\Delta x_3)^2 + \ldots + (\Delta x_n)^2 + (\Delta t)^2 = (\Delta p)^2 \tag{4.13}$$

When the Pythagorean theorem is used as above, the value of $\frac{\partial t}{\partial p}$ is often poorly scaled. To get around this scale factors w_1 and w_2 can be introduced.

$$\frac{w_1}{n}\sum_{i=1}^{n}\left[\frac{\partial x_i}{\partial p}\right]^2 + w_2\left[\frac{\partial t}{\partial p}\right]^2 = 1 \tag{4.14}$$

Experience shows that w_1=0.05 and w_2=0.95 give good results. It is not necessary that w_1 and w_2 sum to unity because they are only arbitrary scale factors. The resulting system of equations is given by

$$\begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \frac{\partial h_1}{\partial x_2} & \frac{\partial h_1}{\partial x_3} & \cdots & \frac{\partial h_1}{\partial x_n} & \frac{\partial h_1}{\partial t} \\ \frac{\partial h_2}{\partial x_1} & \frac{\partial h_2}{\partial x_2} & \frac{\partial h_2}{\partial x_3} & \cdots & \frac{\partial h_2}{\partial x_n} & \frac{\partial h_2}{\partial t} \\ \frac{\partial h_3}{\partial x_1} & \frac{\partial h_3}{\partial x_2} & \frac{\partial h_3}{\partial x_3} & \cdots & \frac{\partial h_3}{\partial x_n} & \frac{\partial h_3}{\partial t} \\ \vdots & \vdots & & & & \vdots \\ \frac{\partial h_n}{\partial x_1} & \frac{\partial h_n}{\partial x_2} & \frac{\partial h_n}{\partial x_3} & \cdots & \frac{\partial h_n}{\partial x_n} & \frac{\partial h_n}{\partial t} \\ \frac{w_1}{n}\frac{\partial x_1}{\partial p} & \frac{w_1}{n}\frac{\partial x_2}{\partial p} & \frac{w_1}{n}\frac{\partial x_3}{\partial p} & \cdots & \frac{w_1}{n}\frac{\partial x_n}{\partial p} & w_2\frac{\partial t}{\partial p} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial p} \\ \frac{\partial x_2}{\partial p} \\ \frac{\partial x_3}{\partial p} \\ \vdots \\ \frac{\partial x_n}{\partial p} \\ \frac{\partial t}{\partial p} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \tag{4.15}$$

The above system must be solved for the solution vector. At first glance this appears to be an iterative procedure because the solution vector is included in the last equation. However, the form of the constraint equation allows the solution to be normalized such that the normalized solution is the desired solution vector.

The solution procedure for the Euler step is then as follows. First assume values for the solution vector. Then solve the system of equations. Normalize the solution according to the formula

$$\left[\frac{\partial x_i}{\partial p}\right] = \frac{\left[\frac{\partial x_{i,c}}{\partial p}\right]}{\sqrt{\frac{w_1}{n}\sum_i \left[\frac{\partial x_{i,c}}{\partial p}\right]^2 + w_2\left[\frac{\partial t_c}{\partial p}\right]^2}} \tag{4.16}$$

$$\left[\frac{\partial t}{\partial p}\right] = \frac{\left[\frac{\partial t_c}{\partial p}\right]}{\sqrt{\frac{w_1}{n}\sum_i \left[\frac{\partial x_{i,c}}{\partial p}\right]^2 + w_2\left[\frac{\partial t_c}{\partial p}\right]^2}} \tag{4.17}$$

The subscript c denotes the calculated values from solving the matrix equations (4.15). A proof is given for this normalization equation in Appendix III.

Instead of using $\frac{\partial x_i}{\partial p}$ and $\frac{\partial t}{\partial p}$ in the predictor step, it is also possible to use $\frac{\partial x_i}{\partial t}$. Let the homotopy equations (4.15) be partitioned into

$$\underline{H}_x + \underline{H}_t = 0 \tag{4.18}$$

where $\underline{H}_x$ is an n X n matrix containing the x_i terms and $\underline{H}_t$ is a column vector containing the t terms. Now differentiate (4.18) with respect to t, and expand $\underline{H}_x$ by the chain rule.

$$\underline{H}'_x \frac{\partial \underline{x}}{\partial t} + \underline{H}'_t = 0 \tag{4.19}$$

Here the prime denotes derivative, and rearranging,

$$\frac{\partial \underline{x}}{\partial t} = -\left[\underline{H}'_x\right]^{-1} \underline{H}'_t \tag{4.20}$$

The benefit of using 4.20 is that $\underline{H}'_x$ is the Jacobian in a standard implementation of Newton's method, and so implementing this in an existing Newton code is made very easy. However, the Jacobian becomes singular at a turning point, and one of the columns of the Jacobian must be removed from the equation set so that Jacobian is no longer rank deficient. This method was not used in this work, because it was felt that since 4.15 is not singular at turning points it was the best choice. Vickery and Taylor however did use this approach with their physical homotopies, and since they did not encounter any turning points 4.20 was a good choice for their work.

4.1.3 Euler Projection

Once the slopes $\frac{\partial x_i}{\partial p}$ and $\frac{\partial t}{\partial p}$ are known a simple Euler projection is done. The distance projected is calculated differently depending on if the current point is near or far from a turning point. The value of $\frac{\partial t}{\partial p}$ indicates whether the current point is close to a turning point because at a turning point, $\frac{\partial t}{\partial p} = 0$. In the program the criteria for being in the neighbourhood of a turning point is that $\left|\frac{\partial t}{\partial p}\right| < 0.1$. When far from a turning point the projected distance is based on a desired value of Δt. The value of Δx_i is calcluated by

$$\Delta x_i = \frac{\left(\frac{\partial x_i}{\partial p}\right) \Delta t}{\frac{\partial t}{\partial p}} \tag{4.21}$$

Since $\frac{\partial t}{\partial p}$ is in the denominator of this equation it is clearly unsuitable close to turning points where $\frac{\partial t}{\partial p}$ approaches zero.

Close to the turning point, the distance projected is based on a desired movement along the path, Δp. The value of Δp used is based on the value from the previous iteration. In this work half of the previous value of Δp was used. If the start of the path is near a turning point then a conservative value of Δp (0.1) should be used. If this fails the value should be halved until a successful step is taken.

The actual projections are

$$\Delta x_i = \left[\frac{\partial x_i}{\partial p}\right] \Delta p \tag{4.22}$$

$$\Delta t = \left[\frac{\partial t}{\partial p}\right] \Delta p \tag{4.23}$$

4.1.4 The Corrector Step

After the Euler projection is made there are different ways to proceed. Most algorithms try to get close to the path again or try to get back on the path exactly. This work followed the example of Vickery and Taylor(1986) who solved the homotopy equations exactly only at the solution. The actual path is followed loosely to reduce the total computation time. No loss of solution accuracy results because exact intermediate solutions along the path are not required. Exact intermediate solutions merely give Euler projections closer to the true tangent vector. Exact projections are not necessary because the purpose of the projection is to predict a point in the vicinity of the homotopy path. In the case of path following with respect to a physical parameter it is important to follow the homotopy path closely because the intermediate solutions do have physical meaning. Note that in the special case where the homotopy path is linear that no correction is necessary because the Euler projection would then be exact. However nearly all paths have curvature.

The correction step is solved using the extended system, except at the solution point where the equations are solved at t=1.0. The extended system is formed by appending the discrete form of the n dimensional Pythagorean theorem to the homotopy equations (equation

4.13).

The purpose of the n dimensional Pythagorean equation is to constrain the movement along the path to Δp, the desired distance to be travelled along the path. The resulting equation set is given by:

$$\begin{aligned} h_1(x_1,x_2,x_3,\ \ldots,\ x_n,t) &= 0 \\ h_2(x_1,x_2,x_3,\ \ldots,\ x_n,t) &= 0 \\ h_3(x_1,x_2,x_3,\ \ldots,\ x_n,t) &= 0 \\ &\vdots \\ h_n(x_1,x_2,x_3,\ \ldots,\ x_n,t) &= 0 \end{aligned} \tag{4.24}$$

$$(\Delta x_1)^2 + (\Delta x_2)^2 + (\Delta x_3)^2 + \ldots + (\Delta x_n)^2 + (\Delta t\ )^2 = (\Delta p\ )^2$$

Note that $\Delta x_i = x_i - x_i^0$, where x_i^0 is the previous point on the path. The Jacobian matrix and right hand side for this system are given by:

$$\begin{bmatrix} \frac{\partial h_1}{\partial x_1} & \frac{\partial h_1}{\partial x_2} & \frac{\partial h_1}{\partial x_3} & \cdots & \frac{\partial h_1}{\partial x_n} & \frac{\partial h_1}{\partial t} \\ \frac{\partial h_2}{\partial x_1} & \frac{\partial h_2}{\partial x_2} & \frac{\partial h_2}{\partial x_3} & \cdots & \frac{\partial h_2}{\partial x_n} & \frac{\partial h_2}{\partial t} \\ \frac{\partial h_3}{\partial x_1} & \frac{\partial h_3}{\partial x_2} & \frac{\partial h_3}{\partial x_3} & \cdots & \frac{\partial h_3}{\partial x_n} & \frac{\partial h_3}{\partial t} \\ & \vdots & & \cdots & \vdots & \\ \frac{\partial h_n}{\partial x_1} & \frac{\partial h_n}{\partial x_2} & \frac{\partial h_n}{\partial x_3} & \cdots & \frac{\partial h_n}{\partial x_n} & \frac{\partial h_n}{\partial t} \\ 2(x_1-x_1^0) & 2(x_2-x_2^0) & 2(x_3-x_3^0) & \cdots & 2(x_n-x_n^0) & 2(t-t^0) \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \\ \\ \Delta x_n \\ \Delta t \end{bmatrix} = \begin{bmatrix} -h_1 \\ -h_2 \\ -h_3 \\ \\ -h_n \\ -\Delta p^2 \end{bmatrix} \tag{4.25}$$

Note that in this formulation, t, the homotopy parameter becomes an unknown and the path length Δp is specified. The resulting system is no longer singular at a turning point.

Following is the algorithm of how the predictor/corrector was implemented.

```
1.  Solve the initial problem at $t_o$.

2.  Calculate the initial Jacobian.

3.  To begin, let $\Delta p$ [illegible]25. If the problem is well posed,
    $dt/dp \cong 1$ and so $\Delta t \cong 0.2$[illegible] If the initial problem starts out
    in a region near a turning point, $dt/dp \cong 0$, and so $\Delta t$ will be
    small.  This is acceptable because small steps are often
    necessary to go around turning points.

4.  Calculate $\frac{\partial x_1}{\partial p}$ and $\frac{\partial t}{\partial p}$ from 4.16.

5.  Take the Euler predictor step, clamping t at $t_f$ if needed.
        $t^{k+1} = t^k + \Delta p * \frac{\partial t}{\partial p}$
        IF $t^{k+1} > t_f$ THEN
            $t^{k+1} = t_f$
            $\Delta p = (t^{k+1} - t^k)/(dt/dp)$
        ENDIF
        $\Delta x_1 = \left[ \frac{\partial x_1}{\partial p} \right] \Delta p$

6.  Take Newton Corrector Step.
        IF error increases GOTO 7
        IF error < tolerance THEN
            GOTO 8
        ELSE
            IF under 5 Newton iterations THEN
                GOTO 6
            ELSE
                GOTO 7
            ENDIF
        ENDIF

7.  Newton Corrector Failed.
    $\Delta p^{k+1} = \Delta p^k/2$
    IF $\Delta p^{k+1} < \Delta p_{min}$ THEN
        Continuation Failed.
    ELSE
        GOTO 5.
    ENDIF
```

8. Newton Corrector Converged to Homotopy Path

```
IF $t^k = t_f$ THEN
    Continuation Solved.
ELSE
    $\Delta p^{k+1} = \Delta p^k * 2$
    IF $\Delta p^k > \Delta p_{max}$ THEN $\Delta p = \Delta p_{max}$
    GOTO 5
ENDIF
```

Figure 4.1 Solution Space for the Functions f(x,y) and g(x,y) of Vasquez et at. (1987)

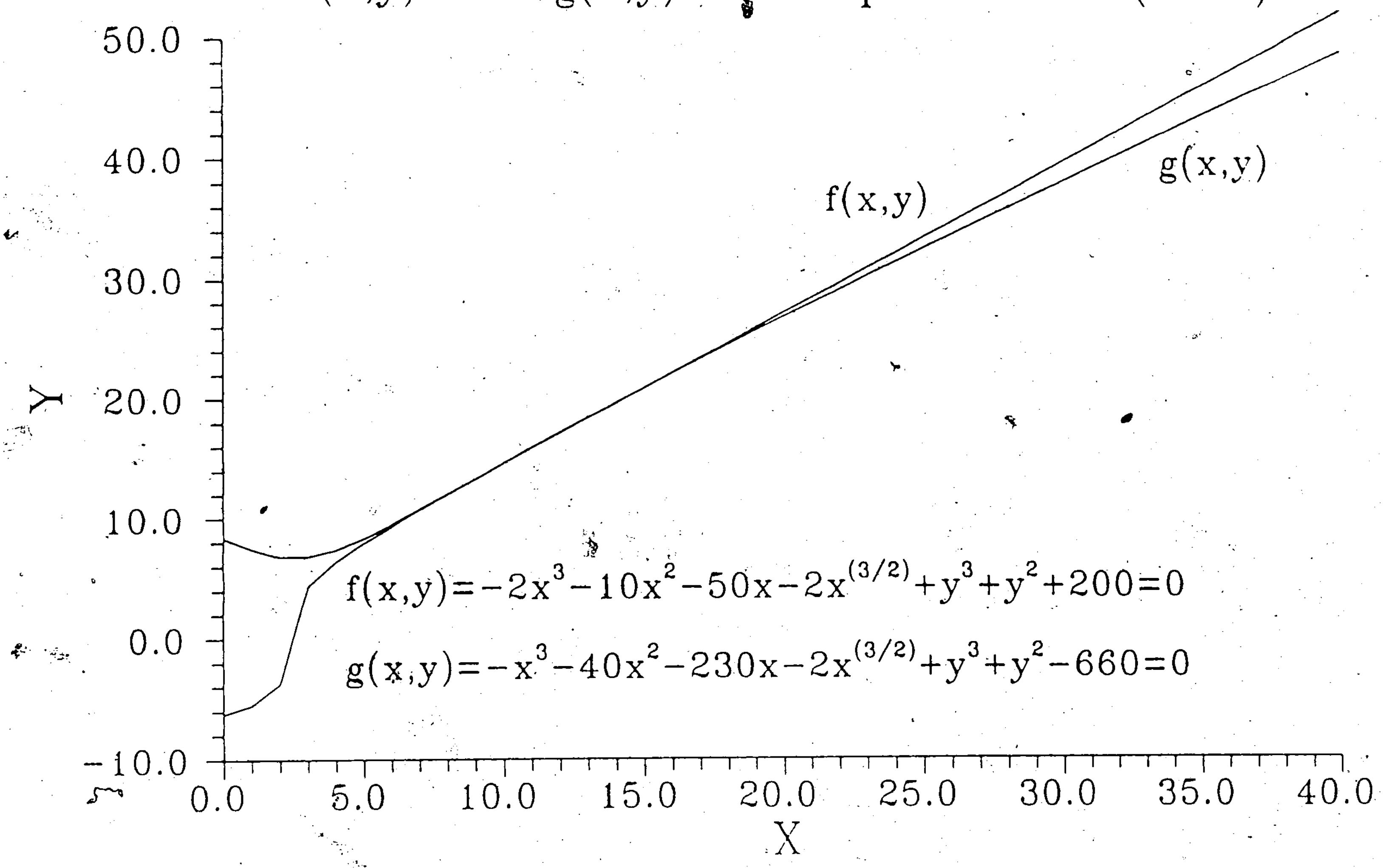
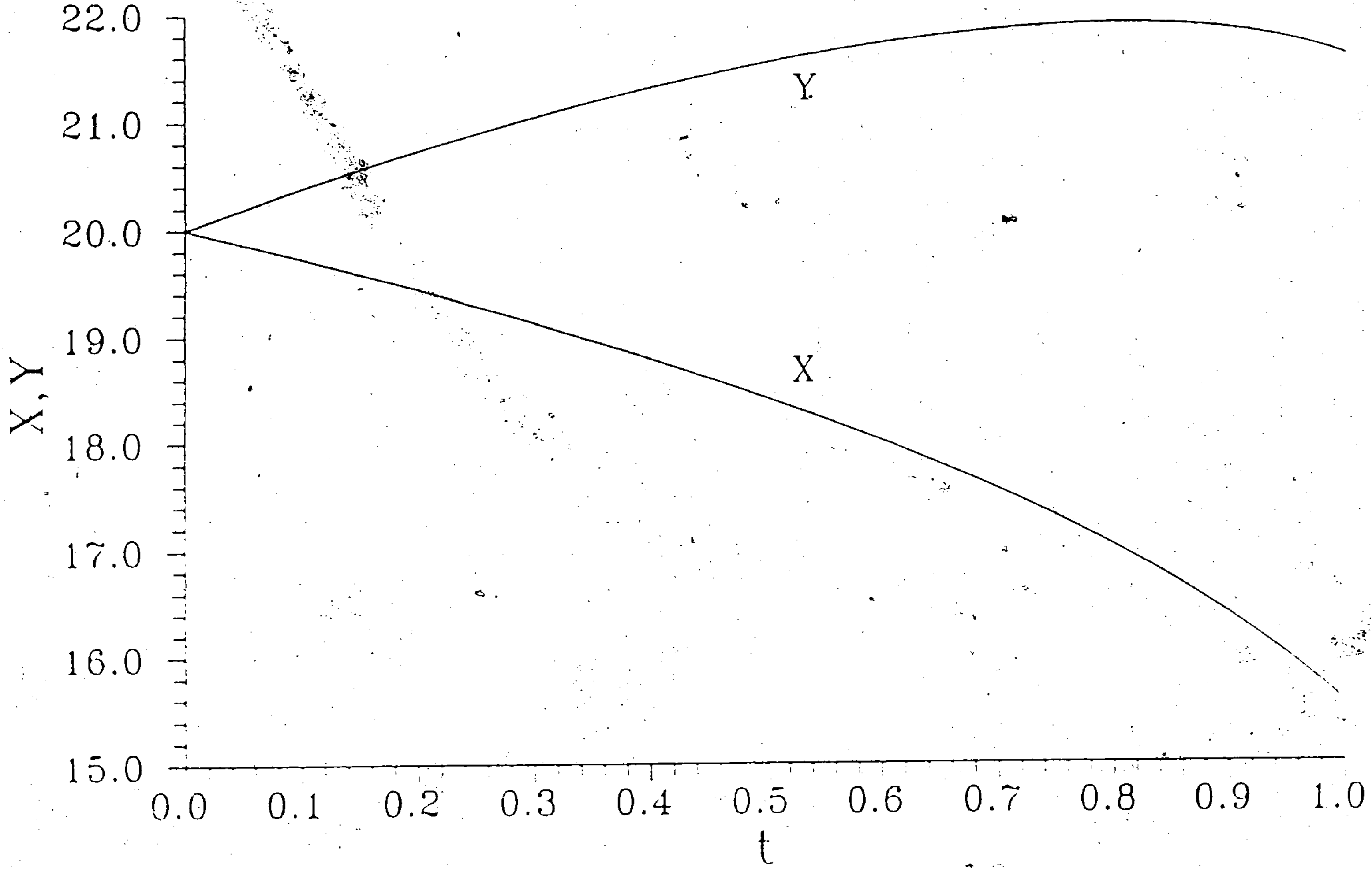


Figure 4.2 Newton Homotopy Starting at (20,20) For Example 2 of Vasquez et al. (1987)



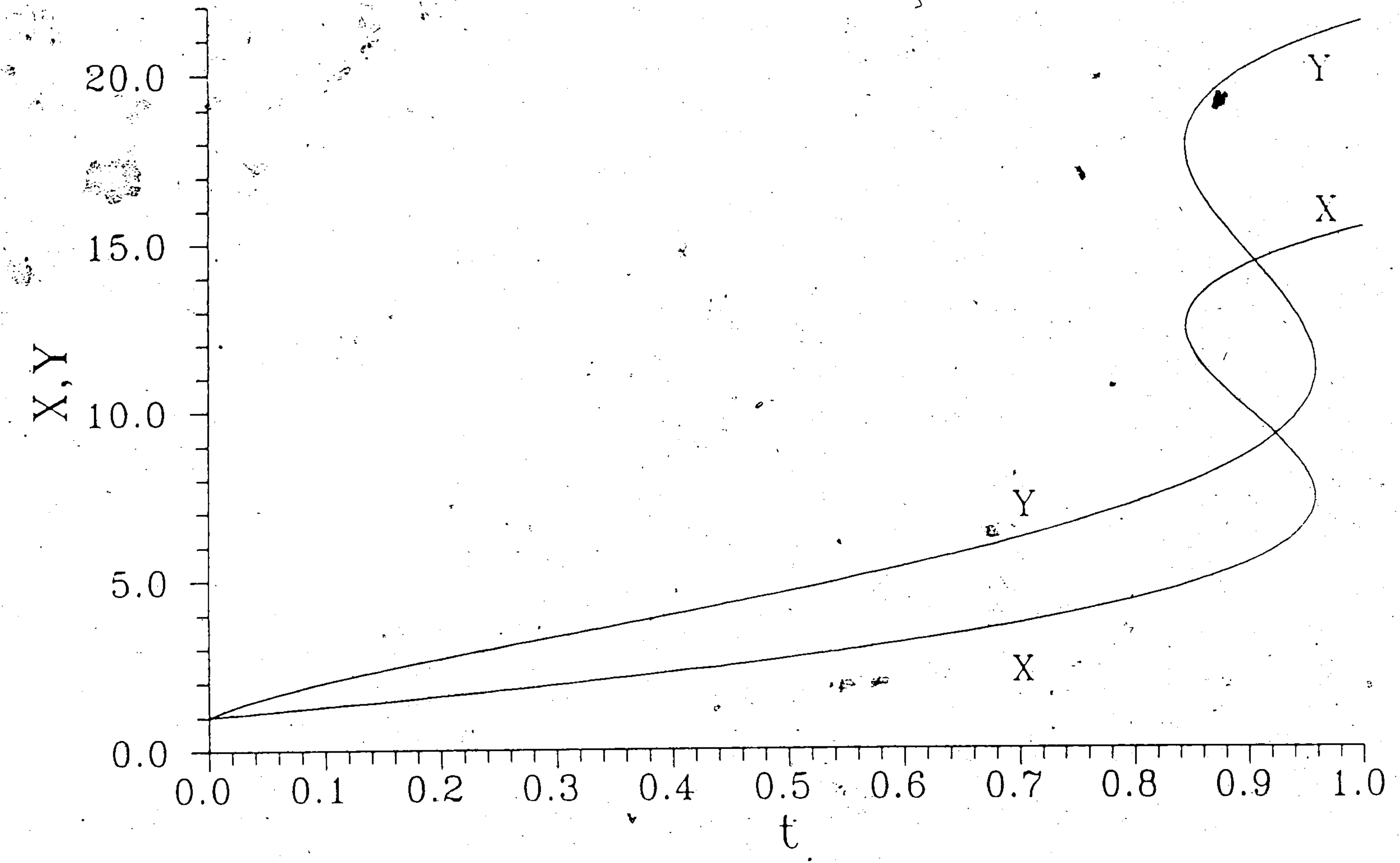
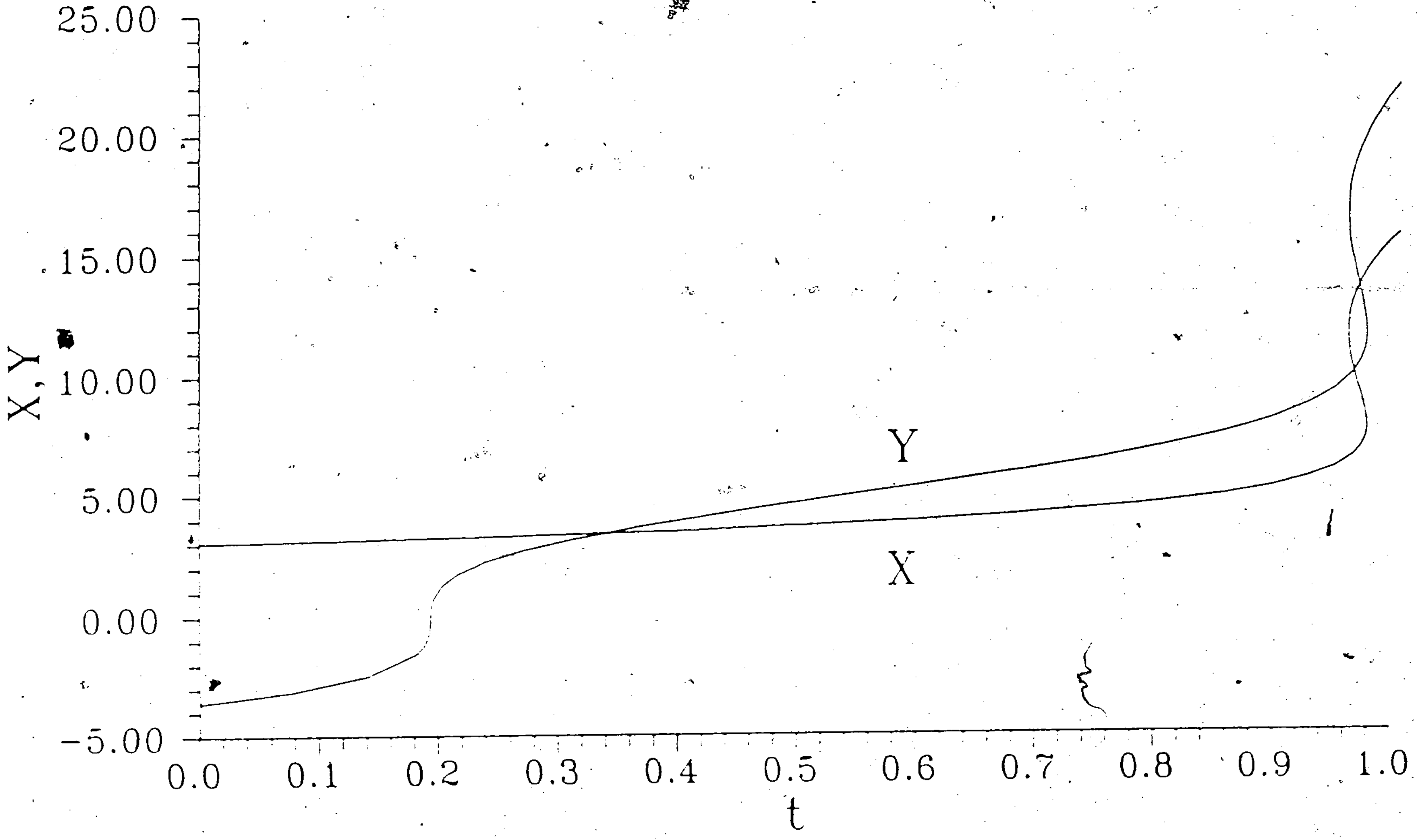


Figure 4.3 Newton Homotopy Starting at (1,1)
For Example 2 of Vasquez et al. (1987)

Figure 4.4 Custom Homotopy For Example 2 of Vasquez et al.



4.6 Homotopy Selection

One current deficiency in the literature is a comparison between physical and mathematical homotopies to aid in homotopy selection. This section will attempt to present an unbiased overview of the strengths and weaknesses of the different physical and mathematical homotopies. The homotopies discussed are limited to those which have been used recently in separation calculations.

Tables 4.1 and 4.2 each address different issues associated with choosing a homtopy and also provide comparisons to Newton's Method and to the new functional transformation method of Vasquez et al. The functional transformation method is an *ad hoc* method for jumping over turning points by modifying the equation set.

If a good initial estimate is available for the problem, then Newton's method will probably work and path following methods are not required. In those cases where good initial estimates are available but Newton's method still fails, they should still be used as a starting point for the continuation algorithm to keep the path short. The closer the solution of the initial problem is to the solution of the final problem the shorter and less tortuous the homotopy path will be.

As mentioned previously, it is important to be able to solve the initial problem. The Newton homotopy can start from any vector of initial estimates. However, the physical homotopies use iterative procedures and so they have the potential of failing at this point. The method of solving the initial problem was found to be quite robust for the hydrocarbon systems studied in this work. Although not pursued in this work, shortcut methods could be used to provide estimates of the vapour and liquid traffic and temperature profiles for solving the initial problem.

The wide boiling hydrocarbon mixture problem is a good test for a distillation algorithm because of the wide range of volatilities present. Unfortunately, no results are available in the literature for using mathematical homotopies to solve these problems. As shown in this work path following in artificial heater/coolers and structure solve these systems reliably. Newton's method often requires damping or line searching techniques to stabilize it when there is not a good initial estimate available.

When solving chemical systems the liquid phase activity coefficients are strong functions of the liquid phase composition. Path following in heater/coolers and structure has not been done with chemical systems yet, but since no provision has been made for the non-idealities of the liquid phase, it will probably perform poorly. Particularly, the method outlined here for solving the initial problem is not appropriate for systems where the liquid phase activity is a strong function of the liquid composition. Kovach and Seider have shown that a combination of the Newton homotopy and a physical homotopy for solving the liquid-liquid equilibrium problem (they used mixed K-values) works very well for chemical systems. Vickery et al. have shown that their physical homotopies also work very well for chemical systems.

One advantage that mathematical homotopies have is that there is no extra work required to implement non standard specification equations. Also, the initial problem is usually trivial to solve. Mathematical homotopies are also appealing from the point of view of finding an algorithm which works well for all types of distillation problems, if any such algorithm will ever be found.

At this point in time, neither mathematical or physical homotopies can be considered superior; each one has its advantages. Depending on the experience of the person implementing the homotopy, one of them will be easier to work with. If only physical homotopies have the ability to detect non-physical specifications and indicate the limiting values of the specification, then this would be an advantage over the mathematical homotopies.

Homotopy	Starting Guess		Solving the Initial Problem	Wide/Narrow Boiling Mixture
	Good	Bad		
Heaters/ Coolers & Structure	help to get close to final solution	homotopy path may be long	easy, but still iterative	good for both
Tray Efficiency	not able to use	no effect	easy, but still iterative	wide boiling mixture will be steep
Thermo-dynamics	helps initial problem	homotopy path may be long	easy, but still iterative	?
Newton Homotopy	makes path short, easy to converge	may have trouble in thermo-dynamics	trivial	should be good for both but no results with rigorous T/D
Other Methods				
Functional Transformation	should not need transformation	may have trouble in T/D	–	?
Newton's Method	converges quickly	may not converge	–	may need damping, line search to help converge
Comments	no need for homotopy methods		potential weakness of physical homotopies	no literature examples using mathematical homotopies

Table 4.1
Comparision of Physical and Mathematical
Homotopies, Functional Transformation Method,
and Newton's Method

	Chemical Systems	Comments
Homotopy		
Heaters/ Coolers & Structure	may need to include K Values or tray efficiency	may have trouble when initial liquid/vapour profile is poor
Tray Efficiency	works best for these systems	not well suited for wide boiling hydrocarbons.
Thermo-dynamics	works best for these systems	no literature examples with non standard specifications
Newton Homotopy	paths are tortuous, requires manual tuning of step size parameters	only universal approach, paths can be long and tortuous
Other Methods		
Functional Transformation	?	distillation examples not yet in literature
Newton's Method	requires a good initial estimate	this should always be tried first
Comments	these are the most difficult systems to solve	

Table 4.2
Comparision of Physical and Mathematical Homotopies; Functional Transformation, and Newton's Method

5.0 Case Studies

The purpose of the case studies presented is twofold. The first is to investigate how path following in artificial heater/coolers, structure and specifications perform when physically infeasible specifications are given. The second is to determine whether physical homotopies can be used to find multiple steady state solutions for interlinked columns. Two different distillation columns were studied using different types of specifications. The columns studied were a simple column with a total condenser and partial reboiler and a distillation column with attached sidestripper.

The Peng-Robinson equation of state was used to calculate fugacities and enthalpy departures for the liquid and vapour phases. Critical constants, acentric factors and ideal gas heat capacities were taken from Reid et al. (1977). All binary interaction parameters for the equation of state were set to zero.

5.1 Case Study 1 : C_3-C_4-C_5-C_6 Splitter

This case study uses a simple C_3-C_4-C_5-C_6 (all normal alkanes) splitter. The column has four equilibrium stages including a total condenser and a partial reboiler. For all runs the feed to the column was an equimolar mixture of C_3-C_4-C_5-C_6 to tray 3 with a total flowrate of 1000 kmol/h. The column pressure is constant at 2048 kPa (300 psia).

Case study 1A investigated the effect of a purity specification which was too high. The column is specified with 50 mole percent of propane in the overhead and a bottom rate of 500 kmol/h. By overall mass balance the distillate rate is also 500 kmol/h. Therefore to satisfy the distillate purity specification there will be 250 kmol/h propane in the distillate. Since there are only 250 kmol/h of propane entering the column, and the purity spec is only satisfied when all of the propane exits the column in the distillate, to achieve this concentration would require propane to be non distributing. Appendix IV shows that in order to achieve this separation 18 Fenske (total reflux) stages are necessary. Since there are only 4 ideal stages at a reflux ratio of 3 the purity specification cannot be achieved.

When Newton's method was used to solve this column the liquid and vapour corrections were very large, since the column was trying to get to infinite reflux in one step. Damping the Newton step does not help with this sort of problem because the Newton corrections are always trying to increase the liquid rates to infinite reflux.

When path following in artificial heater/coolers was used the solution gradually changed as the homotopy path was followed. Figures 5.1 through 5.4 show how the reflux ratio, mole fraction of propane in the distillate, condenser temperature and dt/dp change as the homotopy path was followed. Note that the calculation was terminated at about t=0.23 when the reflux ratio was around fifty and dt/dp was small (approximately 0.001). The algorithm contains a check to stop calculations when dt/dp is less then 0.001 for 5 consecutive iterations. This must be done to avoid stopping prematurely when approaching a very sharp turning point.

Case study 1B considered the effects of having a purity specification that was too low. For this case study the mole fraction of propane in the distillate was specified at 0.25 and the bottoms product rate was specified at 500 kmol/h. To meet the propane purity specification in the distillate requires that 125 kmol/h of propane exit the column in each of the distillate. Since there are only 250 kmol/h of propane in the feed., to maintain overall mass balance 125 kmol/h of propane must exit the column out the bottom product, Since propane is the lightest component it is not physically possible for it to distribute evenly between,the top and bottom products.

To verify that it is physically impossible to have 125 kmol/h of propane in both the distillate and bottoms streams with only 4 equilibrium stages, a simulation was run with a low reflux ratio (0.001). At a low reflux ratio there will be a low separation, and so this provides an estimate for the maximum amount of propane that will exit the column in the bottoms. Appendix V shows that there are still 200 kmol/h of propane in the overhead with this low reflux ratio.

When this problem was solved using Newton's method it 'blew up'. However, when using continuation a smooth path resulted which was easily followed. Figures 5.5 through 5.8 show how the reflux ratio, mole fraction of propane in the distillate, condenser temperature and dt/dp change as the homotopy path is followed. The homotopy path stops abruptly at approximately t=0.22. This occurs when the liquid rate on tray 1 becomes zero. If the liquid and vapour rates were not constrained to be positive, then the rates became negative.

Case Study 2 : Depentanizer

Case study 2 considers a simple depentanizer. The column has 6 components, the normal alkanes propane through octane. The feed has the following mole fractions:

propane	0.05
n-butane	0.15
n-pentane	0.20
n-hexane	0.25
n-heptane	0.25
n-octane	0.10

The feed is bubble point liquid at 1600 kPa. The main column has 10 equilibrium stages including a total condenser and a partial reboiler. The sidestripper has 3 equilibrium stages including a partial reboiler. The sidestripper liquid draw and vapour return are from stage 3 of the main column, where the condenser is stage 1. The feed enters the column on stage 4 and the pressure throughout the column and sidestripper is 1600 kPa.

Case study 2A was done to examine the effect of specifying an octane bottoms purity which was too high. This is similar to case study 1A. In this case study, the specifications are as follows:

1) Distillate Product Rate = 200 kmol/h
2) Mole Fraction n-octane in bottoms = 0.20
3) Liquid Side Draw Rate = 300 kmol/h
4) Sidestripper Product Rate = 200 kmol/h

Figures 5.9 through 5.12 show how dt/dp, reflux ratio, octane mole fraction in the bottoms and the condenser temperature change as the homotopy path is followed. In this case the reflux ratio becomes very large to meet the purity spec, and dt/dp approaches zero at approximately t=0.375.

Case study 2B was also done to examine the effect of having an octane purity spec in the bottoms which was too high, except that the liquid draw rate specification on the draw from the column to the sidestripper was changed to a reflux ratio specification. The reflux ratio was specified at 3.0.

Figures 5.13 through 5.16 show how dt/dp, the tray 3 molar liquid rate, octane mole fraction in the bottoms and the sidestripper product temperature change as the path is followed. The path here stops when the tray 3 liquid rate becomes zero at approximately t=0.52, because the algorithm constrains the liquid and vapour rates to be positive.

Case study 2C was done to compare solution times of Newton's method and path following. The specifications used here were:

1) Propane Purity in Distillate
2) Bottoms Rate = 600 kmol/h
3) Reflux Ratio = 3.0
4) Sidestripper Product Rate = 200 kmol/h

Note that since there are only 3 products and 2 of the rates have been specified that the third (distillate) product rate can be calculated from the overall mass balance. Since the reflux ratio has been specified, the variable which will have the greatest impact on the column is the liquid draw rate from the main column to the sidestripper. This rate will determine the amount of liquid and vapour traffic in the main column below the liquid draw tray (stage 3).

Table 5.1

Equivalent Newton Iterations for Case 2C

	Propane Mole Fraction in Distillate			
	.2200	.2250	.2323	.2350
Newton's Method	5	5	5	7
Heater/Coolers	10	10	10	11
Heater/Coolers and Structure	16	14	14	16

Table 5.1 shows the number of iterations required to solve the column with different propane purity specifications in the distillate. For the cases where path following was used, the path started at t=0.1 and an initial increment of Δp=0.3 was used.

The homotopy paths for the cases in table 5.1 are not shown because they are all smooth and monotonic between the initial and terminal points along the path. Figures 5.17 through 5.20 show the homotopy paths for the case where the propane purity in the distillate is specified at 0.2450. This path turns around, indicating that with 10 equilibrium stages and a reflux ratio of three that this purity cannot be met. Newton's method also fails for this case.

This path is different from those presented in the other case studies, because the constraints of infinite reflux or a liquid rate going to zero do not occur to indicate an infeasible specification. In this case, the path turns around, and the turning point indicates the approximate value of the limiting value. The value is only approximate because the problem being solved is not exactly the same as the desired problem due to the presence of the artificial heater / coolers.

Case study 2D was done to search for multiple solutions. The work of Lin et al. showed that for a column and sidestripper with purity specifications on each of the product streams and a reflux ratio specified that multiple solutions can be found using the Newton homotopy with a square mapping function. This work extended the work of Chavez et al. by finding multiple solutions along the same homotopy path.

Figure 5.21 shows the liquid sidedraw rate and tray 3 liquid rate for path following in heater/coolers, structure and specifications at a reflux ratio of 5. In each case the path stops when the tray 3 liquid rate becomes zero. The adjustments made to all of the variables are scaled such that no variable becomes negative. Note that only one solution is found. Different starting guesses were not tried to see if the algorithm would converge to the other solution for the case where the reflux ratio is 4.

Figure 5.22 shows the homotopy paths at different reflux ratios for the liquid sidedraw rates that result when path following is done in structure and specifications. In this case the path turns around and multiple solutions are found. Multiple solutions are found at reflux ratios of 3 and 4. No solution exists at a reflux ratio of 2.75, although the path also has a turning point. For a reflux ratio of 5 only a single solution is found.

Appendix VII gives the simulation results for the multiple solution case at a reflux ratio of 4.0. The solution of the initial problem is given (t=0), and the column temperature, liquid, vapour, and liquid mole fraction profiles are given for both of the steady state solutions found.

Figure 5.1
Variation of Reflux Ratio
Along the Homotopy Path for Case 1A

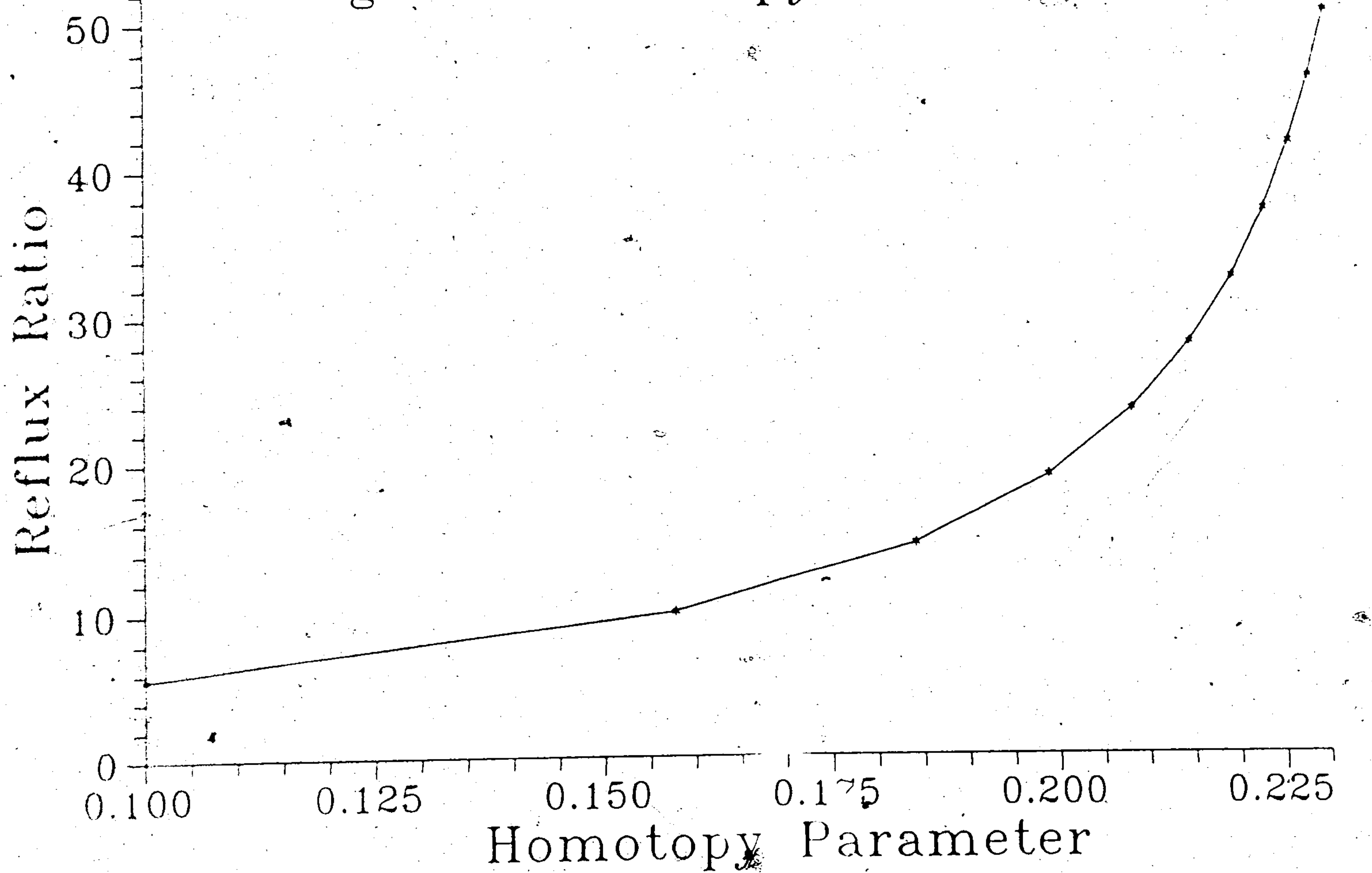


Figure 5.2
Variation of C3 Mole Fraction in Distillate
Along the Homotopy Path

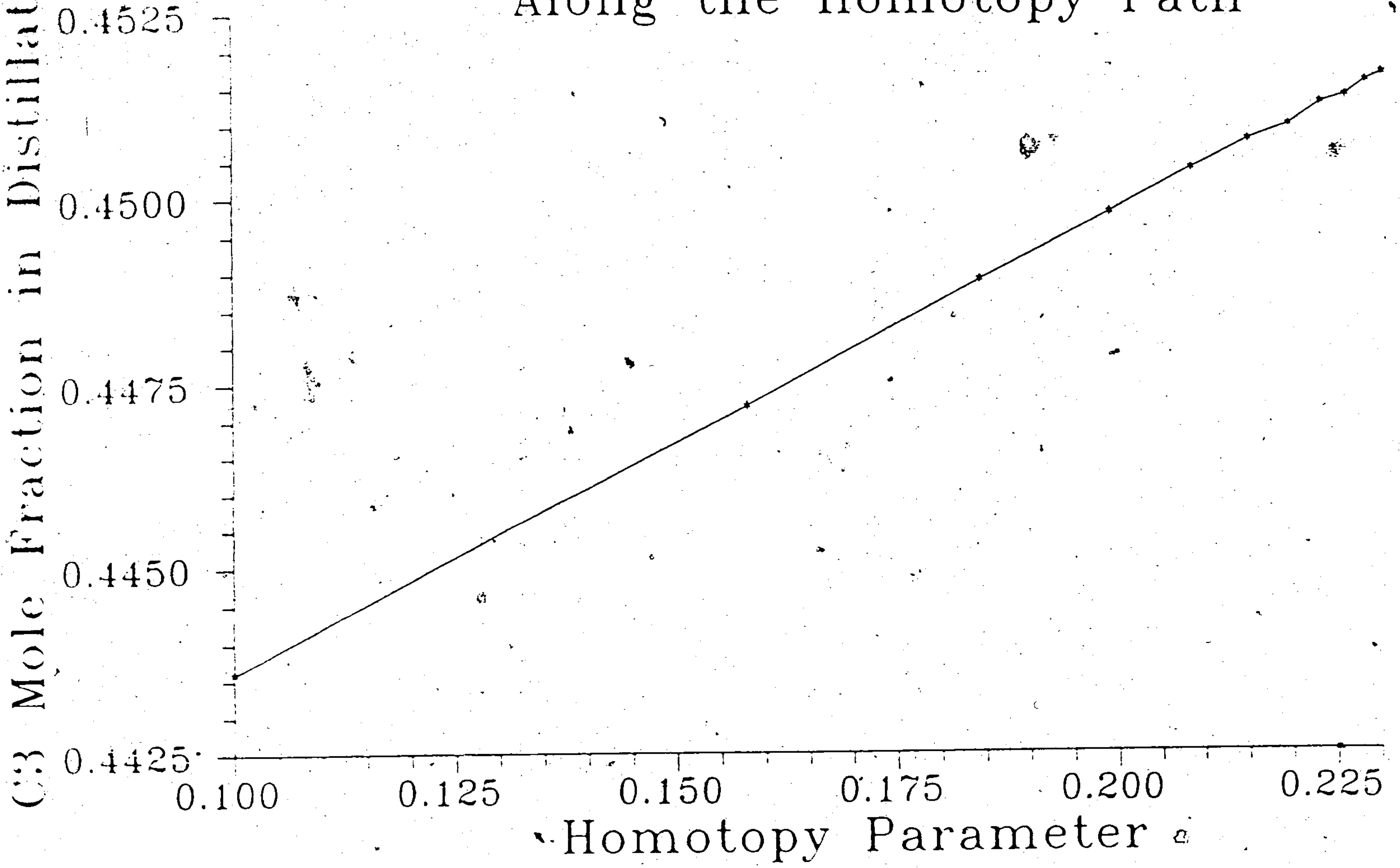


Figure 5.3

Variation of Condenser Temperature Along the Homotopy Path for Case IA

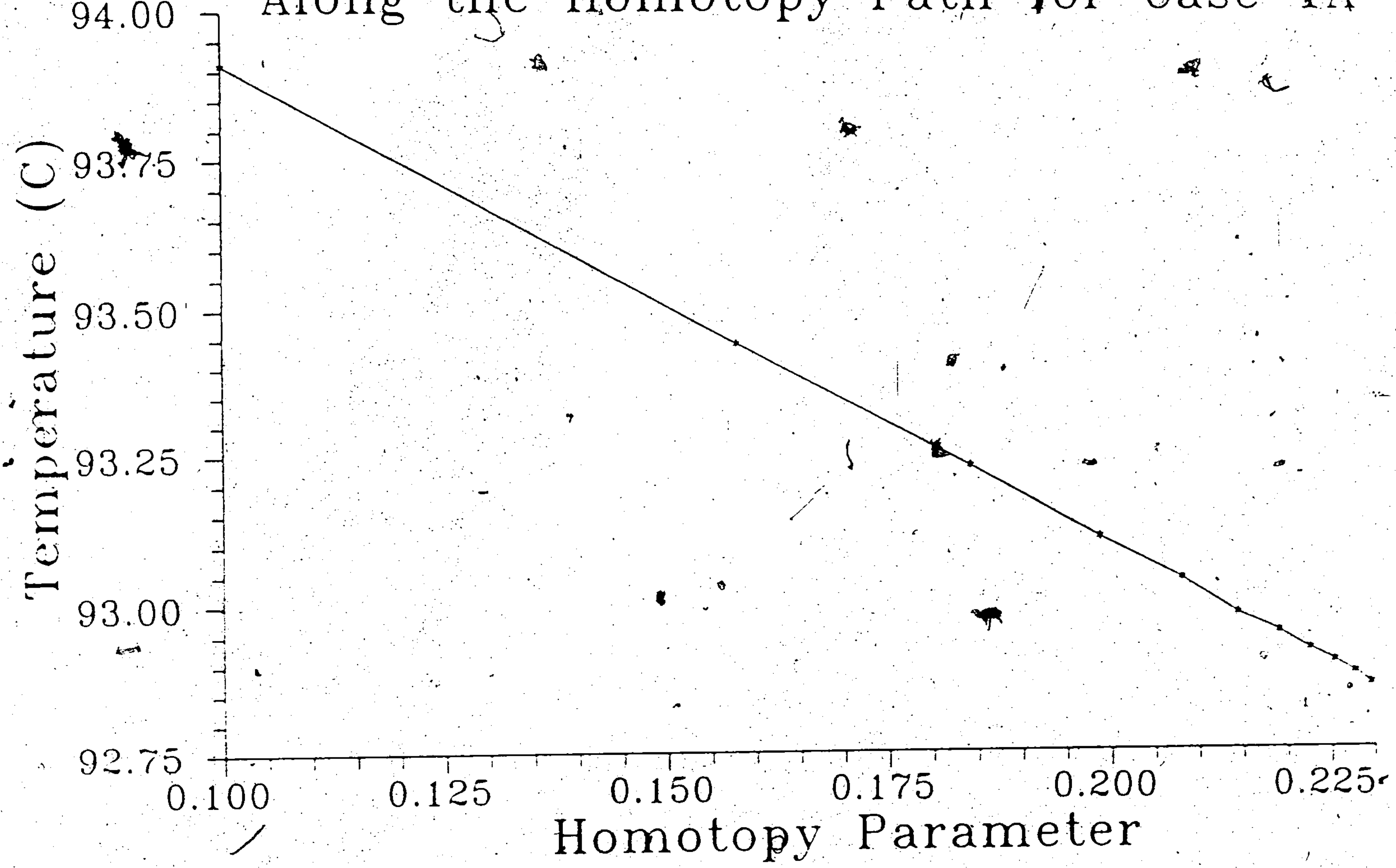


Figure 5.4
Variation of dt/dp Along the
Homotopy Path for Case 1A

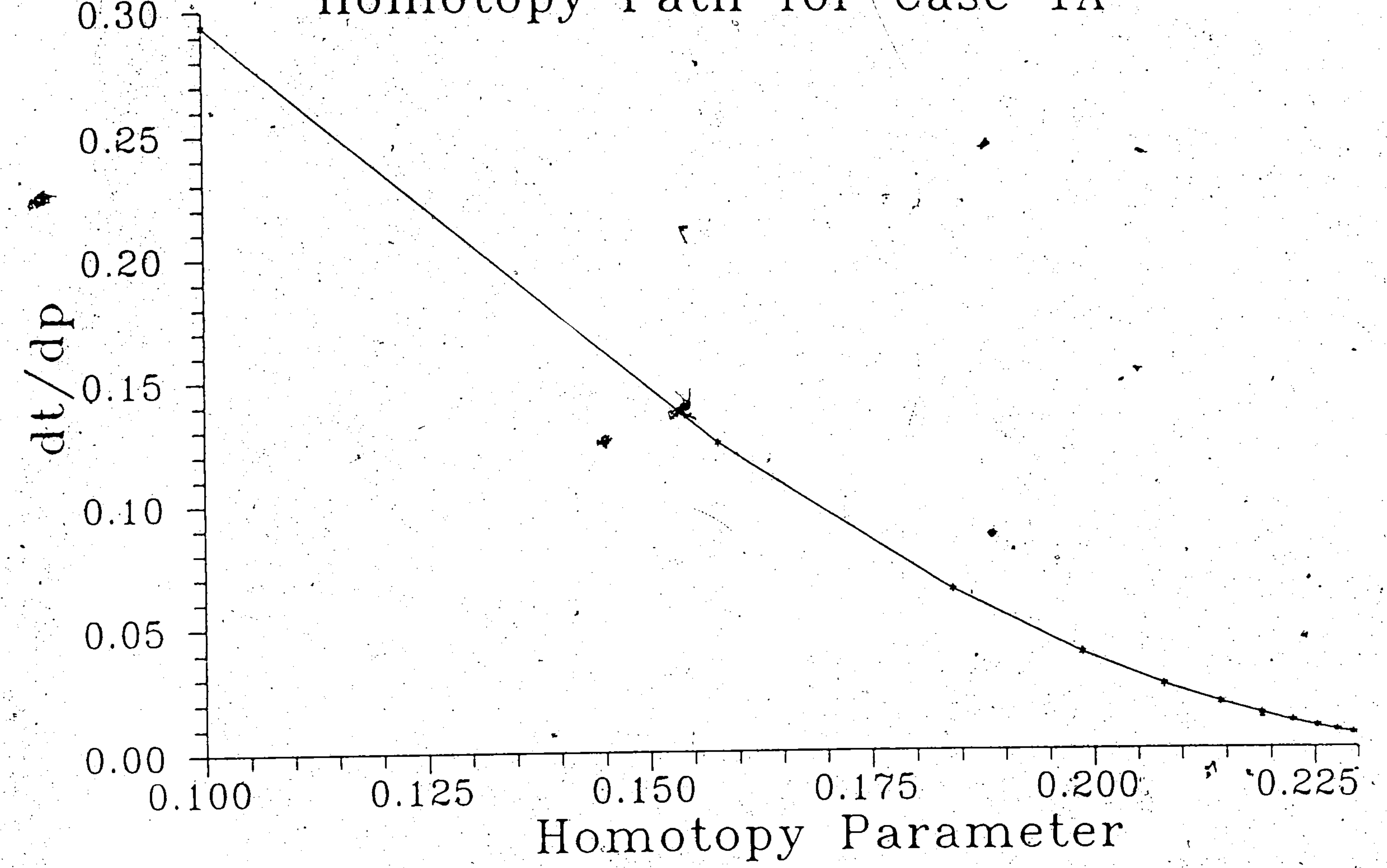


Figure 5.5
Variation of Reflux Ratio Along the Homotopy Path for Case 1B

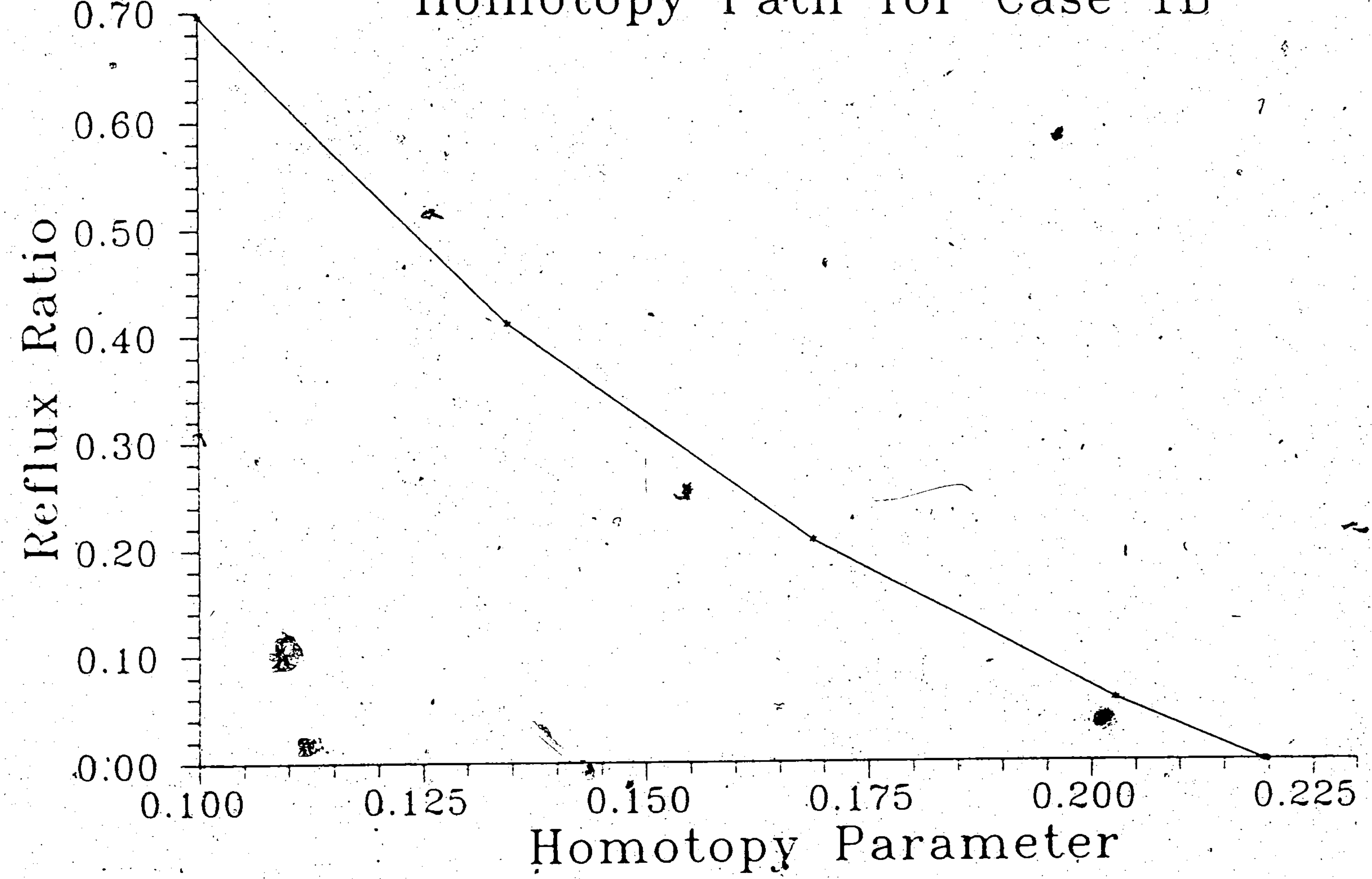


Figure 5.6
Variation of Distillate C3 Mole Fraction
Along the Homotopy Path for Case 1B

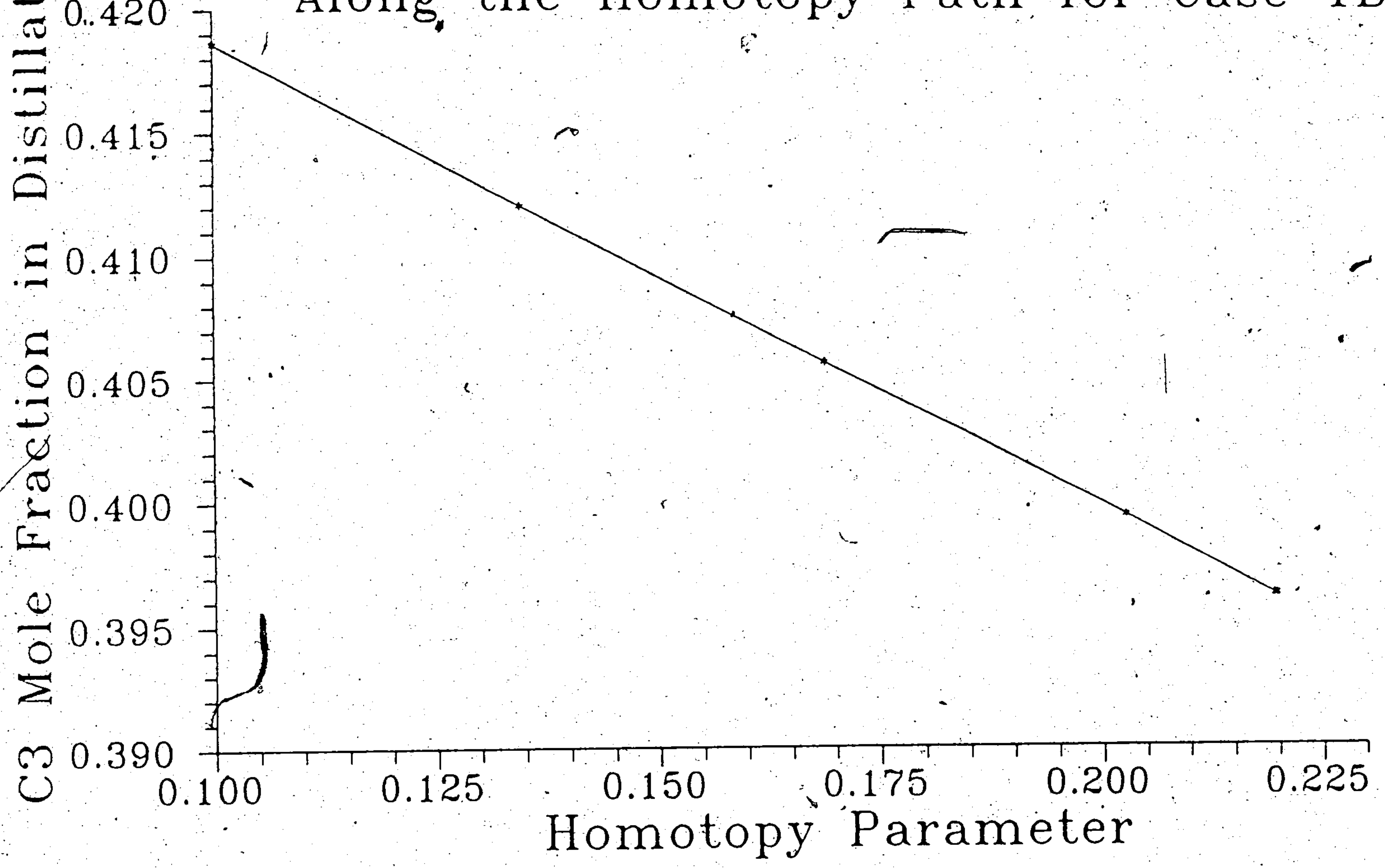


Figure 5.7
Variation of Condenser Temperature Along the Homotopy Path for Case 1B

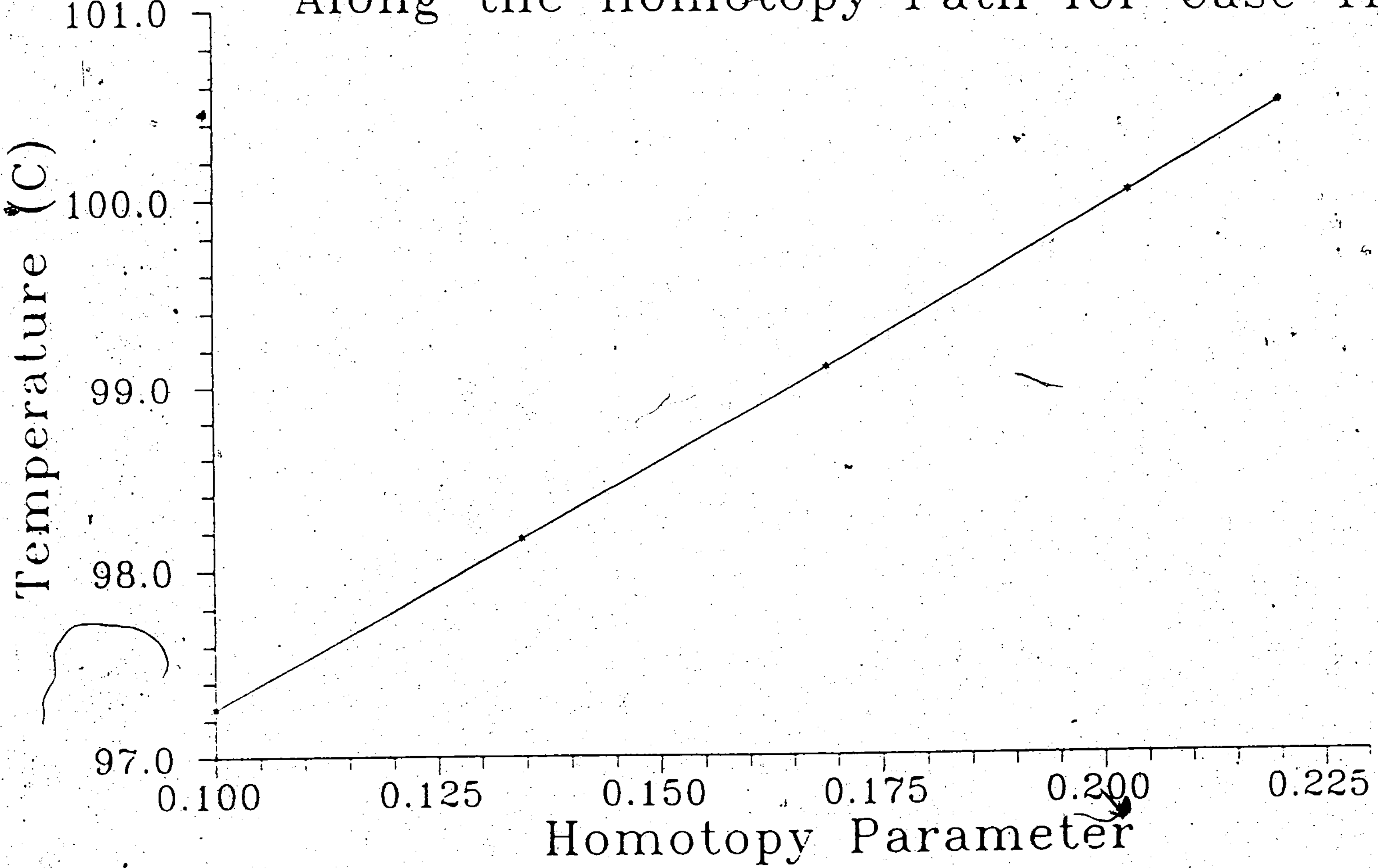


Figure 5.8
Variation of dt/dp Along the
Homotopy Path for Case 1B

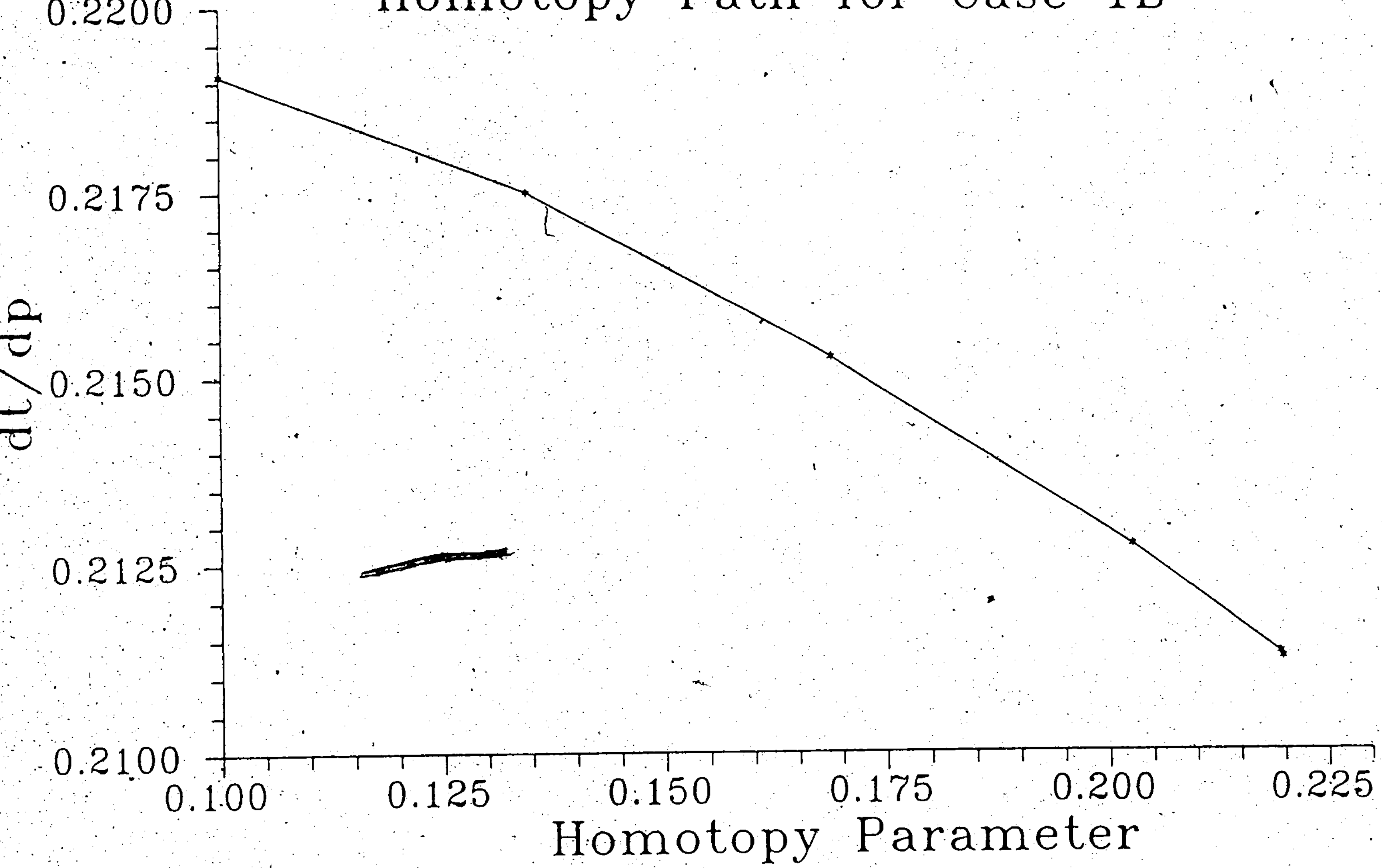


Figure 5.9
Reflux Ratio Along the Homotopy
Path for Case 2A

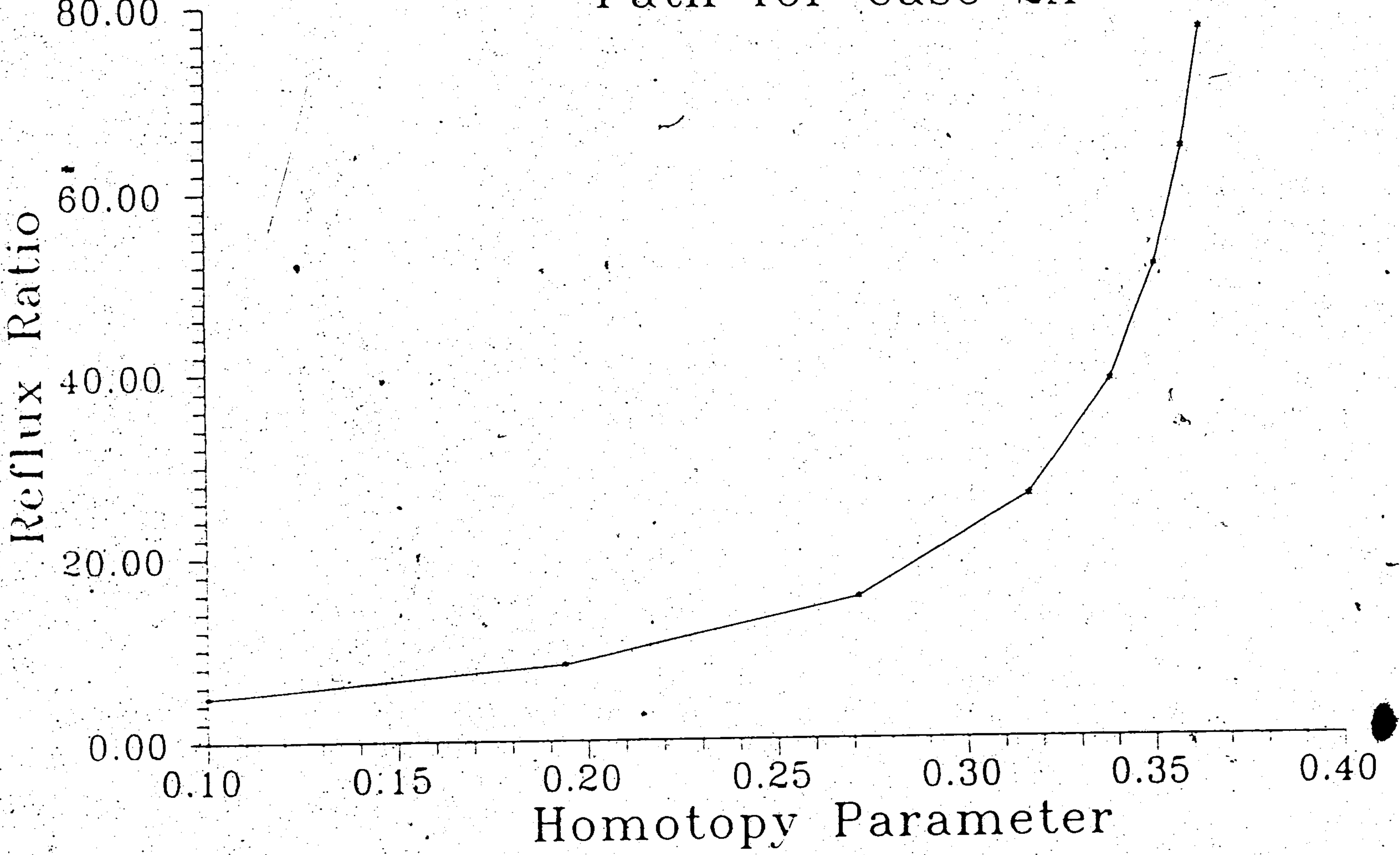


Figure 5.10
NC8 Mole Fraction in Bottoms Along
the Homotopy Path for Case 2A

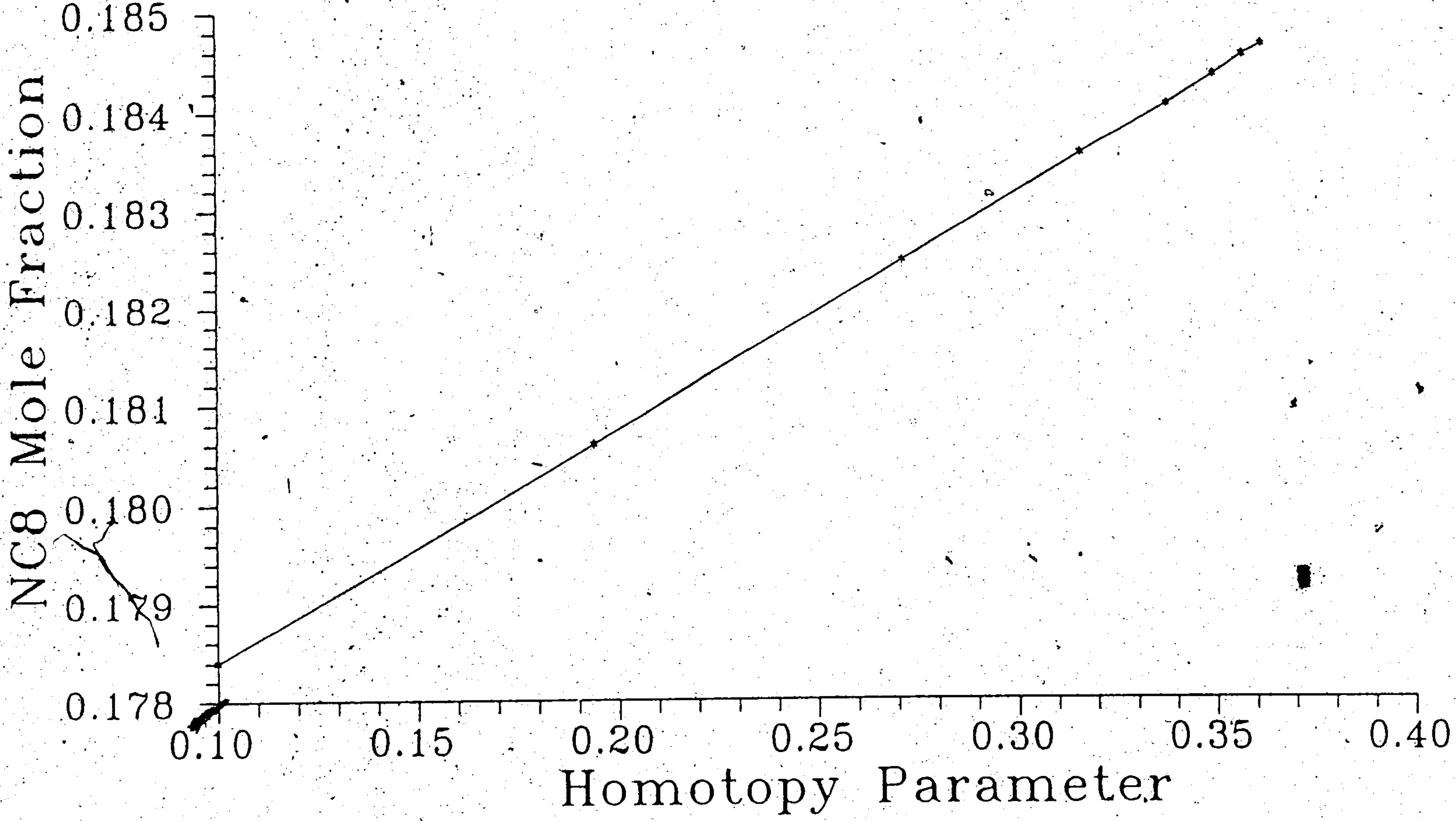


Figure 5.11
Reboiler Temperature Along the Homotopy Path for Case 2A

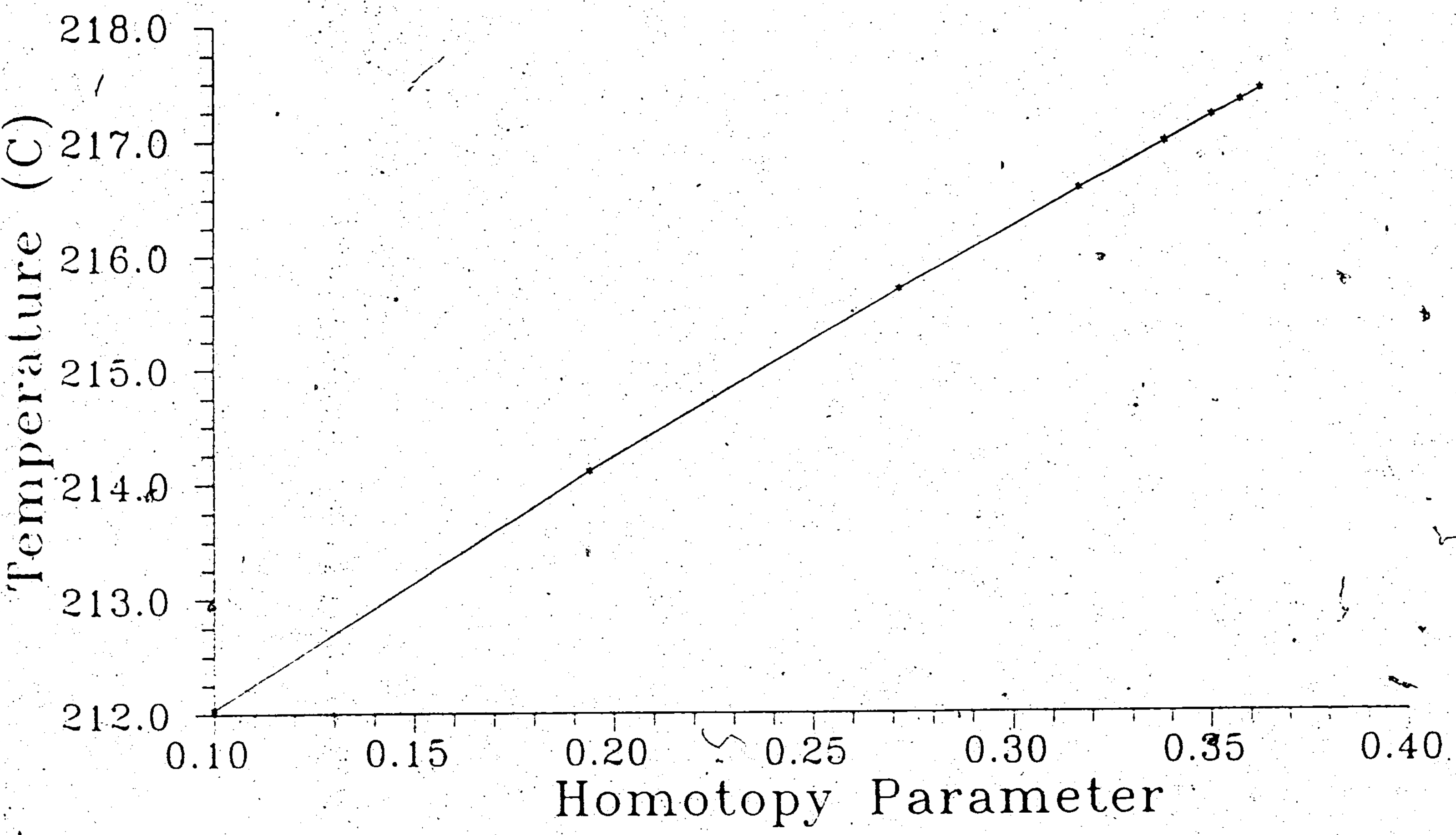


Figure 5.12
dt/dp along the Homotopy Path
for Case 2A

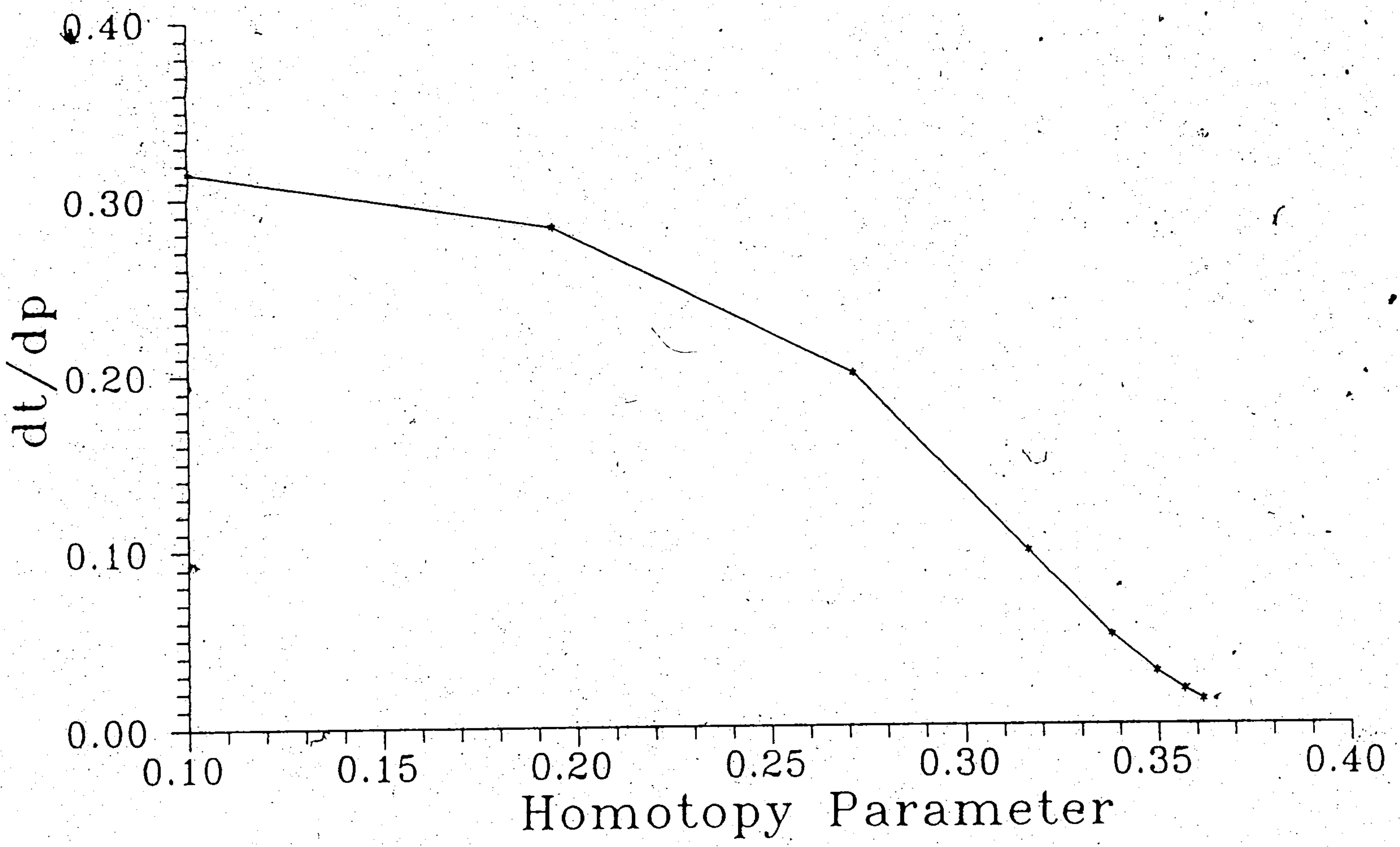


Figure 5.13
Tray 3 Molar Liquid Rate Along the Homotopy Path for Case 2B

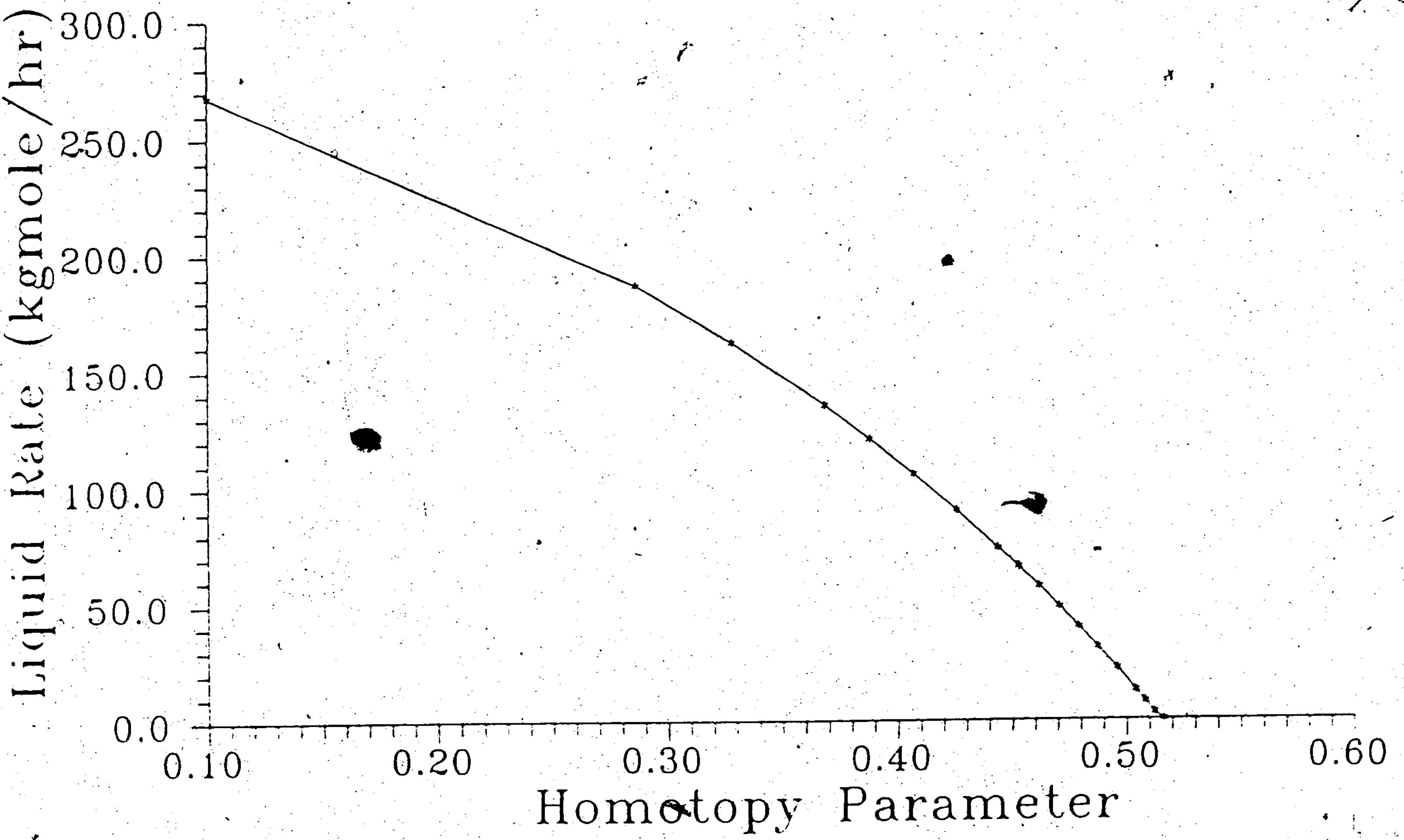


Figure 5.14
Bottoms-NC8 Mole Fraction Along the
Homotopy Path for Case 2B

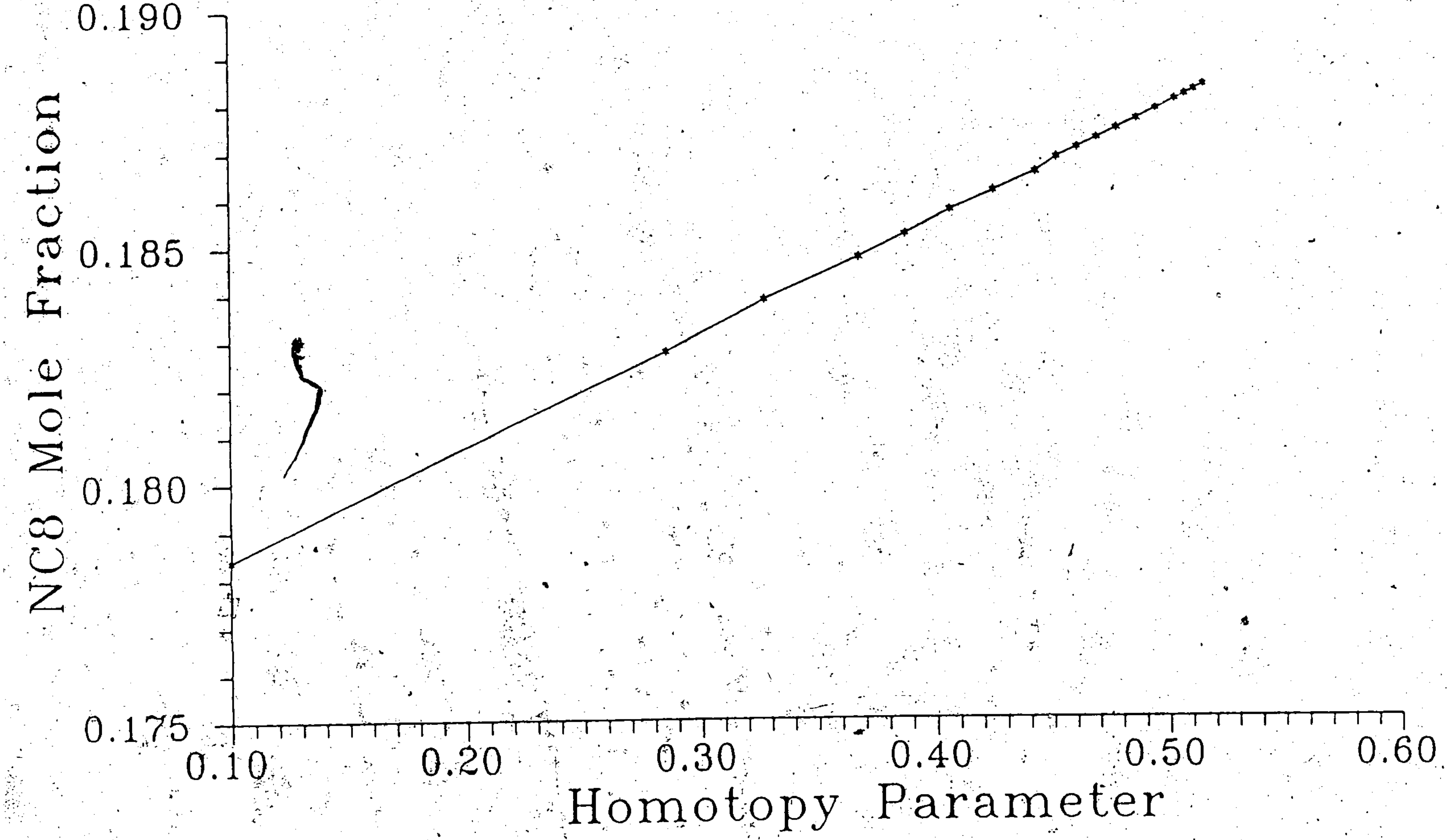
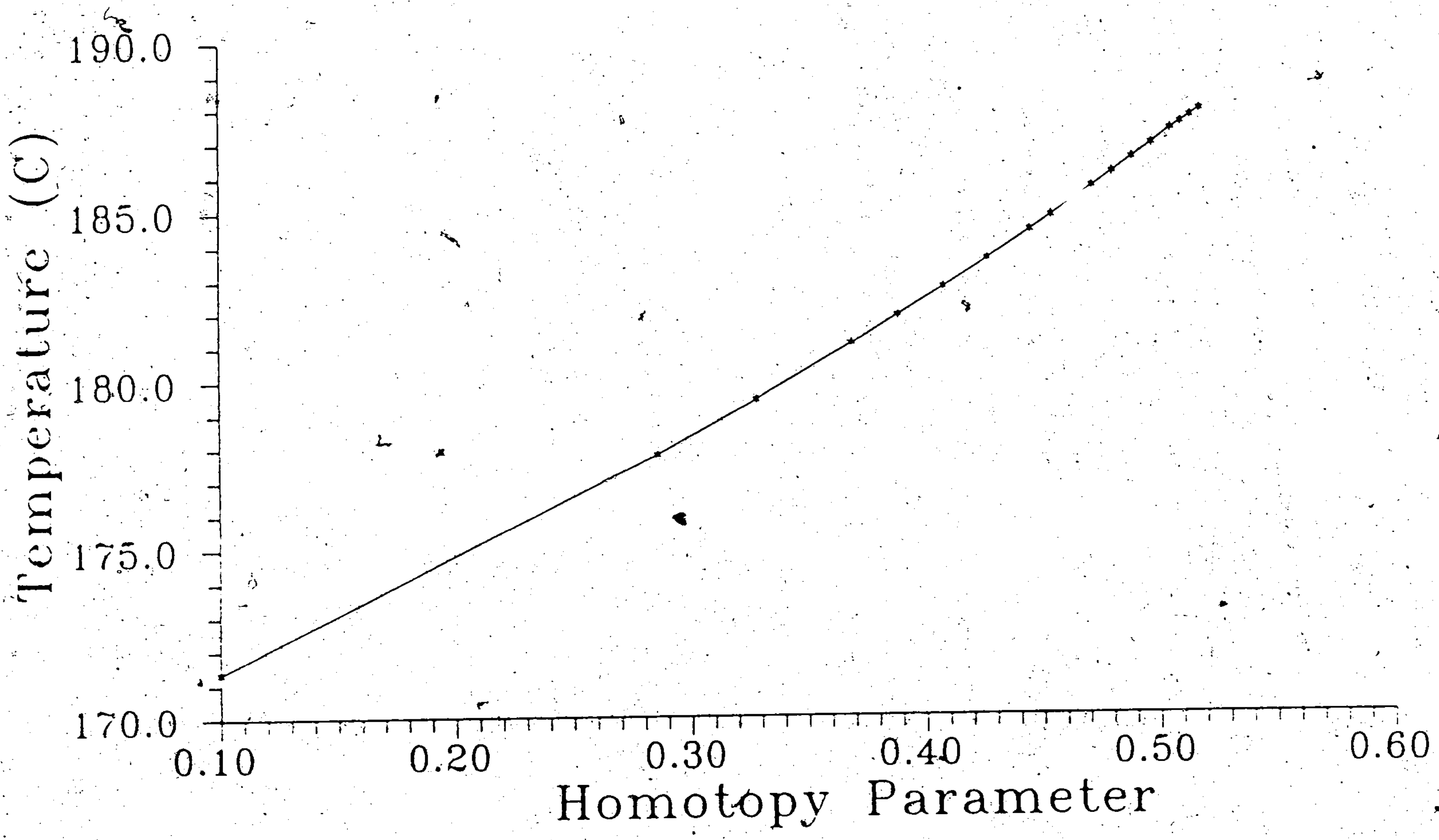


Figure 5.15
Sidestripper Product Temperature
Along the Homotopy Path for Case 2B



K VALUES

```
TRAY    1
 2.3236   1.2291   0.6685   0.3714   0.2078
 0.1187
TRAY    2
 2.7979   1.6044   0.9463   0.5675   0.3433
 0.2109
TRAY    3
 3.0920   1.8675   1.1598   0.7303   0.4643
 0.2989
TRAY    4
 3.2906   2.0589   1.3243   0.8620   0.5668
 0.3767
TRAY    5
 3.3789   2.1757   1.4392   0.9622   0.6499
 0.4430
TRAY    6
 3.4364   2.2599   1.5260   1.0404   0.7166
 0.4977
TRAY    7
 3.4799   2.3274   1.5976   1.1064   0.7742
 0.5457
TRAY    8
 3.5167   2.3869   1.6621   1.1669   0.8278
 0.5912
TRAY    9
 3.5491   2.4425   1.7239   1.2260   0.8810
 0.6370
TRAY   10
 3.5767   2.4956   1.7851   1.2859   0.9360
 0.6850
TRAY   11
 3.1077   1.8860   1.1768   0.7444   0.4754
 0.3073
TRAY   12
 3.1410   1.9226   1.2099   0.7714   0.4966
 0.3235
TRAY   13
 3.2210   2.0067   1.2849   0.8329   0.5452
 0.3608
```

```
                SOLUTION #2

   DISTILLATION BY ARCLENGTH-CONTINUATION

                PENG-ROBINSON EOS


                          --- SOLUTION ---

                          MAIN COLUMN

STAGE  LIQUID  VAPOUR  TEMP   SIDE LI   SIDE VA
          kmol/hr      deg C     kmol/hr

   1   1614.     403.  117.2     0.        0.
   2   1554.    2017.  142.1     0.        0.
   3    224.    1958.  160.4     0.        0.
   4   1305.     867.  175.8     0.        0.
   5   1368.     947.  185.3     0.        0.

   6   1415.    1011.  193.0     0.        0.
   7   1449.    1058.  199.7     0.        0.
   8   1473.    1092.  206.0     0.        0.
   9   1492.    1116.  212.6     0.        0.
  10    357.    1134.  219.7     0.        0.


                CONDENSER DUTY :    -40976.42     MJ/HR
                REBOILER  DUTY :     22876.52     MJ/HR


                          --- SIDESTRIPPER  1---

TRAY     LIQUID     VAPOUR     TEMP
            kmol/hr            deg C

 11      1336.3     1068.7      173.1
 12      1352.1     1096.2      184.9
 13       240.1     1112.0      196.6

                                       SIDESTRIPPERS

  SSTRP        DRAW   RET  TYPE        COL DRAW  PRODUCT RATE

     1           3     3    2             1308.8     240.1

 SIDE    TOP TRAY  BOTTOM TRAY

   1          11         13
```

```
                    LIQUID MOLE FRACTIONS
TRAY    1
 0.1234    0.3563    0.3560    0.1393    0.0233
 0.0017
TRAY    2
 0.0450    0.2285    0.3900    0.2563    0.0715
 0.0087
TRAY    3
 0.0201    0.1401    0.3422    0.3321    0.1397
 0.0257
TRAY    4
 0.0191    0.1019    0.2303    0.3114    0.2494
 0.0879
TRAY    5
 0.0078    0.0647    0.2124    0.3490    0.2748
 0.0913
TRAY    6
 0.0031    0.0388    0.1813    0.3728    0.3065
 0.0976
TRAY    7
 0.0012    0.0221    0.1449    0.3787    0.3443
 0.1088
TRAY    8
 0.0004    0.0120    0.1084    0.3643    0.3860
 0.1288
TRAY    9
 0.0002    0.0062    0.0755    0.3288    0.4262
 0.1632
TRAY   10
 0.0001    0.0029    0.0477    0.2741    0.4562
 0.2190
TRAY   11
 0.0077    0.0840    0.3019    0.3879    0.1850
 0.0336
TRAY   12
 0.0027    0.0458    0.2372    0.4145    0.2483
 0.0515
TRAY   13
 0.0009    0.0224    0.1653    0.4005    0.3232
 0.0876
```

```
          K VALUES

TRAY   1
 2.2883   1.2060   0.6535   0.3618   0.2016
 0.1147
TRAY   2
 2.7399   1.5692   0.9126   0.5433   0.3262
 0.1990
TRAY   3
 3.0365   1.8179   1.1192   0.6989   0.4406
 0.2814
TRAY   4
 3.2960   2.0419   1.3010   0.8392   0.5469
 0.3604
TRAY   5
 3.3778   2.1517   1.4086   0.9324   0.6236
 0.4211
TRAY   6
 3.4327   2.2332   1.4924   1.0074   0.6871
 0.4727
TRAY   7
 3.4752   2.3003   1.5633   1.0723   0.7432
 0.5192
TRAY   8
 3.5126   2.3612   1.6290   1.1336   0.7971
 0.5645
TRAY   9
 3.5476   2.4209   1.6948   1.1959   0.8528
 0.6120
TRAY  10
 3.5794   2.4811   1.7635   1.2626   0.9135
 0.6647
TRAY  11
 3.1981   1.9840   1.2650   0.8167   0.5325
 0.3511
TRAY  12
 3.3297   2.1294   1.3991   0.9293   0.6235
 0.4224
TRAY  13
 3.4415   2.2638   1.5290   1.0427   0.7184
 0.4990
```

Appendix VIII

This appendix contains information about the Fortran program written to do this research. There is a listing and brief explanation of the main variables in the common blocks and a listing of the executive routine that does the path following (Subroutine HTPY01). These subroutines should be useful to anyone considering writing their own continuation algorithm.

Definition of Variables

```
C
     ***** COMMONS IN INCL1.FOR *****
C
  ++++++ REALS +++++++
C
  HLIQU       :   ENTHALPY OF LIQUIDS
  HVAPO       :   ENTHALPY OF VAPOURS
  HLIQ()      :   ENTHALPY OF LIQUID OFF EACH TRAY
  HVAP()      :   ENTHALPY OF VAPOUR OFF EACH TRAY
  DHLIST()    :   DH/DT FOR EACH LIQUID
  DHVAST()    :   DH/DT FOR EACH VAPOUR

  GLOBL1()   :  PACKED VECTOR CONTAINING PHYSICAL CONSTANTS
        GLOBL1(START+1) = ATC OR SQRT(ATC) FOR MIXTURES
        GLOBL1(START+2) = B FOR CUBIC EOS
        GLOBL1(START+3) = M FOR CUBIC EOS
        GLOBL1(START+4) = 1 / CRITICAL TEMPERATURE (K)
        GLOBL1(START+5) = TRUE : CPA    PSEUDO : SG
        GLOBL1(START+6) = TRUE : CPB    PSEUDO : ECN
        GLOBL1(START+7) = TRUE : CPC    PSEUDO : EMPTY
        GLOBL1(START+8) = TRUE : CPD    PSEUDO : EMPTY
        GLOBL1(START+9)= MWT
        GLOBL1(START+10)= NBP (KELVIN)

      NOTE THAT NSIZE GIVES THE SIZE OF EACH COMPONENT
      IN GLOBL1, SO IF NSIZE=10, THE 5TH COMPONENT
      STARTS AT (5-1)*10 + 1 = 41 ( GLOBL1(41) CONTAINS
      ATC FOR THE 5TH COMPONENT.

 GLOBL2()     :  PACKED VECTOR CONTAINING THE ANTOINE
                 COEFFICIENTS A, B, C
 TVEC1()...TVEC6() VECTORS USED FOR TEMPORARY STORAGE
                     AND IN THE SPLINE ROUTINES.
 RTAD()       :  CONTAINS SQRT(A) FOR THE GIVEN CUBIC EOS,
                 FILLED IN GETPQR, AND USED IN FUGCTY
                 AND ENTDEP.
 RKVALS()     :  KVALUES FOR THE GIVEN EOS.  FILLED IN
                 BY FUGCTY AND GTKVALS.  NOTE THAT
                 KVALS() RELATES TO THE MIXTURE
                 IN XMOLE() AND YMOLE().
 IKVALS()     :  IDEAL KVALUES, CALCULATED USING WAGNER VAPOUR
                 PRESSURE EQUATION OF WILLMAN AND TEJA
 KVALS()      :  APPROPRIATE KVALUES, DEPENDING ON IF YOU ARE
                 PATH FOLLOWING IN K (PATHFK) AND IF NOT PATH
                 FOLLOWING, THEN ON WHETHER IDEAL KVALUES OR
                 NON IDEAL KVALUES (KIDEAL) ARE REQUESTED.
 KVALST(,)    :  STORAGE OF KVALES, (TRAY, COMP)
 KRMKIS(,)    :  RIGOROUS K VALUE - IDEAL KVALUE, NEEDED
                 FOR DERIVATIVES WITH RESPECT TO THE HOMOTOPY
```

```
                 PARAMETER.
DKDTS()      :   DERIVATIVE OF K WRT TEMPERATURE.
DKDTST(,)    :   STORAGE OF DKDT FOR EACH TRAY AND COMP
ZLIQ         : LIQUID Z FROM EOS
ZVAP         : VAPOUR Z FROM EOS
T            : TEMPERATURE USED IN THERMODYNAMIC ROUTINES (K)
PRES         : PRESSURE USED IN THERMODYNAMIC ROUTINES (PASCALS)
A, B, C      : EQUATION OF STATE (EOS) CONSTANTS
P, Q, R      : USED TO SOLVE EOS FOR Z
RT, ORT      : RGAS * T (RGAS = 8.3144 J/MOL K) ORT = 1 / RT
ALPHA2       :
DADT         :
Z            : EITHER ZLIQ OR ZVAP DEPENDING ON LIQUID=T OR F
V            : V = ZRT/PRES
LNZ          : LNZ = NATURAL LOG OF Z
ACAP, BCAP   : ACAP = A * PRES * ORT * ORT
CCAP           BCAP = B * PRES * ORT
               CCAP = C * PRES * ORT
C
  +++++++ INTEGERS +++++++++
C
  NDISC      : TOTAL NUMBER OF DISCRETE COMPONENTS
  NTRUE      : NUMBER OF TRUE COMPONENTS
  NPSDO      : NUMBER OF PSEUDO COMPONENTS
  THERMO     :   INDICATES WHICH EOS IS IN USE
                 1 ==> SOAVE REDLICH KWONG
                 2 ==> PENG ROBINSON
                 3 ==> PATEL TEJA
  NSIZE      :   INDICATES THE SIZE OF EACH PARTITION IN GLOBL1
  NSIZE2     : SIZE OF PARTITION OF GLOBL2 (=3)
  START      : USED TO POINT TO STARTING POSITION IN GLOBL1
  START      : USED TO POINT TO STARTING POSITION IN GLOBL2
C
  ++++++++ LOGICAL +++++++++
C
  LIQUID     : TRUE ===> A LIQUID STREAM IS BEING
               EVALUATED ( Z, ENTHALPY )
             : FALSE ==> A VAPOUR STREAM
 PATHFH :  TRUE ==>  PATH FOLLOWING WITH HEATER COOLERS
 PATHFK :  TRUE ==>  PATH FOLLOWING WITH KVALUES
 PATHFS :  TRUE ==> PATH FOLLOWING IN STRUCTURE
 PATHFP :  TRUE ==> PATH FOLLOWING IN PRODUCT PURITY
 FIRSTP :  TRUE ==> HOMOTP = 0.0  (STARTING THE PATH)
 LASTP  :  TRUE ==> HOMOTP = 1.0  (ENDING THE PATH)
 KIDEAL :  TRUE ==>  USE IDEAL KVALUES IN THE CALCULATION
                THIS IS USED FOR THE INITIAL PROBLEM.
 EULER  :  TRUE ==> EULER STEP, DO NOT CALCULATE RHS.
  SVRHS      : TRUE ==> SUB INBIXX INTERCEPTS VALUES AND ADDS THEM
                    TO RHSSTO(). THIS PERMITS THE JACOBIAN WITHOUT
                    THE RHS TO BE SAVED AND USED IN THE EULER
                    CALCULATION.
   ------------- END OF INCL1.FOR ---------------
```

********* VARIABLES IN INCLA.FOR *************

++++++++ REALS +++++++

LIQU() : LIQUID RATE MOLES/TIME FROM EACH TRAY
VAPOUR() : VAPOUR RATE MOLES/TIME FROM EACH TRAY
OHDPUR : OVERHEAD PURITY SPEC
BOTPUR : BOTTOMS PURITY SPEC
OHDPUI : PURITIES FROM INITIAL PROBLEM
BOTPUI : PURITIES FROM INITIAL PROBLEM
REFRAT : REFLUX RATIO
RFRATI : REFLUX RATIO FOR INITIAL PROBLEM
OHDPRI : OVERHEAD RATE FOR INITIAL PROBLEM
BOTPRI : BOTTOMS RATE FOR INTIAL PROBLEM
BOTPRS : BOTTOMS RATE SPECIFICATION
OHDPRS : OVERHEAD RATE SPECIFICATION
FEEDT() : FEED TEMPERATURE, KELVIN
FEEDPR() : FEED PRESSURE, PASCALS
FEEDRA() : FEED RATE, MOLES/TIME
FEEDML(,) : MOLE FRACTION OF EACH FEED COMPONENT
FEEDMW() : MOLECULAR WEIGHT OF EACH FEED
FEEDEN() : FEED ENTHALPY
HTCLIM() : DUTY OF IMAGINARY HEATER / COOLERS
HTCOOL() : DUTY OF REAL HEATER / COOLERS
SIDEDU() : DUTY OF SIDESTRIPPER REBOILER
SIDERA() : RATE OF SIDESTRIPPER PRODUCT
SSPRPU() : SIDESTRIPPER PRODUCT PURITY (MOLE PERCENT)
SIDELI() : RATE OF SIDESTRIPPER DRAW FROM MAIN COLUMN
SIDRAI() : INITIAL PROBLEM SIDESTRIPPER PRODUCT RATES
SSPECI() : PURITY SPEC ON SIDESTRIPPER FOR INITIAL PROBLEM
SIDELL() : VALUE OF SIDESTRIPPER DRAW RATE FROM THE INITIAL PROBLEM
SIDELS() : SPECIFICATION OF SIDESTRIPPER DRAW RATE

PUMPDU() : DUTY OF PUMPAROUND
PUMPRT() : PUMPAROUND RETURN TEMPERATURE
PUMPDT() : PUMPAROUND TEMPERATURE DIFFERENCE
PUMPRA() : PUMPAROUND RATE
PUMPRH() : PUMPAROUND RETURN ENTHALPY
TRAYTK() : TRAY TEMPERATURES, KELVIN
DTDPMN : LOWER VALUE OF DTDPMN WHERE TURNING POINT STARTS
DPMAX : MAXIMUM VALUE OF DELTA P WITHIN PROPER RANGE OF T AS GIVEN BY DPMXRG
DPMXRG : RANGE OF ABS(T) SUCH THAT DELTA P IS CLAMPED
DPINI : INITIAL VALUE OF DP (MAKE DPINI < 0 TO PATH FOLLOW BACKWARDS)
MINSTP : MINIMUM VALUE ALLOWED FOR DELTAP STEP. USED TO DETERMINE WHEN NEWTON'S EXTENDED SYSTEM HAS FAILED
DXDPST() : STORAGE OF DXDP AND DTDP. THIS IS NEEDED SO THAT IT CAN BE USED WHEN A NEW EULER STEP IS TO BE MADE SO THAT THE INITIAL VALUES OF DXDP AND DTDP CAN BE "CLOSE" TO SPEED CONVERGENCE.
RHSSTO() : VECTOR TO STORE THE VALUES FOR THE RIGHT HAND SIDE TO ALLOW THE JACOBIAN TO BE STORED WITHOUT THE RHS FOR THE EULER CALCULATION.

```
HMTMAX      :  WHEN ABS(HOMOTP) > HMTMAX STOP PATH FOLLOWING.
TEXPHC      :  EXPONENT  FOR  HEATERS/COOLERS
TEXPKV      :  EXPONENT  FOR  KVALUES
TEXPST      :  EXPONENT  FOR  STRUCTURE
TEXPPP      :  EXPONENT  FOR  PRODUCT  PURITY
HOEXHC      :  HOMOTP  **  TEXPHC
HOEXKV      :  HOMOTP  **  TEXPKV
HOEXST      :  HOMOTP  **  TEXPST
HOEXPP      :  HOMOTP  **  TEXPST
HODEHC      :  TEXPHC * HOMOTP ** (TEXPHC - 1)
HODEKV      :  TEXPKV * HOMOTP ** (TEXPKV - 1)
HODEST      :  TEXPST * HOMOTP ** (TEXPST - 1)
HODEPP      :  TEXPPP * HOMOTP ** (TEXPPP - 1)
DELTAP      :  THE CHANGE IN P USED TO TAKE EULER STEP
  +++++++ INTEGERS +++++++
NTRAYS      :  TOTAL NUMBER OF TRAYS IN SYSTEM
NTRCOL      :  NUMBER OF TRAYS IN MAIN COLUMN
NTRSSP()    :  NUMBER OF TRAYS IN EACH SIDESTRIPPER
TRYORD()    :  ORDER OF TRAYS IN JACOBIAN
TRAYTP()    :  TRAY TYPES
                1 = SIMPLE TRAY
                2 = TOTAL CONDENSER
                3 = PARTIAL REBOILER
                4 = LIQUID DRAW
                5 = TOP OF SIDESTRIPPER
                6 = CRUDE FEED (VAPOUR FEED AT BOTTOM OF COLUMN,
                     NO REBOILER)
                7 = LIQUID FEED
                8 = VAPOUR FEED TRAY
                9 = LIQUID AND VAPOUR FEED TRAY
               10 = SUPERTRAY
JACSTR()    :  STARTING COLUMN OF EACH TRAY IN THE JACOBIAN
PUMPDR()    :  TRAY FOR PUMPAROUND DRAW
PUMPRE()    :  TRAY FOR PUMPAROUND RETURN
PUMPTY()    :  TYPE OF PUMPAROUND SPECIFICATION
                1 = GIVE DT, Q, FIND FLOW
                2 = GIVE DT, FLOW FIND Q
                3 = GIVE FLOW, Q, FIND DT
                4 = GIVE DT
                5 = GIVE FLOW
                6 = GIVE Q
                7 = SPECIFY NOTHING
NPUMP       :  NUMBER OF PUMPAROUNDS
SIDEDR()    :  TRAY FOR SIDESTRIPPER LIQUID DRAW
SIDERE()    :  TRAY FOR SIDESTRIPPER VAPOUR RETURN
SSRBTY()    : SIDESTRIPPER REBOILER TYPE
               1 = PARTIAL REBOILER
               2 = TOTAL REBOILER
NSIDE       :  NUMBER OF SIDESTRIPPERS
FEEDTP()    : TYPE OF FEED
               1 = SUBCOOLED LIQUID
               2 = LIQUID AT BUBBLE POINT
               3 = VAPOUR AT DEW POINT
               4 = SUPERHEATED VAPOUR
```

```
FEEDTR()    :  FEEDTRAYS
NFEEDS      :  NUMBER OF FEEDS
FEEDPH()    :  FEED PHASE
                 1 = LIQUID
                 2 = VAPOUR
OVHTYP      :  TYPE OF OVERHEAD PRODUCT
                 1 = MOLE / TIME
                 2 = KG / TIME
BOTTYP      :  TYPE OF BOTTOMS PRODUCT
                 1 = MOLE / TIME
                 2 = KG / TIME
REBTYP      :  REBOILER TYPE
               1 = NO REBOILER
               2 = PARTIAL REBOILER
CONTYP      :  CONDENSER TYPE
               1 = TOTAL CONDENSER
NONSTD      :  NUMBER OF NON-STANDARD EQUATIONS OR
               NUMBER OF DEGREES OF FREEDOM
NONSTB      :  NUMBER OF NONSTANDARD EQUATIONS ON THE BORDER
SSSPEC()    :  SPECIFICATION FOR THE TYPES OF SIDESTRIPPERS
               1 ==> PRODUCT RATE KMOLES/TIME
                   EX.  1   50.   -1  (-1 IS A DUMMY ARG)
               2 ==> PURITY SPEC
                   EX.  2   1     0.9
                           WHERE 2 IS OPTION 2
                                 1 IS THE FIRST COMPONENT
                                 0.9 IS THE MOLE FRACTION
               3 ==> BOILING POINT SPEC
                   EX. 3  95.   280.
                           WHERE 3 IS THE OPTION
                                 95. IS 95 WT%
                                 280. IS THE NBP (DEG C)
  4 ===> DUTY
  5 ===> NOTHING
SSPEC2()    :  FOR SPECIFICATIONS OF SIDESTRIPPERS WHICH
               GO ON THE BORDERS OF THE MATRIX
                    1===>  REFLUX RATIO
                    2===>  LIQUID DRAW RATE FROM SIDESTRIPPER
SSPUCO()    :  COMPONENT THAT SIDESTRIPPER PURITY APPLIES TO
TPTRSS()    :  TOP TRAY OF SIDESTRIPPER()
BOTRSS()    :  BOTTOM TRAY OF SIDESTRIPPER()
OHDTYP      :  OVERHEAD SPECIFICATION TYPE (CONDENSER)
               1==>  PRODUCT RATE, MOLES/TIME
               2==>  PRODUCT PURITY
               3==>  DUTY OF CONDENSER
               4==>  REFLUX RATIO
               5==>  BOILING POINT SPEC
               6==>  NONE
BOTTYP      :  BOTTOM SPECIFICATION TYPE (REBOILER)
               1==>  PRODUCT RATE, MOLES/TIME
               2==>  PRODUCT PURITY
               3==>  DUTY OF CONDENSER
               4==>  BOILING POINT SPEC
               5==>  NONE
```

```
OHPUCO     :  COMPONENT THAT OVERHEAD PURITY APPLIES TO
BOPUCO     :  COMPONENT THAT BOTTOMS  PURITY APPLIES TO
CYCLE     :  CYCLE LENGTH FOR WEGSTEIN'S ACCELERATION IN WEGACC
MXFLMB    :  MAXIMUM NUMBER OF ALLOWED FAILS FOR MASBAL
TOTVAR    :  TOTAL NUMBER OF VARIABLES ( INCLUDING HOMOTP ).
 ------------  END OF INCLA.FOR  ----------------

   CODES USED IN SUBROUTINE JACCGEN()
                        1=  RETURN SIZE OF SUBMATRIX
                        2=  INITIALIZE JACOBIAN STRUCTURE
                        3=  ENTER MASS BALANCE COEFFICIENTS
                        4=  CALCULATE IMAGINARY HEATER/COOLERS
                        5=  ENTER PATH FOLLOWING COEFFICIENTS
                        6=  SAVE THE CURRENT POINT ON THE PATH
                        7=  RESTORE THE PREVIOUS POINT ON THE PATH
                        8=  TAKE THE EULER STEP
                        9=  TAKE THE NEWTON STEP
                        10= EVALUATE CONSTRAINT EQUATION FOR
                            THE EXTENDED SYSTEM

 *** LOGICAL ***

  PATHST   ==>  TRUE, PATH FOLLOWING IN STRUCTURE IS DESIRED
                FALSE PATH FOLLOWING IN STRUCTURE IS NOT DESIRED
 PFS1      ==>  TRUE :  SOLVE THE INITIAL (WANG HENKE) PROBLEM
                        WITHOUT THE VAPOUR RETURN FROM THE
                        SIDESTRIPPER TO THE MAIN COLUMN
                FALSE:  SOLVE THE INITIAL (WANG HENKE) PROBLEM
                        WITH    THE VAPOUR RETURN FROM THE
                        SIDESTRIPPER TO THE MAIN COLUMN
 PFS2  ...  ONLY USED WHEN PFS1 = TRUE
            TRUE ==>  PATH FOLLOW FORWARDS IN ORDER TO GET
                      ON THE RIGOROUS PATH
            FALSE ==>  PATH FOLLOW BACKWARDS IN ORDER TO GET
                       ON THE RIGOROUS PATH
 PFS3 ==>   TRUE :  FROM THE FIRST POINT ON THE RIGOROUS
                    PATH, PATH FOLLOW FORWARDS TO TRY TO
                    GENERATE MULTIPLE SOLUTIONS
            FALSE :  FROM THE FIRST POINT ON THE RIGOROUS PATH,
                     PATH FOLLOW BACKWARDS TO TRY TO GENERATE
                     MULTIPLE SOLUTIONS
```

Homotopy Continuation Subroutine

```
      SUBROUTINE HTPY01(KO)
      IMPLICIT REAL*8 (A-Z)
C
C         ---  HOMOTOPY CONTINUATION SUBROUTINE ---
C
C     TAKES EULER STEP AND CORRECTS WITH NEWTONS METHOD.
C     FAR FROM A TURNING POINT THE HOMOTOPY PARAMETER IS
C     NOT SOLVED FOR.
C     LOOPS : TOTAL NUMBER OF STEPS
C     LOOPN : NUMBER OF NEWTON ITERATIONS FOR ONE TRY
C     LOOPNT: TOTAL NUMBER OF NEWTON ITERATIONS
C     LOOPE : NUMBER OF EULER ITERATIONS FOR ONE TRY
C     LOOPET: TOTAL NUMBER OF EULER ITERATIONS
C CONDIV : NUMBER OF CONSECUTIVE DIVERGENCES
C MAXDIV : MAXIMUM NUMBER OF ALLOWED CONSECUTIVE ITERATIONS
C          WHERE THE ALGORITHM IS DIVERGING ( I.E. THE RESIDUAL
C          IS INCREASING )
C          NOTE THAT DIFFERENT VALUES ARE USED FOR THE SIMPLE SYSTEM
C          AND THE EXTENDED SYSTEM
C OLDERR : VARIABLE TO HOLD THE ERROR FROM THE PREVIOUS ITERATION
C
C    MNFAIL : MAXIMUM NUMBER OF NEWTON CORRECTOR FAILURES
C     INCR   :  TRUE ==>  THE PATH WILL CROSS t=1 BY INCREASING
C               THIS IS USED TO DETERMINE WHEN t=1 SHOULD BE
C               SET SO THAT A SOLUTION CAN BE CALCULATED.
C
C               WHEN MULTIPLE SOLUTIONS ARE PRESENT, AFTER THE
C               FIRST SOLUTION, THE PATH MUST TURN AROUND AND
C               CROSSOVER t=1 WHEN t IS DECREASING.(INCR=.FALSE.).
C
C     SOLU   :  TRUE ==>  t=1 AND SO THIS IS A SOLUTION TO THE
C               DESIRED SET OF EQUATIONS.
C
C     FAIL   :  TRUE ==>  NEWTON'S METHOD FAILED
C                              (SIMPLE OR EXTENDED)
C               AND SO THE STEP LENGTH (DP) IS HALVED.
C
C     TURN   :  TRUE ==>  DTDP < DTDPMN AND SO THIS IS ASSUMED TO
C               BE A TURNING POINT.
C
C     ECONV :   TRUE ==>  EULERS METHOD CONVERGED,
C                         SAVE DXDP AND DTDP.
C DERIV     :  .TRUE. ==> UPDATE DERIVATIVES IN GTHERM
C     W1, W2:   WEIGHTS ON DXDP AND DTDP, THIS HELPS TO SCALE DTDP
C  EULTOL   :   TOLERANCE FOR EULERS METHOD
C  NOFAIL   :   THIS IS TRUE WHEN THE CORRECTIONS DONE AFTER THE
C               FIRST EULER PREDICTOR STEP CONVERGE
C               IF THE FIRST CORRECTION STEPS DO NOT CONERGE, THEN
C               THE DELTAP USED TO PREDICT THE NEXT POINT ON THE PATH
C               WAS TOO LARGE (I.E. THE CURVE IS STEEP HERE).
C               THEREFORE DO NOT DOUBLE THE STEP LENGTH WHEN THE
C               SOLUTION DOES CONVERGE.
```

```
      REAL*8 OLDERR
      INTEGER END, I, CODE, KO, LOOPS, LOOPN,
     A   LOOPNT, LOOPE, LOOPET, MNFAIL,
     A   MAXS, MSGLVL, IERR, NEQNS, FUGERR,
     A   CONDIV, MAXDIV, J, K, VATYPE,
     A   VACOMP, VATRAY, SIDE, BOT, TOP
C***
C***
C
      LOGICAL INCR, SOLU, FAIL, TURN, ECONV, DERIV,
     A    DECOMP, NOFAIL
      INCLUDE '[RONB.THESIS.SOURCE]INCL1.VAR'
      INCLUDE '[RONB.THESIS.SOURCE]INCLA.VAR'
C     NOW INSERT COMMONS
C
      COMMON /SPKUSR/ MSGLVL, IERR, MAXS, NEQNS
      INCLUDE '[RONB.THESIS.SOURCE]INCL1.COM'
      INCLUDE '[RONB.THESIS.SOURCE]INCLA.COM'
      COMMON /MA28LL/ DECOMP
C
C     NOW INSERT DATA STATEMENTS
C
      INCLUDE '[RONB.THESIS.SOURCE]INCL1.DAT'
C
      INCR = .TRUE.
      SOLU = .FALSE.
      FAIL = .FALSE.
      TURN = .FALSE.
      SVRHS= .FALSE.
      DEBUG = .FALSE.
      NOFAIL = .TRUE.
C
C     TURN OFF PATH FOLLOWING IN KVALUES...
C     HOPEFULLY ANY HYDROCARBON SYSTEM WILL BE ABLE TO BE
C     SOLVED FOR KVALUES BY INTRODUCING K INCREMENTALLY
      PATHFK = .FALSE.
C
      W1 = EXTWT1
      W2 = EXTWT2
      EULTOL = 1.D-04
      RN = DFLOAT(TOTVAR)
C
C     TOLCON IS THE CONVERGENCE TOLERANCE USED AT T=1.0
C     TOLPAT IS THE CONVERGENCE TOLERANCE USED ALONG THE PATH
      TOLCON = 1.D-05
      TOLPAT = 2.5D-04
      DTDP = ZERO
C
C     MINSTP IS THE MINIMUM ALLOWED STEPLENGTH
      MINSTP = 1.D-6
      DPMXRG = TWO
      TMAX = 15.D0
      OLDERR = 1.D06
      DPMAX = DABS(DPINI)
```

```
      DELTAP = DPINI
      DELTAT = DELTAP
      CONDIV = 0
C     SAVE THE INITIAL POINT ON THE PATH
      CALL JACGEN(6)
      CALL NONSTE(6)
      XVECST(TOTVAR) = ZERO
C
C     HAVE THE HARWELL ROUTINES DO THE DECOMPOSITION FIRST
      DECOMP = .TRUE.
C
C     SET THE SWITCH FOR THE FIRST POINT ON THE PATH
      FIRSTP = .TRUE.
C
C     SET THE NUMBER OF ITERATIONS BEFORE A METHOD FAILS
      MNFAIL = 25
      MNFLSV = MNFAIL
C
C     INITIALIZE TH[illegible]OR THE NUMBER OF SOLUTIONS
      NSOLNS = 0
C
C     IF DT/DP IS BE[illegible]LUE THEN INVOKE THE EXTENDED
C     SYSTEM BECAUSE[illegible]NG POINT IS PROBABLY COMING UP
      DTDPMN = 0.10D0
C
      HODEHC = ONE
      HODEKV = ONE
      HODEST = ONE
      HODEPP = ONE
C
      HOMOTP = ZERO
      HOEXHC = HOMOTP
      HOEXKV = HOMOTP
      HOEXST = HOMOTP
      HOEXPP = HOMOTP
C
      PATHLN = ZERO
C
C     SET PATHFS TO GET ON THE RIGOROUS PATH...
      TEST = DPINI
      PATHFS = .FALSE.
      IF(PFS1) PATHFS = .TRUE.
      DPINI = - DABS(DPINI)
      IF(PFS2) DPINI = DABS(DPINI)
      IF(.NOT. PATHST) DPINI = DSIGN(DPINI, TEST)
C
C     INTITIALIZE THE DERIVATIVES
      DERIV = .TRUE.
      CALL GTHERM(DERIV,FUGERR)
C
C     CALCULATE THE IMAGINARY HEATER/COOLERS WHEN USED
      IF(PATHFH) THEN
      CALL JACGEN(4)
      CALL NONSTE(4)
```

Figure 5.16
dt/dp Along the Homotopy Path
For Case 2B

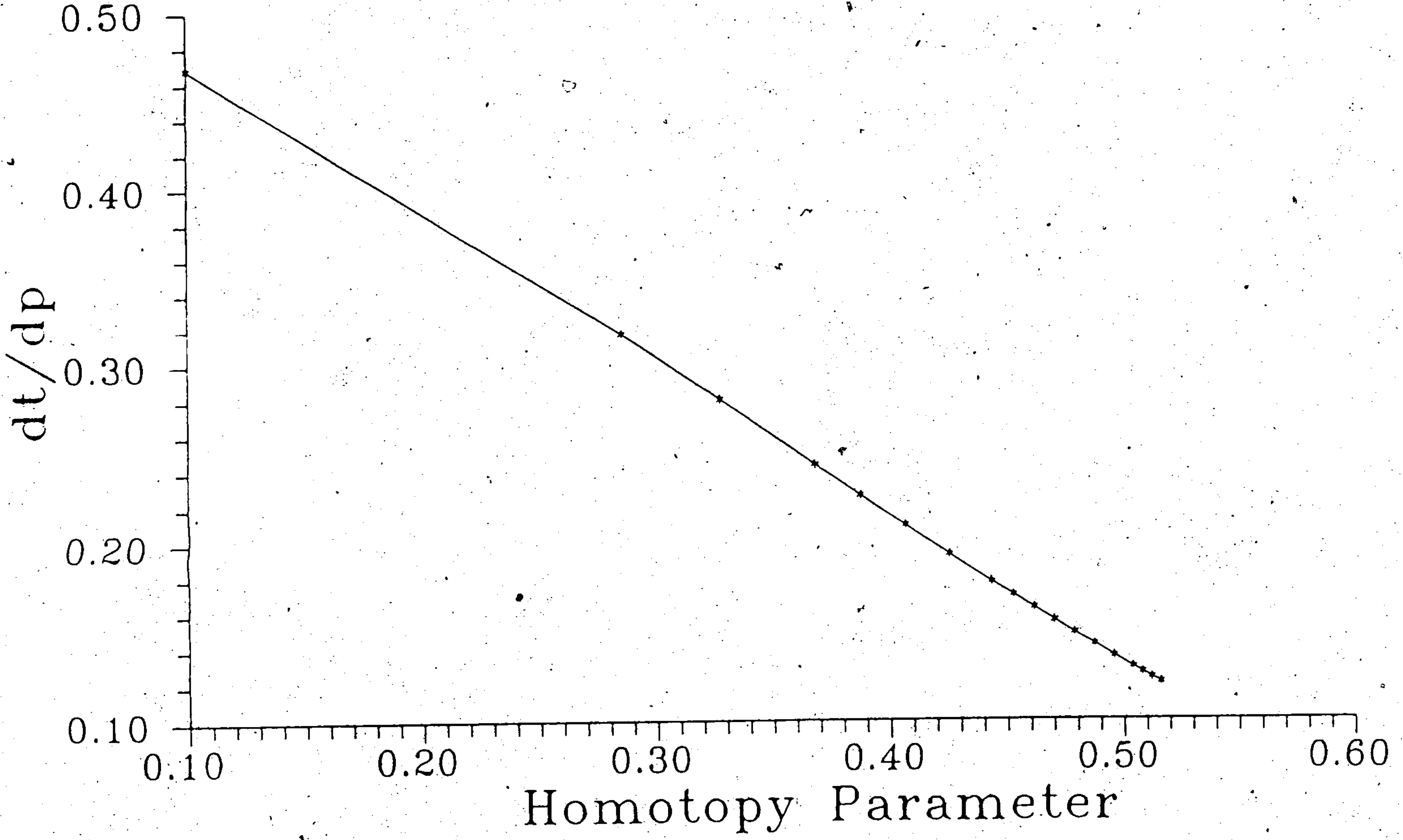


Figure 5.17
Liquid Draw Rate Along the
Homotopy Path for Case 2C

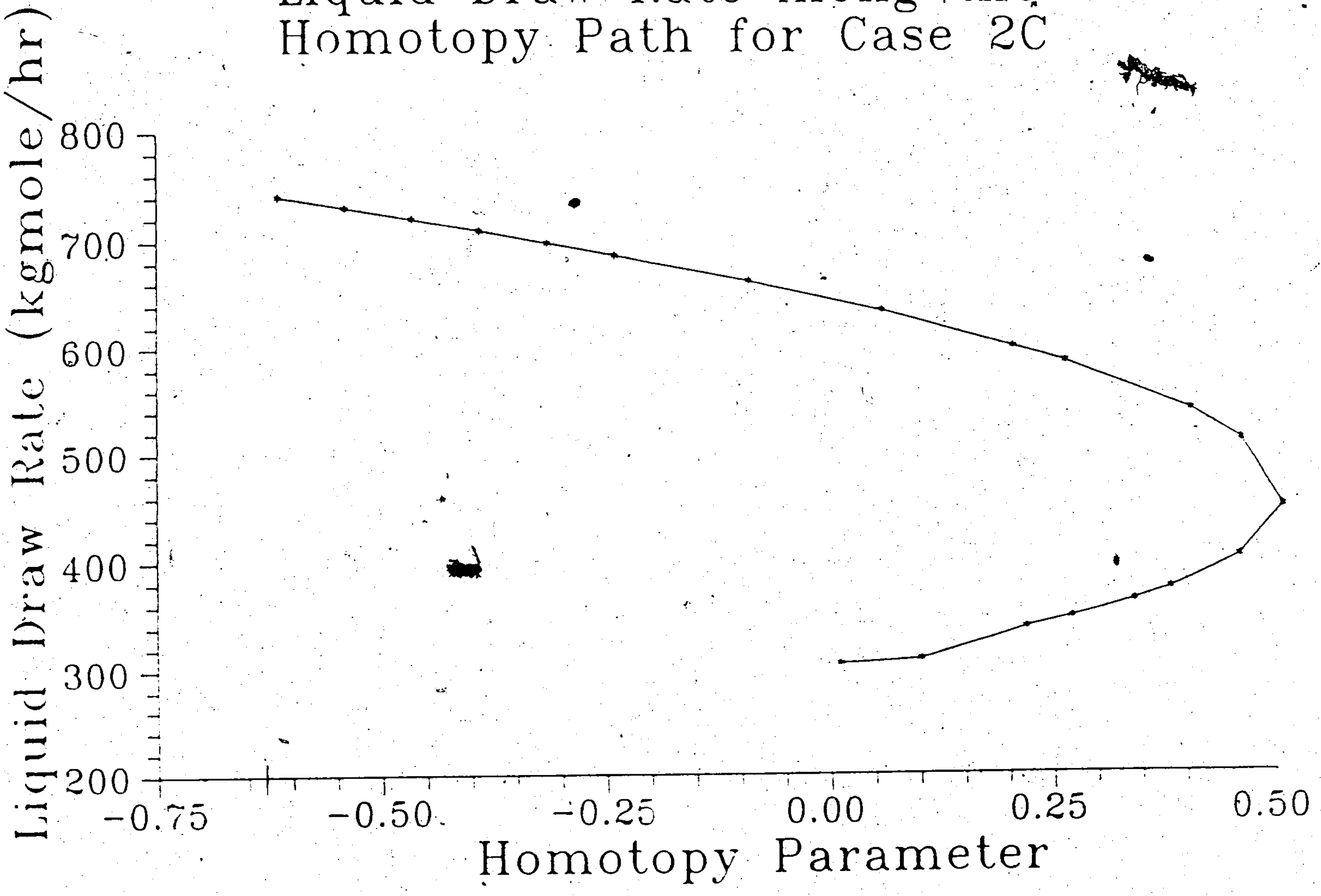


Figure 5.18
Propane Mole Fraction in Distillate
Along the Homotpy Path for Case 2C

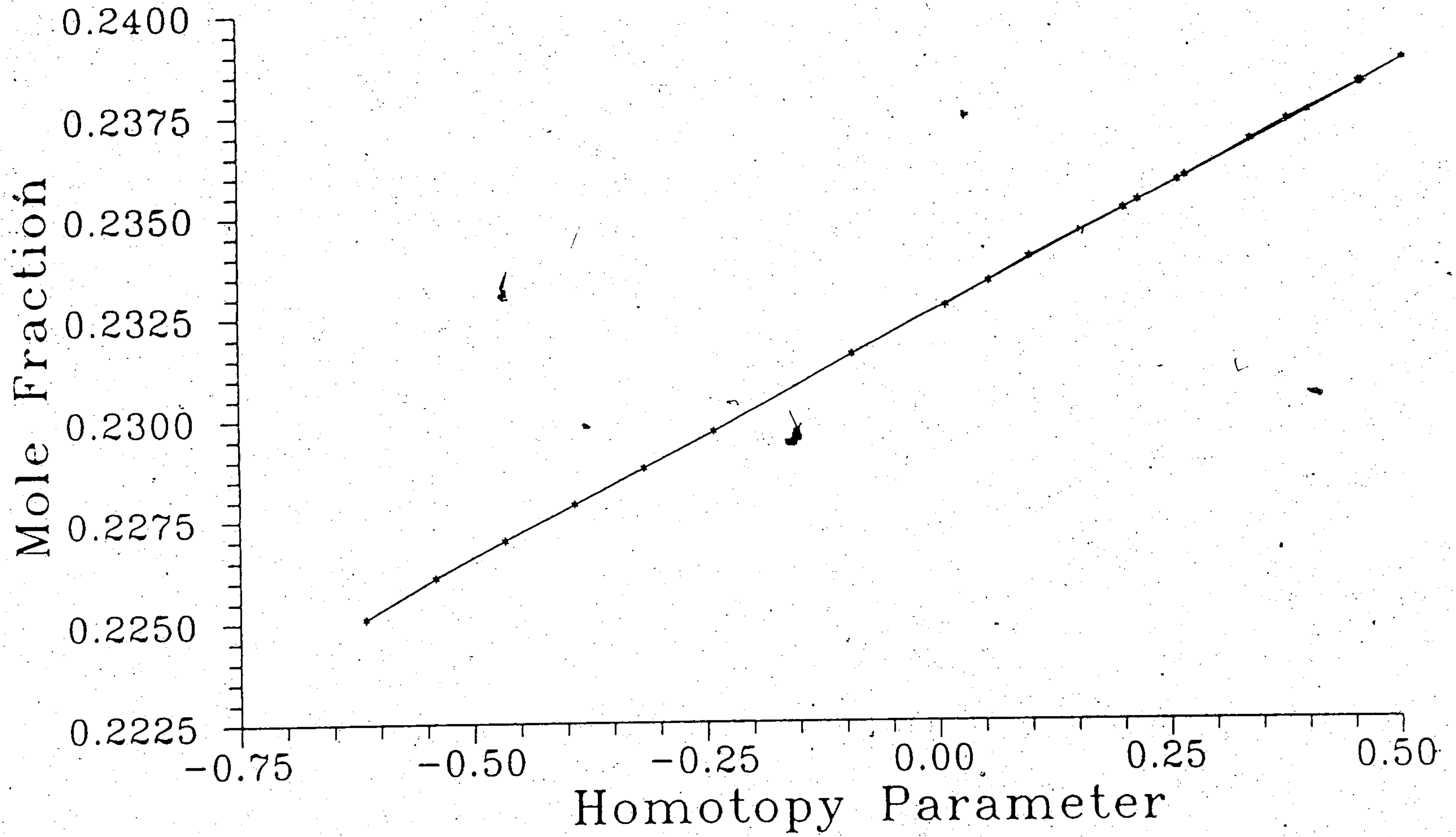


Figure 5.19
Condenser Temperature Along the
Homotopy Path for Case 2C

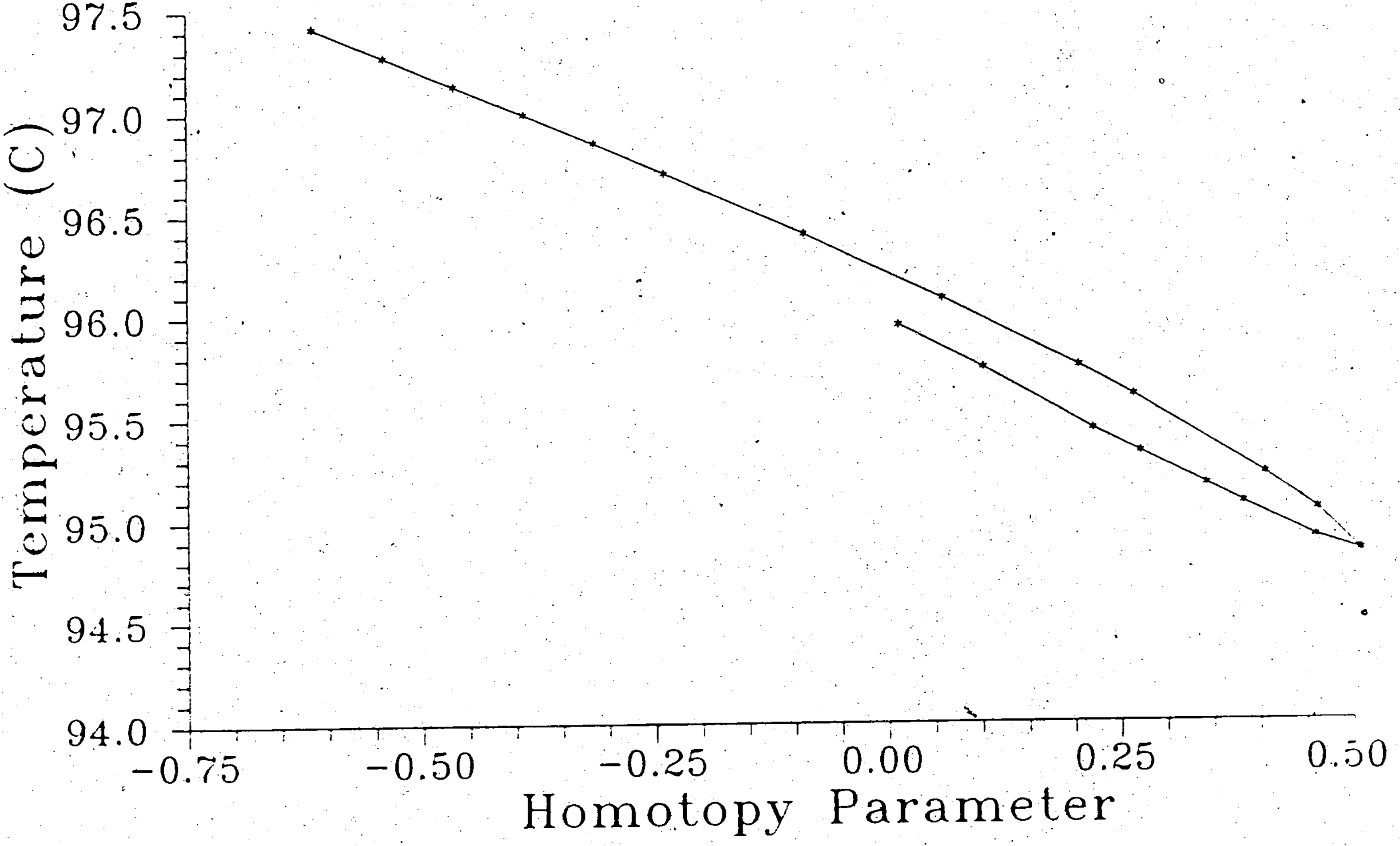


Figure 5.20
dt/dp Along the Homotopy Path for Case 2C

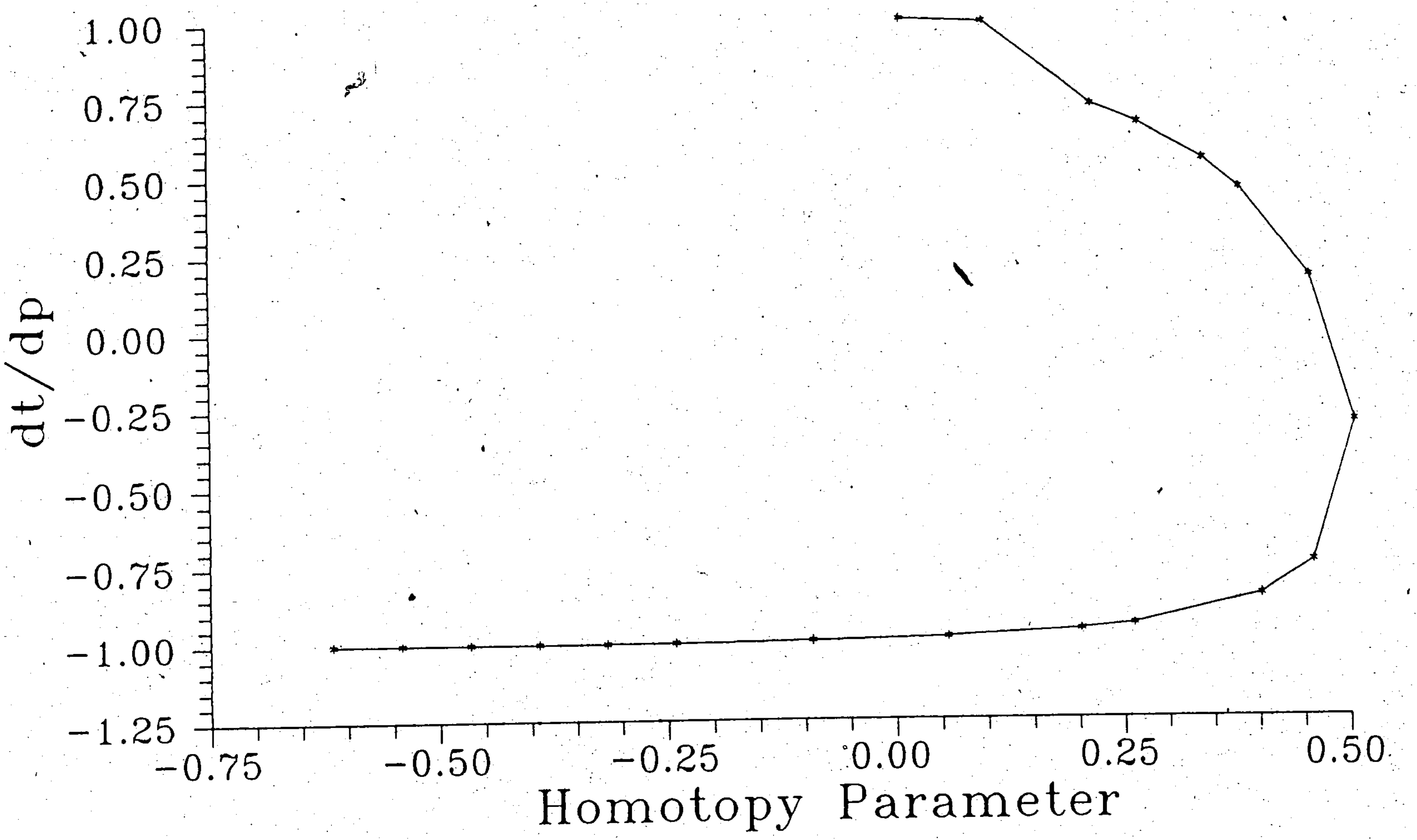


Figure 5.21
Homotopy Paths for Path Following
in Heater/Coolers and Structure

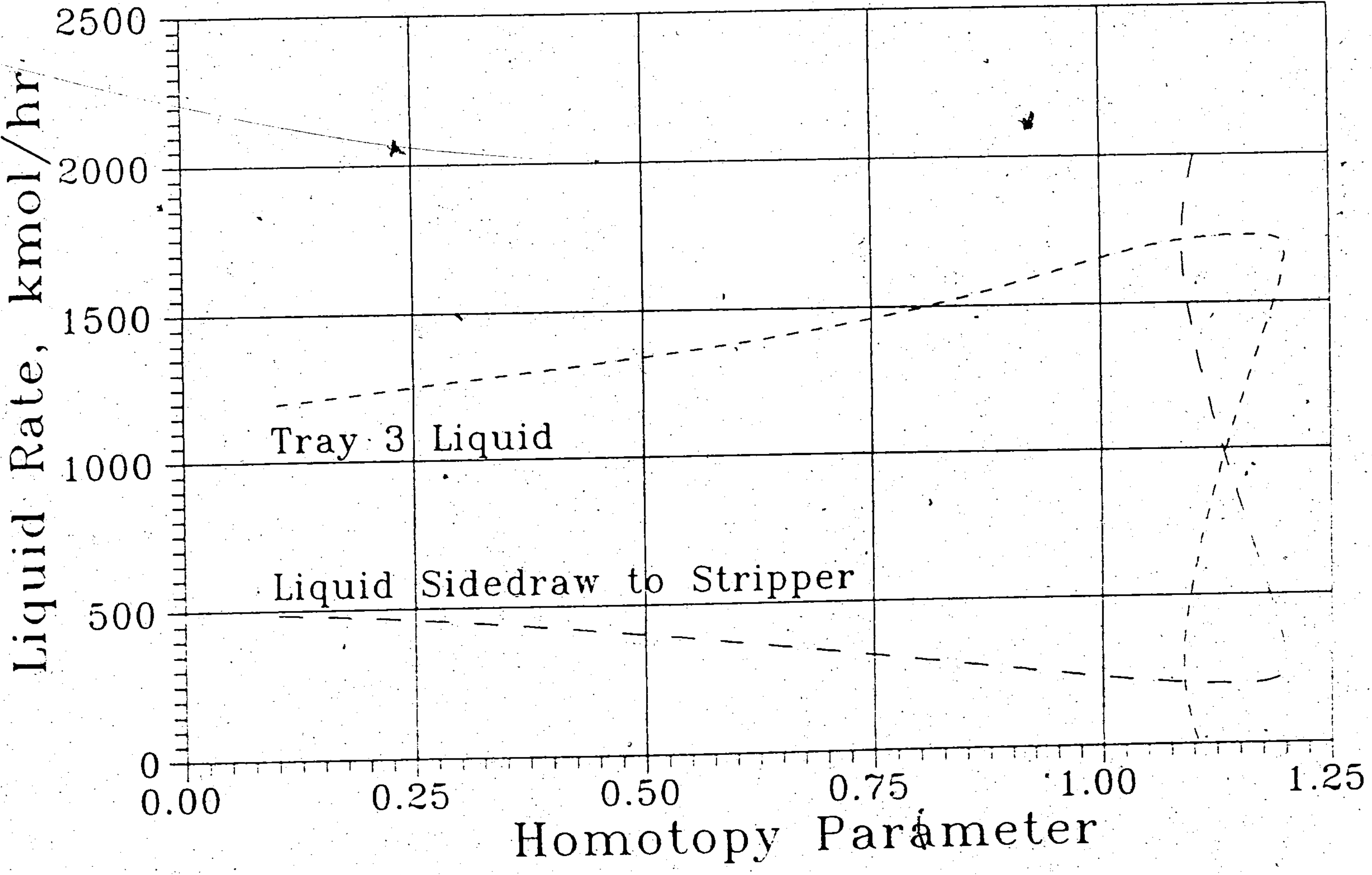
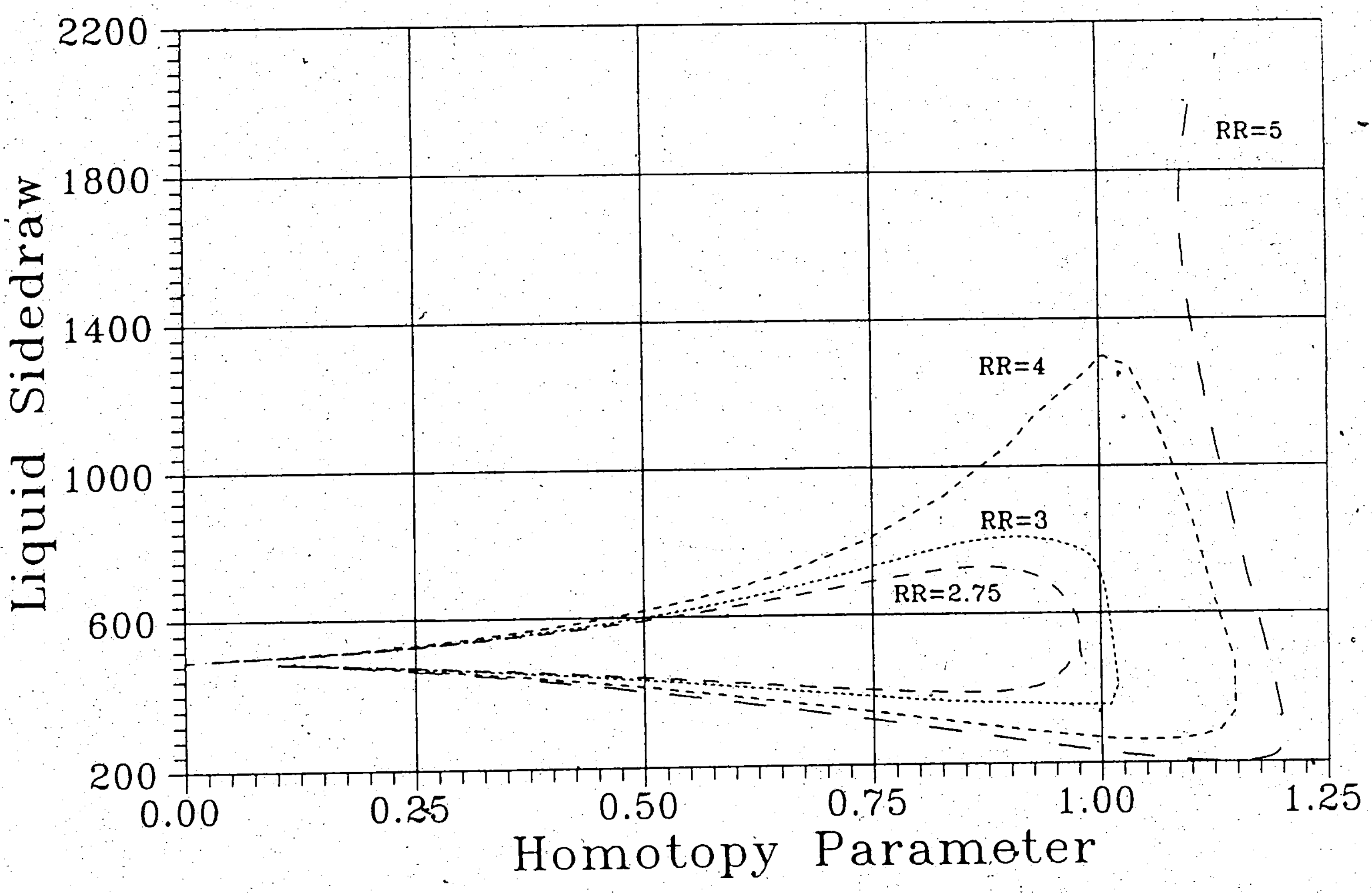


Figure 5.22
Multiple Solution Homotopy Paths at
Different Reflux Ratios



6.0 Discussion of Results

6.1 Case Study 1 : Splitter

Case study 1 used a simple 4 stage distillation column with an equimolar feed of the normal paraffins propane through hexane. The first test done with this column was to examine the behaviour when too high a product purity was specified. Figures 5.1 through 5.4 show how the reflux ratio, condenser temperature, propane mole fraction in the distillate and dt/dp change as the homotopy path is followed. The reflux ratio plot and the propane mole fraction plot give the best information that something is wrong with the specification. Even though the reflux ratio is changing very rapidly, the concentration of propane is barely changing at all. The second indication that something is wrong is that the value of dt/dp is approaching zero. The value of dt/dp is an indicator of the 'stiffness' of the system being solved. Classically, stiffness is indicated by the ratio of the largest to smallest eigenvalue. This first case study is an example of a problem where a limiting specification is indicated by the reflux ratio approaching infinity. Physically, this type of homotopy path can be expected for other types of specifications which require purities beyond the physically limiting purity which is obtained from minimum reflux calculations. For example a true boiling point, a component molar flowrate, or a tray temperature specification may be infeasible if the purity required to satisfy the specification is greater than the purity obtained at total reflux conditions.

Figure 5.2 shows how the mole fraction of propane in the distillate changes as the homotopy path is followed. This path is linear because the mole fraction specification equation changes linearly as the path is followed. It is interesting to note that the condenser temperature also changes linearly as the homotopy path is followed (figure 5.3). This is because the bubble point temperature is a function of the composition. This system is obviously very stiff because although the condenser temperature and propane mole fraction change approximately one percent and one degree Celsius, the reflux ratio changes by an order of magnitude (figure 5.1).

This simple example points out very well the main advantage of continuation methods over Newton's method for solving physical problems of this nature. When this problem is solved by Newton's method, all of the corrections are very large. This is because an infinite amount of reflux is needed to satisfy the specifications, and Newton's method is trying to get there in one large step.

On the other hand, the continuation method is able to make a large correction in reflux rate and small corrections in the mole fractions so that the homotopy path is closely followed. This ability to closely follow the homotopy path is what makes path following a stable and robust solution method.

Since this work focused on problems with physically impossible specifications, it was necessary to come up with a criterion which could be used to check for this condition. The method used here was simply to check the value of dt/dp. If dt/dp was less than a certain value, then the algorithm was stopped with the appropriate warning messages. A minimum value of 0.001 was used here. This approach will fail in the neighborhood of a very sharp turning point because it is possible that dt/dp could get very small as the homotopy path goes around the turning point. The turning points encountered in this work were not sharp, and therefore they could be traversed with large steps. Due to the large steps the absolute value of dt/dp was less than 0.001 for at most one step.

The results of case study 1B are shown in figures 5.5 through 5.8. Case study 1B examines the effect of specifying a mole fraction of propane too small in the distillate. When Newton's method is used to solve this problem the flows become negative and must be reset to small positive values. Newton's method makes these corrections because it is trying to decrease the amount of propane in the distillate to meet the purity specification. However the thermodynamic equilibrium constraints cannot also be met and so Newton's method diverges.

When path following in artificial heater/coolers, the path is followed smoothly until the liquid on tray 1 dries up. The path stops here because the liquid and vapour traffic is constrained to be positive. When the liquid and vapour traffic are not constrained the liquid and vapour rates become negative. This is because the model equations in this form make no difference between positive or negative flows, and so if the liquid and vapour rates are not constrained to be positive, then they may become negative yielding non-physical solutions.

The fact that dt/dp was not close to zero when the path stopped is another indicator that the model equations in this form do not reflect the physical reality that flows cannot be negative. The equations are still mathematically correct because a change in sign corresponds to a change in direction. Although they did not address this problem, Lin and Seader (1987) have cast the equations in a new form which will alleviate this problem. Very simply, they used a square mapping substitution such that the variables are written in terms of new variables x, y, L, V, T where :

$$\mathrm{x} = x^2 \tag{7.1}$$

$$\mathrm{y} = y^2 \tag{7.2}$$

$$\mathrm{L} = L^2 \tag{7.3}$$

$$\mathrm{V} = V^2 \tag{7.4}$$

$$\mathrm{T} = T^2 \tag{7.5}$$

The MESH equations are written in terms of the new variables, thereby preventing the physical quantities from becoming negative. Lin et al. used this in their mathematical homotopy to find multiple solutions by tracking a single homotopy path. If this square mapping function was used with path following in artificial heater coolers it is possible that the path would naturally stop when the liquid rates are zero, or it may turn around. This is an interesting idea for future research. The only drawbacks to this approach are the added non linearity to the equations and the fact that 2^n more solutions are introduced by the square mapping function. However, the results of Lin et al. are encouraging because they were able to find all known solutions on the same homotopy path to the problems they studied.

Case study 1B has shown one example of the second type of limiting case for physically impossible specifications, one of the tray liquid rates drying up. As before, it should be remembered that this could happpen for a wide range of specification types which were not presented here.

6.2 Case Study 2 : Depentanizer

Case studies 2A and 2B with the depentanizer were done to see if path following would give the same type of results as with the splitter in case study 1 when physically impossible high distillate purities were specified. Case study 2C was done to compare Newton's method with path following.

The specifications for Case study 2A were:

1) Octane Purity in Bottoms= 0.200
2) Bottom Product Rate = 600 kgmole/hr
3) Sidestripper Product Rate = 200 kgmole/hr
4) Liquid Draw From Main Column = 300 kgmole/hr

The purity specified can only be reached if all of the octane that enters in the feed exits out the bottoms. This would require an infinite amount of reflux, and as in Case 1A this is what is being approached as the path is followed. Figures 5.9 through 5.12 show how dt/dp, reflux ratio, octane mole fraction in the bottoms and the bottoms temperature change as the path is followed. Path following was discontinued when the reflux ratio reached approximately 80. Note that the data points on the figures give an indication of how the step size decreases as the path becomes steeper.

Case study 2A has shown that paths approaching infinite reflux can be generated for single columns and columns with attached sidestrippers. Therefore path following provides a method of detecting physically impossible specifications for both of these types of columns.

Case study 2B was very similiar to case study 2A. This case study changed the liquid draw rate specification to a reflux ratio specification. The specifications for this case study were:

1) Octane Purity in Bottoms= 0.200
2) Bottom Product Rate = 600 kgmole/hr
3) Sidestripper Product Rate = 200 kgmole/hr
4) Reflux Ratio = 3.0

The reflux ratio specification was introduced to see the effect of limiting the reflux and hence the amount of liquid and vapour traffic in the column.

Figures 5.13 through 5.16 show the results of case study 2B. When the reflux ratio was constrained, the liquid rate on tray 3 became zero as the path was followed. Also, dt/dp changed linearly with t in this case. The octane mole fraction changes linearly with t, as shown in figure 5.14.

These two case studies demonstrate that even with sidestrippers path following provides a method of detecting non-physical specifications. When Newton's method was used on these problems it made very large corrections to the liquid and vapour traffic, and would have offered no information as to why the simulation failed to converge.

Case study 2C was done with the following specifications:

1) Propane Purity in Distillate
2) Bottoms Product Rate = 600 kgmole/hr
3) Sidestripper Product Rate = 200 kgmole/hr
4) Reflux Ratio = 3.0

Table 5.1 shows the number of iterations used by Newton's method, path following in heater/coolers and path following in structure and heater/coolers. For path following the number of iterations was determined by the number of Newton corrector steps that were done. As the table shows, path following in heater/coolers took twice as many iterations as Newton's method, and path following in structure and heater/coolers took three times as many iterations as Newton's method.

Table 6.1
Solution and Initial Liquid Profiles for Case 2C

Tray	Liquid Rate (kgmole/hr) Initial Point for Heater/Coolers Structure	Initial Point for Heater/Coolers	Final Solution
main			
1	600	600	600
2	600	600	537
3	300	300	235
4	1300	1300	1270
5	1300	1300	1308
6	1300	1300	1340
7	1300	1300	1370
8	1300	1300	1395
9	1300	1300	1417
10	500	600	600
side 1	300	300	262
2	300	300	264
3	200	200	200

Path following in heater/coolers and structure took a longer path to reach the solution because the initial point on the path is farther from the solution compared to path following in heater/coolers alone. Table 6.1 shows the solution liquid rate profile for a distillate propane purity of 0.2250 and the starting profiles for both of the path following schemes. Note that Newton's method uses the same starting point as path following in heater/coolers.

Table 6.2
Solution and Initial Propane Mole Fraction Profiles for Case 2C

Tray	Propane Mole Fraction		
	Initial Point for Heater/Coolers Structure	Initial Point for Heater/Coolers	Final Solution
main 1	0.1962	0.2327	0.2250
2	0.0768	0.0984	0.0934
3	0.0361	0.0473	0.0457
4	0.0234	0.0288	0.0300
5	0.0115	0.0164	0.0175
6	0.0055	0.0091	0.0098
7	0.0026	0.0050	0.0052
8	0.0012	0.0026	0.0026
9	0.0005	0.0013	0.0012
10	0.0002	0.0005	0.0005
sid[illegible]	0.0284	0.0384	0.0416
2	0.0203	0.0283	0.0348
3	0.0118	0.0169	0.0235

Table 6.2 shows the propane mole fraction at the solution and also at the starting points for each of the continuation methods. The table shows that path following in heater/coolers and structure results in a starting point which is farther from the solution than path following in heater/coolers alone.

The reason that path following in heater/coolers and structure results in a starting point farther from the solution is because the traffic in the column at the start of the path is significantly different than at the solution. While the goal is that this different problem is easier to solve, it will of necessity result in a homotopy path which is longer than path following in heater/coolers alone.

Case study 2C is an example of where a turning point indicates what the limiting value of a specification is. It is expected that this sort of path is atypical, and results due to the specifications and the location of the feed and draw trays in the column. Since the reflux ratio is a specification it obviously cannot go to infinity. Since the feed to the main column is on tray 3, this helps avoid having tray 3 dry up. Also, as shown by figure 5.17, the liquid draw rate from the main column to the sidestripper decreases as the homotopy path is followed. If the draw rate had increased then one of the trays might have dried up.

Case study 2D was done with the following specifications:

1) Propane Distillate Purity: 0.1234
2) Octane Bottoms Purity: 0.2192
3) Hexane Sidestripper Purity: 0.4005
4) Various Reflux Ratios

Figure 5.21 shows how path following in heater/coolers, structure and specifications solved this problem. Multiple solutions are not found, and the solution that is found is the one closest to the initial estimate. As figure 5.21 shows, the path stops when the tray 3 liquid rate becomes zero. Negative rates and mole fractions are not allowed by reducing the Newton correction, so the path is forced to stop when the liquid rate becomes zero.

This example illustrates one of the potential problems of path following methods. There is no guarantee that the path will remain in a region where all of the independent variables are physically meaningful. It is possible that the tray 3 liquid could have dried up before the solution was reached. Although this was not observed in this work, there may be other distillation problems in which the path strikes the edge of the the region where the independent variables are defined before reaching the solution to the desired problem. However, it is encouraging that all of the path following methods used here always found at least one solution to the problem. As mentioned before, this is where the square mapping function of Lin et al. could be used to ensure that the physical quantities are always positive.

Figure 5.22 shows results obtained by path following in structure and specifications only. Multiple solutions were obtained when this was done, as shown by the plots of liquid sidedraw as a function of the homotopy parameter (figure 5.22). The homotopy paths all start at t=0.1.

The homotopy path for a reflux ratio of 2.75 is included to show that although there is no solution at this reflux ratio, the homotopy path has the same characteristic shape as the other paths. The homotopy path at a reflux ratio of 5.0 shows that there is an upper limiting reflux ratio for which there exists only a single solution. This homotopy path at a reflux ratio of 5.0 stops because the tray 3 liquid became zero.

The initial value of the liquid sidedraw is the same for each reflux ratio because of the way in which the liquid sidedraw rate is initialized. The liquid sidedraw rate is initialized based on the amount of the initial (assumed) sidestripper product. For each of these problems the product rates are initialized to a third of the feed to the column. This was done to represent the worst case where estimates of the product rates are not available. The reflux ratio was initialized to the specified value, so that in effect path following was not done in reflux ratio.

When formulating mathematical models using physical homotopies where it is desired to path follow past t=1, it is important to define the homotopy equations such that the physical system still has meaning when t is greater than 1. This was taken into account when the model equations were developed for this work. For the models developed here, the homotopy parameter is only included in the heat balances (when path following in artificial heater/coolers), the mass and heat balance equations for the tray which the vapour return from the sidestripper returns to, and the specification equations.

The term in the heat balances containing the homotopy parameter is $(1-t)Q_{ar}$. When t is greater than 1, the term $(1-t)$ becomes negative, and this has the effect of changing the sign of the artificial heater / cooler. Since the only difference between the paths in figures 5.21 and 5.22 is that in the latter path following in artificial heater / coolers is not done, there must be some conflict in using the same homotopy parameter in the stage heat balances, mass balance for the vapour return from the sidestripper and the specification equations.

The term in the mass and heat balances for the tray which the vapour from the sidestripper returns to is tV_{ss}, (and $tH^{V}V_{ss}$ in the heat balance) where V_{ss} is the vapour from the top of the sidestripper. When t is greater than 1 this indicates that the feed to the main column is now greater than the vapour product from the top of the sidestripper. Note that only the rate of the vapour return stream is changed by the homotopy parameter, not the composition. Physically this is equivalent to having an external feed to the main column the same composition as the vapour stream from the top of the sidestripper. Note also that as the homotopy path is followed past t=1, that the composition of the vapour product stream is changing, and so the composition of the external feed stream is also changing. While this could not be built, it is still physically meaningful.

The previous heat and mass balance equations do not place any restriction on how much larger than one the homotopy parameter may become. However, for the specification equations, there will be a limiting upper value of the homotopy parameter. For example, for a purity specification, the equation has the form

$$NS = x - (x^{initial} - t(x^{spec} - x^{initial})) = 0$$

or

$$NS = x - x^{initial} + t(x^{spec} - x^{initial}) = 0$$

Here x is some liquid mole fraction, $x^{initial}$ is the liquid mole fraction from the solution of the initial problem and x^{spec} is the specified (desired) value.

If x^{spec} is greater than $x^{initial}$ then in order to satisfy the constraint equation x will have to increase past the specified value. However, there is obviously an upper limit of $x=1$. This upper limit is what causes the homotopy path to turn around. Similarly, for a rate specification there is an upper limit of all of the feed entering the column. For a temperature specification, there is an upper limiting condition of the bubble point of the heaviest component.

A similiar argument holds if x^{spec} is less than $x^{initial}$. There is obviously a lower limit of $x=0$. Rate specifications can also not be less than zero, and temperature specifications will be limited by the bubble point of the lightest component. There are also interactions between the specification equations, and it is possible that some combination of limiting conditions could prevent t from becoming any larger.

7.0 Conclusions and Recommendations

1. It has been shown that for certain types of distillation specifications homotopy continuation can indicate the limiting values of non physical specifications. Three different and easily identifiable characteristics of paths were determined to indicate that the limiting value of a specification may have been reached. These characteristics are the path stopping abruptly, the path turning around, and the path approaching a limiting value asymptotically. However, although the path may exhibit one of these three characteristics, that does not necessarily mean that the path has reached the limiting value of a specification. The path may have a valid turning point, or the path may strike the edge of the domain of definition of the independent variables. The square mapping function of Lin et al. would appear to be a good way to avoid problems of striking the edge of the domain of definition.

2. This study has investigated two new physical homotopies. It has shown that these physical homotopies have computation times two to three times greater than Newton's method.

3. This work confirms the work of Vickery and Taylor that physical homotopies result in simple, smooth paths. This removes the requirement for sophisticated step length predictors, and the manual tuning that these predictors require.

4. This work has shown that path following in the physical structure of a problem is feasible. This is a general concept which may be used to enhance convergence of physical problems which include recycles.

5. This work has shown how path following using physical homotopies can be extended to other types of specifications besides those used by Vickery and Taylor. Other types of specifications are employed by solving the simple problem with an alternate (simpler) set of specifications, usually product rates and reflux ratio. Once the initial problem is solved, then new homotopy equations are formulated for the non standard specifications. This work used simple linear equations such that at the start of the homotopy path the specification is at the value from the solution to the initial problem, and at the end of the homotopy path the equations have the desired values of the specifications.

6. While this work has considered hydrocarbon distillation problems, no problems were considered in which water formed a separate liquid phase. This will typically happen at the condenser of a crude column. This poses a new problem which was not dealt with in this work, namely the appearance and disappearance of the water phase introduces a discontinuity along the homotopy path. This would be an interesting area for future research.

7. When path following in more than one physical quantity (structure, artificial heater/coolers, specifications) it may be beneficial to use multiple homotopy parameters. This would allow the different physical quantities to have different values of $\frac{\partial t_k}{\partial p}$ as the homotopy path is followed. A further modification of $t_k^{n_k}$ would allow the different homotopy parameters to be introduced at different rates by using different values of the exponents n_k. Perhaps the exponents n_k could be changed adaptively to make the path smooth and avoid unnecessary turning points.

8. It must be understood that one piece of information that the path following techniques presented in this thesis do not provide is which specification has a value that is limiting. If there are multiple specifications, only some of the specifications may be limiting. For example, if there were 5 specifications made, and one of them was a purity specification which was greater than the purity achieved at infinite reflux, then only this specification would be considered limiting. Unfortunately, when the path stops at some intermediate value of the homotopy parameter there is nothing to indicate which specification is limiting. Perhaps if different homotopy parameters were used for each specification equation then the limiting specification would reach a maximum value of its homotopy parameter, and the homotopy parameters for the other specifications would proceed to their terminal values.

9. It has been shown that physical homotopies can be used to find multiple solutions along a single homotopy path. This confirms the work of Lin et al. that multiple solutions do exist for a column and sidestripper specified with three product purities and a reflux ratio. For future research this work could be extended to multiple sidestrippers to investigate if the two solutions per liquid/vapour interlink predicted by Chavez et al. can be reproduced with physical homotopies.

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Appendix I

Sample Calculation of Degrees of Freedom for a Total Condenser

The number of degrees of freedom for any system of equations is the number of variables minus the number of equations. For a total condenser, there are 2 streams (inlet and outlet streams) and a heat duty. Each stream has C+2 variables (C component rates, temperature and pressure), so the total number of variables is 2C+5. For equations, there are C component mass balances and an enthalpy balance for a total of C+1 equations. The number of degrees of freedom is given by C+4.

Appendix II

Derivation of Custom Homotopy for Example 2 of Vasquez et al.

The functions to be solved are :

$$f_1(x,y) = y^3 + y^2 -2x^3 -10x^2 -2x^{3/2} - 50x + 200 = 0 \qquad (1)$$

$$f_2(x,y) = y^3 + y^2 -x^3 -40x^2 -2x^{3/2} + 230x - 660 = 0 \qquad (2)$$

At this point it helps to know what kind of answer you are looking for before you start. It is desired to find a homotopy such that at t=0 the solution can be easily found. A good candidate then for the initial homotopy would be to include only linear terms from the original equations so that a linear system could be solved. This would avoid any difficulty in getting on the homotopy path. Such a homotopy would take the general form:

$$h_1(x,y,t) = a_1x + a_2y + a_3 + t(a_4y^n + a_5x^m) = 0 \qquad (3)$$

$$h_2(x,y,t) = b_1x + b_2y + b_3 + t(b_4y^p + b_5x^q) = 0 \qquad (4)$$

Here a_i, b_i, n, m, p and q are constants.

Examination of the equations f_1 and f_2 reveals that there is no linear term in y. However, as long as the same term (y^2 or y^3) appears in both equations, the value of y^2 or y^3 can be solved for directly. Choosing the y^2 term, the homotopy equations at t=0 become:

$$h_1(x,y,t=0) = -50x + y^2 + 200 = 0 \qquad (5)$$

$$h_2(x,y,t=0) = 230x + y^2 - 660 = 0 \qquad (6)$$

(3) - (4) gives

$$-280x + 860 = 0 \qquad (7)$$

Therefore $x=\frac{860}{280} \cong 3.0714$. Substituting the value of x back into equation 3 results in $y^2 = -46.43$ and so it would appear that this approach will only work with complex numbers. However, remembering that y^3 could have been chosen instead of y^2, it is apparent that y^3 is a better choice. If there was no y^3 term available another approach would have been necessary. Now equations 3 and 4 can be rewritten with y^3:

$$h_1(x,y,t=0) = -50x + y^3 + 200 = 0 \tag{8}$$

$$h_2(x,y,t=0) = 230x + y^3 - 660 = 0 \tag{9}$$

Once again $x=3.0714$. Now $y^3=-46.43$ and therefore $y=-3.5908$. The homotopy equations are given by:

$$h(x,y,t) = -50x + y^3 + 200 + t(y^2 - 2x^3 - 10x^2 - 2x^{3/2}) = 0 \tag{10}$$

$$h(x,y,t) = 230x + y^3 - 660 + t(y^2 - x^3 - 40x^2 - 2x^{3/2}) = 0 \tag{11}$$

The Jacobian elements are given by:

$$\frac{\partial h_1}{\partial x} = -50 + t(-6x^2 - 20x - 3x^{1/2}) \tag{12}$$

$$\frac{\partial h_1}{\partial y} = 3y^2 + 2ty \tag{13}$$

$$\frac{\partial h_1}{\partial t} = y^2 - 2x^3 - 10x^2 - 2x^{3/2} \tag{14}$$

$$\frac{\partial h_2}{\partial x} = 230 + t(-3x^2 - 80x - 3x^{1/2}) \tag{15}$$

$$\frac{\partial h_2}{\partial y} = 3y^2 + 2ty \tag{16}$$

$$\frac{\partial h_2}{\partial t} = y^2 - x^3 - 40x^2 - 2x^{3/2} \tag{17}$$

At this point the methods outlined in section 5.1 can be used to solve the homotopy equations. The main difference between this custom homotopy and the Newton homotopy is that the starting point for this homotopy is fixed, whereas for the Newton homotopy the starting point is an arbitrary choice.

Appendix III

Example Calculation Showing that Normalization Results in Euler Solution After One Iteration

A simple 2X2 system will be solved to show that the Euler calculation is not an iterative process. Consider the system of equations

$$ax_1 + bx_2 = 0 \tag{1}$$

$$x_1^2 + x_2^2 = 1 \tag{2}$$

This is the same form as the system of equations 4.16. In matrix form:

$$\begin{bmatrix} a & b \\ x_1 & x_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{3}$$

While this appears to be a system of equations requiring an iterative solution procedure, the nature of equation 2 can be exploited to normalize the solution after one iteration such that the resulting normalized values are the correct solution to the system of equations. While this is being done here for a 2X2 system of equations, the math is general and so it also applies to any NXN system of equations.

Let c and d be the initial estimates of x_1 and x_2 respectively. Also let w_1 and w_2 be the initial solution for x_1 and x_2. In matrix form this is given by:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{3}$$

Solving for w_1 and w_2 using determinants:

$$D = ad - bc \; ; \; D_1 = -b \; ; \; D_2 = a$$

This results in

$$w_1 = \frac{-b}{ad - bc} \tag{4}$$

$$w_1 = \frac{a}{ad - bc} \tag{5}$$

Since at the solution equation 2 must be true, at this point it is suggested to solve for x_1 and x_2 with the following normalizations:

$$x_1 = \frac{w_1}{\sqrt{w_1^2 + w_2^2}} \tag{6}$$

$$x_2 = \frac{w_2}{\sqrt{w_1^2 + w_2^2}} \tag{7}$$

Substituting in values for w_1 and w_2 from (4) and (5) into (6) and (7) gives x_1 and x_2 as functions of a and b only. These substitutions result in the following:

$$x_1 = \frac{-b}{\sqrt{a^2 + b^2}} \tag{8}$$

$$x_2 = \frac{a}{\sqrt{a^2 + b^2}} \tag{9}$$

If these are the correct values for x_1 and x_2 then substitution of these quantities back into (3) and resolving for x_1 and x_2 should give exactly the same result. Substituting (8) and (9) into (3) gives

$$\begin{bmatrix} a & b \\ \dfrac{-b}{\sqrt{a^2 + b^2}} & \dfrac{a}{\sqrt{a^2 + b^2}} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{10}$$

Solving once again by determinants:

$$D = \frac{a^2 + b^2}{\sqrt{a^2 + b^2}} \tag{11}$$

$$D_1 = -b \qquad D_2 = a \tag{12}$$

Now solving for x_1 and x_2 from the determinants:

$$x_1 = \frac{-b\sqrt{a^2 + b^2}}{a^2 + b^2} \tag{13}$$

$$x_2 = \frac{a\sqrt{a^2 + b^2}}{a^2 + b^2} \tag{14}$$

$$x_1 = \frac{-b}{\sqrt{a^2 + b^2}} \tag{15}$$

$$x_2 = \frac{a}{\sqrt{a^2 + b^2}} \tag{16}$$

Therefor since x_1 and x_2 are the same from equations (8),(9) and (14),(16) it has been shown that a system of equations of the form in equation (1) can be solved in one iteration by normalizing the sum of the squares after the calculation.

Appendix IV

In order to establish limits for the operation of the distillation columns in case studies 1 and 2, minimum reflux calculations were done using Underwoods method, and Fenske calculations were done to determine the minimum number of stages for which the separations could be done. The calculations were done using PROCESS.

The calculations show that 18 Fenske stages are needed to perform the separation specified in case study 1A. This shows that the solution with 4 stages is infeasible. Following is are the results from PROCESS.

PROCESS INPUT FILE

```
VERSION 3.02, VAX     7Z                        TM
SIMULATION SCIENCES INC.                 PROCESS  INPUT LISTING PAGE    1

  TITLE PROJ=THESIS, PROB=THESIS, DATE=JUNE 88, USER=RON
  DIME SI TEMP=C ENER=KJ TIME=HR PRES=KPA
  PRINT STREAM=PART INPUT=NONE
  COMP
    LIBI 1 PROPANE / 2 NC4 / 3 NC5 / 4 NC6
  THERMO
    METHODS SYSTEM=PR
  STREAM
    PROP STRM=FEED PRES=2048 LFRAC=1.0 COMP= 250 / 250 / 250 / 250
  UNIT OPS
   SHORTC
     FEED FEED
     PROD STRM=OVHD PHASE=L RATE=500 PRES=2048.
     PROD STRM=BTTM PHASE=L RATE=500 PRES=2048.
     COND TYPE=3 $ TOTAL CONDENSER
     CALC MODEL=1 TRIAL=100 KEYL=2 KEYH=3 MMMIN=1.01
     SPEC STRM=OVHD         RATE=500 ATOL=0.0001
     SPEC STRM=OVHD COMP=1 RATE=250 ATOL=0.0001
  END
```

PROCESS SOLUTION

```
                 **** PROBLEM SOLUTION REACHED ****

VERSION 3.02, VAX     77                      TM
SIMULATION SCIENCES INC.                 PROCESS              PAGE   2
PROJECT  THESIS                        UNIT  1 -                     RON
PROBLEM  THESIS                           SOLUTION             JUNE 88

           SHORTCUT DISTILLATION UNIT    1,
1 FEED STREAMS

  FEED FEED IS LIQUID STREAM
2 PRODUCTS AND NOS OF TRAYS AT TOTAL REFLUX
  PRODUCT     ---      MATERIAL BALANCES         ---      SECTION   NO OF
             KG MOLS/HR      M  KGS/HR        M3/HR                 TRAYS

   OVHD          500.000         25.590        46.712         1     18.30
   BTTM          500.000         39.547        61.170
  TOTAL         1000.000         65.137       107.882                18.30
3 SPECIFICATIONS
  PARAMETER        SPECIFICATION     SPEC        CURRENT      ERROR
    TYPE               TYPE          VALUE        VALUE

  STRM OVHD   ML RATE             0.5000E+03  0.5000E+03  0.000E+00
  STRM OVHD  COMP ML RATE         0.2500E+03  0.2500E+03 -0.305E-04

SUMMARY OF UNDERWOOD CALCULATIONS
  MINIMUM REFLUX RATIO       1.72896
  FEED CONDITION Q           1.00002
  FENSKE MINIMUM TRAYS      18.29815

VERSION 3.02, VAX     77                      TM
SIMULATION SCIENCES INC.                  PROCESS                PAGE   3
PROJECT  THESIS                                                        RON
PROBLEM  THESIS                            SOLUTION              JUNE 88
                      STREAM COMPONENT FLOW RATES -  KG MOLS/HR
 STREAM ID                          BTTM          FEED          OVHD
        NAME
        PHASE                      LIQUID        LIQUID        LIQUID

  1 PROPANE                        0.0002      250.0000      250.0000
  2 NC4                            2.4927      250.0000      247.5074
  3 NC5                          247.5076      250.0000        2.4823
  4 NC6                          249.9996      250.0000        0.0003
 TOTALS, KG MOLS/HR,             500.0000     1000.0000      500.0000
 TEMPERATURE, DEG C              184.7341      122.5275       82.7791
 PRESSURE, KPA                  2048.0000     2048.0000     2048.0000
 H, MM KJ  /HR                    19.9148       20.9624        5.8601
 MOLECULAR WEIGHT                 79.0945       65.1375       51.1804
 MOL FRAC LIQUID                   1.0000        1.0000        1.0000
 RECYCLE CONVERGENCE               0.0000        0.0000        0.0000
```

Appendix V

In order to verify the results that the simulation of Case Study 1B are infeasible, the column was run with a fixed overhead rate of xxx and a reflux ratio of 0.001. With this low reflux ratio there is still about 200 kgmole/hr of propane in the overhead of the column. This shows that it is infeasible to obtain 125 kgmole/hr of propane in the overhead and bottoms of the column. Following are the results of the simulation using PROCESS.

PROCESS INPUT FILE

```
VERSION 3.02, VAX     77                    TM
SIMULATION SCIENCES INC.            PROCESS   INPUT LISTING   PAGE   1

TITLE PROJ=THESIS, PROB=EXAMPLE, DATE=APRIL 88, USER=RON
DIME SI TEMP=C ENERGY=KJ TIME=HR PRES=KPA
PRINT INPUT=NONE STREAM=PART
COMP
  LIBI 1 PROPANE / 2 NC4 / 3 NC5 / 4 NC6
THERMO
  METHODS SYSTEM=PR
STREAM
  PROP STRM=FEED PRES=2048 LFRAC=1.0 COMP= 250 / 250 / 250 / 250
UNIT OPS
 COLUMN
   FEED  FEED, 2
   PARA  TRAY=4
   PROD  OVHD=OVHD,500 BTMS=BTMS,500
   PSPEC DPCOL=0 TOP=2048
   COND  TYPE=3
   HEAT 1 1 / 2 4
   VARY HEAT=1 2
   SPEC  RRATIO=0.001
   SPEC  STRM=OVHD RATE=500
   ESTI MODEL=1
END
```

```
                **** PROBLEM SOLUTION REACHED ****
VERSION 3.02, VAX     77                       TM
SIMULATION SCIENCES INC.               PROCESS                     PAGE   2
PROJECT  THESIS                      UNIT  1 -                          RON
PROBLEM  EXAMPLE                          SOLUTION                 APRIL 88
           I SUMMARY FOR COLUMN     UNIT  1 -
  1 TOTAL NUMBER OF ITERATIONS
         FAST METHOD    -                                            0
         SURE METHOD                                                 3
  2 COLUMN SUMMARY
TRAY  TEMP  PRESSURE       NET FLOW RATES, KG MOLS/HR          HEAT(COOL)ER
                        LIQUID    VAPOR                            DUTIES
      DEG C    KPA     PHASE(L)  PHASE(V)   FEED     PRODUCT   MM KJ  /HR

 1     98.5  2048.00       0.5                          500.0L    -9.0731
 2    128.9  2048.00    1014.7     500.5  1000.0L
 3    138.9  2048.00    1037.3     514.7
 4    153.5  2048.00               537.3                500.0L    10.4558

3 FEED AND PRODUCT STREAMS                         FLOW RATES    HEAT RATES
                                                   KG MOLS/HR    MM KJ  /HR
  * FEED STREAMS:              (FROM UNIT, UID)
  FEED IS LIQUID TO TRAY   2                          1000.000       20.9624
  * PRODUCT STREAMS:
  BTMS IS LIQUID FROM TRAY    4                        500.000       14.7984
  OVHD IS LIQUID FROM TRAY    1                        500.000        7.5471
  OVERALL MASS BALANCE, (FEEDS - PRODUCTS)      0.00000E+00
  OVERALL HEAT BALANCE, (HIN - HOUT)                              -0.43488E-03

4 SPECIFICATION VALUES
  PARAMETER TRAY COMP. SPECIFICATION  SPECIFIED   CALCULATED
    TYPE     NO   NO       TYPE         VALUE       VALUE
  TRAY LIQD   1        MOL RATE RATIO 0.1000E-02  0.1000E-02
  STRM OVHD   1        MOL RATE       0.5000E+03  0.5000E+03
5 REFLUX RATIOS
                                                REFLUX RATIOS
                                        MOLAR      WEIGHT    STD L VOL
     REFLUX / FEED STREAM FEED         0.0005      0.0004     0.0005
     REFLUX / LIQUID DISTILLATE        0.0010      0.0010     0.0010
```

```
VERSION 3.02, VAX    77                          TM
 SIMULATION SCIENCES INC.                  PROCESS                   PAGE  3
 PROJECT  THESIS                       UNIT  1 -                          RON
 PROBLEM  EXAMPLE                              SOLUTION               APRIL 88
                          IIB TRAY VAPOR     RATES AND DENSITIES
 TRAY  M  KGS/HR       MW        M STD        Z        M ACTUAL      ACTUAL
                                  M3/HR                 M3/HR    KGS/M  M3
2       28.986   57.915      11.218  0.70888         0.579    50051.262
3       31.356   60.918      11.536  0.69861         0.601    52131.707
4       35.245   65.595      12.043  0.68112         0.634    55602.004
                       IIC TRAY LIQUID    RATES AND DENSITIES
TRAY  M  KGS/HR       MW      STD DRY LV    STD DRY     ACTUAL        ACTUAL
                               M3/HR       KGS/M3     M3/HR        KGS/M3

1         0.029  57.915        0.050    576.454       0.063     457.671
2        67.534  66.556      110.903    608.945     147.463     457.970
3        71.424  68.856      115.808    616.747     157.045     454.801
4        36.180  72.360       57.648    627.601      80.397     450.017
VERSION 3.02, VAX    77                          TM
SIMULATION SCIENCES INC.                  PROCESS                 PAGE  4
PROJECT  THESIS                                                       RON
PROBLEM  EXAMPLE                              SOLUTION              APRIL 88
                         STREAM COMPONENT FLOW RATES -  KG MOLS/HR
  STREAM ID                         BTMS         FEED         OVHD

          NAME
          PHASE                    LIQUID       LIQUID       LIQUID

    1 PROPANE                     44.0360     250.0000     205.9629
    2 NC4                        101.1999     250.0000     148.7997
    3 NC5                        158.0482     250.0000      91.9522
    4 NC6                        196.7158     250.0000      53.2852
  TOTALS, KG MOLS/HR             500.0000    1000.0000     500.0000
  TEMPERATURE, DEG C             153.5054     122.5275      98.4985
  PRESSURE, KPA                 2048.0000    2048.0000    2048.0000
  H, MM KJ  /HR                   14.7984      20.9624       7.5471
  MOLECULAR WEIGHT                72.3598      65.1375      57.9153
  MOL FRAC LIQUID                  1.0000       1.0000       1.0000
  RECYCLE CONVERGENCE              0.0000       0.0000       0.0000
```

Appendix VI

Verification of Program

An example is presented to verify that the results produced by the research code. The results were compared to the commercial simulator PRO/II, from Simulation Sciences. The agreement between the two is very good. Both runs were done using the Peng-Robinson equation of state. The problem presented is the distillation column with sidestripper from case study two. Ideal gas enthalpy coefficients from this work are from Reid et al. (1977), and PRO/II uses proprietary correlations. However, for the alkane mixture in the feed the ideal gas enthlapy coefficients are reliabe. First the PRO/II results are presented, then the input file for the thesis code, and then the results for the thesis code.

PRO/II Input File

```
TITLE PROJ=THESIS, PROB=EXAMPLE, DATE=APRIL 88, USER=RON
DIME SI TEMP=C DUTY=KJ/HR PRES=KPA
PRINT FRACTIONS, EXTEN
COMP
  LIBI 1 PROPANE / 2 NC4 / 3 NC5 / 4 NC6 / 5 NC7 / 6 NC8
THERMO
  METHODS SYSTEM=PR
STREAM
  PROP STRM=FEED PRES=1600 LFRAC=1.0 COMP=5 / 15 / 20 / 25 / 25 / 10
                 RATE=1000
UNIT OPS
  COLUMN UID=C1 NAME=MAIN
    PARA TRAY=10
    FEED FEED 4 / SVAP 3
    PROD OVHD=DIST 400 BTMS=BOTT 400 LDRAW=SLIQ 3 400
    COND TYPE=3 PRES=1600
    PSPEC TOP=1600 DPCOL=0
    HEAT 1 1 / 2 10
    VARI HEAT=1,2
    SPEC RRATIO VALUE=3
    SPEC STRM=DIST RATE VALUE=400.
    ESTI MODEL=1 CTEMP=120 RTEMP=150
    PRINT ITER=1 PROP=NONE
  SIDESTRIPPER
    PARA TRAY=3
    FEED SLIQ 1
    PROD OVHD=SVAP,200 BTMS=SPRD,300
    PSPEC TOP=1600 DPCOL=0
    HEAT 1 3
    VARI HEAT=1
    SPEC STRM=SPRD RATE VALUE=200
    PRINT PROP=NONE
```

```
                              PRO/II RESULTS

SIMULATION SCIENCES INC.                           TM
PROJECT  THESIS                              PRO/II   VERSION 1.01
PROBLEM  EXAMPLE                                     OUTPUT
PLANT/CASE                                       COLUMN SUMMARY
=================================================================
                                             UNIT 1, 'C1', 'MAIN'

COLUMN SUMMARY

                           ----------- NET FLOW RATES --------  HEATER
 TRAY    TEMP   PRESSURE   LIQUID    VAPOR     FEED  PRODUCT   DUTIES
         DEG C    KPA                    KG-MOL/HR             M*KJ/HR
------ -------- --------  --------  --------        -------- -------
     1   118.5  1600.00    1200.0                     400.0L -33.1602
     2   145.0  1600.00    1154.2    1600.0
     3   163.3  1600.00     731.8    1554.2   200.0V  400.0L
     4   177.4  1600.00    1843.6    1331.8  1000.0L
     5   187.6  1600.00    1929.7    1443.6
     6   195.5  1600.00    1991.9    1529.7
     7   202.3  1600.00    2034.8    1591.9
     8   208.6  1600.00    2063.4    1634.9
     9   214.9  1600.00    2082.4    1663.4
    10   221.5  1600.00              1682.4               400.0L  33.2251

 SIDESTRIPPER

 1/ 11   168.2  1600.00     408.0             400.0L  200.0V
 2/ 12   174.5  1600.00     414.2     208.0
 3/ 13   183.8  1600.00               214.2               200.0L  -4.5428

FEED AND PRODUCT STREAMS

   TYPE     STREAM     PHASE     FROM   TO     FLOW RATES    HEAT RATES
                                 TRAY  TRAY    KG-MOL/HR      M*KJ/HR
 --------  --------  --------    ----  ----   ------------  ----------
  FEED      SVAP      VAPOR               3         200.00      9.8987
  FEED      FEED      LIQUID              4        1000.00     35.3436
  PRODUCT   DIST      LIQUID        1               400.00      8.1904
  PRODUCT   SLIQ      LIQUID        3               400.01     13.7019
  PRODUCT   BOTT      LIQUID       10               400.00     23.4150

 SIDESTRIPPER

  FEED      SLIQ      LIQUID             11         400.01     13.7019
  PRODUCT   SVAP      VAPOR        11               200.00      9.8987
  PRODUCT   SPRD      LIQUID       13               200.01      8.3459

 OVERALL MASS BALANCE, (FEEDS - PRODUCTS)            0.000
 OVERALL HEAT BALANCE, (H(IN) - H(OUT)  )                       -0.0001
```

```
SPECIFICATIONS

 PARAMETER TRAY  COMP.  SPECIFICATION  SPECIFIED   CALCULATED
   TYPE     NO    NO        TYPE         VALUE        VALUE
 --------- ---- ------- ------------- ----------  ----------
 UNIT C1     1                RRATIO     3.000E+00   3.000E+00
 STRM DIST   1          MOL RATE         4.000E+02   4.000E+02
 STRM SPRD  13          MOL RATE         2.000E+02   2.000E+02
 STRM SLIQ   3   1   6  MOL RATE         4.000E+02   4.000E+02

STREAM ID                  BOTT        DIST        FEED         SLIQ
       NAME
       PHASE             LIQUID      LIQUID      LIQUID       LIQUID

   1  PROPANE            0.0120     49.3743     50.0000       8.4165
   2  NC4                0.7117    138.6017    150.0000      53.7646
   3  NC5               14.2989    136.8927    200.0000     123.8684
   4  NC6              108.3501     61.5425    250.0000     134.7431
   5  NC7              188.9555     12.5309    250.0000      65.6934
   6  NC8               87.6687      1.0530    100.0000      13.5253

TOTAL RATE,KG-MOL/HR 399.9969    399.9951   1000.0001     400.0113
TEMPERATURE, C       221.4982    118.4668    164.0412     163.3220
PRESSURE, KPA       1600.0000   1600.0000   1600.0000    1600.0000
ENTHALPY, M*KJ/HR     23.4150      8.1904     35.3436      13.7019
MOLECULAR WEIGHT      98.4010     66.9755     83.3730      80.4307
MOLE FRACTION LIQUID   1.0000      1.0000      1.0000       1.0000

                  STREAM MOLAR COMPOSITIONS - FRACTIONS
==================================================================

STREAM ID                 BOTT        DIST        FEED         SLIQ
       NAME
       PHASE            LIQUID      LIQUID      LIQUID       LIQUID

   1  PROPANE       2.9911E-05      0.1234      0.0500       0.0210
   2  NC4           1.7792E-03      0.3465      0.1500       0.1344
   3  NC5               0.0357      0.3422      0.2000       0.3097
   4  NC6               0.2709      0.1539      0.2500       0.3368
   5  NC7               0.4724      0.0313      0.2500       0.1642
   6  NC8               0.2192  2.6326E-03      0.1000       0.0338

TOTAL RATE,KG-MOL/HR 399.9969    399.9951   1000.0001     400.0113
TEMPERATURE, C       221.4982    118.4668    164.0412     163.3220
PRESSURE, KPA       1600.0000   1600.0000   1600.0000    1600.0000
ENTHALPY, M*KJ/HR     23.4150      8.1904     35.3436      13.7019
MOLECULAR WEIGHT      98.4010     66.9755     83.3730      80.4307
MOLE FRACTION LIQUID   1.0000      1.0000      1.0000       1.0000
```

Input File for Continuation Method

```
C      SIMPLE SIDESTRIPPER FOR USE IN THESIS
C
C           RWB>THESIS>SIDE01.DAT
C
C
C    THERMO TYPE    1=SRK      2=PR       3=PT
      2
C
C    #TRAYS IN MAIN COLUMN
     10
C
C    NUMBER OF FEEDS
     1
C
C    FEEDSTAGE
     4
C
C    FEEDTYPE
C    1=SUBCOOLED LIQ  2=LIQ AT BUBBLE  3=VAP AT DEW  4=SUP HT VAP
     2
C
C    FEED TEMP AND PRES    DEG C   KPA
  173.D0   1600.D0
C
C    FEED FLOW RATE        KG / HR
     1000.0D0
C
C    #DISCRETE COMPONENTS AND LIBID'S
     6
 132 0.05
 181 0.15
 223 0.20
 271 0.25
 308 0.25
 354 0.10
C
C    CRUDE TBP CURVE      1=NO   2=YES
     1
C
C    OVERHEAD SPEC  1=RATE 2=PURITY 3=DUTY 4=REFRAT 5=BP 6=NONE
C    EX  1   100.   -1
C        2     2   0.95
C        3   1.D06   -1
C        4   1.      -1
C        5   495.    95.
C        6   -1.     -1.
         2   1   0.1234D0  -1.  -1.
C
C    CONDENSER TYPE  1=TOTAL
     1
C
```

```
C       BOTTOM SPEC   1=RATE 2=PURITY 3=DUTY 4=BP 5=NONE
C       EX  1    100.   -1
C           2      2.   0.95
C           3    1.D06  -1
C           4    495.    95.
C           5    -1.     -1.
            1 400.D0  -1    -1
C
C       REBOILER TYPE    1=NO REBOILER  2=PARTIAL
        2
C
C       NUMBER OF PUMPAROUNDS
        0
C
C       NUMBER OF SIDESTRIPPERS
        1
C
C       SIDESTRIPPER #1
C
C       1=PRODUCT RATE  2=PURITY 3=BOILING PT 4=DUTY
C      EX     1    100.    -1.          5=LIQ DRAW
C             2      2.     0.95        6=REFLUX RATIO
C             3    495.     95.
C             4    1.0E6    -1.
C             5    -1.      -1.
              1     200.D0  -1.   -1.       1 <=  N  <= 4
              6    3.D0      -1.   -1.       5 <= N <= 6, OR 1
C
C       LIQUID DRAW AND VAPOUR RETURN TRAY
        3    3
C
C       NUMBER OF TRAYS IN SIDESTRIPPER ( INCLUDING REBOILER )
        3
C
C       TOP AND BOTTOM TRAY TEMP ESTIMATES (MAIN COLUMN).
        75.D0      250.D0
C
C       SPRTYP  :   TYPE OF SOLUTION THAT SPARSPAK USES 1<= N <= 3
        1
C
C       CYCLE ( FOR WEGS ACC ) AND MXFLMB ( MX ITERS IN INIT PROB)
        6   20
C
C       PATH FOLLOWING SWITCHES   HC   ST
    T   T
C
C       EXPONENTS FOR PATH FOLLOWING KV   HC   PP ST
        1.0D0  1.0D0  1.0D0  1.0D0
C
C       INITIAL VALUE OF DP    (DP < 0 TO PATH FOLLOW BACKWARDS)
        0.25D0
C
C       WEIGHTING FOR EXTENDED SYSTEM
            0.10D0     0.90D0
```

Output From Continuation Method

Note that part of the input file is echoed in the output along with additional feed information.

```
C        SIMPLE SIDESTRIPPER FOR USE IN THESISC
C              RWB>THESIS>SIDE01.DAT
C
C
C      THERMO TYPE     1=SRK      2=PR       3=PT
                   2
C
C      #TRAYS IN MAIN COLUMN
                  10
C
C      NUMBER OF FEEDS
                   1
C
C      FEEDSTAGE
                   4
C
C      FEEDTYPE
C      1=SUBCOOLED LIQ  2=LIQ AT BUBBLE  3=VAP AT DEW  4=SUP HT VAP
                   2
C
C      FEED TEMP AND PRES     DEG C   KPA
             173.0000             1600.000
C
C      FEED FLOW RATE         KG / HR
             1000.000
C
C      #DISCRETE COMPONENTS AND LIBID'S
                   6
                 132         0.5000000E-01
                 181         0.1500000
                 223         0.2000000
                 271         0.2500000
                 308         0.2500000
                 354         0.1000000
C
C      CRUDE TBP CURVE       1=NO     2=YES
                   1
                                  ***** FEED  1 *****
                                  DISCRETE COMPONENTS
    NAME      FORMULA   LIBID       MWT        NBP K     MOLE FRAC
   Propane       C3H8     132      44.097     231.10    0.0500    3.0
   n-Butane      C4H10    181      58.124     272.70    0.1500    3.9
   n-Pentane     C5H12    223      72.151     309.20    0.2000    4.9
   n-Hexane      C6H14    271      86.178     341.90    0.2500    5.9
   n-Heptane     C7H16    308     100.205     371.60    0.2500    6.8
   n-Octane      C8H18    354     114.232     398.80    0.1000    7.8
          AVERAGE MOLECULAR WEIGHT   83.373
```

```
                  *** PENG ROBINSON EOS ***
  THE FEED IS LIQUID AT THE BUBBLE POINT
  THE BUBBLE POINT TEMPERATURE IS   163.89 C  AT  1600. KPa

  THE ENTHALPY OF THE BUBBLE POINT LIQUID IS   21768. J / MOLE
  THE ENTHALPY OF THE BUBBLE POINT VAPOUR IS   34968. J / MOLE
     Z LIQUID :  0.0777      Z VAPOUR :  0.7465
C
C     OVERHEAD SPEC  1=RATE 2=PURITY 3=DUTY 4=REFRAT 5=BP 6=NONE
C     EX  1   100.   -1
C         2     2   0.95
C         3   1.D06  -1
C         4   1.      -1
C         5   495.    95.
C         6   -1.     -1.
      2     1.000       0.1234       -1.000
C
C     CONDENSER TYPE, 1=TOTAL
                  1
C
C     BOTTOM SPEC  1=RATE 2=PURITY 3=DUTY 4=BP 5=NONE
C     EX  1   100.   -1
C         2     2   0.95
C         3   1.D06  -1
C         4   495.    95.
C         5   -1.     -1.
      1     400.0       -1.000       -1.000
C
C     REBOILER TYPE   1=NO REBOILER  2=PARTIAL
                  2
C
C     NUMBER OF PUMPAROUNDS
                  0
C
C     NUMBER OF SIDESTRIPPERS
                  1
C
C     SIDESTRIPPER #1
C
C     1=PRODUCT RATE  2=PURITY 3=BOILING PT 4=DUTY
C    EX     1   100.   -1.           5=LIQ DRAW
C           2     2.     0.95        6=REFLUX RATIO
C           3   495.    95.
C           4   1.0E6   -1.
C           5   -1.     -1.
              1          200.0000          -1.000000
              6          3.000000          -1.000000
C
C     LIQUID DRAW AND VAPOUR RETURN TRAY
                  3              3
C
C     NUMBER OF TRAYS IN SIDESTRIPPER ( INCLUDING REBOILER )
                  3
C
```

```
 C     TOP AND BOTTOM TRAY TEMP ESTIMATES (MAIN COLUMN)
            75.00000              250.0000
 C
 C     SPRTYP  :  TYPE OF SOLUTION THAT SPARSPAK USES 1<= N <= 3
                  1
 C
 C     CYCLE ( FOR WEGS ACC ) AND MXFLMB ( MX ITERS IN INIT PROB)
                  6               20
 C
 C     PATH FOLLOWING SWITCHES  HC  ST
             T           T
 C
 C     EXPONENTS FOR PATH FOLLOWING KV  HC  PP ST
          1.0000      1.0000      1.0000      1.0000
 C
 C     INITIAL VALUE OF DP   (DP < 0 TO PATH FOLLOW BACKWARDS)
           0.2500000
 C
 C     WEIGHTING FOR EXTENDED SYSTEM
           0.1000000           0.9000000


                          *** CONVERGED ***
                  T= 0.1000
   T(1) =  398.05     T(10) =  501.89 K


                          *** CONVERGED ***
                  T= 0.2713
   T(1) =  396.71     T(10) =  500.32 K


                          *** CONVERGED ***
                  T= 0.4662
   T(1) =  395.50     T(10) =  498.93 K


                          *** CONVERGED ***
                  T= 0.6605
   T(1) =  394.28     T(10) =  497.54 K


                          *** CONVERGED ***
                  T= 0.8527
   T(1) =  393.00     T(10) =  496.13 K


                          *** CONVERGED ***
                  T= 1.0000
   T(1) =  391.57     T(10) =  494.52 K
```

```
        DISTILLATION BY ARCLENGTH-CONTINUATION
                   PENG-ROBINSON EOS

                              --- SOLUTION ---

                              MAIN COLUMN

STAGE  LIQUID  VAPOUR  TEMP
         kmol/hr       deg C

   1    1200.    400.   118.4
   2    1154.   1600.   145.0
   3     738.   1554.   163.2
   4    1848.   1338.   177.2
   5    1931.   1448.   187.3

   6    1991.   1531.   195.2
   7    2032.   1591.   202.0
   8    2060.   1632.   208.3
   9    2080.   1660.   214.7
  10     400.   1680.   221.4


                   CONDENSER DUTY     -33180.39      MJ/HR
                   REBOILER  DUTY      33398.30      MJ/HR

                              --- SIDESTRIPPER  1---

TRAY      LIQUID      VAPOUR     TEMP
                kmol/hr          deg C

 11         399.7       192.2       167.8
 12         405.4       199.7       173.9
 13         200.0       205.4       183.1

  SIDESTRIPPERS
  SSTRP        DRAW    RET   TYPE            COL DRAW   PRODUCT RATE

     1           3       3    1                 392.2       200.0

 SIDE    TOP TRAY   BOTTOM TRAY

   1          11           13
```

```
                 LIQUID MOLE FRACTIONS
                    MAIN COLUMN

TRAY   1
 0.1234   0.3458   0.3410   0.1564   0.0308
 0.0026
TRAY   2
 0.0441   0.2158   0.3611   0.2765   0.0899
 0.0125
TRAY   3
 0.0209   0.1340   0.3090   0.3395   0.1628
 0.0337
TRAY   4
 0.0148   0.0903   0.2350   0.3445   0.2408
 0.0746
TRAY   5
 0.0056   0.0529   0.2030   0.3842   0.2749
 0.0795
TRAY   6
 0.0021   0.0294   0.1628   0.4029   0.3151
 0.0877
TRAY   7
 0.0007   0.0157   0.1228   0.3990   0.3601
 0.1016
TRAY   8
 0.0003   0.0080   0.0873   0.3732   0.4063
 0.1249
TRAY   9
 0.0001   0.0039   0.0582   0.3279   0.4474
 0.1625
TRAY  10
 0.0000   0.0018   0.0357   0.2678   0.4750
 0.2197

                    SIDESTRIPPER

TRAY  11
 0.0125   0.1128   0.3105   0.3588   0.1708
 0.0346
TRAY  12
 0.0068   0.0857   0.2939   0.3835   0.1912
 0.0389
TRAY  13
 0.0031   0.0548   0.2465   0.4015   0.2385
 0.0554
```

```
                         K VALUES
                           MAIN COLUMN
TRAY   1
 2.3160   1.2237   0.6648   0.3689   0.2062
 0.1176
TRAY   2
 2.7969   1.6023   0.9442   0.5657   0.3419
 0.2099
TRAY   3
 3.0884   1.8599   1.1519   0.7234   0.4587
 0.2946
TRAY   4
 3.2949   2.0536   1.3160   0.8536   0.5594
 0.3705
TRAY   5
 3.3809   2.1683   1.4289   0.9518   0.6405
 0.4351
TRAY   6
 3.4371   2.2516   1.5147   1.0290   0.7063
 0.4889
TRAY   7
 3.4798   2.3188   1.5861   1.0947   0.7634
 0.5364
TRAY   8
 3.5163   2.3785   1.6509   1.1554   0.8171
 0.5818
TRAY   9
 3.5492   2.4353   1.7139   1.2156   0.8711
 0.6282
TRAY  10
 3.5779   2.4907   1.7776   1.2778   0.9281
 0.6779

                           SIDESTRIPPER

TRAY  11
 3.1408   1.9183   1.2046   0.7665   0.4925
 0.3203
TRAY  12
 3.2113   1.9953   1.2743   0.8239   0.5380
 0.3552
TRAY  13
 3.3164   2.1098   1.3790   0.9115   0.6086
 0.4104
```

Appendix VII

This appendix presents the results for the multiple solution case at a reflux ratio of 4.0. First the input echo is given (some of the feed data is included) then the solution to the initial problem (t=0), then the two solutions are given.

Input File

```
C
C      THERMO TYPE     1=SRK      2=PR       3=PT
                2
C
C      #TRAYS IN MAIN COLUMN
                10
C
C      NUMBER OF FEEDS
                1
C
C      FEEDSTAGE
                4
C
C      FEEDTYPE
C      1=SUBCOOLED LIQ  2=LIQ AT BUBBLE  3=VAP AT DEW  4=SUP HT VAP
                2
C
C      FEED TEMP AND PRES     DEG C   KPA
         173.0000            1600.000
C
C      FEED FLOW RATE        KG / HR
         1000.000
C
C      #DISCRETE COMPONENTS AND LIBID'S
                6
              132        0.5000000E-01
              181        0.1500000
              223        0.2000000
              271        0.2500000
              308        0.2500000
              354        0.1000000
C
C      CRUDE TBP CURVE      1=NO    2=YES
                1
```

```
                          ***** FEED  1 *****


                          DISCRETE COMPONENTS

 NAME      FORMULA    LIBID      MWT        NBP K    MOLE FRAC
Propane     C3H8       132      44.097     231.10    0.0500    3.0
n-Butane    C4H10      181      58.124     272.70    0.1500    3.9
n-Pentane   C5H12      223      72.151     309.20    0.2000    4.9
n-Hexane    C6H14      271      86.178     341.90    0.2500    5.9
n-Heptane   C7H16      308     100.205     371.60    0.2500    6.8
n-Octane    C8H18      354     114.232     398.80    0.1000    7.8

      AVERAGE MOLECULAR WEIGHT   83.373


                    *** PENG ROBINSON EOS ***
THE FEED IS LIQUID AT THE BUBBLE POINT
THE BUBBLE POINT TEMPERATURE IS   163.89 C   AT   1600. KPa

THE ENTHALPY OF THE BUBBLE POINT LIQUID IS   21768. J / MOLE
THE ENTHALPY OF THE BUBBLE POINT VAPOUR IS   34968. J / MOLE


      Z LIQUID :  0.0777      Z VAPOUR :  0.7465

C
C     OVERHEAD SPEC  1=RATE 2=PURITY 3=DUTY 4=REFRAT 5=BP 6=NONE
C     EX  1   100.   -1
C         2     2   0.95
C         3   1.D06  -1
C         4   1.     -1
C         5   495.   95.
C         6   -1.    -1.
     2    1.000        0.1234       -1.000
C
C     CONDENSER TYPE  1=TOTAL
                 1
C
C     BOTTOM SPEC  1=RATE 2=PURITY 3=DUTY 4=BP 5=NONE
C     EX  1   100.   -1
C         2     2   0.95
C         3   1.D06  -1
C         4   495.   95.
C         5   -1.    -1.
     2    6.000        0.2192       -1.000
C
C     REBOILER TYPE   1=NO REBOILER  2=PARTIAL
                 2
C
C     NUMBER OF PUMPAROUNDS
                 0
```

```
C
C     NUMBER OF SIDESTRIPPERS
                 1
C
C     SIDESTRIPPER #1
C
C     1=PRODUCT RATE  2=PURITY 3=BOILING [illegible] DUTY
C    EX     1   100.    -1.          5=LIQ DRAW
C           2     2.    0.495        6=REFLUX RATIO
C           3   495.    95.
C           4   1.0E6   -1.
C           5   -1.     -1.
            2          4.000000             0.4005000
            6          4.000000            -1.000000
C
C     LIQUID DRAW AND VAPOUR RETURN TRAY
                 3             3
C
C     NUMBER OF TRAYS IN SIDESTRIPPER ( INCLUDING REBOILER )
                 3
C
C     TOP AND BOTTOM TRAY TEMP ESTIMATES (MAIN COLUMN)
            75.00000          250.0000
C
C     SPRTYP  :  TYPE OF SOLUTION THAT SPARSPAK USES 1<= N <= 3
                 1
C
C     CYCLE ( FOR WEGS ACC ) AND MXFLMB ( MX ITERS IN INIT PROB)
                 6             20
C
C     PATH FOLLOWING SWITCHES  HC  ST
             F         T
C
C     EXPONENTS FOR PATH FOLLOWING KV  HC  PP  ST
          1.0000      1.0000      1.0000      1.0000
C
C     INITIAL VALUE OF DP   (DP < 0 TO PATH FOLLOW BACKWARDS)
            0.1000000
C
C     WEIGHTING FOR EXTENDED SYSTEM
            0.1000000          0.9000000
```

```
                     SOLUTION OF THE INITIAL PROBLEM
                                 (T=0)


     DISTILLATION BY ARCLENGTH-CONTINUATION

                    PENG-ROBINSON EOS


                                --- SOLUTION ---

                                  MAIN COLUMN

   STAGE  LIQUID  VAPOUR  TEMP  SIDE LI  SIDE VA
            kmol/hr       deg C    kmol/hr

      1    1333.    333.  123.5     0.       0.
      2    1333.   1667.  156.0     0.       0.
      3     833.   1667.  1[illegible]7.8     0.       0.
      4    1833.   1667.  191.8     0.       0.
      5    1833.   1667.  205.8     0.       0.

      6    1833.   1667.  215.4     0.       0.
      7    1833.   1667.  222.6     0.       0.
      8    1833.   1667.  228.4     0.       0.
      9    1833.   1667.  233.5     0.       0.
     10     167.   1667.  238.1     0.       0.

                                --- SIDESTRIPPER  1---

   TRAY     LIQUID     VAPOUR     TEMP
                kmol/hr           deg C

    11        500.0      166.7      180.3
    12        500.0      166.7      184.2
    13        333.3      166.7      191.4
```

```
                              SIDESTRIPPERS

SSTRP      DRAW   RET  TYPE        COL DRAW  PRODUCT RATE

   1         3      3    2          500.0     333.3

SIDE   TOP TRAY  BOTTOM TRAY

  1        11         13


                      LIQUID MOLE FRACTIONS

      TRAY    1
       0.1237   0.3049   0.2874   0.2027   0.0745
       0.0067
      TRAY    2
       0.0411   0.1725   0.2687   0.3086   0.1828
       0.0262
      TRAY    3
       0.0174   0.0964   0.2058   0.3346   0.2860
       0.0598
      TRAY    4
       0.0112   0.0617   0.1496   0.3096   0.3613
       0.1066
      TRAY    5
       0.0035   0.0286   0.1004   0.2926   0.4385
       0.1365
      TRAY    6
       0.0011   0.0128   0.0636   0.2557   0.4938
       0.1731
      TRAY    7
       0.0003   0.0056   0.0387   0.2111   0.5264
       0.2179
      TRAY    8
       0.0001   0.0024   0.0227   0.1664   0.5363
       0.2721
      TRAY    9
       0.0000   0.0010   0.0129   0.1256   0.5246
       0.3358
      TRAY   10
       0.0000   0.0004   0.0070   0.0907   0.4938
       0.4080
      TRAY   11
       0.0128   0.0878   0.2051   0.3415   0.2920
       0.0607
      TRAY   12
       0.0086   0.0740   0.1971   0.3500   0.3064
       0.0639
      TRAY   13
       0.0048   0.0526   0.1701   0.3509   0.3438
       0.0778
```

```
                K VALUES

TRAY    1
 2.4310    1.2977    0.7127    0.3996    0.2257
 0.1301
TRAY    2
 3.0079    1.7682    1.0695    0.6568    0.4072
 0.2560
TRAY    3
 3.3111    2.0647    1.3238    0.8591    0.5632
 0.3732
TRAY    4
 3.4671    2.2383    1.4850    0.9955    0.6743
 0.4609
TRAY    5
 3.5457    2.3748    1.6329    1.1325    0.7938
 0.5604
TRAY    6
 3.5758    2.4526    1.7256    1.2235    0.8766
 0.6320
TRAY    7
 3.5894    2.5036    1.7903    1.2892    0.9381
 0.6864
TRAY    8
 3.5966    2.5413    1.8401    1.3411    0.9876
 0.7309
TRAY    9
 3.6001    2.5715    1.8815    1.3851    1.0302
 0.7698
TRAY   10
 3.6006    2.5965    1.9174    1.4241    1.0686
 0.8052
TRAY   11
 3.3318    2.0936    1.3525    0.8840    0.5837
 0.3894
TRAY   12
 3.3653    2.1381    1.3962    0.9220    0.6151
 0.4144
TRAY   13
 3.4285    2.2198    1.4765    0.9923    0.6738
 0.4616
```

```
                  SOLUTION #1

     DISTILLATION BY ARCLENGTH-CONTINUATION

                  PENG-ROBINSON EOS

                           --- SOLUTION ---

                           MAIN COLUMN

  STAGE  LIQUID  VAPOUR  TEMP  SIDE LI  SIDE VA
          kmol/hr        deg C    kmol/hr

     1    1580.    395.   118.8    0.       0.
     2    1531.   1976.   145.2    0.       0.
     3    1239.   1926.   163.9    0.       0.
     4    2373.   1821.   178.0    0.       0.
     5    2471.   1954.   188.3    0.       0.

     6    2539.   2053.   196.4    0.       0.
     7    2584.   2121.   203.2    0.       0.
     8    2614.   2166.   209.6    0.       0.
     9    2634.   2195.   215.8    0.       0.
    10     419.   2215.   222.3    0.       0.


                 CONDENSER DUTY :   -40948.78    MJ/HR
                 REBOILER  DUTY :    43675.42    MJ/HR

                           --- SIDESTRIPPER  1---

  TRAY    LIQUID    VAPOUR     TEMP
              kmol/hr          deg C

    11      271.3      83.1      165.4
    12      274.0      85.3      168.3
    13      186.1      87.9      174.9


                                 SIDESTRIPPERS

   SSTRP      DRAW  RET  TYPE        COL DRAW  PRODUCT RATE

     1         3     3    2           269.1     186.1

  SIDE    TOP TRAY  BOTTOM TRAY

    1         11        13
```

LIQUID MOLE FRACTIONS

```
TRAY    1
  0.1234    0.3396    0.3421    0.1642    0.0285
  0.0022
TRAY    2
  0.0441    0.2117    0.3615    0.2893    0.0830
  0.0104
TRAY    3
  0.0195    0.1274    0.3082    0.3610    0.1547
  0.0292
TRAY    4
  0.0124    0.0820    0.2363    0.3739    0.2311
  0.0644
TRAY    5
  0.0044    0.0456    0.1950    0.4130    0.2717
  0.0703
TRAY    6
  0.0016    0.0242    0.1500    0.4261    0.3182
  0.0799
TRAY    7
  0.0005    0.0123    0.1088    0.4141    0.3684
  0.0959
TRAY    8
  0.0002    0.0061    0.0747    0.3797    0.4177
  0.1217
TRAY    9
  0.0001    0.0029    0.0484    0.3277    0.4594
  0.1616
TRAY   10
  0.0000    0.0013    0.0291    0.2641    0.4856
  0.2198
TRAY   11
  0.0156    0.1216    0.3109    0.3664    0.1561
  0.0293
TRAY   12
  0.0113    0.1083    0.3083    0.3789    0.1628
  0.0304
TRAY   13
  0.0066    0.0818    0.2824    0.4003    0.1906
  0.0382
```

```
      ENDIF
C
C     PRINT OUT INITIAL DATA
      TV1 = TRAYTK(1) - 273.15D0
      TV2 = TRAYTK(NTRCOL) - 273.15D0
      WRITE(9,52) HOMOTP, MOLEST(1,1), MOLEST(NTRCOL,NDISC),
     A   LIQU(1), VAPOUR(1), LIQU(NTRCOL), VAPOUR(NTRCOL),
     A  TV1, TV2
C
      WRITE(11,52) HOMOTP, DTDP, MOLEST(1,1), MOLEST(1,6),
     A             MOLEST(10,1), MOLEST(10,6)
C
C
C     SKIP IF THERE ARE NO SIDESTRIPPERS
      IF(NSIDE.EQ.0) GOTO 8711
      SIDE = 1
      BOT = BOTRSS(1)
      TOP = TPTRSS(1)
      TV1 = TRAYTK(TOP) - 273.15D0
      TV2 = TRAYTK(BOT) - 273.15D0
C
C     SET UP COUNTERS
 8711 LOOPE  = 0
      LOOPET = 0
      LOOPN  = 0
      LOOPNT = 0
      LOOPS  = 0
      ERROR = 1.D06
C
C     CHECK FOR NEWTON'S METHOD
      IF(NEWTON) WRITE(6,7)
      IF(NEWTON) WRITE(*,7)
 7    FORMAT(//,' ',T10,'*** NEWTON''S METHOD ***',//)
      IF(NEWTON) GOTO 205
C
C     ESTIMATE DXDP
      DTDP = 1.0D0
      DXDPST(TOTVAR) = DTDP
      TV1 = DSQRT((ONE - W2*DTDP*DTDP)*RN/(W1*(TOTVAR-1)))
      END = TOTVAR - 1
      DO 10 I = 1, END
         DXDPST(I) = TV1
 10   CONTINUE
C
C     INITIALIZE DP, INITIAL STEP LENGTH
      DP = DPINI
C
C     GENERATE THE JACOBIAN, EXCEPT FOR THE LAST ROW
      CODE = 5
C
C     PREVENT THE RHS FROM BEING INPUT
      INRHS = .FALSE.
C
C     ZERO OUT THE B VECTOR WHICH HOLDS THE DH/DT COLUMN
```

```
      DO 20 I = 1, ASIZE
         BVEC(I) = ZERO
 20   CONTINUE
C
C***
C     THIS DEBUG SHOULD PRODUCE RHSSTO() = 0
C     BECAUSE THIS POINT SHOULD BE ON THE PATH
C     ( TO GET THINGS STARTED )
      DEBUG = .FALSE.
      IF(DEBUG) THEN
      INRHS = .TRUE.
      SVRHS = .TRUE.
      CALL DUMP(9)
      DO 774 I = 1, TOTVAR
         RHSSTO(I) = ZERO
 774  CONTINUE
      ENDIF
C***
      CALL JACGEN(CODE)
      CALL NONSTE(CODE)
C***
C
C     RESET THE VALUE OF INRHS
      INRHS = .TRUE.
C
C     GOTO 100 TO DO INITIAL EULER PREDICTION.
C     GOTO 240 TO SKIP EULER PREDICTION AND JUST
C     TRY TO SOLVE FOR THE POINT ON THE RIGOROUS PATH AT T=0.1
C
C     GOTO 100
      GOTO 240
C
C     ----- GO HERE WHEN CONVERGED -----
C
 40   LOOPS = LOOPS + 1
      WRITE(KO, 50)HOMOTP, TRAYTK(1),
     A             NTRCOL, TRAYTK(NTRCOL)
C     WRITE(9 , 50)HOMOTP, TRAYTK(1),
C    A             NTRCOL, TRAYTK(NTRCOL)
      WRITE(*, 50) HOMOTP, TRAYTK(1), NTRCOL, TRAYTK(NTRCOL)
 50   FORMAT(//,' ',T30,'*** CONVERGED ***',/,' ',T20,'T=',F7.4,
     A /,' ',T10,'T(1) = ',F7.2,5X,'T(',
     A       I2,') = ',F7.2,' K')
C
C     PRINT OUT
      TV1 = TRAYTK(1) - 273.15D0
      TV2 = TRAYTK(NTRCOL) - 273.15D0
      WRITE(10,2111) HOMOTP, DTDP, MOLEST(1,1), MOLEST(10,6),
     A                MOLEST(13,4), SIDELI(1)*1000.0, LIQU(3)*1000.0
 2111 FORMAT(1X,5F8.4,2F8.2)
      WRITE(9,52) HOMOTP, MOLEST(1,1), MOLEST(NTRCOL,NDISC),
     A  LIQU(1), VAPOUR(1), LIQU(NTRCOL), VAPOUR(NTRCOL),
     A  TV1, TV2
      WRITE(11,52) HOMOTP, DTDP, MOLEST(1,1), MOLEST(1,6),
```

```
     A                MOLEST(10,1), MOLEST(10,6)
 52   FORMAT('  ',10(F8.4,2X))
C
C     IF THERE ARE NO SIDESTRIPPERS, SKIP THE PRINT
      IF(NSIDE.EQ.0) GOTO 8712
      SIDE = 1
      BOT = BOTRSS(1)
      TOP = TPTRSS(1)
      TV1 = TRAYTK(TOP) - 273.15D0
      TV2 = TRAYTK(BOT) - 273.15D0
C###
      WRITE(9,52) HOMOTP, SIDELI(SIDE), LIQU(BOT), VAPOUR(TOP),
     A        MOLEST(TOP,1), MOLEST(BOT,1), MOLEST(TOP,2),
     A        MOLEST(BOT,2), TV1, TV2
      WRITE(11,52) HOMOTP, MOLEST(13,1), MOLEST(13,6)
 8712 CONTINUE
C
C     IF USING NEWTON'S METHOD THEN RETURN
      IF(NEWTON) RETURN
C
C     CHECK TO SEE IF DELTAT IS BELOW MINSTP.  THIS MAY HAPPEN
C     IF THE CURVE IS GETTING STEEPER BUT SINCE THE PREDICTIONS
C     ARE SHORTER THE NEWTON CORRECTORS ARE ALWAYS CONVERGING
C     SO THAT THE MINIMUM STEP CHECK IS NEVER DONE AT THE
C     PLACE WHERE NEWTON'S METHOD FAILS.  IT IS MORE APPROPRIATE
C     TO DO THE CHECK HERE SO THAT THE LAST KNOWN POINT ON THE
C     PATH IS RECORDED.
C
C     NOTE THAT THE VALUE OF DTDP CAN'T BE INCLUDED IN THE CHECK
C     BECAUSE WHEN FLOWS GO NEGATIVE, DTDP MAY STILL BE IN THE
C     NEIGHBOURHOOD OF 1 BUT THE PATH CANNOT ADVANCE BECAUSE THE
C     LIQUID AND VAPOUR TRAFFIC ARE CONSTRAINED TO BE POSITIVE.
C     THIS IS A PLACE WHERE THE SQUARE MAPPING FUNCTION WOULD
C     PERHAPS FORCE THE FUNCTION TO TURN AROUND, IN WHICH CASE
C     DTDP WOULD APPROACH ZERO.  IF THE SQUARE MAPPING FUNCTION
C     IS IMPLEMENTED THE CHECK FOR DTDP SHOULD NOT BE DONE EITHER.
C     IF(DABS(DELTAT) .LT. MINSTP .AND. ABS(DTDP) .LT. 0.1) GOTO 404
      IF( ABS(DELTAT) .LT. MINSTP ) GOTO 404
C     RESET COUNTERS
      LOOPE = 0
      LOOPN = 0
      CONDIV = 0
      OLDERR = 1.D06
      FIRSTP = .FALSE.
C
C     SAVE THE TOTAL PATH LENGTH
      PATHLN = PATHLN + DABS(DELTAP)
C
C     SAVE THE CURRENT CONVERGED POINT ON THE PATH
      CODE = 6
      CALL JACGEN(CODE)
      CALL NONSTE(CODE)
      XVECST(TOTVAR) = HOMOTP
      DXDPST(TOTVAR) = DTDP
```

```
      IF(.NOT.SOLU) GOTO 100
C
C     ---------------------------
C     --- EQUATIONS SOLVED WITH t=1 ---
C     ---------------------------
C
C     PRINT OUT THE SOLUTION TO THE EQUATIONS
      CALL PRINT1(6)
      CALL PRINT1(7)
      CALL DUMP(6)
C     CALL DUMP(7)
C
      WRITE(6,70)
 70   FORMAT(' ',T30,25('*'),/,' ',T30,25('*'),/,' ',T30,'SYSTEM',
     A    ' SOLVED FOR t = 1',/,' ',T30,25('*'),/,' ',T30,25('*'))
C
C     WRITE OUT THE VALUES OF DX(I)/DP
      WRITE(9,'(1X,//,1X,T30,''DXDP VALUES'')')
      DO 71 I = 1, TOTVAR
         WRITE(9,7171) I, DXDPST(I)
 7[illegible]E
[illegible]X,T5,'DX(',I3,') / DP = ',G15.7)
C
C     NEWTON'S METHOD WORKED...
      IF(NEWTON) WRITE(6,72)
 72   FORMAT(' ',//,' ',T10,
     A '*** NEWTON''S METHOD CONVERGED ***',//)
C
C     THAT'S ALL FOLKS...
      SOLU = .FALSE.
      NSOLNS = NSOLNS + 1
      IF(INCR) THEN
         INCR = .FALSE.
      ELSE
         INCR = .TRUE.
      ENDIF
      IF (NSOLNS .GT. 1) RETURN
C     RETURN
C
C
C     **************
C     EULER STEP
C     **************
C
 100  LOOPE = LOOPE + 1
      LOOPET = LOOPET + 1
C
      DEBUG = .FALSE.
      IF(DEBUG) THEN
        CALL JACGEN(5)
        CALL NONSTE(5)
        DEBUG = .FALSE.
        STOP 0123
      ENDIF
```

```
C
C     FILL IN CONSTRAINT ROW IN JACOBIAN.
      TV1 = W1 / RN
      DO 105 I = 1, ASIZE
         CVEC(I) = DXDPST(I) * TV1
 105  CONTINUE
C
      ALPHA = DXDPST(TOTVAR) * W2
C
C     ENTER THE RHS FOR THE CONSTRAINT ROW
      RHO1 = ONE
C
C     SOLVE
      IF(LOOPE.EQ.1) GOTO 110
        CALL BORDR2
        GOTO 111
C
 110  CALL INBI(1,ZERO,SPRSTR)
      CALL BORDER
 111  CONTINUE
C
      IF(IERR.NE.0) THEN
         WRITE(*,*) ' HTPY01 ''STOP 123'' IERR = ',IERR
         STOP 123
      ENDIF
C
C     CONVERGED?
      SUM = ZERO
      END = TOTVAR - 1
      DO 130 I = 1, ASIZE
         SUM = SUM + SPRSTR(I) * SPRSTR(I)
 130  CONTINUE
      SUM = SUM * W1 / RN + W2*EPSLON*EPSLON
      EULTST = DABS(SUM-ONE)
      ECONV = .FALSE.
      IF((DABS(EULTST).LT.EULTOL) .OR. (LOOPE.GE.7))
     A                               ECONV = .TRUE.
C
C     NORMALIZE THE SOLUTION
C***
C     WRITE(9,88)
C88   FORMAT(' ',//,' ',T10,'*** EULER''S TEST ***',
C    A      //,' ',T10,' I - 1 ',T30,' I ',
C    A         T50,'REL DIFF',/)
C***
      SUM = ONE / DSQRT(SUM)
      DO 160 I = 1, ASIZE
         DXDPST(I) = SPRSTR(I) * SUM
C***
C     IF(LOOPE.EQ.1) GOTO 159
C     DENOM = SPRSTR(I)
C     IF(DENOM.EQ.ZERO) DENOM = ONE
C     TEST = (OLDEUL(I) - SPRSTR(I)) / DENOM
C     WRITE(9,89) I, OLDEUL(I), SPRSTR(I), TEST
```

```
C89   FORMAT(' ',I3,T5,3(G15.7,5X))
C     OLDEUL(I) = SPRSTR(I)
C     GOTO 160
C
C159  OLDEUL(I) = SPRSTR(I)
C***
 160  CONTINUE
C
      DTDP = EPSLON * SUM
      DXDPST(TOTVAR) = DTDP
C
C
      IS THIS A TURNING POINT?
      TURN = .FALSE.
      IF(DABS(DTDP) .LT. DTDPMN) TURN = .TRUE.
      IF(ECONV) GOTO 190
C
C     ---------------------------
C     -- EULER'S NOT CONVERGED YET
C     ---------------------------
C
      WRITE(6,180) LOOPET, LOOPE, EULTST, DTDP
C     WRITE(7,180) LOOPET, LOOPE, EULTST, DTDP
C     WRITE(9,180) LOOPET, LOOPE, EULTST, DTDP
 180  FORMAT(1H ,T10,'EULER : TOTAL LOOPS',
     A       I3,3X,'LOOPS',I3,/,' ',T10,'ERROR',
     A       E11.4,5X,'DTDP ',E11.4)
C
C     CHECK TO SEE IF EULERS METHOD IS CONVERGING
      IF(LOOPE.LT.10) GOTO 100
C
C     NOT CONVERGING
      WRITE(6,181) LOOPE
 181  FORMAT(' ',//,' ',40('*'),//,' ',T20,'EULER''S FAILED ',
     A   'TO CONVERGE AFTER ',I3,' ITERS',//,' ',40('*'),/)
      RETURN
C
C     -------------------------
C     --- EULER'S CONVERGED ---
C     -------------------------
C
 190  WRITE(6,180) LOOPET, LOOPE, EULTST, DTDP
      WRITE(*,195) LOOPE, DTDP
      WRITE(6,195) LOOPE, DTDP
C     WRITE(7,180) LOOPET, LOOPE, EULTST, DTDP
      DEBUG = .FALSE.
      IF(DEBUG) WRITE(9,180) LOOPET, LOOPE, EULTST, DTDP
 195  FORMAT(' ',T5,'*** EULER''S CONVERGED *** LOOP =',
     A    I3,5X,'DTDP = ',F8.4)
C***
C      DEBUG = .TRUE.
C      IF(DEBUG) THEN
C      WRITE(9,196) (I,DXDPST(I), I=1,TOTVAR)
C196   FORMAT(' ',T10,'HTPY01 : DX/DP(',I2,') =',G15.7)
```

```
C        DEBUG = .FALSE.
C        WRITE(9,*)' HTPY01 : DT/DP = ',DTDP
C        ENDIF
C***
C
C       SAVE DT/DP
        DXDPST(TOTVAR) = DTDP
C
C       GET THE NEW VALUES OF DELTAP AND DELTAT
C       DOUBLE THE VALUE OF DELATP ONLY IF NOFAIL=TRUE,
C       I.E. IF THE NEWTON CORRECTIONS CONVERGED AFTER
C       THE FIRST EULER PREDICTION
        IF(NOFAIL) THEN
          DELTAP = DELTAP * TWO
          IF(ABS(DELTAP) .LT. 0.001) DELTAP= DSIGN(0.001D0,DELTAP)
          DP = DABS(DELTAP)
          IF((DP.GT.DPMAX) .AND. (DABS(HOMOTP).LT.DPMXRG))
       A      DELTAP = DSIGN(DPMAX,DELTAP)
        ENDIF
C
C####   THIS IS TO PREVENT T FROM BEING PROJECTED PAST
C        T = 1 AND GETTING A SOLUTION...  IT LOOKS LIKE THE
C        PATH WANTS TO TURN AROUND
        DLTPSV = DELTAP
        IF(HOMOTP .GT. 0.99 .AND. HOMOTP .LT. 1.01) THEN
           DELTAP = 0.01
        ELSE
           DELTAP = DLTPSV
        ENDIF
C####
C
C       GET NEW DELTAT USING NEW DELTAP AND NEW DT/DP
        DELTAT = DTDP * DELTAP
C
C       CHECK TO SEE IF THE PREDICTED VALUE OF T IS PAST T=1,
C       IF SO, RESET DELTAT AND DELTAP SUCH THAT THE PROJECTED
C       POINT WILL BE CLOSE TO THE SOLUTION.
C###
        IF(1.GT.2) THEN
        TV1 = HOMOTP + DELTAT
C       IF(((TV1.GT.0.95) .AND. (DTDP.GT.0.6)) .OR.
C       A                    (TV1.GT.0.995)).AND. INCR) THEN
         IF( TV1 .GT. 0.999999999D0 .AND. INCR ) THEN
            DELTAT = ONE - HOMOTP
            DELTAP = DELTAT / DTDP
            SOLU = .TRUE.
            WRITE(*,713)TV1
            WRITE(6,713)TV1
 713        FORMAT(' T PROJECTED TO : ',F7.3,':ATTEMPT TO SOLVE AT T=1')
        ENDIF
         IF(.NOT. INCR .AND. TV1 .LE. 1.0D0) THEN
            DELTAT = ONE - HOMOTP
            DELTAP = DELTAT / DTDP
            SOLU = .TRUE.
```

```
             WRITE(*,713)TV1
             WRITE(6,713)TV1
          ENDIF
          ENDIF
C####
C
C         RESET NOFAIL
          NOFAIL = .TRUE.
C
          DEBUG = .FALSE.
          IF(DEBUG) THEN
            WRITE(9,1271) (I,DXDPST(I), I=1, TOTVAR)
 1271       FORMAT(' ',//,' ',T20,'EULER''S CONVERGED',/,' ',
     A      500(/,' ',T10,I5,5X,F8.4))
          ENDIF
C
C         GET THE INITIAL VALUE OF DT AND DP
          IF(.NOT. FIRSTP) GOTO 202
          FIRSTP = .FALSE.
C
C         TURNING POINT?
          IF(TURN) GOTO 200
C
C         CURVE IS FLAT
          DELTAP = DELTAT / DTDP
          GOTO 201
C
C         TURNING A CORNER OR NEWTON'S FAILED
  200     DELTAT = DELTAP * DTDP
C
C         NOW CHECK THE SIGNS
C         THE SIGN OF DPINI IN THE INPUT FILE IS GIVEN
C         T[illegible] DELTAT TO SOLVE THE INITIAL PROBLEM
  201     DELTAT = DSIGN(DELTAT, DPINI)
          TV1 = DTDP * DELTAT
          DELTAP = DSIGN(DELTAP, TV1)
C
C         PRINT OUT THE INITIAL VALUES OF DELTAP AND DELTAT
          WRITE(6,9024) DELTAT, DELTAP
 9024     FORMAT(/,' ',T10,'** HTPY01 ** ',/,' ',T10,'INITIAL ',
     A      'VALUES OF DELTAT AND DELTAP ARE...',
     A      /,' ',T10,2(G15.7,2X),/)
C
C***
C         THIS DEBUG SKIPS THE EULER UPDATE TO CHECK THE JACOBIAN
C         THIS DEBUG IS ONLY APPLICABLE FOR THE FIRST POINT ALONG
C         THE PATH.
C         IF(1.LT.2) GOTO 240
C***
C
C         NOW PROCEED DIRECTLY TO THE EULER STEP
  202     HOMOTP = HOMOTP + DELTAT
C
C###
```

```
C      WHEN T CROSSES OVER 1 PRINT OUT THE SOLUTION BUT DON'T FORCE
C      A SOLUTION AT T=1.0
       IF(INCR .AND. HOMOTP .GT. 1.00D0) THEN
          CALL PRINT1(7)
          CALL DUMP(7)
          INCR = .FALSE.
       ELSEIF( .NOT. INCR .AND. HOMOTP .LT. 1.0D0) THEN
          CALL PRINT1(7)
          CALL DUMP(7)
          INCR = .TRUE.
       ENDIF
       HOEXHC = HOMOTP
       HOEXST = HOMOTP
       HOEXKV = HOMOTP
       HOEXPP = HOMOTP
       IF(SOLU) GOTO 205
       GOTO 235
C
C      UPDATE THE VALUE OF DELTAT USING THE NEW DTDP
C      WHEN  IT IS NECESSARY TO ADVANCE IN INCREMENTS OF
C      DELTAP ALONG THE CURVE.
 4312  IF((FAIL .OR. TURN) .AND. (.NOT. SOLU))
     A             DELTAT = DTDP * DELTAP
C
C      UPDATE THE VALUE OF DELTAP WHEN THE CURVE IS FLAT
C      OR WHEN THE ALGORITHM IS TRYING TO COMPUTE A
C      SOLUTION POINT.
C
C***
       TV1 = DELTAP
       IF( SOLU .OR. (.NOT.(FAIL.OR.TURN)))
     A                    DELTAP = DELTAT / DTDP
C
C      THIS IS DONE SO THAT DELTAP DOES NOT CHANGE SIGN
C      ONCE THE PATH IS BEING TRAVERSED IN A CERTAIN
C      DIRECTION
       DELTAP = DSIGN(DELTAP, TV1)
C***
C
C      MAKE SURE THE SIGNS OF DTDP, DELTAP, AND DELTAP ARE
C      CONSISTENT
       TV1 = DTDP * DELTAP
       DELTAT = DSIGN(DELTAT, TV1)
C
C      TEST TO SEE IF THIS WAS A SOLUTION POINT.
C      IF SO, DELTAT NEEDS TO BE RESET
       IF(.NOT. SOLU) GOTO 203
       WRITE(6,1110)
 1110  FORMAT(' CHECK1')
       WRITE(6,7192)
       WRITE(6,1110)
 7192  FORMAT(' ',/,T10,'*** JUST SOLVED SYSTEM AT T = 1.0')
C
C      PATH FOLLOWING PAST T=1 TO LOOK FOR MULTIPLE SOLUTIONS.
```

```
C     SET THE SIGN OF DPINI
      PATHFS = .TRUE.
      DELTAP = DABS(DPINI)
      DELTAT = DTDP * DELTAP
C
C     LET'S GET THE SIGNS RIGHT... PFS3 = TRUE ==> DELTAT > 0
      DELTAT = -DABS(DELTAT)
      IF(PFS3) DELTAT = DABS(DELTAT)
      TV1 = DELTAT * DTDP
      DELTAP = DSIGN(DELTAP,TV1)
C
C     RESET SOLU AND INCR
      SOLU = .FALSE.
C
C     NOTE THAT INCR = TRUE ONLY WHEN THE HOMOTOPY PARAMETER
C     IS LESS THAN ZERO AND WILL BE APPROACHING FROM THAT 'SIDE'
C     OF T=1.
      INCR = .TRUE.
      HOMOTP = ONE + DELTAT
      WRITE(6,5512) HOMOTP, ONE, DELTAT
 5512 FORMAT(' ',/,T10,'HOMOTP, ONE, DELTAT',3(F7.4,2X))
      IF(HOMOTP.GT.ONE) INCR = .FALSE.
C
      WRITE(6,7712) HOMOTP, INCR, SOLU
 7712 FORMAT(' ',/,'  ** HOMOTP, INCR, SOLU ...',F7.4,L4,L4)
      HOMOTP = ONE
C
C
C     GO HERE AFTER THE NEWTON CORRECTOR STEP HAS FAILED, AND
C     A NEW SMALLER STEP IS BEING TRIED.  AT THIS POINT HOMOTP
C     HAS THE VALUE FROM THE LAST POINT ON THE PATH.
C
C     UPDATE THE HOMOTOPY PARAMETER
 203  HOMOTP = HOMOTP + DELTAT
      HOEXHC = HOMOTP
      HOEXKV = HOMOTP
      HOEXST = HOMOTP
      HOEXPP = HOMOTP
      WRITE(6,204) DELTAT, DELTAP, HOMOTP
C     WRITE(9,204) DELTAT, DELTAP, HOMOTP
 204  FORMAT(' ',3X,'** HTPY01 ** DT, DP, T',
     A     1X,E11.4,1X,E11.4,1X,E11.4)
C
C     PATH CROSSING OVER T=1?
      SOLU = .FALSE.
C####
      IF(.NOT. DEBUG ) GOTO 220
C####
      IF((INCR).AND. (HOMOTP.LT.0.9999999D0)) GOTO 220
      IF((.NOT.INCR).AND. (HOMOTP.GT.1.000000001D0)) GOTO 220
C
C     JUST CROSSED OVER T=1, TRY TO SOLVE
C
      WRITE(*,8891) HOMOTP
```

```
      WRITE(6,8891) HOMOTP
 8891 FORMAT(' ',T10,'** T = ',F7.5,' JUST CROSSED OVER :',
     A   /,' ',T10,'SET T=1.0 AND TRY TO SOLVE',/)
C
      DELTAT = ONE - XVECST(TOTVAR)
      DELTAP = DELTAT / DTDP
      DELTAP = DSIGN(DELTAP, DPINI)
C
C     GO HERE WHEN USING NEWTON'S METHOD
 205  SOLU = .TRUE.
      HOMOTP = ONE
      LASTP = .TRUE.
C
      HOEXHC = ONE
      HOEXKV = ONE
      HOEXST = ONE
      HOEXPP = ONE
C
      HODEHC = TEXPHC
      HODEKV = TEXPKV
      HODEST = TEXPST
      HODEPP = TEXPPP
C
C     SKIP THE EULER PREDICTOR STEP FOR NEWTON'S METHOD
      IF(NEWTON) GOTO 240
      GOTO 230
C
C     SET UP HOMOTOPY PARAMETERS
 220  IF(HOMOTP .EQ. ZERO) GOTO 229
      TV1 = ONE
      IF(HOMOTP.LT.ZERO) TV1 = -ONE
      HOMOTP = DABS(HOMOTP)
C
      HOEXHC = TV1 * HOMOTP ** TEXPHC
      HOEXKV = TV1 * HOMOTP ** TEXPKV
      HOEXST = TV1 * HOMOTP ** TEXPST
      HOEXPP = TV1 * HOMOTP ** TEXPPP
C
      HODEHC =  TEXPHC * HOMOTP ** (TEXPHC - ONE)
      HODEKV =  TEXPKV * HOMOTP ** (TEXPKV - ONE)
      HODEST =  TEXPST * HOMOTP ** (TEXPST - ONE)
      HODEPP =  TEXPPP * HOMOTP ** (TEXPPP - ONE)
C
      HOMOTP = TV1 * HOMOTP
      GOTO 230
C
 229  HOEXHC = ZERO
      HOEXKV = ZERO
      HOEXST = ZERO
      HOEXPP = ZERO
C
      HODEHC = ONE
      HODEKV = ONE
      HODEST = ONE
```

```
      HODEPP = ONE
  230 CONTINUE
C
C     --- TAKE THE EULER STEP ---
C***
      DEBUG = .FALSE.
      IF(DEBUG) THEN
      WRITE(9,444)
  444 FORMAT(1H ,T10,'** HTPY01 **     BEFORE EULER STEP')
      DEBUG = .FALSE.
      ENDIF
C***
  235 CODE = 8
      CALL JACGEN(CODE)
      CALL NONSTE(CODE)
C
C     NOTE THAT THE HOMOTOPY PARAMETER WAS UPDATED BACK AT
C     STATEMENT 203.  THIS IS NECESSARY TO CHECK IF THE
C     NEW VALUE CROSSED OVER T=1, THE SOLUTION POINT.
C***
      DEBUG = .FALSE.
      IF(DEBUG) THEN
      WRITE(9,445)
  445 FORMAT(1H ,T10,'** HTPY01 **      AFTER EULER STEP')
      ENDIF
C***
C
C     ***************
C     NEWTON'S METHOD
C     ***************
C
C     GO HERE TO BEGIN ANOTHER ITERATION OF NEWTONS METHOD,
C     SIMPLE OR EXTENDED SYTEM.  THIS IS THE CORRECTION STEP.
C
C     ZERO OUT STORAGE OF RHS IN RHSSTO()
C
  240 DO 233 I =1, ASIZE
        RHSSTO(I) = ZERO
        BVEC(I) = ZERO
        CVEC(I) = ZERO
  233 CONTINUE
      RHSSTO(TOTVAR) = ZERO
C
C***
C      IF(ABS(HOMOTP) .GT. 0.5D0 .AND. .NOT. SOLU .AND. DEBUG) THEN
      IF(ABS(HOMOTP) .GT. 0.5D0 .AND. .NOT. SOLU ) THEN
C      THIS WAS AN IDEA THAT DIDN'T WORK TOO WELL BUT
C      IS BEING KEPT ON THE BACK BURNER
C
C      FIND DELTAT TO SATISFY THE EXTENDED SYSTEM
C      CONSTRAINT EQUATION.  THIS SHOULD REDUCE/PREVENT
C      THE HOMOTOPY PARAMETER FROM OSCILLATING.
       SUMEXS = ZERO
       CALL JACGEN(10)
```

```
      CALL NONSTE(10)
      DELTSV = DELTAT
      TV1 = (DELTAP*DELTAP - W1/RN*SUMEXS) / W2
      IF (TV1 .GT. ZERO .OR. ABS(DTDP) .LT. 0.10D0 .OR.
     A                       ERROR .LT. 1.D-03) THEN
C       DELTAT = DSQRT(TV1)
        GOTO 1235
      ELSE IF(ABS(TV1) .GT. 0.01D0) THEN
        WRITE(*,'(A)') ' INITIAL DELTA T SQUARED WAS NEGATIVE...'
        SUM = ZERO
        DO 1234 I = 1, ASIZE
           SUM = SUM + (DXDPST(I)*DXDPST(I)) / (DTDP*DTDP)
 1234   CONTINUE
        TV1 = DELTAP*DELTAP / (W1*SUM/RN + W2)
        DELTAT = SQRT(TV1)
        WRITE(*,'(A,F8.4)')' DELTAT CORRECTED TO ',DELTAT
      ENDIF
C
C     NOW APPLY THE SIGN OF EPSLON TO THE NEW VALUE
C     EPSLON IS THE CALCULTATED VALUE OF DELTAT
      TV1 = DTDP * DELTAP
C
C     PREVENT OSCILLATIONS...
C      IF( ABS(DELTAT / TV1) .GT. 5.D0) DELTAT = TV1
      DELTAT = DSIGN(DELTAT, TV1)
      HOMOSV = HOMOTP
      HOMOTP = XVECST(TOTVAR) + DELTAT
C     HOMOTP = HOMOTP         + DELTAT
      WRITE(*,'(A,2F8.4)') ' OLD AND NEW T :',HOMOSV,HOMOTP
C
C     MAKE SURE T ISN'T BEING PROJECTED PAST THE SOLUTION
C         IF(INCR .AND. HOMOTP .GT. ONE) THEN
C            HOMOTP = HOMOSV + DELTSV
CC           IF(HOMOTP .GT. ONE) HOMOTP = XVECST(TOTVAR) + DTDP*DELTAP
C            IF(HOMOTP .GT. ONE) HOMOTP = (ONE+HOMOSV)/2.0
C            WRITE(*,'(A,F8.4)')' NEW T FROM PROJECTION = ',HOMOTP
C            GOTO 1235
C         ENDIF
C###     THIS IF HAS BEEN REMOVED EFFECTIVELY
C         IF(INCR .AND. HOMOTP .GT. ONE) THEN
C            HOMOTP = XVECST(TOTVAR) + DTDP * DELTAP
C            WRITE(*,'(A,F8.4)')' NEW T FROM PROJECTION = ',HOMOTP
C         ENDIF
C
C         IF(.NOT. INCR .AND. HOMOTP .LT. ONE) THEN
C            HOMOTP = XVECST(TOTVAR) + DTDP * DELTAP
C            WRITE(*,'(A,F8.4)')' NEW T FROM PROJECTION = ',HOMOTP
C         ENDIF
     ENDIF
C ***
 1235   DEBUG = .FALSE.
C
C    GENERATE THE JACOBIAN (EXCEPT FOR THE LAST ROW)
     CODE = 5
```

```
      INRHS = .TRUE.
C
C     GET THE THERMODYNAMIC PROPERTIES AT THESE CONDX
      CALL GTHERM(DERIV,FUGERR)
C
C     CHECK TO SEE IF ANY OF THE TEMPERATURES ARE GOING
C     SUPERCRITICAL.  IF SO, TRY AGAIN WITH A SMALLER
C     STEP LENGTH ALONG THE PATH.
      IF(FUGERR.NE.0) WRITE(6,430) FUGERR
C     IF(FUGERR.NE.0) WRITE(7,430) FUGERR
C     IF(FUGERR.NE.0) WRITE(9,430) FUGERR
  430 FORMAT(' ',//,' ',T10,'*** GTHERM FOUND SUPERCRITICAL',
     A  ' TEMPERATURE(S) ',/,' ',T10,'ERR = ',I6,/)
      IF((FUGERR.NE.0) .AND. (.NOT. NEWTON)) GOTO 411
C***
C     DEBUG = .FALSE.
C     WRITE(9,8877)
C8877 FORMAT(' ',//,' ',T20,'** GENERATE JACOBIAN **',/)
C     CALL DUMP2(9)
C***
C
C***
C     THIS DEBUG IS USED TO SAVE THE RHS IN RHSSTO(), IT
C     MAY BE PRINTED OUT LATER.
      SVRHS = .TRUE.
C***
      IF(.NOT.FIRSTP) DEBUG = .FALSE.
      IF(DEBUG) THEN
        CALL DUMP(9)
      ENDIF
      CALL JACGEN(CODE)
      CALL NONSTE(CODE)
C
      IF(.NOT.FIRSTP) DEBUG = .FALSE.
      IF(DEBUG) THEN
         WRITE(9,8713) (I, RHSSTO(I), I=1, ASIZE)
 8713    FORMAT(' ',//,' ',T20,'RHS VECTOR FOR A MATRIX',/,' ',
     A              500(' ',/,T10,I4,5X,G15.7))
C     STOP 1212
      IF(.NOT.FIRSTP) STOP 1212
      ENDIF
C
C***
C     NOW PUT THE RHS BACK IN
      SVRHS = .FALSE.
      DO 234 I = 1, ASIZE
         CALL INBI(I,RHSSTO(I), SPRSTR)
  234 CONTINUE
C***
C
C     FLAT, SOLU  . OR ..  TURN, FAIL  ?
C
C***
C     THIS DEBUG FORCES THE EXTENDED SYSTEM TO BE INVOKED
```

```
C     ( NOTE THAT THE SIMPLE SYSTEM WILL BE INVOKED
C     IN ORDER TO SOLVE THE EQUATIONS AT T=1.0 )
C     IF(.NOT. SOLU) GOTO 290
C
C     MODIFY IF CHECK SO THAT WHEN SOLVING FIRST POINT ON PATH
C     SIMPLE SYSTEM IS USED
      IF((.NOT. SOLU) .AND. (.NOT.FIRSTP)) GOTO 290
C***
C     IF((FAIL.OR.TURN) .AND. (.NOT.SOLU)) GOTO 290
C
C     CURVE IS FLAT OR THIS IS A SOLUTION POINT
C
C     SOLVE THE SIMPLE SYSTEM ( NO CONSTRAINT ROW)
      I = MSGLVL
      MSGLVL = MSGSOL
      CALL SPRSOL(SPRSTR, SPRTYP)
      MSGLVL = I
      IF(IERR.NE.0) STOP 8181
C
C     UPDATE THE SOLUTION
      CODE = 9
      CALL JACGEN(CODE)
      CALL NONSTE(CODE)
C
C     CONVERGED ?
      SUM1 = ZERO
      SUM2 = ZERO
      MAXRSD = ZERO
      MAXRS2 = ZERO
      DO 237 I = 1, ASIZE
         TEST2 = DABS(SPRSTR(I))
         SUM1 = SUM1 + TEST2
         TEST = DABS(RHSSTO(I))
         SUM2 = SUM2 + TEST
C
C     LOOK FOR THE LARGEST RESIDUAL
         IF(TEST.LT.MAXRSD) GOTO 236
            J = I
            MAXRSD = TEST
C
 236     IF(TEST2.LT.MAXRS2) GOTO 237
              K = I
              MAXRS2 = TEST2
 237  CONTINUE
C
      WRITE(6,238) J, RHSSTO(J)
      WRITE(*,238) J, RHSSTO(J)
 238  FORMAT(' ',T5,'EQUATION ',I4,' HAD THE LARGEST',
     A      ' RESIDUAL ',G15.7)
C
C     FIND THE VARIABLE WITH THE LARGEST DELTA
      CALL FINDVA(K, VATYPE, VACOMP, VATRAY, VALUE)
      IF(VATYPE.EQ.1) WRITE(6,1111) SPRSTR(K), VATRAY, VACOMP,
     A                         VALUE
```

```
      IF(VATYPE.EQ.2) WRITE(6,1112) SPRSTR(K), VATRAY,
     A       VALUE
      IF(VATYPE.EQ.3) WRITE(6,1113) SPRSTR(K), VATRAY,
     A         VALUE
      IF(VATYPE.EQ.4) WRITE(6,1114) SPRSTR(K), VATRAY,
     A          VALUE
      IF(VATYPE.EQ.5) WRITE(6,1115) VALUE, VATRAY, HTCOOL(VATRAY)
C
 1111 FORMAT(' LARGEST DELTA OF ',E11.4,' FOR X(',I3,',',I3,
     A         ') = ',E11.4)
 1112 FORMAT(' LARGEST DELTA OF ',E11.4,' FOR LIQUID(',I3,') = ',
     A         ,E11.4)
 1113 FORMAT(' LARGEST DELTA OF ',E11.4,' FOR VAPOUR(',I3,') = ',
     A         E11.4)
 1114 FORMAT(' LARGEST DELTA OF ',E11.4,' FOR TEMP(',I3,') = ',
     A         F8.2,' (C)')
 1115 FORMAT(' LARGEST DELTA OF ',E11.4,' FOR HTCOOL(',I3,') = ',
     A         E11.4)
C
C     CHECK TO SEE HOW LARGE THE LARGEST DELTA WAS.
C     IF IT WAS TOO BIG, FAIL AND INVOKE THE EXTENDED SYSTEM.
      TV1 = DABS(SPRSTR(K))
      IF((TV1 .GT. 1000.D0) .AND. (.NOT. NEWTON))GOTO 411
C
C
      SUM1 = SUM1 / RN
      SUM2 = SUM2 / RN
C     ERROR = (SUM1 + SUM2) * 0.5D0
      ERROR = SUM2
C
C     CHECK TO SEE IF THE RESIDUAL IS INCREASING AND IF SO,
C     HOW MANY CONSECUTINVE TIMES HAS THIS HAPPENED
C     IF TOO MANY, FAIL AND INVOKE THE EXTENDED SYSTEM
C     DO NOT DO THIS CHECK FOR THE FIRST POINT ON THE PATH
      MAXDIV = 4
      IF(.NOT.FIRSTP) THEN
C
C     THIS ALLOWS A 25% INCREASE IN THE ERROR
      TV1 = ERROR / (OLDERR*1.25D0)
      OLDERR = ERROR
      IF(TV1 .GE. ONE ) CONDIV = CONDIV + 1
      IF(TV1 .LT. ONE ) CONDIV = 0
      IF(CONDIV.GE.MAXDIV) WRITE(6,7129) MAXDIV
      IF(CONDIV.GE.MAXDIV) WRITE(*,7129) MAXDIV
 7129 FORMAT(/,' ',T10,'MAXIMUM NUMBER OF CONSECUTIVE ',
     A  'RESIDUAL',/,' ',T10,' INCREASES (',I3,') REACHED :',
     A  /,' ',T10,'FAIL AND INVOKE EXTENDED SYSTEM',/)
C
C     IF MAXIMUM NUMBER OF INCREASES IS GREATER THAN THAT
C     ALLOWED, NEWTON'S METHOD FAILS.
      IF((CONDIV .GE. MAXDIV) .AND. (.NOT. NEWTON)) GOTO 411
C     IF((CONDIV .GE. MAXDIV) .AND. NEWTON) RETURN
C
      ENDIF
```

```
C
C      PRINT
       LOOPN = LOOPN + 1
       LOOPNT = LOOPNT + 1
       WRITE(*,241) ERROR, LOOPN, HOMOTP
       WRITE(6,241) ERROR, LOOPN, HOMOTP
 241   FORMAT(' ',2X,'**NEWTON''S SIMPLE SYSTEM : ERROR = ',E11.4,
      A   /,' ',T10,'LOOP =',I3, ' FOR T= ',F7.4,/)
C
C      CONVERGED ?
C
C      SET THE TOLERANCE SO THAT ALONG THE CURVE THE TOLERANCE
C      IS LOOSER AND AT THE SOLUTION THE TOLERANCE IS TIGHT
       TOL = TOLPAT
       IF(SOLU) TOL = TOLCON
       IF(.NOT. SOLU .AND. ABS(DELTAP) .LT. 0.01) TOL = TOL * 2.0D0
       IF(ERROR.LT.TOL) GOTO 40
C
C      NEWTON'S METHOD FAILED ?
       IF(SOLU) THEN
           MNFAIL = 25
       ELSE
           MNFAIL = 10
       ENDIF
       IF(LOOPN.LE.MNFAIL) GOTO 240
       MNFAIL = 10
C
C      NEWTON'S METHOD FAILED.
       FAIL = .TRUE.
       CONDIV = 0
       OLDERR = 1.D06
       DELTAP = DELTAP * 0.5D0
       DELTAT = DELTAT * 0.5D0
C
       IF(.NOT.NEWTON) THEN
       WRITE(6,243)
       WRITE(*,243)
 243   FORMAT(' ',T10,'** NEWTON''S METHOD : ',
      A'          'SIMPLE SYSTEM * FAILED *')
       ENDIF
       LOOPN = 0
C
C      IF NEWTONS METHOD, THEN DOUBLE THE NUMBER OF ITERATIONS
C      THAT IT GETS TO TRY AND CONVERGE
C
C      ALSO DO THIS WHEN PATH FOLLOWING AND A FEW MORE ITERATIONS
C      ARE NEEDED TO CONVERGE
       IF((NEWTON .OR. SOLU) .AND. (MNFAIL.EQ.MNFLSV)) THEN
                MNFAIL = 2 * MNFLSV
                GOTO 240
       ELSE IF(NEWTON) THEN
          WRITE(7,*)' NEWTON''S METHOD FAILED'
          CALL DUMP(7)
                STOP 1234
```

```
      ENDIF
C
C     RESTORE THE POINT ON THE PATH
      CODE = 7
      CALL JACGEN(CODE)
      CALL NONSTE(CODE)
      HOMOTP = XVECST(TOTVAR)
      DTDP = DXDPST(TOTVAR)
C
C     TRY IT AGAIN
      GOTO 203
C
C     ----- EXTENDED SOLUTION -----
C
 290  LOOPN = LOOPN + 1
      LOOPNT = LOOPNT + 1
      IF(LOOPN.EQ.1) WRITE(6,291)
 291  FORMAT('-',//,' ',T10,'EXTENDED SYSTEM REQUIRED')
C
C     ENTER ROW IN JACOBIAN FOR EXTENDED SYSTEM
      FACTR1 = W1 / RN * TWO
      SUMEXS = ZERO
      CALL JACGEN(10)
      CALL NONSTE(10)
C
C     ADD COEF IN LAST ROW FOR THE HOMOTOPY PARAMETER
      ALPHA = W2 * TWO * DELTAT
C
C     FINISH OFF THE RHS OF THE CONSTRAINT EQUATION
      TEST1 = W2 * DELTAT * DELTAT
      RHO1 = SUMEXS * W1 / RN + TEST1 - DELTAP * DELTAP
C
C     CHANGE THE SIGN OF RHO1 TO DRIVE NEWTON'S METHOD
      RHO1 = - RHO1
C
C     SOLVE
      CALL BORDER
      IF(IERR.NE.0) STOP 8282
C
C***
C     WRITE(9,8712)
C8712 FORMAT(' ',/,' ',T20,'** NEWTON EXTENDED SYSTEM **',
C    A  /)
C     WRITE(9,782) (I,SPRSTR(I), I=1, ASIZE)
C782  FORMAT(' ','** HTPY01 ** DELTA X(',I2,') =',G15.7)
C***
C     NEWTON UPDATE
      CODE = 9
      CALL JACGEN(CODE)
      CALL NONSTE(CODE)
C
C***
C     THIS WAS AN IDEA THAT DIDN'T WORK TOO WELL BUT
C     IS BEING KEPT ON THE BACK BURNER
```

```
C
C     FIND DELTAT TO SATISFY THE EXTENDED SYSTEM
C     CONSTRAINT EQUATION.  THIS SHOULD REDUCE/PREVENT
C     THE HOMOTOPY PARAMETER FROM OSCILLATING.
C     SUMEXS = ZERO
C     CALL JACGEN(10)
C     CALL NONSTE(10)
C     TV1 = (DELTAP*DELTAP - W1/RN*SUMEXS) / W2
C     DELTAT = 0.1D0
C     IF(TV1 .LT. 1.D-20) GOTO 292
C     DELTAT = DSQRT(TV1)
C
C     NOW APPLY THE SIGN OF EPSLON TO THE NEW VALUE
C     EPSLON IS THE CALCULTATED VALUE OF DELTAT
C     DELTAT = DSIGN(DELTAT, EPSLON)
C292  CONTINUE
C
C   --- WELL, THIS UPDATE OF DELTAT MIGHT STILL COME IN
C       HANDY, ...  IT SEEMS TO OSCILLATE A LOT, BUT
C       PERHAPS IT SHOULD BE INVOKED WHEN THE PROBLEM
C       IS NOT CONVERGING. ---
C     EPSLON = DELTAT
C
C     CLAMP THE VALUE OF EPSLON, THE CORRECTION TO THE
C     HOMOTPY PARAMETER.  IF HOMOTPY = ZERO, THEN SKIP
C     THE TEST.
C      IF(DABS(HOMOTP) .LT. 0.1D0) GOTO  297
C
C      TEST = 0.5D0 * DABS(HOMOTP)
C      IF(DABS(EPSLON).GT.TEST) EPSLON = DSIGN(TEST,EPSLON)
C 297  CONTINUE
C
      HOMOLD = HOMOTP
      HOMOTP = HOMOTP + EPSLON * TMAX
C
C     DON'T LET T DIGRESS
C
C     CHECK TO SEE IF T HAS GONE LESS THAN WHERE IT WAS.
       IF(INCR .AND. DTDP.GT.0.1D0 .AND. HOMOTP .LT. XVECST(TOTVAR))
     A            HOMOTP = XVECST(TOTVAR) + DTDP * DELTAP * TMAX
C
       IF(.NOT. INCR .AND. DTDP .LT. ZERO .AND. ABS(DTDP) .GT. 0.1D0
     A                              .AND. HOMOTP .GT. XVECST(TOTVAR))
     A            HOMOTP = XVECST(TOTVAR) + DTDP * DELTAP * TMAX
C
C
C     NOTE THAT ALTHOUGH IT WOULD BE NICE TO CLAMP
C     THE VALUE OF T AT 1.0 AT THIS POINT IF THE SOLUTION
C     POINT IS APPARENTLY BEING SKIPPED OVER, THIS CANNOT
C     BE DONE BECAUSE THE EXTENDED SYSTEM EQUATION
C     DICTATES HOW FAR ALONG THE PATH THE NEXT SOLUTION
C     WILL BE ACCORDING TO THE VALUE OF DELTAP, AND SO
C     DELTAT MUST BE ALLOWED TO FLOAT TO MEET THIS
C     CONDITION
```

```
C
      DELTAT = HOMOTP * XVECST(TOTVAR)
C
C     UPDATE HOMOTP ETC. AND APPLY CORRECT SIGN
      TV1 = ONE
      IF(HOMOTP.LT.ZERO) TV1 = -ONE
      HOMOTP = DABS(HOMOTP)
C
      HOEXHC = TV1 * HOMOTP
      HOEXKV = TV1 * HOMOTP
      HOEXST = TV1 * HOMOTP
      HOEXPP = TV1 * HOMOTP
C
      HODEHC =  TEXPHC * HOMOTP ** (TEXPHC - ONE)
      HODEKV =  TEXPKV * HOMOTP ** (TEXPKV - ONE)
      HODEST =  TEXPST * HOMOTP ** (TEXPST - ONE)
      HODEPP =  TEXPPP * HOMOTP ** (TEXPPP - ONE)
C
      HOMOTP = TV1 * HOMOTP
C
C
C     CHECK TO SEE IF T > 1.  IF SO, SET SOLU=TRUE.
C     THIS IS NECESSARY IN CASE THE EULER PROJECTION
C     PUTS T CLOSE TO 1 (I.E. T=0.97 OR SO) AND THEN
C     WHEN SOLVING THE EXTENDED SYSTEM THE FINAL POINT
C     ON THE PATH IS PAST T = 1.
C     IF(HOMOTP.GE.ONE) SOLU = .TRUE.
C
C     CONVERGED ?
      SUM1 = ZERO
      SUM2 = ZERO
      MAXRSD = ZERO
      MAXRS2 = ZERO
      DO 300 I = 1, ASIZE
         TEST2 = DABS(SPRSTR(I))
         SUM1 = SUM1 + TEST2
         TEST = DABS(RHSSTO(I))
         SUM2 = SUM2 + TEST
C
C     LOOK FOR THE LARGEST RESIDUAL
         IF(TEST.LT.MAXRSD) GOTO 301
            J = I
            MAXRSD = TEST
C
 301     IF(TEST2.LT.MAXRS2) GOTO 300
            K = I
            MAXRS2 = TEST2
 300  CONTINUE
      WRITE(6,238) J, RHSSTO(J)
C
C     FIND THE VARIABLE WITH THE LARGEST DELTA
      CALL FINDVA(K, VATYPE, VACOMP, VATRAY, VALUE)
      IF(VATYPE.EQ.1) WRITE(6,1111) SPRSTR(K), VATRAY, VACOMP,
     A                        VALUE
```

```
      IF(VATYPE.EQ.2) WRITE(6,1112) SPRSTR(K), VATRAY,
     A     VALUE
      IF(VATYPE.EQ.3) WRITE(6,1113) SPRSTR(K), VATRAY,
     A         VALUE
      IF(VATYPE.EQ.4) WRITE(6,1114) SPRSTR(K), VATRAY,
     A           VALUE
      IF(VATYPE.EQ.5) WRITE(6,1115) VALUE, VATRAY, HTCOOL(VATRAY)
C
C
C
      SUM1 = (SUM1 + DABS(EPSLON)) / RN
      SUM2 = (SUM2 + DABS(RHO1))   / RN
C     ERROR = (SUM1 + SUM2) * 0.5D0
      ERROR = SUM2
C
      WRITE(6,401) LOOPN, ERROR, HOMOTP, DELTAP, DELTAT
C     WRITE(9,401) LOOPN, ERROR, HOMOTP, DELTAP, DELTAT
      WRITE(*,401) LOOPN, ERROR, HOMOTP, DELTAP, DELTAT
  401 FORMAT(' ',T30,'** NEWTON''S EXTENDED SYSTEM **',/,' ',
     A  T5,'LOOPN : ',I3,3X,'ERROR : ',E11.4,3X,'t : ',F9.4,
     A  /,' ',T5,'DEL P : ',F8.5,5X,'DEL T : ',F8.5,/)
      FAIL = .FALSE.
C
C
C     CHECK TO SEE IF THE RESIDUAL IS INCREASING AND IF SO,
C     HOW MANY CONSECUTINVE TIMES HAS THIS HAPPENED
C     IF TOO MANY, THE EXTENDED SYSTEM FAILS FOR THIS STEP
      MAXDIV = 3
C
C     THIS ALLOWS A 25% INCREASE IN ERROR
      TV1 = ERROR / (OLDERR*1.25D0)
      OLDERR = ERROR
      IF(TV1 .GE. ONE ) CONDIV = CONDIV + 1
      IF(TV1 .LT. ONE ) CONDIV = 0
      IF(CONDIV.GE.MAXDIV) WRITE(6,7129) MAXDIV
      IF(CONDIV.GE.MAXDIV) WRITE(*,7129) MAXDIV
      IF(CONDIV .GE. MAXDIV) GOTO 409
C
C     SET THE TOLERANCE SO THAT ALONG THE CURVE THE TOLERANCE
C     IS LOOSER
      TOL = TOLPAT
      IF(.NOT. SOLU .AND. ABS(DELTAP) .LT. 0.01) TOL = TOL * 2.0D0
      IF(SOLU) TOL = TOLCON
C
C     CHECK TO SEE IF THE VALUE OF T HAS GONE PAST 1.0.
C     IF IT HAS, THEN SET THE HOMOTOPY PARAMETER AT 1.0 AND
C     SOLVE THE SIMPLE SYSTEM
      IF(HOMOTP.GT.ONE .AND. ABS(DELTAT).LT.2.D-06
     A                  .AND. HOMOTP .LT. 1.01D0) THEN
C         SOLU = .TRUE.
        LOOPN  = 0
        HOMOTP = ONE
        HOEXST = ONE
        HOEXHC = ONE
```

```
        HOEXKV = ONE
        HOEXPP = ONE
        HODEST = ONE
        HODEHC = ONE
        HODEKV = ONE
        HODEPP = ONE
        WRITE(*,*)'T CROSSED [illegible]VER 1, SWITCHING TO SIMPLE SYSTEM AT T=1'
        WRITE(*,*)
        GOTO 240
      ENDIF
      IF(ERROR.LT.TOL) GOTO 40
      FAIL = .TRUE.
C
C     --- NOT CONVERGED YET ---
C
C
C     NEWTON'S METHOD FAILED ?
      IF(LOOPN .LE. MNFAIL) GOTO 240
C
C     SET NOFAIL = FALSE, A SHORTER EULER PREDICTION IS NEEDED
      NOFAIL = .FALSE.
C
C     IS THE MINIMUM STEP LENGTH TOO SMALL?
      TV1 = DABS(DELTAT)
      TV2 = DABS(DELTAP)
C
C     SEE THE NOTE IN THE START OF THE CODE WHICH DOES THIS
C     CHECK AS TO WHY THE VALUE OF DTDP SHOULD NOT BE CHE[illegible]KED.
C     IF(TV1 .GT. MINSTP .AND. ABS(DTDP) .GT. 0.1) GOTO 4[illegible]9
      IF(TV1 .GT. MINSTP .OR. TV2 .GT. 0.001D0) GOTO 409
C
C     WRITE OUT THE VALUES OF DX/DP TO SEE IF THEY CAN
C     OFFER ANY INSIGHT
 404  WRITE(6,402) (I,DXDPST(I), I=1,ASIZE)
C     WRITE(7,402) (I,DXDPST(I), I=1,ASIZE)
C     WRITE(9,402) (I,DXDPST(I), I=1,ASIZE)
 402  FORMAT(' ',//,'NEWTON''S EXTENDED SYSTEM FAILED ',
     A 'BECAUSE',
     A ' THE STEP SIZE IS TOO SMALL...',/,' ',T10,'ARC-LENGTH',
     B ' CONTINUATION FAILED',/,' ',T10,
     C 'IF YOU WANT TO SPEND SOME MORE MONEY', /,' ',T10,
     D 'MAKE MINSTP SMALLER AND RECOMPILE',
     A  //,' ',T10,'THE DX/DP VALUES ARE',
     C /,255(/,' ',T10,'I = ',I4,4X,G15.7))
C
      WRITE(6,501) DTDP
C     WRITE(7,501) DTDP
C     WRITE(9,501) DTDP
 501  FORMAT(' ',//,' ',T10,'DTDP = ',G15.7,//)
      RETURN
C
C     NEWTON'S METHOD EXTENDED SYSTEM FAILED,
C     HALVE THE STEP SIZE AND TRY IT AGAIN
C
```

```
 409  WRITE(*,410) HOMOTP, DELTAP, DELTAT
      WRITE(6,410) HOMOTP, DELTAP, DELTAT
C     WRITE(7,410) HOMOTP, DELTAP, DELTAT
C     WRITE(9,410) HOMOTP, DELTAP, DELTAT
 410  FORMAT(' ',//,' ',T10,'*** NEWTON''S EXTENDED ',
     A   'SYSTEM FAILED ***',/,' ',T10,'T = ',F8.4,
     B   3X,'DP = ',F8.5,3X,'DT = ',F8.5)
 411  LOOPN = 0
      LOOPE = 0
      CONDIV = 0
      OLDERR = 1.D06
      FAIL = .TRUE.
C
C     IS THE MINIMUM STEP LENGTH TOO SMALL?
C     I KNOW THIS IS REDUNDANT, BUT WE HAVE TO CHECK
C     DELTAT WHEN THE STEP CRASHES DUE TO SUPERCRITICAL
C     TEMPERATURES AND EXCEEDING THE MAXIMUM NUMBER OF
C     CONSECUTIVE DIVERGENCES...
      TV1 = DABS(DELTAT)
      IF(TV1 .LT. MINSTP) GOTO 404
C
      DELTAP = DELTAP * 0.5D0
      DELTAT = DELTAP * DTDP
      WRITE(6,420) DELTAP, DELTAT, DTDP
C     WRITE(7,420) DELTAP, DELTAT, DTDP
 420  FORMAT(/,' ',T10,'NEW VALUES ARE : DP DT DT/DP :',
     A   /,' ',T10,3(G12.5,2X),/)
C
C     RESTORE THE PREVIOUS POINT ON THE PATH
      CALL JACGEN(7)
      CALL NONSTE(7)
      HOMOTP = XVECST(TOTVAR)
      DTDP = DXDPST(TOTVAR)
C
C     TAKE SHORTER EULER STEP FROM PREVIOUS POINT ON THE PATH
      GOTO 203
C
      END
```