Feasibility Analysis, Dynamics, and Control of Distillation Columns With Vapor Recompression.

Edgar Hernandez

Louisiana State University and Agricultural & Mechanical College

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FEASIBILITY ANALYSIS, DYNAMICS, AND CONTROL OF DISTILLATION COLUMNS WITH VAPOR RECOMPRESSSION

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Chemical Engineering

by

Edgar Hernandez

B.S. Chem. Eng., Univ. of Puerto Rico at Mayaguez, May 1977
M.S. Chem. Eng., Louisiana State University, May 1980
M.S. Ind. Eng., Louisiana State University, Dec. 1980
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ABSTRACT

The conventional distillation system owes its existence to its simplicity, low investment, and inexpensive energy. Inexpensive energy is something that belongs to the past. Therefore, vapor recompression has indeed become more attractive despite the more complex flow arrangements.

In this research, a steady state model was developed to study the effect of different variables on the feasibility of heat pump installations. As expected, the heat pump system favored the close boiling mixture against the wide boiling mixture. A relationship between the savings and the thermodynamic availability of the mixture was devised. The savings were also found to be very sensitive to the relative cost of steam and electricity. A possible way of predicting the pressure effect on the heat pump feasibility based on the Antoine equation for the vapor pressure of the key components was also devised.

A dynamic model of a distillation column with a heat pump system was developed which includes pressure dynamics in the compressor suction and in the compressor discharge. Pressure dynamics are included in order to study the effect of pressure variations on the overall control strategy. This model was used to perform dynamic and control studies.

The presence of stiff differential equations in the dynamic model justified a search for a more efficient
integration technique. The LSODE computer software package was found to be the most effective numerical integration package for our system.

Basic distillation control schemes which utilize pressure to manipulate the trim cooler outflow were successfully implemented. No interaction was found between the pressure control loop and the product composition control loop. On the other hand, some interaction was observed when the temperature was used to indirectly control the composition. This interaction was found to be closely related to the relative magnitude of the sample time of the pressure controller to the sample time of the temperature controller.

Vapor recompression is a feasible way of economizing energy on a distillation unit. The outlook for the use of the heat pump concept has now induced process engineers to consider its applications.
CHAPTER 1

INTRODUCTION

Most of the interest and attention in recent studies is being devoted to energy conservation. During the past decade the price of oil has increased considerably. Two reasons for the sharp increase in the price of oil were: the Arab embargo in 1973, and the Iran crisis in 1979, which made the U.S. to look for alternate sources of energy and for energy conservation. Consequently, distillation became a focal point of many studies because:

1. Distillation is the most widely used unit operation for separating components in a mixture.
2. Distillation is a heavy consumer of energy.

To have an idea of how much energy is consumed in a distillation process, in 1976 the U.S. distillation energy consumption was estimated to be nearly 3% of the entire national energy consumption. If 10% of the energy used in distillation is saved, energy consumption would be reduced by nearly 100,000 bbl/day of oil which represents about 0.5% of the entire national production (Mix, Dweck, and Weinberg, 1978). This is one of the reasons, distillation has been a subject of continuous research. Figure 1.1 shows a typical distillation column.

The purpose of this dissertation is to investigate the feasibility, dynamics, and control of a distillation column.
Figure 1.1 Conventional Distillation Column
when it is integrated for energy conservation with special interest on heat pump installations.

Basically, energy integration is divided in two major categories: multiple effect systems and vapor recompression. Figure 1.2 shows an example of a multiple effect system applied to a distillation column. The multiple effect distillation is analogous to the multiple effect evaporation. The multiple effect system presented in Figure 1.2 is called the single source, single load system (Buckley, 1978). The source column is the one that supplies the energy to the system. The load column is the one that removes the heat from the system. In this scheme the bottom stream of the source column is the feed stream to the load column. The top stream of the source column serves to drive the reboiler of the load column. There are a wide variety of multiple effect arrangements besides the one described above.

Figure 1.3 shows an example of a vapor recompression system also applied to a distillation column. This system is commonly referred to as a heat pump system. This is the most simple heat pump arrangement. It uses an external refrigerant for heating and cooling. The column condenser is cooled with evaporating refrigerant at relatively low pressure and the column reboiler is heated with condensing refrigerant at relatively high pressure. This system is highly recommended when the column fluid is highly corrosive and it can not be used as a working fluid.
Figure 1.2 Multiple Effect Distillation Arrangement
Figure 1.3 Heat Pump with External Refrigerant
Another type of heat pump system is shown in Figure 1.4. This is a heat pump system with reboiler liquid flashing. In this system, the reboiler is eliminated by flashing the reboiler liquid across an expansion valve. This arrangement eliminates the use of a reboiler.

Figure 1.5 shows another example of a heat pump system. This is a heat pump system with compression of overhead vapor. This scheme is appropriate when the column fluid is itself a fairly good refrigerant and it is not highly corrosive. This particular scheme eliminates the use of the overhead condenser. The vapor from the top of the column is compressed in order to drive the reboiler of the same column. A trim cooler is normally used to remove the excess energy developed in the system. This heat pump arrangement is the one being studied throughout this research.

The heat pump principle involves the use of a compressor to recycle the latent heat in the vapor from the top of the tower at conditions suitable enough to drive the reboiler at the bottom of the tower. Some of the key variables in analyzing a heat pump installation on a distillation column include the pressure difference between the top and the bottom of the tower, the absolute pressure level of the tower, which affects both the relative volatility and the compression ratio, the temperature difference in the reboiler vs the horse power to provide it, and the size of the duty involved.

There are several factors that must be considered
Figure 1.4 Heat Pump with Reboiler Liquid Flashing
Figure 1.5 Heat Pump with Compression of Overhead Vapor
regardless of the scheme under study. These are:

1. Reserve capacities which may be required:
   Extra heating capacity
   Extra cooling capacity
   Extra process equipment capacity

2. Interactions -- elaborated heat recovery schemes are often highly interactive.

3. Overall material balance -- How to maintain it?

4. Overall heat balance -- How to maintain it?

5. Economics -- Is it feasible?

The analysis presented in this dissertation is divided in three parts. These are:

1. Effect of column variables on a heat pump installation. This study is based on steady state analysis. (Chapter 2)

2. Economic evaluation of a distillation column with a heat pump. This study is also based on steady state analysis. (Chapter 3)

3. Dynamics and control studies of a distillation column with a heat pump. This study is based on a dynamic model of a distillation column which includes a heat pump unit. (Chapter 5.)

One of the most relevant work done in this area, is the work done by Quadri (1981). He wrote two papers dealing with process design and process optimization of a heat pump installation with particular reference to propylene-propane splitters. In part 1 he discussed alternative process
schemes and a computer oriented calculation method for the design optimization of heat pump splitters. The computer calculation method was also general enough to be applicable to rectification cases other than propylene-propane. The design optimization was performed case by case. In part 2, the results of the optimization obtained by applying the calculation method to an industrial propylene-propane splitter were illustrated and the instrument control systems were discussed based on data and experience from the design and early operation of a similar unit by the author. Finally, the economics of the heat pump rectification was compared against alternative systems.

The difference between Quadri's work and the work in this research is in the heat pump configuration used. His scheme does not have a recycle of vapor to the compressor. It also appears that the products are taken off from the column at the highest pressure. In the system studied in this research the vapor generated in the flash is recycled back to the compressor. The advantage of recycling back the flashed vapor is that for some binary systems the vapor from the top of the column is not enough to drive the reboiler of the column; therefore, requiring the use of a trim reboiler to compensate for the extra energy needed. Benzene-Toluene is an example of such a system.

The work done by Null (1976) included the study of some of the variables that affect the heat pump installations of distillation columns. In his work he studied different
overhead condensation temperatures, different reboiler temperatures, the temperature driving force for heat transfer and different cooling media. His work involved an economic evaluation by comparing the available capital resulting from utility savings with that required to install a heat pump system. The definition of available capital depends on the type of installation, and on the utilities capital allocation policy of the company. According to Null, in a new installation, where neither a heat pump nor a conventional design has been previously selected, the available capital is to be applied to the difference between the cost of the heat exchangers for the heat pump system plus the compressor and the heat exchangers for the conventional column. In a replacement situation, the conventional column has already been built. Therefore, the available capital is applied toward the total cost of the exchangers and the compressor for the heat pump system. He described the methods used and the results obtained in a study conducted to develop guidelines to conditions under which heat pump systems might be economical substitute for conventional distillation processes. He concluded that heat pumps have extensive applicability to distillation specially in new process design. The range of applications is diminished in replacement situations.

Null's economic evaluation differs from the one in this research in that he considered available capital at a fixed return of investment to determine feasibility while in this
research feasibility was based on the calculated rate of return. Inflation was a factor considered which was not considered in Null's evaluation. The economic evaluation in this research was performed by doing a cash flow type of analysis where our main product was the energy savings. Also, different variables were considered in this research which were not considered in Null's article.

Additional work was done by Danziger (1979). His work dealt primarily with vapor recompression as applied to a pilot plant distillation column. He performed an energy and economic analysis for both the conventional and the heat integrated column as applied to pilot plants. He was able to come up with savings of over 80% for a system of cis/trans decalin.

None of the literature reviewed deals directly with the dynamics and control of distillation columns with a heat pumps. Only Quadri discussed briefly about control strategies, but it has not yet been examined by a computer simulation effort. Therefore, one of the major contributions of this research is in the area of process dynamics and control.

In order to study any control system by computer simulation, a dynamic model of a distillation column is required. The particular control system requires a distillation model with pressure dynamics included. This is necessary to be able to close the energy balance through pressure control. An attempt was made previously by Stewart
(1981) to include the pressure control as an integral part of the overall control scheme in a conventional distillation column. This objective is carried on throughout this research. Pressure control is included as an integral part of the overall control scheme, but for a distillation column with a heat pump installation.

In an effort to make the simulation run faster different integration methods were tested. Among the integration methods tested were Runge-Kutta forth order, EPISODE (Byrne, 1979) and LSODE (Hindmarsh, 1980). The last two are computer software packages based on Gear's method (Hindmarsh, 1979) for solving stiff differential equations. Stiff differential equations are those that contain widely separated eigenvalues. The numerical integration is discussed in Chapter 4.

This research program which was initiated by this work was not an exhaustive study on heat pump installations. The ultimate goal of this research program is the completion of a definitive study on heat integration systems for energy conservation, in order to evaluate its feasibility, operation and control problems. This study was considered the first step in a complete research program on heat integration on distillation columns, laying the groundwork for future studies.
CHAPTER 2

EFFECT OF COLUMN VARIABLES ON HEAT PUMP INSTALLATIONS

As mentioned before among the most important variables that affect the heat pump installations are:

1. Pressure drop across the column
2. Absolute pressure of the tower
3. Approach temperature in the reboiler/condenser

The purpose in this chapter is to develop the necessary tools needed to perform the above mentioned studies. Among the tools needed are:

1. A design program to estimate number of trays, reflux ratio and feed tray location of a distillation column for a given separation based on shortcut calculation methods. A mechanical design of the column with the heat pump system is also needed.
2. A steady state distillation routine to perform distillation calculations.
3. A steady state routine for the heat pump system.

The purpose of the design program is to come up with a reasonable design of a distillation column based on shortcut methods.

The steady state routine for the distillation column is based on the well known Thiele-Geddes method. This method is chosen because its simplicity allowing more
computer time for the heat pump system, and because our prime interest is to evaluate the heat pump installation and not to perform rigorous studies on distillation which are well known.

The steady state routine for the heat pump system models the compression of the vapor at the top of the column which is used to drive the reboiler of the column. In this process a considerable amount of energy in the reboiler can be saved, but a more expensive electrical energy is used in the compressor. Only economics dictates its feasibility. The economics of heat pump installations are discussed in Chapter 3.

Both the conventional column routine and the heat pump routine are included in one single program, so that the comparison studies are done simultaneously. The steady state distillation routine was tested against the distillation routine developed by Wang (1981). An agreement of less than 1% was obtained between both programs. The heat pump routine was successfully tested against cases obtained from the literature (Quadri, 1981).

The following assumptions were made in the development of the steady state computer model:

1. The stages were considered to be in equilibrium
2. Complete mixing per stage
3. Adiabatic stages
4. No heat of mixing
5. Total condenser for the conventional column
6. Partial reboiler for the conventional column
7. Saturated liquid feed
8. One feed and two products (distillate and bottom)
9. K-values are calculated using Raoult's law
   \[ K(i) = \frac{PS(i)}{PT} \]
   where PS is the component vapor pressure and PT is the total pressure.
10. Liquid and vapor enthalpies are calculated using polynomial equations for the liquid and vapor heat capacities.
   \[ C = A + B T + C T^2 + D T^3 \]
   where \( T \) is temperature in degrees Kelvin.
11. Adiabatic compression with polytropic efficiency of 75%
12. One stage centrifugal compressor
13. Adiabatic flash
14. Condenser side of the reboiler/condenser is a total condenser and the reboiler side is a partial reboiler

The computer technique used in this research is based on a method proposed by Thiele and Geddes and modified by others (Lyster, Sullivan, Billingsley, and Holland, 1959) to solve multicomponent distillation problems. The following column specifications are needed:

1. Number of stages in each column section
2. Quantity, composition and thermal condition of the feed
3. Column pressure or pressure profile
4. Type of overhead condenser
5. Reflux ratio
6. Distillate flowrate

To start the successive approximations, the temperature, liquid and vapor profiles are assumed. The convergence method is then concerned in the way in which the profiles are adjusted to meet the specified distillate rate at the specified reflux rate. This method is the so called Theta method (Lyster, Sullivan, Billingsley and Holland, 1959) which relates the calculated values to the corrected values for the new iteration. The convergence is aided by Newton-Raphson. Since this method is well known, it will not be discussed in details. The distillation routine works as follows:

1. Read input data
2. Initialize liquid and vapor profiles assuming equal molar overflow.
3. Initialize the temperature profile based on the bubble point of the two key components.
4. Initialize the pressure profile using a linear pressure drop between the top and the bottom of the column.
5. Using Thiele-Geddes algorithm solve for the compositions from the bottom up to the feed tray and from the top down to the feed tray.
6. Correct the compositions using the Theta method.
7. Obtain a new temperature profile, using a bubble point procedure
8. Simultaneously, solve the heat balance and the material balance on each stage to get a new liquid and vapor profiles.
9. If the summation equation is not met for the liquid compositions in each tray, return to step 5.
10. Print out the results of distillation routine and transfer data to the compressor routine.

The compressor routine uses the results obtained from the distillation routine to determine the power requirements on the compressor and the energy savings obtained by implementing the heat pump system on a conventional distillation column. The compressor routine works as follows:

1. Transfer of necessary data from the distillation routine
2. Initialize the amount of vapor flashed in the reflux drum
3. Assume a compressor outlet pressure, and calculate the compressor outlet bubble point temperature.
4. Check if the bubble point temperature meets the specified approach temperature in the reboiler/condenser. If not the secant method is used to get a new outlet pressure, then return to step 3.
5. If the approach temperature is met, calculate the amount of liquid flashed in the reflux drum once
the pressure is brought back to the column top pressure.

6. If the liquid flashed plus the condensate of the trim cooler is not equal to the distillate plus the reflux flowrate, return to step 2 with the calculated amount of vapor flashed.

7. Printout results and store results for plotting purposes and for the dynamic program.

8. Return back to the main program to check if more cases are going to be run.

The location of the trim condenser was decided based on economic considerations. Preliminary economic calculations said that it is more economical to have the trim condenser before the compressor rather than having it after the compressor (See Figure 2.1) The reason for this is that at higher pressure, for the same heat load, the temperature driving force is larger compared with that at lower pressure. This means that if the overall heat transfer coefficient does not change significantly the high pressure system requires a smaller heat exchanger than at a lower pressure. However, the capital savings obtained in the trim condenser by locating it after the compressor does not compensate for the extra energy consumption of having a higher flow through the compressor. For this reason, in this particular arrangement, it is more economical to have the trim condenser before the compressor rather than after the compressor. The trim condenser condensates part of the
Figure 2.1 Heat Pump with Compression of Overhead Vapor

with Possible Trim Cooler Locations
top vapor in order to close the overall energy balance.

In order to make comparison studies, the product conditions of the column with heat pump should be the same as the product conditions of the conventional column. To accomplish this, the reflux rate was modified in such a way to keep column products the same as the base case column products. The base case conditions are shown in Tables 2.1 and 2.2. All comparisons are made based on these column conditions as reference points.

In this part of the research, two binary systems were tested: Benzene-Toluene and Methanol-Ethanol. These two binary mixtures were chosen because they behave fairly ideal and also because one mixture is a close boiling mixture while the other is a relatively wide boiling mixture. The boiling range for the Methanol-Ethanol mixture is about 14 K while for the Benzene-Toluene system, the boiling range is about 30 K. Scientists have claimed that heat pump installations are more suitable for close boiling mixtures than for wide boiling mixtures. Therefore it is expected to save more energy with the Methanol-Ethanol mixture than with the Benzene-Toluene mixture.

It was mentioned before that the electric cost is more expensive than the steam (689.5 KPA) cost per unit energy basis. In order to account for this fact, a cost factor was developed based on the cost of electricity and steam. This factor is the ratio between the electric cost and the steam cost. According to the literature (Peters and Timmerhaus,
<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Stages</td>
<td>15</td>
</tr>
<tr>
<td>Feed Tray Location</td>
<td>9</td>
</tr>
<tr>
<td>Feed Rate</td>
<td>1000 g-moles/min.</td>
</tr>
<tr>
<td>Feed Rate Composition</td>
<td>50% Benzene, 50% Toluene</td>
</tr>
<tr>
<td>Quality of Feed</td>
<td>Saturated liquid</td>
</tr>
<tr>
<td>Distillate Rate</td>
<td>500 g-moles/min.</td>
</tr>
<tr>
<td>Distillate Composition</td>
<td>94.2% Benzene, 5.8% Toluene</td>
</tr>
<tr>
<td>Quality of Distillate</td>
<td>Saturated liquid</td>
</tr>
<tr>
<td>Bottoms rate</td>
<td>500 g-moles/min.</td>
</tr>
<tr>
<td>Bottoms Composition</td>
<td>5.8% Benzene, 94.2% Toluene</td>
</tr>
<tr>
<td>External Reflux Ratio</td>
<td>1.2</td>
</tr>
<tr>
<td>Top Pressure</td>
<td>101.3 KPA (1 atm)</td>
</tr>
<tr>
<td>Pressure Drop per Tray</td>
<td>0</td>
</tr>
<tr>
<td>Steam Pressure</td>
<td>689.5 KPA (100 psig)</td>
</tr>
<tr>
<td>Cooling Water Inlet</td>
<td>299.8 K (80 F)</td>
</tr>
<tr>
<td>Cooling Water Temperature</td>
<td>22.2 K (40 F)</td>
</tr>
<tr>
<td>Polytropic Efficiency</td>
<td>75%</td>
</tr>
<tr>
<td>Approach Temperature on Reboiler/Condenser</td>
<td>5.0 K (9 F)</td>
</tr>
</tbody>
</table>
### TABLE 2.2

**METHANOL-ETHANOL COLUMN SPECIFICATIONS**

**FOR THE STEADY STATE MODEL**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Stages</td>
<td>15</td>
</tr>
<tr>
<td>Feed Tray Location</td>
<td>9</td>
</tr>
<tr>
<td>Feed Rate</td>
<td>1000 g-moles/min.</td>
</tr>
<tr>
<td>Feed Rate Composition</td>
<td>50% Methanol, 50% Ethanol</td>
</tr>
<tr>
<td>Quality of Feed</td>
<td>Saturated liquid</td>
</tr>
<tr>
<td>Distillate Rate</td>
<td>500 g-moles/min.</td>
</tr>
<tr>
<td>Distillate Composition</td>
<td>94.7% Methanol, 5.3% Ethanol</td>
</tr>
<tr>
<td>Quality of Distillate</td>
<td>Saturated liquid</td>
</tr>
<tr>
<td>Bottoms Rate</td>
<td>500 g-moles/min.</td>
</tr>
<tr>
<td>Bottoms Composition</td>
<td>5.3% Methanol, 94.2% Ethanol</td>
</tr>
<tr>
<td>External Reflux Ratio</td>
<td>4.5</td>
</tr>
<tr>
<td>Top Pressure</td>
<td>101.3 KPA (1 atm)</td>
</tr>
<tr>
<td>Pressure Drop per Tray</td>
<td>0</td>
</tr>
<tr>
<td>Steam Pressure</td>
<td>689.5 KPA (100 psig)</td>
</tr>
<tr>
<td>Cooling Water Inlet</td>
<td>299.8 K (80 F)</td>
</tr>
<tr>
<td>Cooling Water Temperature Rise</td>
<td>22.2 K (40 F)</td>
</tr>
<tr>
<td>Polytropic Efficiency</td>
<td>75%</td>
</tr>
<tr>
<td>Approach Temperature on Reboiler/Condenser</td>
<td>5.0 K (9 F)</td>
</tr>
</tbody>
</table>
1980), it was found that this ratio varies from 3.92 to 5.34 for self generated electricity and from 5.86 to 10.42 for purchased electricity. Only self generated electricity was considered in this research. The same approach followed for the self generated electricity alternative can be used when the purchased electricity alternative is considered. Savings were estimated in the following fashion:

\[
\% \text{ Savings} = (1 - \frac{W}{Q}) \times (\text{Factor}) \times 100
\]

\[\text{c b}\]

where:

\[W = \text{compressor work}\]
\[Q = \text{Reboiler load}\]

\[\text{Factor} = \text{cost ratio of electricity to steam}\]

If this factor is greater than \(\frac{Q}{W}\), then the heat pump system is not economically feasible under the stated conditions. A cost factor greater than one means that the electrical energy costs more than steam energy. Therefore, reducing the amount of savings. The higher this factor is the more infeasible becomes the heat pump installation. This study did not consider any capital cost needed to implement the heat pump installation. The study considering capital cost associated with the implementation of the heat pump system is discussed in Chapter 3.
Column Pressure

The column pressure effect on the energy savings, column differential temperature between the top and the bottom of the column, reboiler load and the compressor work were studied for both mixtures. In order to keep product specifications the same as the base case, the reflux rate was adjusted as the column pressure was increased.

Figure 2.2 shows the effect in the energy savings when the column pressure was increased from 101.3 KPA (1 atm) to 506.5 KPA (5 atm) for the system Benzene-Toluene. Curve No. 1 represents the savings when a factor of 1 is used. Curve No. 2 represents the savings when the lower limit cost factor of 3.92 was applied. Curve No. 3 represents the savings when the upper limit cost factor of 5.34 was applied.

As noticed, savings of over 80% can be achieved by implementing a heat pump system. Once the cost factor is applied, the savings drop drastically but they are still in the feasible region. Cooling water savings were considered negligible compared to the savings in steam. In the case where a refrigerant is used as a cooling media, the savings in cooling can become significant.

The Benzene-Toluene system appears to favor a lower operating pressure as shown on Figure 2.2. On the other hand, Methanol-Ethanol system appears to favor a higher operating pressure as shown on Figure 2.3. This is caused by the effect of the pressure on the saturation temperature of
Figure 2.2 Column Pressure vs Energy Savings for Benzene-Toluene System
Figure 2.3 Column Pressure vs Energy Savings for Methanol-Ethanol System
the components involved. For the Benzene-Toluene system, the saturation temperature of Benzene and Toluene tends to get further apart as the pressure of the system is increased. On the other hand, for Methanol-Ethanol system, the saturation temperature of Methanol and Ethanol tends to get closer as the pressure of the system is increased. This effect can also be noticed on Figure 2.4 where the column differential temperature between the top and bottom of the column for the Benzene-Toluene system increases as the column pressure is increased. Figure 2.5 shows the opposite behavior for the Methanol-Ethanol system as the column pressure is increased. A theoretical explanation was derived to explain this behavior.

If the Antoine equation is re-arranged to solve for the saturation temperature, the following expression is obtained:

\[ T = \frac{B}{(A - \ln P) - C} \]  

(2.2)

where:

- \( A, B, C \) = Antoine Equation Constants
- \( P \) = Saturation Pressure (mm hg)
- \( T \) = Saturation Temperature (K)

Taking the difference between the saturation temperature of the two key components yields:
Figure 2.4 Column Pressure vs Column Delta T for Benzene-Toluene System
Figure 2.5 Column Pressure vs Column Delta T for Methanol–Ethanol System
\[ \Delta T = \frac{B}{(A - \ln P)} - \frac{B}{(A - \ln P)} - \Delta C \quad (2.3) \]

where:

\[ \Delta T = \text{Saturation temperature difference between} \]

the heavy component (2) and the light component (1) \( T_2 - T_1 \)

\[ \Delta C = \text{Difference between the } C \text{ constants} \ (C_2 - C_1) \]

Differentiate equation 2.3 with respect to pressure and rearrange,

\[ P \left( \frac{d \Delta T}{dP} \right) = \frac{B}{(A - \ln P)} - \frac{B}{(A - \ln P)} \quad (2.4) \]

Therefore, substituting the Antoine constants in equation 2.4 gives you the slope of the curve of saturation temperature difference vs pressure as a function of pressure. By using the above equations, it might be possible to predict beforehand the pressure effect on the heat pump feasibility for a particular binary system. This peculiarity was not mentioned before in the literature surveyed.

Figures 2.6 and 2.7 show that the reboiler load increases as the column pressure increases for both systems.
Figure 2.6 Column Pressure vs Reboiler Load for Benzene-Toluene System
Figure 2.7 Column Pressure vs Reboiler Load for
Methanol-Ethanol System
Figure 2.8 and 2.9 show that the compressor work also increases as the column pressure increases for both systems.

Tray pressure drop

The tray pressure drop effect on the energy savings were studied for both systems. Figure 2.10 shows the effect in the energy savings when the tray pressure drop is increased from 0 to 1.333 kPa (0.013 atm) for the Benzene-Toluene system. It shows that the energy savings decreases somewhat linearly when the tray pressure drop is increased. The same happens for the Methanol-Ethanol system as shown on Figure 2.11. This means that heat pump systems are favored by low pressure drop trays. The reboiler load and the compressor work behaved the same way as in the column pressure studies.

Approach Temperature in Reboiler/Condenser

Figure 2.12 and 2.13 show the effect of the reboiler/condenser approach temperature to the Benzene-Toluene system and for the Methanol-Ethanol system respectively. This variable appears to be the one that has the largest effect on the energy savings than the one previously studied. In this study, the approach temperature of the reboiler/condenser was increased from 5 K to 50 K. The figures show that the energy savings dropped drastically as the approach temperature is increased. This is a result of having to
Figure 2.8 Column Pressure vs Compressor Work for Benzene-Toluene System
Figure 2.9 Column Pressure vs Compressor Work for Methanol-Ethanol System
Figure 2.10  Tray Pressure Drop vs Energy Savings for Benzene-Toluene System
Figure 2.11 Tray Pressure Drop vs Energy Savings for Methanol-Ethanol System
Figure 2.12 Reboiler/Condenser Approach Temperature vs Energy Savings for Benzene-Toluene System
Figure 2.13 Reboiler/Condenser Approach Temperature vs Energy Savings for Methanol-Ethanol System
increase the work in the compressor for the same reboiler load. A large temperature approach will require a small heat transfer area, but a large compressor capacity. Since the approach temperature is the variable having the largest effect on the heat pump economics, a complete economic analysis including capital investment is performed in Chapter 3 to find out the return on capital investment.
CHAPTER 3

ECONOMIC EVALUATION OF A DISTILLATION COLUMN
WITH A HEAT PUMP INSTALLATION

No project is complete unless some kind of economic evaluation is made. It was found in the previous chapter that of the variables studied the one having the largest effect on the heat pump system being studied was the approach temperature of the reboiler/condenser. Therefore, the purpose in this chapter is to come up with a more detailed economic evaluation of the heat pump system when the approach temperature of the reboiler/condenser is increased.

To compare the cost of a column with a heat pump system against a conventional column, the amount of new capital needed to implement the heat pump system needs to be determined and compared against the savings in utility costs. The extra capital needed to implement the heat pump system is determined by the difference between the capital investment in a distillation column with heat pump and that in a conventional column. The net result is the capital needed to be invested in compression and heat transfer equipment for the heat pump installation. It was assumed that other design changes are negligible compared to the one previously mentioned.

A zero allocation credit in utilities capital was
considered. This means that although credit for utilities not used can be claimed, the fact is that the utilities capital has already been spent and the heat pump installation will not reduce it. However, if this release of capacity in steam and cooling water is needed elsewhere in the plant, its allocation should be properly credited to the heat pump system.

Energy tax credit was not considered in this research, because of the different variations in which this credit is applied. However, if a project is feasible without the tax credit being considered, then it may become more feasible once the tax credit is applied. On the other hand, if a project is not feasible considering a zero tax credit, it may become feasible once the tax credit is applied.

According to Pavone and Patrick (1981) in order to qualify for the energy tax credit, capital projects must meet the criteria written into the law. Eligible investments are limited to:

1. Alternative energy property, solar or wind energy
2. Specially defined energy property
3. Recycling equipment
4. Shale-oil producing equipment

The alternative energy property includes combustion equipment plus the auxiliary pollution control hardware necessary for firing fuels other than oil and gas or their derivatives. Facilities for producing geothermal energy, and certain hydroelectric generating equipment.
Specially defined energy property refers to equipment used for increasing the energy efficiency of an existing facility such as waste heat boiler, economizers as well as heat pump systems, etc.

Recycling equipment is limited to facilities for sorting, preparing and recycling solid waste for conversion into energy.

Shale-oil producing equipment is defined to include production and extraction equipment but exclude equipment for downstream processing such as refining.

Most chemical-process industries investments are entitled to a standard 10% tax credit. Facilities satifying the Energy Tax Act and Windfall Profit Tax Act definitions (except for public utilities facilities) are entitled to an additional 10% credit or a total of 20%.

The economic evaluation was performed by doing a rate of return analysis. Kuri's (1980) cost estimation and economic evaluation programs were used for this study. The compressor costs were obtained from Peters and Timmerhaus (1980). The feasibility was determined by the alternative having the largest rate of return. This analysis differs slightly from Null's (1976) analysis where the rate of return was already fixed and the availability of capital was determined based on that.

In this evaluation, the steam and cooling water savings were considered our main products, with the power spent in the compressor as fixed operating costs. The difference in
capital investment between the column with heat pump and the conventional column is the capital investment needed to implement the heat pump installation. Table 3.1 shows a summary of the economic factors assumed.

Table 3.2 shows a summary of the heat transfer and compression requirements for the conventional column system. The cost of the column itself is not included in the economic evaluation because it is assumed to be the same for both the conventional case and the heat pump case. The reboiler is assumed to be a partial thermosyphon reboiler using steam of 689.5 KPA (100 psig). The condenser is assumed to be a total condenser using cooling water at 299.8 K (80 F) with a temperature rise of 22.2 K (40 F).

Tables 3.3 and Table 3.4 show a summary of the compression and heat transfer requirements for the heat pump installation under study for both binary systems. The heat transfer requirements for the reboiler/condenser decreases while the heat transfer requirements for the trim cooler increases as the reboiler/condenser approach temperature is increased for the Benzene-Toluene mixture. For the Methanol-Ethanol mixture, the heat transfer requirements in the reboiler/condenser decreases, then after 15 K the reboiler/condenser heat transfer requirements is constant. On the other hand the compression requirements increases with the reboiler/condenser approach temperature for both mixture.

Table 3.5 and 3.6 show the savings and costs incurred by implementing the heat pump installation for both systems.
### TABLE 3.1

**ECONOMIC FACTORS ASSUMED**

<table>
<thead>
<tr>
<th>Factor</th>
<th>Assumed Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost Reference Date</td>
<td>January 1981</td>
</tr>
<tr>
<td>Cost of 689.5 KPA Steam</td>
<td>$0.007 / kw-hr</td>
</tr>
<tr>
<td>(100 psig steam)</td>
<td></td>
</tr>
<tr>
<td>Cost of Power</td>
<td>$0.034 / kw-hr</td>
</tr>
<tr>
<td>Cost of Cooling Water</td>
<td>$0.032 / metric ton</td>
</tr>
<tr>
<td>Running Hours per Year</td>
<td>8000</td>
</tr>
<tr>
<td>Depreciation Factor (Straight line)</td>
<td>10% of differential</td>
</tr>
<tr>
<td>Salvage Value</td>
<td>10% of differential</td>
</tr>
<tr>
<td>Income Tax Rate</td>
<td>50%</td>
</tr>
<tr>
<td>Inflation Rate</td>
<td>10%</td>
</tr>
</tbody>
</table>
**TABLE 3.2**

**CONVENTIONAL COLUMN HEAT TRANSFER REQUIREMENTS**

<table>
<thead>
<tr>
<th>System</th>
<th>Reboiler Area 2 M</th>
<th>Condenser Area 2 M</th>
<th>Water Required Kg/hr</th>
<th>Steam Required Kg/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>31.81</td>
<td>43.85</td>
<td>22570.</td>
<td>989.</td>
</tr>
<tr>
<td>Toluene</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>112.08</td>
<td>230.06</td>
<td>67670.</td>
<td>3057.</td>
</tr>
<tr>
<td>Ethanol</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reb./Cond. Appr. Temp. K</td>
<td>Reb./Cond. Area 2 M</td>
<td>Trim Cooler Area 2 M</td>
<td>Compressor Power KWatts</td>
<td>Cooling Water Kg/hr</td>
</tr>
<tr>
<td>-------------------------</td>
<td>---------------------</td>
<td>----------------------</td>
<td>-------------------------</td>
<td>--------------------</td>
</tr>
<tr>
<td>1</td>
<td>375.26</td>
<td>4.43</td>
<td>65.40</td>
<td>2179.</td>
</tr>
<tr>
<td>2</td>
<td>294.27</td>
<td>4.62</td>
<td>67.86</td>
<td>2272.</td>
</tr>
<tr>
<td>3</td>
<td>240.28</td>
<td>4.81</td>
<td>70.33</td>
<td>2365.</td>
</tr>
<tr>
<td>4</td>
<td>205.18</td>
<td>5.00</td>
<td>72.80</td>
<td>2459.</td>
</tr>
<tr>
<td>5</td>
<td>178.19</td>
<td>5.18</td>
<td>75.31</td>
<td>2554.</td>
</tr>
<tr>
<td>15</td>
<td>78.30</td>
<td>7.10</td>
<td>100.67</td>
<td>3493.</td>
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<tr>
<td>20</td>
<td>62.10</td>
<td>8.10</td>
<td>114.09</td>
<td>3987.</td>
</tr>
</tbody>
</table>
### TABLE 3.4

**HEAT PUMP SYSTEM HEAT TRANSFER AREA AND COMPRESSION REQUIREMENTS FOR METHANOL-ETHANOL SYSTEM**

<table>
<thead>
<tr>
<th>Reb./Cond. Appr. Temp. K</th>
<th>Reb/Cond. Area M</th>
<th>Trim Cooler Area M</th>
<th>Compressor Power Kwatts</th>
<th>Cooling Water Kg/hr</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>284.86</td>
<td>12.25</td>
<td>94.25</td>
<td>3603.</td>
</tr>
<tr>
<td>2</td>
<td>253.70</td>
<td>13.22</td>
<td>101.50</td>
<td>3889.</td>
</tr>
<tr>
<td>3</td>
<td>227.00</td>
<td>14.20</td>
<td>108.79</td>
<td>4177.</td>
</tr>
<tr>
<td>4</td>
<td>204.74</td>
<td>15.18</td>
<td>116.09</td>
<td>4465.</td>
</tr>
<tr>
<td>5</td>
<td>186.94</td>
<td>16.16</td>
<td>123.79</td>
<td>4754.</td>
</tr>
<tr>
<td>10</td>
<td>127.54</td>
<td>21.11</td>
<td>161.07</td>
<td>6210.</td>
</tr>
<tr>
<td>15</td>
<td>114.70</td>
<td>26.12</td>
<td>198.36</td>
<td>7683.</td>
</tr>
<tr>
<td>20</td>
<td>114.70</td>
<td>31.21</td>
<td>234.89</td>
<td>9181.</td>
</tr>
</tbody>
</table>
TABLE 3.5

HEAT PUMP SYSTEM SAVINGS AND COSTS
FOR BENZENE-TOLUENE SYSTEM

<table>
<thead>
<tr>
<th>R/C Appr. Temp K</th>
<th>Savings in CW Steam $/Yr</th>
<th>Electric Cost $/Yr</th>
<th>Compressor Costs $</th>
<th>Heat pump Exchangers Cost $</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$36,930</td>
<td>$17,890</td>
<td>$186,230</td>
<td>$81,030</td>
</tr>
<tr>
<td>2</td>
<td>$36,910</td>
<td>$18,560</td>
<td>$188,790</td>
<td>$66,220</td>
</tr>
<tr>
<td>3</td>
<td>$36,880</td>
<td>$19,230</td>
<td>$191,350</td>
<td>$56,560</td>
</tr>
<tr>
<td>4</td>
<td>$36,860</td>
<td>$19,910</td>
<td>$193,920</td>
<td>$50,360</td>
</tr>
<tr>
<td>5</td>
<td>$36,830</td>
<td>$20,590</td>
<td>$196,500</td>
<td>$45,630</td>
</tr>
<tr>
<td>10</td>
<td>$36,710</td>
<td>$24,050</td>
<td>$209,600</td>
<td>$33,420</td>
</tr>
<tr>
<td>15</td>
<td>$36,590</td>
<td>$27,520</td>
<td>$222,820</td>
<td>$28,230</td>
</tr>
<tr>
<td>20</td>
<td>$36,460</td>
<td>$31,190</td>
<td>$236,760</td>
<td>$25,370</td>
</tr>
</tbody>
</table>
Table 3.6

Heat pump system savings and costs for methanol-ethanol system

<table>
<thead>
<tr>
<th>R/C Appr. Temp K</th>
<th>Savings in CW Steam $/Yr</th>
<th>Electric Cost $/Yr</th>
<th>Compressor Costs $</th>
<th>Heat pump Exchangers Cost $</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$115,210</td>
<td>$25,870</td>
<td>$216,550</td>
<td>$64,530</td>
</tr>
<tr>
<td>2</td>
<td>$115,140</td>
<td>$27,850</td>
<td>$224,070</td>
<td>$58,950</td>
</tr>
<tr>
<td>3</td>
<td>$115,060</td>
<td>$29,850</td>
<td>$231,640</td>
<td>$54,280</td>
</tr>
<tr>
<td>4</td>
<td>$114,990</td>
<td>$31,840</td>
<td>$239,220</td>
<td>$50,700</td>
</tr>
<tr>
<td>5</td>
<td>$114,910</td>
<td>$33,840</td>
<td>$246,820</td>
<td>$47,930</td>
</tr>
<tr>
<td>10</td>
<td>$114,550</td>
<td>$44,030</td>
<td>$285,530</td>
<td>$39,240</td>
</tr>
<tr>
<td>15</td>
<td>$113,170</td>
<td>$54,220</td>
<td>$324,240</td>
<td>$38,610</td>
</tr>
<tr>
<td>20</td>
<td>$113,790</td>
<td>$64,410</td>
<td>$362,950</td>
<td>$40,160</td>
</tr>
</tbody>
</table>
The total exchanger cost decreases and compressor cost increases when the approach temperature is increased. The net savings in steam and cooling water decreases as approach temperature is increased. Electric cost increases with approach temperature.

Table 3.7 shows the heat pump economic evaluation summary for both binary systems. The internal rate of return is tabulated against the reboiler/condenser approach temperature. The optimum region was found to lie between 0 and 1 K for both mixtures. For the Methanol-Ethanol system a 13.9% rate of return is obtained for an approach temperature of 1 K. The rate of return decreases as the approach temperature is increased in both systems. This is because the increase in compressor costs are more significant than the decrease in heat transfer costs. Also the electric costs increases more than the savings in steam and cooling water.

In summary, the heat pump feasibility strongly depends on the thermodynamic availability of the mixture and on the relative cost between steam and electricity. The overall temperature driving force that the compressor has to overcome is a combination of the saturation temperature difference between the key components, the temperature difference cause by the pressure drop on the trays and the approach temperature on the reboiler/condenser. As expected, the heat pump installation favored the closed boiling mixture against the wide boiling mixture.
## TABLE 3.7

**HEAT PUMP ECONOMIC EVALUATION**

<table>
<thead>
<tr>
<th>Reb/Cond Approach Temp. \ K</th>
<th>Internal Rate of Return \ %</th>
<th>Reb/Cond Approach Temp. \ K</th>
<th>Internal Rate of Return \ %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-6.69</td>
<td>1</td>
<td>13.95</td>
</tr>
<tr>
<td>2</td>
<td>-6.69</td>
<td>2</td>
<td>13.31</td>
</tr>
<tr>
<td>3</td>
<td>-6.70</td>
<td>3</td>
<td>12.60</td>
</tr>
<tr>
<td>4</td>
<td>-6.91</td>
<td>4</td>
<td>11.82</td>
</tr>
<tr>
<td>5</td>
<td>-7.18</td>
<td>5</td>
<td>10.99</td>
</tr>
<tr>
<td>10</td>
<td>-9.00</td>
<td>10</td>
<td>6.70</td>
</tr>
<tr>
<td>15</td>
<td>&lt; -10</td>
<td>15</td>
<td>2.26</td>
</tr>
<tr>
<td>20</td>
<td>&lt; -10</td>
<td>20</td>
<td>-1.35</td>
</tr>
</tbody>
</table>
NUMERICAL INTEGRATION PROCEDURE

The fact that the simulation model was taking excessive computer time, the need for a search of a more efficient integration technique was greatly justified in this research. The main reason for the excessive computer is the presence of stiff differential equations in the heat pump model. Stiff differential equations are those equations that contain widely separated eigenvalues.

Stiff problems are relatively expensive to solve and the expense depends more strongly on the tolerance desired. The user's meaning of "accuracy" can affect the results considerably. A common one is to measure the relative error to the maximum (absolute) value of the solution component seen so far in the integration. Another one is a combination of absolute error and error relative to the solution magnitude. It is important to be able to specify error tolerances for each component of the solution because scaling components often differ radically for stiff systems. To be able to do this, one must use a suitable error control, so that during transient, accuracy dominates the choice of the step size rather than stability. As a result, the transient becomes a relatively expensive part of the integration for most codes.

One of the common problems with some of the codes is
that one can get reasonable looking results which are not close to the desired solution. This difficulty can arise in a number of ways. The most common one is the step control phase that can make the step so large that an active region of the solution is missed entirely, and a formula that is stable for unstable problems completely ignores an increasing component of the solution. Therefore a conservative tolerance is always required. If the interest is only in the equilibrium behavior and it is known that the errors will be damped, then computer time can be reduced by computing the transient crudely.

Among the integration methods tested were Runge-Kutta fourth order, LSODE (Hindmarsh, 1980) and EPISODE (Byrne, 1979), the last two being computer software packages based on Gear's method for solving a system of differential equations. LSODE is an acronym for Livermore Solver of Ordinary Differential Equations. EPISODE is an acronym for Effective Package for the Integration of Systems of Ordinary Differential Equations.

The plans are not to discuss all three methods in detail, but to show their effectiveness in our system and by working two example problems with different degrees of stiffness. LSODE and EPISODE are very complicated computer packages and they are not easy to follow, therefore discussion will be limited to the extent of the references encountered.

The Runge-Kutta method attempts to obtain greater
accuracy and at the same time avoid the need for higher derivatives. It has an advantage that it is self-starting (i.e., it requires only the value of function at a given point in time to find the value of the function and its derivative at the next point in time. This method is purely explicit and suitable for non-stiff differential equations. It needs a relatively small step size for stiff differential equations in order to get an accurate stable solution, therefore requiring a considerable amount of computer time.

LSODE and EPISODE are modified versions of the GEAR's package (Hindmarsh, 1979), which is based on the early work of C.W. Gear (1971). The GEAR'S package is a general purpose package, variable-step, variable-order, ODE solver, with eight different options, for solving both stiff and non-stiff type of problems.

A system of ordinary differential equations can be written as follows:

\[
\dot{y} = \frac{dy}{dt} = f(y, t) \tag{4.1}
\]

where:

\[
\begin{align*}
\dot{y} &= \text{vector of derivatives} \\
y &= \text{vector of state variables} \\
t &= \text{independent variable}
\end{align*}
\]

with initial conditions \( y(t_0) = y_0 \), where \( y_0, \dot{y}_0, \) and \( f_0 \) are vectors of length \( N \).
The basic method in the GEAR package are linear multistep methods. Multistep methods are iterative methods refering to predictor-corrector methods rather than methods such as Runge-Kutta which are pure explicit in nature. These methods use information about the solution at more than one point. This package uses two types of multistep methods. The first is based on the Adams formulas,

\[ y = y + h \sum_{i=0}^{q-1} B_i \cdot y_{n-i} \quad (1 < g < 12) \quad (4.2) \]

and the second is based on the Backward Differentiation Formulas (BDF's),

\[ y = \sum_{i=1}^{q} A_i \cdot y_{n-i} + h \cdot B \cdot y_0 \quad (1 < q < 5) \quad (4.3) \]

where:
- \( h \) = step size in \( t \)
- \( q \) = order of the method
- \( y \) = approximation for \( y(t) \)
- \( y_k \) = denotes \( f(y_k, t) \)
- \( A, B \) = parameters

For both methods, it is usually necessary to determine the Jacobian matrix, which is a \( N \times N \) matrix of partial derivatives of \( y \)

\[ J = \frac{\partial y^i}{\partial y^j} \quad i,j = 1, N \quad (4.4) \]
where:

\[ J = \text{Jacobian Matrix (Matrix of partial derivatives)} \]

According to Hindmarsh, the Adams methods are suitable for non-stiff problems, and the BDF methods are suitable for stiff problems. Both methods are implicit, therefore requiring the solution of a system of algebraic equations. Independently of the method used, there are four corrector iteration options for the solution of the algebraic system:

1. Functional (or fixed point) iteration, which uses no Jacobian information
2. Chord (or modified Newton) iteration with a user supplied Jacobian. The Jacobian matrix is factored into upper and lower triangular matrices.
3. Chord iteration with an internally generated approximation to the Jacobian. Same as 2, but with a finite difference approximation of the Jacobian.
4. Chord iteration with a diagonal approximation to the Jacobian (generated internally).

The second and third options involve the use of a \( N \times N \) Newton matrix \( P = I - h \cdot B \cdot J \), where \( I \) is the Identity matrix.

The package uses a so-called Nordsieck history array, of size \( N \times (q+1) \), containing \( y \) and the scaled approximations to its derivatives up to order \( q \). There is a control of the estimated local truncation error, which causes \( h \) and \( g \) to be varied dynamically throughout the
integration, in an attempt to complete the problem in the minimum number of step evaluations.

The efficiency of the GEAR'S package is enhanced by the way it updates the matrices involved. The matrices J and P are updated whenever the scalar $h * B$ has changed by $30\%$ or more since the last evaluation. This update process also occurs if there has been a failure to achieve corrector convergence, or if 20 steps have been taken without an update. A failure to converge usually is an indication that the Jacobian matrix is inaccurate for some reason. Typically, it takes about 5 to 10 steps between Jacobian evaluations. The Jacobian is only used for modified Newton iterations in solving the algebraic system. Therefore, inaccuracies in the Jacobian do not affect the accuracy of the computed solution. They only affect the rate of convergence for obtaining the solution.

The choice of the method depends on the problem and the stiffness involved. As mentioned before, there are eight different methods, four corrector iteration options for each basic method (Adams and BDF methods). A two digit flag (HF) is used to distinguish between the methods. The first digit in HF stands for the basic methods; 1 for Adams method (for non-stiff systems) and 2 for BDF method (for stiff systems). The second digit stands for the iteration method; 0 for functional iteration, 1 for chord iteration with user supplied Jacobian, 2 for chord iteration with an internally generated Jacobian, and 3 for chord iteration with a
diagonal approximation of the Jacobian. Therefore, $MF = 10$ means that Adams method with functional iteration is going to be used.

The prime consideration regarding the MF choice is stiffness. If the problem is not stiff and the Jacobian cannot be obtained easily the best choice is $MF = 10$. If the Jacobian can be easily obtained then choose $MF = 11$. If the problem is stiff and the user has no knowledge that it is stiff, then try $MF = 10$ and look at the behavior of the computed solution and the step sizes used. It is also possible to have a problem which is non-stiff initially and stiff later, in this case the solution procedure can begin with $MF = 10$ and then change to $MF = 20$ for example. There are other versions of GEAR that can handle special type of problems as for example problems with banded Jacobian matrix and problems with sparse Jacobian matrix.

LSODE is the newest version of GEAR. It has the same capabilities of GEAR and many others has been added as for example an internally computed initial step size.

EPISODE resembles GEAR, but it is based on totally variable-step formulas. These formulas can be written as follows:
\[ y = \sum_{i=0}^{n-1} A_i \cdot y_n - i + h \sum_{i=0}^{n-i} B_i \cdot y_n - i \] (4.5)

where the step size \( h = t_n - t_{n-1} \) is variable from step to step, as are the coefficients \( A \) and \( B \).

These formulas correspond to those used in GEAR, with the following definitions:

- \( K_1 = q, K_2 = 0 \) for BDF, order \( (1 < q < 5) \)
- \( K_1 = 1, K_2 = q-1 \) for Adams, order \( (1 < q < 12) \)

Two problems were tested in this research. The first one with a stiffness of 10 to 1 and the second with a stiffness of 1000 to 1.

1. \( (\frac{DY}{DT})^2 + 11 \frac{DY}{DT} + 10 Y = 0 \)

with initial conditions:

\( \frac{DY}{dT} = -1 \) and \( Y = 1 \)

The solution is:

\[ Y = A_0 \exp(-10T) + B \exp(-T) \quad A_0, B = 1 \]
2. \[(DY/DT)^2 + 1001 \frac{DY}{DT} + 1000 Y = 0\]

with initial conditions:

\[\frac{DY}{dT} = -1 \text{ and } Y = 1\]

The solution is:

\[Y = A \exp(-1000 T) + B \exp(-T) \quad A=0, B=1\]

Table 4.1 shows the results obtained for problem No. 1 using the different options available in LSODE package. It shows that for this particular problem the Adam's method was faster than the BDF method. Of the iteration methods used, the triangular matrix approximation of the Jacobian was the fastest of all. This is true because the triangular matrix approximation did fewer function evaluations for the same Jacobian evaluations compared to the iteration method with exact Jacobian. This may not be true for other types of problems. Normally, it is expected the option with exact Jacobian be the fastest of all for most problems, since errors are minimized when the exact Jacobian is known. The option with no Jacobian calculation was the slowest of all. The ratio of the cpu time between the slowest option and the fastest option is about twice. It means that the computer time can be improved significantly if the right method is chosen.
Table 4.2 shows the results obtained for problem No. 1 using the different options of EPISODE package. The fastest iteration method was again the triangular matrix approximation and the slowest iteration method was the option with the approximated Jacobian matrix.

Table 4.3 shows the results obtained using the Runge-Kutta fourth order method with variable step-size. As noticed, this method was the slowest of all and also the less accurate. The cpu time ratio varied from 200 to 1000 times higher than the one obtained with the previous methods. This ratio may change when the size of the system and the accuracy are increased.

The cpu time does not change significantly when the stiffness is changed from 10 to 1 to a stiffness of 1000 to 1 for both LSODE and EPISODE packages. The conclusions are basically the same as the one obtained previously. The results are shown in Tables 4.4 and 4.5.

The cpu time was about twice when the Runge-Kutta method is used in the stiff problem. The results are shown in Table 4.6.

Overall, LSODE happens to be the fastest and the most accurate integration package for this particular problem. The fact that it calculates the initial step size makes this package more versatile than EPISODE. EPISODE is very sensitive to the initial step size. For the heat pump system the computer time was improved by order of magnitude over that on the Runge-Kutta method and about twice as fast.
over EPISODE.

Hindmarsh (1979) concluded in his article that for fairly smooth solutions, LSODE is more efficient than EPISODE, but for problems requiring frequent drastic step size changes, EPISODE is likely to be more efficient. The reason for this has to do with the fact that changing \( h, A \) and \( B \) in every step can make the Newton iteration matrix less accurate, thus requiring more frequent updates than LSODE.

One must be careful when dealing with very large systems. Most of the time, it is difficult to obtain an exact Jacobian for the system of interest; therefore, there are two options left to be used, either let the program approximate the Jacobian or not use the Jacobian at all. It turns out that for some problems, the option with no Jacobian calculation is the best way to go, because of the time involved in calculating the approximated Jacobian. Also an inaccurate Jacobian leads to more iterations per step.

LSODE package is now available at the computer center of Louisiana State University for your use. It can be accessed under SYS2.FORTLIB library.
## Table 4.1

**Results of the Numerical Integration of**

\[(DY/DT)^2 + 11*DY/DT + 10*Y = 0\]

**Using LSODE Computer Package**

<table>
<thead>
<tr>
<th>Time</th>
<th>Error</th>
<th>MF = 10</th>
<th>CPU = 0.32 secs</th>
<th>Time</th>
<th>Error</th>
<th>MF = 11</th>
<th>CPU = 0.18 secs</th>
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</thead>
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<td></td>
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<td></td>
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<td>0.8479495E-6</td>
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</tr>
<tr>
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<td></td>
<td></td>
<td>100.00</td>
<td>0.2377205E-6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Number of Steps** = 158  
**Number of F evaluations** = 264  
**Number of J Evaluations** = 0

**Number of Steps** = 52  
**Number of F Evaluations** = 66  
**Number of J Evaluations** = 12
### TABLE 4.1 (Cont.)

<table>
<thead>
<tr>
<th>MF = 12</th>
<th>CPU = 0.18 secs</th>
<th>MF = 13</th>
<th>CPU = 0.14 secs</th>
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</thead>
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<td>Time</td>
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<td>Time</td>
<td>Error</td>
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Number of Steps = 52  
Number of F evaluations = 90  
Number of J Evaluations = 12

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</thead>
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<td>Time</td>
<td>Error</td>
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</table>

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Number of F evaluations = 289  
Number of J Evaluations = 0
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<th>Time</th>
<th>Error</th>
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<td>0.8657623E-9</td>
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</table>

Number of Steps = 70  
Number of F evaluations = 109  
Number of J Evaluations = 13
TABLE 4.2

RESULTS OF THE NUMERICAL INTEGRATION OF
(DY/DT)**2 + 11*DY/DT + 10*Y = 0
USING EPISODE COMPUTER PACKAGE

<table>
<thead>
<tr>
<th>Time</th>
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<td>100.00</td>
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</table>

Number of Steps = 163  Number of Steps = 92
Number of F evaluations = 276  Number of F Evaluations = 171
Number of J Evaluations = 0  Number of J Evaluations = 36
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<tr>
<th>MF = 12</th>
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</thead>
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<td>Time</td>
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<td>Time</td>
<td>Error</td>
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Number of F evaluations = 489
Number of J evaluations = 51

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</table>

Number of Steps = 159
Number of F evaluations = 255
Number of J evaluations = 0

Number of Steps = 44
Number of F evaluations = 86
Number of J evaluations = 23
## TABLE 4.2 (cont.)

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</table>

Number of Steps = 48  Number of Steps = 50
Number of F evaluations = 110  Number of F Evaluations = 89
Number of J Evaluations = 20  Number of J Evaluations = 19

MF = 22  CPU = 0.16 secs  MF = 23  CPU = 0.14 secs
### TABLE 4.3

RESULTS OF THE NUMERICAL INTEGRATION OF

\[(\frac{dy}{dt})^2 + 11\cdot\frac{dy}{dt} + 10\cdot y = 0\]

USING RUNGE-KUTTA FOURTH ORDER

<table>
<thead>
<tr>
<th>Time</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>-0.19800799D-04</td>
</tr>
<tr>
<td>0.10</td>
<td>0.96376006D-02</td>
</tr>
<tr>
<td>1.00</td>
<td>0.42727396D-01</td>
</tr>
<tr>
<td>10.00</td>
<td>0.67063253D-04</td>
</tr>
<tr>
<td>100.00</td>
<td>0.61044736D-04</td>
</tr>
</tbody>
</table>

Number of steps = 715993

Number of F Evaluations = 2863972

number of J Evaluations = 0

CPU Time (secs) = 82.36
TABLE 4.4

RESULTS OF THE NUMERICAL INTEGRATION OF

\[(dy/dt)^2 + 1001*dy/dt + 1000*y = 0\]

USING LSODE COMPUTER PACKAGE

<table>
<thead>
<tr>
<th>MF = 10</th>
<th>CPU = 0.34 secs</th>
<th>MF = 11</th>
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</tr>
</thead>
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<td>Time</td>
<td>Error</td>
</tr>
<tr>
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<td>-0.6891866E-6</td>
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<tr>
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<td>-0.4311054E-5</td>
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<td>-0.9594766E-5</td>
</tr>
<tr>
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<td>0.4777035E-4</td>
<td>1.00</td>
<td>-0.2500855E-5</td>
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<tr>
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</table>

Number of Steps = 158  Number of Steps = 70
Number of F evaluations = 264  Number of F Evaluations = 99
Number of J Evaluations = 0  Number of J Evaluations = 18
TABLE 4.4 (cont.)

<table>
<thead>
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<th>Time</th>
<th>Error</th>
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Number of Steps = 59  Number of Steps = 52
Number of F evaluations = 121  Number of F Evaluations = 78
Number of J Evaluations = 18  Number of J Evaluations = 12

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<th>Error</th>
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Number of Steps = 181  Number of Steps = 70
Number of F evaluations = 289  Number of F Evaluations = 83
Number of J Evaluations = 0  Number of J Evaluations = 13
TABLE 4.4 (cont.)

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<th>Time</th>
<th>Error</th>
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<td>0.8658087E-9</td>
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Number of Steps       =    70  Number of Steps       =    74
Number of F evaluations = 109  Number of F Evaluations = 103
Number of J Evaluations = 13   Number of J Evaluations = 13
TABLE 4.5

RESULTS OF THE NUMERICAL INTEGRATION OF
\[(\frac{dy}{dt})^2 + 1001 \cdot \frac{dy}{dt} + 1000 \cdot y = 0\]
USING EPISODE COMPUTER PACKAGE

<table>
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<th>Time</th>
<th>Error</th>
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<tbody>
<tr>
<td>0.01</td>
<td>0.1963540E-4</td>
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<td>0.1963858E-4</td>
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<tr>
<td>0.10</td>
<td>-0.1041523E-5</td>
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<tr>
<td>1.00</td>
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<td>1.00</td>
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</tr>
<tr>
<td>10.00</td>
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<td>100.00</td>
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</table>

MF = 10           CPU = 0.34 secs           MF = 11           CPU = 1.32 sec

Number of Steps = 163  Number of Steps = 424
Number of F evaluations = 276  Number of F Evaluations = 568
Number of J Evaluations = 0  Number of J Evaluations = 65
<table>
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<tr>
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<tr>
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</table>

Number of Steps = 269  
Number of F evaluations = 464  
Number of J Evaluations = 51

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<th>Time</th>
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<tr>
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Number of Steps = 159  
Number of F evaluations = 255  
Number of J Evaluations = 0

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<td>Error</td>
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<td>0.2508143E-5</td>
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<tr>
<td>100.00</td>
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<td>100.00</td>
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Number of Steps = 44  
Number of F Evaluations = 86  
Number of J Evaluations = 23

<table>
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<tr>
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<th>MF = 21</th>
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<td>Time</td>
<td>Error</td>
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<tr>
<td>0.01</td>
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<tr>
<td>1.00</td>
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<td>1.00</td>
<td>-0.2521410E-3</td>
</tr>
<tr>
<td>10.00</td>
<td>0.1245148E-3</td>
<td>10.00</td>
<td>0.1593867E-4</td>
</tr>
<tr>
<td>100.00</td>
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<td>100.00</td>
<td>-0.6308208E-7</td>
</tr>
</tbody>
</table>

Number of Steps = 48  
Number of F Evaluations = 70  
Number of J Evaluations = 20
<table>
<thead>
<tr>
<th>Time</th>
<th>Error</th>
<th>Time</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
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<td>0.01</td>
<td>0.2969306E-4</td>
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<tr>
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<td>100.00</td>
<td>0.5263628E-6</td>
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</table>

Number of Steps = 48  Number of Steps = 50
Number of F evaluations = 110  Number of F Evaluations = 89
Number of J Evaluations = 20  Number of J Evaluations = 19
### Table 4.6

**Results of the Numerical Integration of**

\[(\frac{dy}{dt})^2 + 1001 \cdot \frac{dy}{dt} + 1000 \cdot y = 0\]

**Using Runge-Kutta Fourth Order**

<table>
<thead>
<tr>
<th>Time</th>
<th>Error</th>
</tr>
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<tr>
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<tr>
<td>100.00</td>
<td>0.61044502D-04</td>
</tr>
</tbody>
</table>

- **Number of Steps** = 1742664
- **Number of F Evaluations** = 6970656
- **Number of J Evaluations** = 0
- **CPU time (secs)** = 199.15
CHAPTER 5

DYNAMICS AND CONTROL OF A DISTILLATION COLUMN WITH A HEAT PUMP INSTALLATION

In this chapter, the dynamic behavior of a distillation column with a heat pump installation was studied. Dynamic studies are always important in order to understand the process as it varies with time and also to see how the system behaves when disturbances are present. As mentioned before, none of the literature reviewed examined the dynamic behavior of distillation columns with heat pump systems by a simulation effort. Therefore, these studies constitutes the major contribution of this research.

A dynamic model of a distillation column with a heat pump system needs to be developed and implemented. The distillation model was based on a similar model presented in Luyben (1975). A very good agreement was obtained between his results and the results obtained in this research. This model will be used to make open loop studies and control studies on the system. In developing a model for control studies, the goal is to include enough details to realistically model the area of interest but exclude minor or peripheral effects that would have little or no effect in the final conclusions. A compromise is always made between the accuracy and optimum use of computer time.
Dynamic Model Simplifying Assumptions

A. Assumptions in the Column:

1. There is one feed and two products (distillate and bottom)
2. No pressure drop across the column, but it varies with time according to the pressure dynamics of the compressor suction.
3. The liquid in each tray is perfectly mixed and incompressible.
4. The vapor and liquid are in thermal and phase equilibrium.
5. Vapor-liquid equilibrium relationship is assumed to obey Raoult's law.
6. Adiabatic column operation (no heat lost or gained through the column wall)
7. Tray hydraulics are assumed to follow Francis weir relationship.
8. Enthalpy dynamics are negligible compared to the material balance dynamics. Therefore, they become algebraic equations.
9. Vapor holdup is included as part of the compressor suction holdup.
B. **Assumptions in the Compressor**

1. Adiabatic compression
2. One stage centrifugal compressor
3. Constant compressor speed
4. Compressor dynamics are negligible (i.e., the compressor dynamics are so fast that can be considered to be at steady state at each point in time)
5. Compressor fluid properties are calculated at inlet conditions.

C. **Assumptions in the Reboiler/Condenser**

1. The reboiler side of the reboiler/condenser is a partial reboiler, the condenser side of the reboiler/condenser is a total condenser.
2. Dead time in the liquid line from the bottom of the column to the reboiler and back to the column is negligible.
3. Perfect mixing is assumed in the reboiler
4. Dynamic lag in heat transfer from the condenser side of the reboiler/condenser to the reboiler side of the reboiler/condenser is negligible.
5. There is no "swell" behavior in the reboiler liquid due to increased vaporization rates.
6. No pressure drop is assumed. The pressure is equal to the compressor discharge pressure.
7. Vapor holdup is included as part of the
compressor discharge volume.

8. Liquid holdup is negligible.

D. **Assumptions in the Trim Condenser**

1. A flooded condenser is assumed at constant coolant rate and constant coolant inlet temperature. Only liquid is removed from it.
2. Vapor holdup of the condenser is included as part of the compressor suction vapor holdup.
3. No pressure drop across the condenser, the pressure is equal to the suction pressure of the compressor.
4. The dynamic lag in heat transfer from the condenser vapor to the coolant is negligible.
5. The condensate will be mixed with the flashed liquid in the accumulator.

E. **Assumptions in the reflux accumulator**

1. Vapor holdup of the accumulator is included as part of the compressor suction vapor holdup.
2. The pressure in the accumulator is equal to the suction pressure of the compressor.
3. Perfect mixing is assumed.
4. A steady state flash is assumed.
5. The expansion valve dynamics are considered negligible.
Dynamic Model Development

A. Reboiler Material Balance

Overall Material Balance:

\[ \frac{dM}{dt} = L - V - B \]

Component Material Balance:

\[ \frac{dM_x}{dt} = L_x - V y - B x \]

B. Overall Material Balance on Each Tray

First Tray:

\[ \frac{dM}{dt} = L + V - V - L \]

Second Tray to Tray N-1:

\[ \frac{dM}{dt} = L + V - L - V \]

where: \( q \) is defined as the fraction of feed which is liquid. It has the following numerical limits:
\[ q = 1 \text{ saturated liquid feed} \]
\[ 0 < q < 1 \text{ liquid and vapor feed} \]
\[ q = 0 \text{ saturated vapor feed} \]

and \( U \) and \( V \) are parameters to identify different sections of the column. They are as follows:

\[ U = 1 \text{ for the feed tray} \]
\[ U = 0 \text{ for all other trays} \]
\[ U = 1 \text{ for the feed tray plus 1} \]
\[ U = 0 \text{ for all other trays} \]

C. Component Material Balance on Each Tray

First Tray:

\[ \frac{dH_x}{dt} = L_x + V y - L_x - V y \]
\[ 1 \quad 1, j \quad 2 \quad 2, j \quad b \quad b, j \quad 1 \quad 1, j \quad 1 \quad 1, j \]

Second Tray to Tray \( N-1 \)

\[ \frac{dH_x}{dt} = L_x + V y - L_x \]
\[ n \quad n, j \quad n+1 \quad n+1 \quad n-1 \quad n-1, j \quad n \quad n, j \]

\[ - V y + U q F x + U (1-q) F y \]
\[ n \quad n, j \quad 1 \quad f, j \quad 2 \quad f, j \]
D. Material Balance in Compressor Suction

Overall Material Balance:

\[
\frac{dM}{dt} = V_s + V_n - V_{fl} - V_{tc} - V_c
\]  \hspace{1cm} (5.7)

\[
M = \frac{P \bar{V}}{R'T}
\]  \hspace{1cm} (5.8)

Component Material Balance:

\[
\frac{dM_y}{dt} = V_y s + V_y n - V_y fl - V_y tc - V_y c
\]  \hspace{1cm} (5.9)

E. Material Balance in Compressor Discharge

Including the Reboiler/Condenser

Overall Material Balance:

\[
\frac{dM}{dt} = V_c - L_{r,c}
\]  \hspace{1cm} (5.10)

\[
M = \frac{P \bar{V}}{R'T}
\]  \hspace{1cm} (5.11)

Component Material Balance:

\[
\frac{dM_y}{dt} = V_{y,c} - L_{r,c}
\]  \hspace{1cm} (5.12)
F. **Material Balance in Trim Condenser**

Overall Material Balance:

\[
\frac{dM}{dt} = V - L
\]

\[\text{tc} \quad \text{tc} \quad \text{tc}\]  \hspace{1cm} (5.13)

Component Material Balance:

\[
\frac{dM_{x}}{dt} = V_{y} - L_{x}
\]

\[\text{tc} \quad \text{tc,} \quad j \quad \text{tc} \quad \text{n,} \quad j \quad \text{tc} \quad \text{tc,} \quad j\]  \hspace{1cm} (5.14)

G. **Material Balance in Reflux Accumulator**

Overall Material Balance:

\[
\frac{dM}{dt} = L + L - R - D
\]

\[d \quad \text{fl} \quad \text{tc} \]  \hspace{1cm} (5.15)

Component Material Balance:

\[
\frac{dM_{x}}{dt} = L_{x} + L_{x} - (R - D)_{x}
\]

\[d \quad d, \quad j \quad \text{fl} \quad \text{fl,} \quad j \quad \text{tc} \quad \text{tc,} \quad j \quad d, \quad j\]  \hspace{1cm} (5.16)

H. **Reboiler/Condenser Energy Balance**

Reboiler Side:

\[
V = \frac{(Q - L)_{b} (h - h_{b})}{(H - h_{b})}
\]

\[b \quad b \quad 1 \quad b \quad 1 \quad b \quad b\]  \hspace{1cm} (5.17)
I. **Energy Balance on Each Tray**

First Tray:

\[ V = \frac{(L \ (h - h) + V \ (H - h))}{(H - h)} \]  
\[ \text{First Tray:} \]

Second Tray to Tray N-1:

\[ V = \frac{(L \ (h - h) + V \ (H - h))}{(H - h)} \]  
\[ + U \ q \ F(h - h) + U \ (1-q) \ F(H - h)) / (H - h) \]

where:

q and U are defined as before.

J. **Energy Balance in Compressor Suction**

\[ H = \frac{(V \ H + V \ H - V \ H)}{(V + V - V)} \]  
\[ \text{J. Energy Balance in Compressor Suction} \]

K. **Energy Balance in Compressor**

\[ W = V \ (H - H) \]  
\[ \text{K. Energy Balance in Compressor} \]
1. Energy Balance in Compressor Discharge

Including the Reboiler/Condenser

Condenser Side:

\[ L = \frac{Q}{(H - h)} \quad (5.22) \]

\[ \text{Condenser Side:} \]

H. Energy Balance in Trim Condenser

\[ V = \frac{Q}{(H - h)} \quad (5.23) \]

\[ \text{Trim Condenser:} \]

N. Energy Balance in Accumulator

\[ h = \frac{(L h + L h)}{(H - D)} \quad (5.24) \]

\[ \text{Accumulator:} \]

O. Reboiler/Condenser Heat Load

\[ Q = U A \frac{LMTD}{(T + T)} \quad (5.25) \]

\[ \text{Reboiler/Condenser Heat Load:} \]

where:

\[ \text{LMTD} = \frac{(T + T)}{2 - T} \quad (5.26) \]

\[ \text{LMTD:} \]

P. Trim Condenser Heat Load

\[ Q = U A \frac{LMTD}{(T + T)} = \frac{mc}{(T - T)} \quad (5.27) \]

\[ \text{Trim Condenser Heat Load:} \]
This equation is solved for the coolant outlet temperature. Coolant rate is kept constant.

where:

\[ \text{LMTD} = \frac{T - \bar{T}}{t_c} \quad \text{(5.28)} \]

- \( C \) = Coolant heat capacity
- \( m \) = Coolant mass flow rate
- \( \bar{T} \) = Average process temperature
- \( \bar{T} \) = Average coolant temperature
- \( T \) = Inlet coolant temperature
- \( T \) = Outlet coolant temperature

Q. Steady State Flash Calculations

A steady state flash is assumed at each point in time. The expansion valve dynamics are assumed negligible.

Overall Material Balance:

\[ L = V + L \quad \text{(5.29)} \]
Component Material Balance:

\[ \sum_{rc} \sum_{j} L_x^{rc,j} = V_y^{fl,fl,j} + \sum_{fl} L_x^{fl,fl,j} \]  
(5.30)

Energy Balance:

\[ \sum_{rc} \sum_{fl} L_h^{rc,fl} = V_H^{fl,fl} + \sum_{fl} L_h^{fl,fl} \]  
(5.31)

R. Vapor-Liquid Equilibrium Relationship

Raoult's law was used to describe the vapor-liquid equilibrium relationship.

\[ \phi_y^j P^o_j = \gamma^x_j P^o_j \]  
where: \( \phi = 1 \)  
(5.32)

\[ \gamma_j^x = 1 \]  
(5.33)

The vapor pressure of the pure components are calculated as a function of temperature using Antoine equation,

\[ P^o_j = \exp( A_j - B_j / (T_j + C_j) ) \]  
(5.33)

where:

\( A, B, C \) are the Antoine constant obtained from Reid (Reid, Prausnitz, and Sherwood, 1977)
\[ \frac{\Delta H}{\Delta H} = A' + B'(Q/Q_c) + C'(Q/Q_d)^2 \] (5.34)

where:

- \( A', B', C' \) = Performance curves constants
- \( \Delta H_c \) = Compressor head \((H - H_d)\)
- \( \Delta H_d \) = Compressor head at design conditions
- \( Q_c \) = Compressor volumetric flow at inlet conditions
- \( Q_d \) = Compressor volumetric flow at design inlet conditions

**T. Compressor Volumetric Flow**

\[ Q = \frac{V R^c T}{P_c c s s} \] (5.35)

**U. Compressor Discharge Temperature**

\[ T = T_d (P_d / P)^{k-1/k_n} \] (5.36)

where:

- \( P \) is in MM Hg
- \( T \) is in K
\[ k = \frac{C}{(C - R')} \]  \hspace{1cm} (5.37)

\[ n = \text{polytropic efficiency} \]

\[ R' = \text{gas law constant (1.987 cal/g-mole K)} \]

\textbf{W. Enthalpy Equations}

The enthalpy of a mixture is a function of temperature, pressure and composition of a mixture. However, enthalpy is not a strong function of pressure, therefore it is assumed to be a function of temperature and composition only.

For a pure vapor, the molar enthalpy is given by:

\[ \bar{H} = \int_{T_p}^{T} C \frac{v}{T \cdot p} \, dT + \Delta \bar{H}_{\text{vap}} \]  \hspace{1cm} (5.38)

\[ \Delta \bar{H}_{\text{vap}} / R'T = 7.08 (1 - T) \]

\[ + 10.95 \omega (1 - T) \]  \hspace{1cm} (5.39)

where:

\[ T_c = \text{pure component critical temperature (K)} \]

\[ T_r = \text{reduced reference temperature } \left( \frac{T}{T_{\text{ref}}} \right) \]

\[ \omega = \text{composition} \]
\[ T = \text{reference temperature} \ (298. \ K) \]
\[ \omega = \text{component acentric factor} \]

Likewise, for a pure liquid, the molar enthalpy is given by:

\[
\overline{\Delta h} = \int_{T_{\text{ref}}}^{T} C_1^P \, dT
\]

(5.40)

\[ C_v^V \text{ and } C_v^L \text{ are polynomial functions of temperature for both vapor and liquid respectively.} \]

\[
C_v^V = A_v^V + B_v^V T + C_v^V T^2 + D_v^V T^3
\]

(5.41)

\[
C_v^L = A_l^V + B_l^V T + C_l^V T^2 + D_l^V T^3
\]

(5.42)

where:

\[ A_v^V, B_v^V, C_v^V \text{ and } A_l^V, B_l^V, C_l^V \text{ are constants for the heat capacity equations of both vapor and liquid respectively.} \]

They can be obtained from Reid, Prausnitz, and Sherwood (1977), and Yaws (1977) respectively. Equation 5.39 was also obtained from Reid, Prausnitz, and Sherwood.
If ideal solutions are assumed, then the molar enthalpies of the liquid and vapor mixtures on tray \( n \) can be calculated by:

\[
\begin{align*}
\bar{h}_n &= \sum_{j=1}^{J} x_{n,j} \bar{h}_{n,j} \quad (5.43) \\
\bar{H}_n &= \sum_{j=1}^{J} y_{n,j} \bar{H}_{n,j} \quad (5.44)
\end{align*}
\]

where:

\( \Delta \bar{H} \) is the heat of vaporization of the \( \text{vap} \) pure component at the reference temperature.

I. Liquid Flow rates Over the Weir

The flow rate over the weir can be calculated using the well known Francis formula.

\[
L = \frac{3}{2} K \frac{1}{1 \text{ \text{cm}}} (h_{\text{ow}}) \quad (5.45)
\]

where:

\( h_{\text{ow}} \) = height of liquid over weir (cm)

\( K = 1102.25 \), the units are consistent with the units listed here.
\[ L = \text{liquid flow rate (g-moles/min.)} \]
\[ W = \text{weir length (cm)} \]
\[ \rho_{l} = \text{average molar density (g-moles/cm)} \]

\section*{Y. Molecular Weight and Density of Mixtures}

The molecular weight of each stream is simply a weighted average of the pure components molecular weights.

\[ MW = \sum_{j=1}^{J} x_{j} MW_{j} \quad (5.46) \]

where:

\[ MW_{j} = \text{the pure component molecular weight.} \]

The mixing rule used to calculate the molar density of the liquid mixture was a weighted average of the pure component molar densities.

\[ \rho_{l} = \sum_{j=1}^{J} x_{j} \rho_{l,j} \quad (5.47) \]
\[ \rho = \frac{1}{\rho_l} \] (5.48)

where:

\[ \rho_l = \text{the pure component liquid molar density}. \]

The vapor density of the mixture is estimated using the ideal vapor relationship.

\[ \rho = \frac{P \text{MW}}{R T} \] (5.49)

where:

\[ \text{MW} = \text{average molecular weight of the vapor mixture} \]

2. **Bubble Point Temperature Calculation**

The bubble point temperature of the liquid on tray \( n \) is determined by:

\[ \sum_{j=1}^{J} y_{n,j} = 1 \] (5.50)

\[ y_{n,j} = \frac{P^{o} x_{n,j}}{P} \] (5.51)

Since the above equations are implicit in \( T \), an iterative technique was used to determine the bubble point temperature on tray \( n \). The procedure
begins by choosing an initial guess \( T^i \), which
is 0.1 K greater than the temperature from the
previous time step \( T^{i-1} \). The next best value
was then calculated by:

\[
T^n = T^n - \frac{\ln(f(T)^i)}{SLOPE^n} \quad (5.52)
\]

where:

\[
SLOPE = \frac{\ln(f(T)^{i-1})}{(T^n - T^n)} \quad (5.53)
\]

\( f(T) \) is defined as the summation of the \( y_{n,j} \) at
\( n \) temperature \( T \). The next calculation was based on
\( T^i \) and \( T^{i+1} \). These calculations will continue
until the desired tolerance is met.
**Dynamic Studies**

The control system modeled in this research is based on a proven similar control system proposed by Quadri (1981). Figure 5.1 shows a simplified scheme of the instrument control system for a distillation column with a heat pump system used in this research. As noticed, the control scheme is very similar to the control scheme for a conventional distillation column. The level controller in the accumulator regulates the distillate flowrate while the reflux rate is on flow control. The reboiler/condenser heat transfer rate is controlled at a constant value. The energy balance is closed by the column top pressure controller, regulating the trim cooler heat transfer rate. The material balance is closed by the column bottom level controller regulating the bottom product flowrate. The coolant flowrate and temperature are kept constant. The feed temperature is also kept constant.

Figure 5.2 shows the same control arrangement as in Figure 5.1 except that the distillate composition is controlled by the reflux rate. The rest of the control scheme remains the same.

The control arrangement used in Figure 5.3 is basically the same as the control scheme shown on Figure 5.2, except that instead of controlling the composition, the top tray temperature is used as the controlled variable.

In practice, the severe interactions between the two product purity control loops prevent the use of two tightly
Figure 5.1 Control Scheme No. 1
Figure 5.2 Control Scheme No. 2
Figure 5.3 Control Scheme No. 3
tuned control loops on each product. Therefore, only one product quality can be controlled, while the other must be left essentially uncontrolled.

**Open Loop Case Studies**

One of the most important phases of process control is the study of the open loop behavior of the process under consideration. The open loop response curves are commonly referred to as process reaction curves. They are necessary in order to have an idea of how the process reacts to different disturbances. They are used to determine the parameters that characterize the process (i.e., process gain, process time constants and process dead time). These parameters can be used to determine the controller settings.

Table 5.1 shows the column physical data used for the dynamic and control studies in this research. A Benzene-Toluene mixture is the system used for these studies. The reason for the choice of this particular system is because it behaves fairly ideal and because of relatively easy separation.

The response to a step change in the feed composition, feed rate, reflux rate, and trim cooler outflow on different column variables were examined. For all cases, the step change is made after 10 minutes of simulation to assure that the system is at steady state when the change is made.
Table 5.1

**PHYSICAL DATA USED IN DYNAMIC STUDIES**

**Column Design Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Ideal Stages</td>
<td>-- 15</td>
</tr>
<tr>
<td>Feed Tray Location</td>
<td>-- 9</td>
</tr>
<tr>
<td>Column I.D.</td>
<td>-- 0.7620 m</td>
</tr>
<tr>
<td>Tray Spacing</td>
<td>-- 0.6096 m</td>
</tr>
<tr>
<td>Weir Length</td>
<td>-- 0.6096 m</td>
</tr>
<tr>
<td>Weir Height</td>
<td>-- 0.0508 m</td>
</tr>
<tr>
<td>Effective Height for Heat Transfer on Trim Cooler</td>
<td>-- 0.5199 m</td>
</tr>
<tr>
<td>Number of Tubes in Trim Cooler</td>
<td>-- 137</td>
</tr>
<tr>
<td>Trim Cooler Tubes O.D.</td>
<td>-- 0.01905 m</td>
</tr>
<tr>
<td>Trim Cooler Shell I.D.</td>
<td>-- 0.38735 m</td>
</tr>
<tr>
<td>Overall Condensing Heat Transfer Coefficient</td>
<td>-- 1135.6 J / m * sec * K</td>
</tr>
<tr>
<td>Effective Height for Heat Transfer on Reboiler/Condenser</td>
<td>-- 1.4427 m</td>
</tr>
<tr>
<td>Number of Tubes in Reboiler/Condenser</td>
<td>-- 1049</td>
</tr>
<tr>
<td>Reboiler/Condenser Tubes O.D.</td>
<td>-- 0.01905 m</td>
</tr>
<tr>
<td>Reboiler/Condenser Shell I.D.</td>
<td>-- 0.99060 m</td>
</tr>
<tr>
<td>Overall Reboiler Heat Transfer Coefficient</td>
<td>-- 1419.5 J / m * sec * K</td>
</tr>
<tr>
<td>Polytropic Efficiency</td>
<td>-- 0.75</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>-- 2.4</td>
</tr>
</tbody>
</table>
**TABLE 5.1 (cont.)**

**Steady State Flow and Component Data**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed Rate</td>
<td>1000.0 g-moles/min</td>
</tr>
<tr>
<td>Feed Composition</td>
<td>50 mole % Benzene 50 mole % Toluene</td>
</tr>
<tr>
<td>Feed Temperature</td>
<td>365.26 K (bubble point)</td>
</tr>
<tr>
<td>Distillate Rate</td>
<td>507.0 g-moles/min</td>
</tr>
<tr>
<td>Distillate Composition</td>
<td>92.77% Benzene 7.23 mole % Toluene</td>
</tr>
<tr>
<td>Bottoms Rate</td>
<td>493.0 g-moles/min</td>
</tr>
<tr>
<td>Bottoms Composition</td>
<td>5.89 mole % Benzene 94.11 mole % Toluene</td>
</tr>
<tr>
<td>Reflux Rate</td>
<td>600.0 g-moles/min</td>
</tr>
<tr>
<td>Column Pressure</td>
<td>101.858 kpa</td>
</tr>
<tr>
<td>Cooling Water Inlet Temperature</td>
<td>299.82 K</td>
</tr>
<tr>
<td>Accumulator Holdup</td>
<td>1390.0 m</td>
</tr>
<tr>
<td>Column Bottom Holdup</td>
<td>1390.0 m</td>
</tr>
<tr>
<td>Compressor suction Vapor Holdup</td>
<td>47750.0 m</td>
</tr>
<tr>
<td>Compressor Discharge Vapor Holdup</td>
<td>10000.0 m</td>
</tr>
<tr>
<td>Trim Cooler Holdup</td>
<td>480.0 m</td>
</tr>
</tbody>
</table>
Open Loop Response to Feed Composition

The open loop response to a step change of 10% in the Benzene feed composition was examined. The feed composition was changed from 50 mole% Benzene, 50 mole% Toluene to 55 mole% Benzene and 45 mole% Toluene. The feed temperature was kept constant. Both the distillate rate and the bottoms rate were in tight level control while the reflux rate was in tight flow control. The pressure controller used to manipulate the trim cooler outflow was held in manual keeping the trim cooler outflow at a constant rate.

Figure 5.4 shows the effect on the column variables to the change in Benzene feed composition. As you can see, some interesting results were obtained in this study. As expected, an increase in the the light component composition (in this case Benzene) in the feed stream increases the light component composition everywhere in the column. Therefore, it is expected a monotonic increase of the Benzene in both the distillate and the bottoms streams as shown on Figure 5.4a and 5.4b. Since the feed temperature is kept constant, the feed stream gets partially vaporized when the change in composition occurs; therefore, increasing the vapor rate in the rectifying section; hence, the pressure of the column as shown on Figure 5.4d. Since the effect of composition is not felt by the bottoms in about 1.5 minutes after the change was made the bottoms temperature increases because of the increase in pressure.
Figure 5.4a Open Loop Response to a Change in Feed Composition
Figure 5.4b Open Loop Response to a Change in Feed Composition
Figure 5.4c  Open Loop Response to a Change in Feed Composition
Figure 5.4d Open Loop Response to a Change in Feed Composition
Figure 5.4e  Open Loop Response to a Change in Feed Composition
Figure 5.4f  Open Loop Response to a Change in Feed Composition
right after the change was made as shown on Figure 5.4c. After that period, the composition effect is felt by the bottoms which brings down its temperature. Since the pressure continues to increase, both the bottoms and top tray temperatures will eventually increase to a new steady state value.

The increase in pressure effect on the bottoms temperature combined with the composition effect caused what some people have called double inverse response which is observed in the bottoms temperature. This double inverse action was observed by Stewart (1981) and mentioned by others (Rademaker, Rijnsdorp, and Maarleveld, 1975). They indicated that this behavior may be expected for flooded condenser operation whenever a relatively large upset occurs in the energy balance. In this case it appears to be a combination of two opposing effects. The increase in composition effect that tends to decrease the bubble point temperature and the effect of the increase in pressure that tends to increase the bubble point temperature. This effect occurred during the first 20 minutes after the change was made. This behavior was also observed in the trim cooler heat load response.

An inverse response behavior is observed in the reboiler/condenser heat load as shown on Figure 5.4e. This inverse response occurs because initially the bottoms temperature increased responding to the increase in pressure; therefore, decreasing the heat load. The heat load
then increases to a new steady state value. This behavior is quite different from the behavior in a conventional distillation column because in a conventional distillation column the increase in light component composition in the bottoms decreases the bubble point temperature. In this case the bottoms temperature increases because the column pressure increases. The reboiler heat load increases not because the bottoms temperature decreases but because the temperature of the condenser side of the reboiler/condenser increases more than the temperature of the reboiler side, therefore increasing the temperature driving force and consequently the heat load.

The inverse response in the heat load causes an inverse response in the distillate rate as shown on Figure 5.4a. This is because a decrease in the reboiler/condenser heat load decreases the rate of condensation in the condenser side of the reboiler/condenser, causing a reduction in the feed rate to the flash; therefore, a decrease in the distillate rate. The distillate rate will then increase to a new steady state value as shown on Figure 5.4a. The bottoms rate decreases to satisfy the material balance as shown on Figure 5.4b.

The trim cooler heat load decreases right after the change was made because of the decrease in the top tray temperature that made the trim cooler temperature driving force to decrease as shown on Figure 5.4e. The amount of vapor condensed in the trim cooler increased causing the the
liquid level to rise bringing the heat load down, close to its original value. This is because the rate of condensation has to equal the trim cooler outflow which is held constant.

Open Loop Response to Feed Rate

The open loop response to a 10% increase in feed rate was also examined. The feed rate underwent a change from 1000 g-moles/min. to 1100 g-moles/min. The feed temperature and composition stayed the same. The control scheme remained the same as the scheme used for the previous study.

Figure 5.5 shows the open loop response on the column variables to this change. An increase of the feed rate decreases the reboiler temperature causing a drop in the compressor discharge and suction pressures as shown on Figure 5.5c and 5.5d. The bottoms temperature goes down because of the increase in light component composition as shown on Figure 5.5c. The bottoms temperature follows the behavior of the compressor discharge pressure while the top tray temperature follows the behavior of the compressor suction pressure as shown on Figure 5.5d. The bottoms rate experiences a sudden increase in rate as shown on Figure 5.5b. The bottoms rate is brought back from its initial peak because of the increase in reboiler/condenser heat load that increases the rate of vaporization. The increase in top tray temperature is helped by the increase
Figure 5.5a Open Loop Response to a Change in Feed Rate
Figure 5.5b Open Loop Response to a Change in Feed Rate
Figure 5.5c  Open Loop Response to a Change in Feed Rate
Figure 5.5d Open Loop Response to a Change in Feed Rate
Figure 5.5e  Open Loop Response to a Change in Feed Rate
Figure 5.5f: Open Loop Response to a Change in Feed Rate
in pressure and by the increase of heavy components in the top tray as noticed on Figures 5.5a, 5.5c and 5.5d. The trim cooler heat load goes up because of the increase in top tray temperature but it is brought back down because of the increase in the molar holdup in the trim cooler that causes a decrease in the heat transfer area as shown in Figures 5.5e and 5.5f as before.

Open Loop Response to reflux rate

The open loop response to a step change in reflux rate was examined. The reflux rate underwent a 10% change from 600 g-moles/min. to 660 g-moles/min. Both the reflux controller and the pressure controller are kept in manual. The rest of the control scheme remains the same as in the previous cases.

Figure 5.6 shows the response of column variables to such a change. The immediate effect of a reflux rate change is a decrease in the accumulator level. Since the distillate rate is in level control with the accumulator a drop in the level causes a drop in the distillate rate, so to maintain the level at the steady state value as shown on Figure 5.6a. To maintain the material balance, the bottoms rate increases as observed on Figure 5.6b. The increase in the reflux brought more light component to the top tray and everywhere in the column; therefore decreasing the bubble point temperature as shown on Figure 5.6c. The decrease in the
Figure 5.6a Open Loop Response to a Change in Reflux Rate
Figure 5.6b  Open Loop Response to a Change in Reflux Rate
Figure 5.6c  Open Loop Response to a Change in Reflux Rate
Figure 5.6d Open Loop Response to a Change in Reflux Rate
Figure 5.6e  Open Loop Response to a Change in Reflux Rate
Figure 5.6f  Open Loop Response to a Change in Reflux Rate
temperature in the bottoms causes the reboiler heat load to increase as shown on Figure 5.6e increasing the vapor rate; therefore causing the column pressure to increase to a new steady state value as shown on Figure 5.6d

Open Loop Response to Trim Cooler Outflow

Figure 5.7 shows the open loop response to a 10% change in trim cooler outflow. The trim cooler outflow underwent a change from 130.45 g-moles/min to 143.5 g-moles/min. The pressure controller was kept in manual, with the rest of the control scheme the same as before.

An increase in trim cooler outflow, decreases the level in the trim cooler which at the same time exposes more area for heat transfer as shown on Figure 5.7f. Having more area for heat transfer, the trim cooler heat load increases, increasing the rate of vapor condensed to match the trim cooler outflow as shown on Figure 5.7e. Since the rate of vapor condensation increased, the column pressure decreased as noticed on Figure 5.7d. The top tray and bottoms temperatures decrease because of the decrease in pressure as shown on Figure 5.7c. The reboiler/condenser heat load increases to a new steady state because of the decrease in the bottoms temperature that increases the temperature driving force as shown on Figure 5.7e.

The distillate rate increases because of the increase in the accumulator level as shown on Figure 5.7a. To meet
Figure 5.7a Open Loop Response to a Change in Trim Cooler Outflow
Figure 5.7b Open Loop Response to a Change in Trim Cooler Outflow
Figure 5.7c  Open Loop Response to a Change in Trim Cooler Outflow
Figure 5.7d Open Loop Response to a Change in Trim Cooler Outflow
Figure 5.7e  Open Loop Response to a Change in Trim Cooler Outflow
Figure 5.7f  Open Loop Response to a Change in Trim Cooler Outflow
the material balance the bottoms rate levels out at a lower steady state value. The light component composition decreases for both the distillate and bottoms streams as shown on Figures 5.7a and 5.7b.

In summary, some unanticipated results were obtained in these studies. Unexpected behavior were observed in some of the variables as compared to a conventional distillation column. An example of such a behavior was seen in the reboiler/condenser heat load response to a change in feed composition.

As seen so far, the apparent cause of the double reverse action are due to opposing effects by both the composition effect and the pressure effect on the equilibrium behavior. Also, natural self regulation mechanism combined with the non linearities of the system may have their effect in this phenomenon. This phenomenon may have adverse contribution to tuned control loops.

It was found that the stability of the model depends on the tolerance chosen for the pressure dynamics because the pressure dynamics are the ones that contribute to the stiffness of the system.
Control Studies

As mentioned before, the process reaction curves can be used to determine the parameters for the controllers to be used. Proportional-integral (PI) digital controllers are used in the control schemes shown previously. The velocity algorithm used for a PI digital controller looks as follows:

\[ U = U + K \left( e_n - e_{n-1} + \left( \frac{T}{T} \right) e_n \right) \]  \hspace{1cm} (5.54)

where:

- \( e_n \) = Error signal at sample \( n \)
- \( e_{n-1} \) = Error signal at sample \( n-1 \)
- \( K \) = Controller proportional gain
- \( T \) = Sample time
- \( T \) = Controller reset time
- \( R \) = \( U_n \) = Value of the control variable at sample \( n \)
- \( U_{n-1} \) = Value of the control variable at sample \( n-1 \)

The parameters of the digital controller must be tuned in order to obtain the desired response. There are several tuning algorithms that can be used to tune digital controllers. Among these algorithms are:

1. Ziegler-Nichols Quarter Decay Ratio
2. Minimum Integral Absolute Value of the Error (IAE) Regulator

3. Minimum IAE tracking

4. Loop Compensation 5% Overshoot

5. Dahlin Algorithm

One of the advantages of these algorithms is that the proportional gain, reset time and derivative time correspond closely to the parameters of the analog controllers. Thus the techniques that have been developed to tune analog controllers can be used to tune digital controllers. The only special consideration is the sample time. All these algorithms are based on approximating the process reaction curve to a first order system plus dead time.

The tuning algorithm that gave the best results was the Dahlin algorithm. The main reason for that is because of an adjustable parameter built in the algorithm that allows the refinement of the tuning parameters based on the results obtained.

The Dahlin algorithm for tuning a Proportional-Integral digital controller is as follows:

\[
K_p K_c = \frac{a}{1 - a} \ast \frac{(1 - q)}{1 + N(1 - q)} \quad (5.55)
\]

\[
T_R = \frac{a}{1 - a} \ast T \quad (5.56)
\]

where:

\[
a = \exp(-T/\tau)\]

\[
K_c = \text{Proportional gain}\]
$K = $ Process gain
$P$
$N = $ integer $(\theta / T)$ truncated
$g = \exp(-\lambda T)$ is a tuning parameter
$T = $ Sample time
$R$
$T = $ Reset time
$R$
$\theta = $ Process dead time
$\tau = $ Process time constant
$\lambda = $ Dahlin tuning parameter

**Pressure Control**

The control scheme shown on Figure 5.1 is subject to a change in feed composition in order to study its closed loop behavior. The distillate and bottom rates are on tight level control, the reflux rate is on tight flow control and a proportional-integral (PI) digital controller is used to control the column pressure by manipulating the trim cooler outflow. The coolant rate and temperature are kept constant.

Based on the open loop response curve to a change in the trim cooler outflow on the column pressure the following process parameters were determined:

- Process Steady State Gain = -3.678 mm Hg * min. 
  ------------------------
  g-moles
- Process Time Constant = 16.5 min.
- Process Dead Time = 3.0 min.
Based on these process parameters, the following tuning parameters for the pressure controller were determined:

Controller Proportional Gain = \(-0.05352\) g-moles
\[\text{min} \times \text{mm hg}\]

Controller Reset Time = 14.58 min.

Controller Sample Time = 4.0 min.

Figure 5.8 shows the response of the system with the control scheme shown on Figure 5.1 when a change in the feed composition is made, with the pressure controller on line.

As the pressure increases, the trim cooler outflow increases to expose more area for heat transfer; therefore, bringing the pressure down to its initial steady state value. The maximum value of the pressure is reached in about 35 minutes as shown on Figure 5.8d. The pressure levels out in approximately 175 minutes. The distillate and bottoms composition are basically unaffected by the pressure control loop as shown on Figures 5.8a and 5.8b. Both the top tray and the bottoms temperature are significantly affected by the pressure control loop. The fact that the pressure controller affected the top tray temperature means that some interaction might be expected when this variable is used as a controlled variable and the pressure controller is on. The same conclusion can be derived for the bottoms temperature. The pressure controller action can be observed on the trim cooler outflow curve shown on Figure 5.8e.
<table>
<thead>
<tr>
<th>DISTILLATE MOLE FRACTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
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<table>
<thead>
<tr>
<th>DISTILLATE FLOW RATE</th>
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<tbody>
<tr>
<td>0.00</td>
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</table>

Figure 5.8a System Response of Control Scheme No. 1 to a Change in Feed Composition
Figure 5.8b System Response of Control Scheme No. 1 to a Change in Feed Composition
Figure 5.8c Open Loop Response of Control Scheme No. 1 to a Change in Feed Composition
Figure 5.8d System Response of Control Scheme No. 1 to a Change in Feed Composition
Figure 5.8e System Response of Control Scheme No. 1 to a Change in Feed Composition
These particular studies show that pressure control can be successfully achieved by using the trim cooler outflow as the manipulated variable. They also show that some interaction might be expected when either the top tray temperature or the bottoms temperature is used as the controlled variable. Little interaction is expected when either the distillate composition or the bottoms composition is used as the controlled variable.

**Composition Control**

The control scheme shown on figure 5.2 is subject to a change in feed composition. The distillate and bottom rates are on tight level control. Two (PI) digital controllers are used to control the column pressure and the distillate composition.

In order to implement the control scheme of Figure 5.2 the composition controller needs to be tuned. This controller is tuned with the pressure controller in manual in order to avoid possible interactions which in this case does not make any difference because it was observed in the previous case that the distillate composition is not affected by the pressure controller.

Based on the open loop response curve to a change in the reflux rate on the distillate composition, the following process parameters were determined:

\[
\text{Process Steady State Gain} = 0.0046 \text{ min.}^{-1} \text{g-moles}
\]
Process Time Constant = 9.75 min.
Process Dead Time = 2.25 min.

Based on these process parameters, the following tuning parameters for the composition controller were determined:

Controller Proportional Gain = 5.0609 g-moles
Controller Reset Time = 9.50 min.
Controller Sample time = 0.5 min.

As noticed, a small sample time was used for the composition controller. In reality such a small sample time can not be used because of the delay in the analysis system. The reasons for using such a small sample time was to be able to get a faster response on the system. Therefore the tuning parameters were modified by trial and error in order to get a faster response in the composition.

Figure 5.9 shows the system response when both the pressure controller and the composition controller are on line. As observed before, no interaction is expected when these two controllers are on line. The light component composition reached its maximum peak in about 35 minutes, leveling out in about 175 minutes as shown on Figure 5.9a. The column pressure reaches its peak in about 35 minutes, leveling out in about 175 minutes as shown on Figure 5.9d.
Figure 5.9a System Response of Control Scheme No. 2 to a Change in Feed Composition
Figure 5.9b System Response of Control Scheme No. 2 to a Change in Feed Composition
Figure 5.9c  System Response of Control Scheme No. 2 to a Change in Feed Composition
Figure 5.9d System Response of Control Scheme No. 2 to a Change in Feed Composition
Figure 5.9e System Response of Control Scheme No. 2 to a Change in Feed Composition
REFLUX FLOWRATE

TIME (MINS)

550.00 600.00 625.00
575.00

Figure 5.9f System Response of Control Scheme No. 2 to
a Change in Feed Composition
The distillate and bottoms flow rates were not greatly affected by these control loops as shown on Figures 5.9a and 5.9b. The action of the digital controller is similar to the one observed previously. The action of the digital controller action in the reflux rate is not noticed because of the small sample time used as shown on Figure 5.9f.

The closed loop response to a change in feed rate on this control scheme was also examined. The results are shown on Figure 5.10.

**Temperature Control**

The control scheme shown on figure 5.3 is also subject to a change in feed composition. The distillate and bottom rates are on tight level control. Two PI digital controllers are used to control the column pressure and the top tray temperature. The column pressure is controlled with the trim cooler outflow as before. The top tray temperature is controlled with the reflux rate.

In order to implement the control scheme of Figure 5.3 the temperature controller also needs to be tuned. This controller is tuned with the pressure controller in manual.

Based on the open loop response curve to a change in the reflux rate on the top tray temperature, the following process parameters were determined:
Figure 5.10a System Response of Control Scheme No. 2 to a Change in Feed Rate
Figure 5.10b. System Response of Control Scheme No. 2 to a Change in Feed Rate
Process Steady State Gain = \(-0.0130\) min. K g-moles

Process Time Constant = 7.0 min.
Process Dead Time = 0.25 min.

Based on these process parameters, the following tuning parameters for the temperature controller were determined:

Controller Proportional Gain = \(-0.52695\) g-moles min. K

Controller Reset Time = 6.75 min.
Controller Sample time = 0.5 min.

Figure 5.11 shows the system response when both the pressure controller and the temperature controller were on line. As expected, some interaction was observed when the two controllers were on line. This explains the oscillatory behavior of the system compared to the previous scheme as shown on Figure 5.11c and 5.11d. The temperature reaches its maximum value in about 20 minutes, then it reaches a minimum value in about 50 minutes, oscillating around the set point as shown on Figure 5.11c. The amplitude of the oscillation decreases as time increases. The pressure reaches its maximum value in about 40 minutes, oscillating around the set point as shown on Figure 5.11d.

The closed loop response to a change in feed rate on this control scheme was also examined. The results are shown on Figure 5.12.
Figure 5.11a System Response of Control Scheme No. 3 to a Change in Feed Composition
Figure 5.11b  System Response of Control Scheme No. 3 to a Change in Feed Composition
Figure 5.11c  System Response of Control Scheme No. 3 to a Change in Feed Composition
Figure 5.11d  System Response of Control Scheme No. 3 to a Change in Feed Composition
Figure 5.12a  System Response of Control Scheme No. 3 to a Change in Feed Rate
Figure 5.12b System Response of Control Scheme No. 3 to a Change in Feed Rate
CHAPTER 6

SUMMARY AND CONCLUSIONS

The primary purpose of this research was to investigate the feasibility, dynamics and control of distillation columns with heat pump installations. A steady state model of a distillation column with a heat pump was developed to study the economic feasibility of heat pumps in distillation columns. This model was used to study the effect of different variables to the heat pump feasibility. The effect of column pressure, tray pressure drop, and reboiler/condenser approach temperature to heat pump installations was investigated. It was found that the heat pump feasibility strongly depends on the thermodynamic availability of the mixture and on the relative cost between steam and electricity. The overall temperature driving force that the compressor has to overcome was found to be a combination of the saturation temperature difference between the key components, the temperature difference caused by the pressure drop on the trays and the approach temperature on the reboiler/condenser.

A possible way of predicting the pressure effect on the heat pump feasibility was also devised based on the Antoine equation for vapor pressure. Therefore, the pressure effect on heat pump installations can be predicted beforehand by using the Antoine constants without having to do rigorous
calculations.

It was found that of the variables studied, the reboiler/condenser approach temperature was the one that have the largest effect on heat pump installations feasibility. This is because the increase in compressor costs are more significant than the decrease in the heat transfer requirements. Also, electric costs increases more than the savings in steam and cooling water. As expected, the heat pump installations favored the closed boiling mixture against the wide boiling mixture. Therefore, for very difficult separations where a considerable amount of energy is used in the reboiler, the heat pump concept might be a feasible way of reducing the energy consumption considerably.

A search for a more efficient integration technique was made in order to reduce the computer time usage. The reasons for the excessive computer time was the presence of stiff differential equations in the heat pump model. It was found that the equations that mostly contributed to the stiffness of the system were the pressure dynamic equations. In order to minimize the stiffness of the system a greater vapor holdup was used in the compressor suction and in the compressor discharge. This change can be done as long as the dynamic of the system is not significantly affected. This change is purely for mathematical purposes and not for physical purposes. The main reason for the change is that the computer time is greatly reduced. For our cases, the
vapor holdup in both the compressor suction and the compressor discharge was increased by a factor of 10 to reduce the computer time by a factor of 2. Runge-Kutta fourth order, LSODE and EPISODE were the integration methods tested in this research. The last two are computer software packages based of Gear's method for the integration of ordinary differential equations. It was found the last two methods were an order of magnitude faster than the Runge-Kutta method. For the system studied in this research, LSODE was found to be the most effective.

A dynamic model of a distillation column with a heat pump was developed to perform dynamic and control studies. This model utilizes the trim cooler outflow to control the pressure of the column. Until recently, pressure has been assumed constant in most complex dynamic models. The elimination of this assumption has allowed us to study pressure control as an integral part of the overall column control strategy.

Open loop responses were obtained to changes on feed composition, feed rate, reflux rate, and trim cooler flow out in order to understand the column behavior. A double reverse action was observed which appears to be caused by two opposing effects, the effect of pressure and composition in the equilibrium temperature.

The control schemes studied were essentially the same as the control schemes encountered on conventional distillation columns. Pressure control was successfully
included as part of the overall control strategy. The top tray temperature controller and the distillate composition controller were successfully implemented. Some interaction was observed between the pressure controller and the top tray temperature controller when both controllers are on automatic. No interaction was observed between the composition controller and the pressure controller. We found that the interaction between the pressure controller and the temperature controller can be minimized by increasing the sample time of the pressure controller relative to the sample time of the temperature controller.

**Recommendations for Future Research**

This study was considered as a first step in a complete research program on heat integration systems on distillation columns, laying the groundwork for future studies. Having looked at the economic feasibility of heat pumps as a way of saving energy in a distillation unit and the fact that cheap energy is no longer available, it is greatly justified to continue further studies on this particular area. The following areas are recommended as material for further research.

1. Modify the present model to work for non-ideal systems (e.g., azeotropic mixtures).
2. Study different control arrangements other than the basic control schemes studied in this research.
(e.g., ratio control, feedforward control, etc.).

3. Make decoupling studies between the pressure control loop and the temperature control loop to eliminate the interaction between them.

4. Compressor dynamics might be included in the present model and maybe use the compressor speed as a manipulative variable to control the vapor rate in the column.

5. Modify the model to consider different heat pump arrangements other than the compression of the overhead vapor as illustrated in Chapter 1 and compare to the one studied in this research.

6. Initiate dynamic studies on multiple effect arrangements which can also be used to save a considerable amount of energy.
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>A&lt;sub&gt;rc&lt;/sub&gt;</td>
<td>Reboiler/Condenser area</td>
</tr>
<tr>
<td>A&lt;sub&gt;t&lt;/sub&gt;</td>
<td>Tray area</td>
</tr>
<tr>
<td>A&lt;sub&gt;tc&lt;/sub&gt;</td>
<td>Trim condenser area</td>
</tr>
<tr>
<td>B</td>
<td>Bottoms rate</td>
</tr>
<tr>
<td>C&lt;sub&gt;L&lt;/sub&gt;</td>
<td>Heat capacity of the liquid</td>
</tr>
<tr>
<td>C&lt;sub&gt;P&lt;/sub&gt;</td>
<td>Heat capacity of the vapor</td>
</tr>
<tr>
<td>C&lt;sub&gt;C&lt;/sub&gt;</td>
<td>Heat capacity of the coolant</td>
</tr>
<tr>
<td>D</td>
<td>Distillate rate</td>
</tr>
<tr>
<td>F</td>
<td>Feed rate</td>
</tr>
<tr>
<td>H&lt;sub&gt;H&lt;/sub&gt;</td>
<td>Pure component liquid enthalpy</td>
</tr>
<tr>
<td>h</td>
<td>Enthalpy of the liquid mixture</td>
</tr>
<tr>
<td>H&lt;sub&gt;H&lt;/sub&gt;</td>
<td>Pure component vapor enthalpy</td>
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<tr>
<td>H</td>
<td>Enthalpy of the vapor mixture</td>
</tr>
<tr>
<td>H&lt;sub&gt;b&lt;/sub&gt;</td>
<td>Enthalpy of the bottoms vapor mixture</td>
</tr>
<tr>
<td>h&lt;sub&gt;b&lt;/sub&gt;</td>
<td>Enthalpy of the bottoms liquid mixture</td>
</tr>
<tr>
<td>h&lt;sub&gt;d&lt;/sub&gt;</td>
<td>Enthalpy of the distillate liquid mixture</td>
</tr>
<tr>
<td>H&lt;sub&gt;dc&lt;/sub&gt;</td>
<td>Enthalpy of the vapor mixture in compressor discharge</td>
</tr>
<tr>
<td>H&lt;sub&gt;f&lt;/sub&gt;</td>
<td>Enthalpy of the feed vapor mixture</td>
</tr>
</tbody>
</table>
\( h \) = Enthalpy of the feed liquid mixture

\( h_{fl} \) = Enthalpy of the flash liquid mixture

\( H_{fl} \) = Enthalpy of the flash vapor mixture

\( h_{rc} \) = Enthalpy of the liquid mixture in reboiler/condenser

\( H_{s} \) = Enthalpy of the vapor mixture in compressor suction

\( h_{tc} \) = Enthalpy of the liquid mixture in trim cooler

\( H_{n} \) = Enthalpy of the vapor mixture in tray \( n \)

\( h_{n} \) = Enthalpy of the liquid mixture in tray \( n \)

\( \Delta H_{vap} \) = Pure component heat of vaporization

\( h_{ow} \) = Liquid height over weir

\( L_{fl} \) = Liquid rate from flash

\( L_{n} \) = Liquid rate from tray \( n \)

\( L_{rc} \) = Liquid rate from reboiler/condenser

\( L_{tc} \) = Liquid rate from trim cooler

\( l_{w} \) = Length of weir

\( LMTD_{rc} \) = Temperature driving force on reboiler/condenser

\( LMTD_{tc} \) = Temperature driving force on trim cooler

\( M_{b} \) = Liquid Molar holdup in the column base
$M_{ld}$ = Liquid Molar holdup in the reflux accumulator

$M_{dc}$ = Vapor Molar holdup in the compressor discharge

$M_{ln}$ = Liquid molar holdup on tray n

$M_{ms}$ = Vapor Molar holdup in the compressor suction

$M_{tc}$ = Liquid Molar holdup in the trim cooler

$M_{Wj}$ = Pure component molecular weight

$M_{Wl}$ = Average molecular weight of liquid phase

$M_{Wv}$ = Average molecular weight of vapor phase

$n$ = Polytropic efficiency

$P$ = Pressure

$P_{dc}$ = Compressor discharge pressure

$P_{oj}$ = Pure component vapor pressure

$P_{jn}$ = Pressure on tray n

$P_s$ = Compressor suction pressure

$Q_{eb}$ = Reboiler/condenser heat load

$Q_c$ = Volumetric flow through the compressor

$Q_{tc}$ = Trim cooler heat load

$g$ = Feed quality

$R$ = Reflux rate
\[ R' = \text{Gas law constant} \]
\[ T_{c} = \text{Pure component critical temperature} \]
\[ T_{dc} = \text{Compressor discharge temperature} \]
\[ T_{n} = \text{Temperature on tray n} \]
\[ T_{\text{ref}} = \text{Reference temperature} \]
\[ T_{r} = \text{Pure component reduced temperature} \]
\[ T_{s} = \text{Compressor suction temperature} \]
\[ T_{wi} = \text{Inlet coolant temperature} \]
\[ T_{wo} = \text{Outlet coolant temperature} \]
\[ U_{rc} = \text{Reboiler/condenser heat transfer coefficient} \]
\[ U_{tc} = \text{Trim cooler heat transfer coefficient} \]
\[ V_{b} = \text{Bottoms vapor rate} \]
\[ V_{c} = \text{Vapor rate through the compressor} \]
\[ \bar{V}_{dc} = \text{Vapor holdup in compressor discharge} \]
\[ V_{fl} = \text{Vapor rate in flash} \]
\[ V_{n} = \text{Molar vapor rate from tray n} \]
\[ \bar{V}_{s} = \text{Vapor holdup in compressor suction} \]
\[ V_{tc} = \text{Vapor rate in trim condenser} \]
\[ W_c = \text{Compressor work} \]
\[ x_j = \text{Liquid mole fraction of component } j \]
\[ x_{b,j} = \text{Liquid mole fraction of component } j \text{ in bottoms} \]
\[ x_{d,j} = \text{Liquid mole fraction of component } j \text{ in distillate} \]
\[ x_{f,j} = \text{Liquid mole fraction of component } j \text{ in feed} \]
\[ x_{fl,j} = \text{Liquid mole fraction of component } j \text{ in flash} \]
\[ x_{n,j} = \text{Liquid mole fraction of component } j \text{ in tray } n \]
\[ x_{rc,j} = \text{Liquid mole fraction of component } j \text{ in reboiler/condenser} \]
\[ x_{tc,j} = \text{Liquid mole fraction of component } j \text{ in trim cooler} \]
\[ y_j = \text{Vapor mole fraction of component } j \]
\[ y_{b,j} = \text{Vapor mole fraction of component } j \text{ in bottoms} \]
\[ y_{dc,j} = \text{Vapor mole fraction of component } j \text{ in compressor discharge} \]
\[ y_{f,j} = \text{Vapor mole fraction of component } j \text{ in feed} \]
\[ y_{fl,j} = \text{Vapor mole fraction of component } j \text{ in flash} \]
\[ y_{n,j} = \text{Vapor mole fraction of component } j \text{ in tray } n \]
\[ y_{s,j} = \text{Vapor mole fraction of component } j \text{ in compressor suction} \]
Subscripts:

\( b \) = Bottoms
\( c \) = Compressor
\( d \) = Distillate
\( dc \) = Compressor discharge
\( f \) = Feed
\( fl \) = Flash
\( j \) = Component number
\( l \) = Liquid phase
\( n \) = Tray number
\( s \) = Compressor suction
\( tc \) = Trim condenser
\( v \) = Vapor phase
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VITA

Edgar Hernandez was born on June 16, 1954 in Bronx, New York. His parents moved to Cabo Rojo, Puerto Rico when he was a young child. He attended the public schools in Cabo Rojo, graduating from Luis M. Marin High School in May 1972.

He then enrolled in the University of Puerto Rico at Mayaguez where he finished the degree of Bachelor of Science in Chemical Engineering in December 1976. He received his degree in May 1977. He worked with Union Carbide Caribe during the summer of 1976.

In November 1975, he married the former Estella Chelune which brought two beautiful children Ricky and Rebecca.

From December 1976 to August 1978, he worked with PPG Industries Caribe as a Chemical Engineer.

In August 1978, he joined the Chemical Engineering department at Louisiana State University. In May 1980, he received the degree of Master of Science in Chemical Engineering. In December 1980, he received the degree of Master of Science in Industrial Engineering. During his graduate work, he was admitted to the PHI LAMBDA UPSILON honorary chemical society.

He is at the present a candidate for the degree of Doctor of Philosophy in Chemical Engineering.
Candidate: Edgar Hernandez

Major Field: Chemical Engineering

Title of Thesis: Feasibility Analysis, Dynamics, and Control of Distillation Columns with Vapor Recompression

Approved:

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

Date of Examination:

November 25, 1981