1981


William Bell Stewart Jr
Louisiana State University and Agricultural & Mechanical College

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SIMULATION AND EVALUATION OF DISTILLATION CONTROL SYSTEMS WHICH CONTROL PRESSURE WITH REBOILER HEAT

The Louisiana State University and Agricultural and Mechanical Col. Ph.D. 1981

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Simulation and Evaluation of Distillation Control Systems Which Control Pressure With Reboiler Heat

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 William Bell Stewart, Jr.
B.S., Chem. Engr., Louisiana State University, 1975
M.S., Chem. Engr., Louisiana State University, 1977
May 1981
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ABSTRACT

A recent industrial development in distillation control strategy is to involve pressure control as an integral part of an overall control strategy, rather than as an external feature. This approach is not to simply maintain column pressure, but to manipulate other variables using the pressure as a controlled variable.

In order to study control systems which utilizes this approach, a rigorous non-linear multicomponent dynamic distillation model which includes pressure dynamics was developed. The model was based on total mole, component, and enthalpy balances as well as phase equilibrium relationships and tray hydraulics on each stage. The differential equations of this model were integrated by an algorithm developed in this research which gives second-order truncation accuracy with only one functional evaluation per time step, making it roughly twice as fast as the equivalent unmodified predictor-corrector method.

A simple control scheme which utilized pressure to manipulate reboiler heat was devised based on literature and tested. This control scheme included material balance control to maintain the top product purity. Open-loop and closed-loop responses to column upsets were examined and compared.
INTRODUCTION

Distillation column control has evolved over the years to be fairly sophisticated in many aspects. Historically, however, the control of the column pressure has been more-or-less an "added-on" feature with no ties to the remainder of the column control system. That is, the function of the column pressure controller has been to maintain a constant pressure without directly affecting the control loops concerned with product purity.

A recent development has been to involve the pressure control system in the overall column control system. A control system outlined by Wright and Johncock (28,29) maintains the pressure at the top of the column by manipulating the reboiler heat input. Thus, the pressure control becomes an integral part of the energy balance loop. The entire control system described by Wright and Johncock is semi-empirical. That is, although it is based on logical control concepts, the control system does not owe much to modern control theory. Even though this system has apparently met with success in practice, it has not been examined by a computer simulation effort. The basic thrust of this research was to begin a computer simulation study of the column pressure-reboiler heat control system.

In order to study any control system by computer simulation, a dynamic process model is required. The
particular control system of interest in this research required a comprehensive dynamic distillation model which includes pressure dynamics, which is a very rare commodity. A few linearized models have been presented in the literature (see Chapter 1). However, linearized models are approximations which, for complicated systems such as distillation columns, may not behave at all properly. The superposition principle is characteristic of linearized modeling, but simple experiments with non-linear distillation models reveal that the responses of column variables to the manipulated variable are far from additive. This is more especially true of models which exhibit high non-linearlity, such as a distillation column's pressure dynamics. This is particularly unfavorable when a new steady state is reached because the linearization would no longer be about the about the operating conditions. Therefore, this research began with the development of a unique non-linear unsteady-state distillation model which includes pressure dynamics on each tray in the column. A model of this type has never been reported in the literature. The object of the simulation effort was to make the model represent the pressure variations in an acceptable physical representation so that the column responses to control would be correct, without attempting to reproduce the results of a specific existing column. This approach is typical of models developed for control studies. As long as the
components are modeled in an acceptable and physically correct manner, then the dynamic behavior of the model can be expected to be representative of actual columns. (For example, when a stirred tank reactor model is used, the control system overall behavior is typical, even though no reactor will behave exactly as a stirred tank.)

The distillation column model was developed to simulate multicomponent distillations with rigorous tray and downcomer hydraulics. It performs total material, component, and heat balances on each stage as well as solving equilibrium relationships. These balances and relationships are solved in a unique manner to accommodate the inclusion of the pressure dynamics. Another feature of this model is that the equilibrium relationships are integrated, rather than solved iteratively on each time step, saving significant computer (cpu) time. The model is discussed in detail in Chapter 2.

During the process of making the simulations faster, a novel integration algorithm was developed to integrate the large, stiff system of differential equations of the distillation model with as little cpu time as possible. This algorithm, named the Johnson-Stewart Modified Euler (JSME) technique, is based on the Improved Euler predictor-corrector method, but computes the derivatives only with the predicted values of the integrated variables, rather than with both the predicted and corrected values as does the improved Euler algorithm. This is a very beneficial
feature, since the evaluation of the derivatives takes considerably more computer time than the integration procedure itself. In essence, this algorithm provides the same second-order accuracy of the improved Euler algorithm requiring only half the computer time. The concept can also be applied to higher order predictor-corrector schemes with the same result, a 50% reduction in computer time for equivalent accuracy. The JSME integration method was compared with the Improved Euler, Runge-Kutta, and Hamming algorithms, and was seen to be the most efficient in integrating the differential equations of the dynamic distillation model. This algorithm is discussed in Chapter 3.

The control system simulated analog control as used by Wright and Johncock. The system devised was straightforward, apart from the new pressure control loop. The distillate product composition was controlled through inferential control by manipulating the distillate rate to maintain the top temperature constant. This concept of manipulating product rates, rather than internal flows (reflux and boilup rates) to control one product purity is frequently termed "material balance control". Two very important advantages of material balance control of product composition are that the control loops exhibit considerably less interaction than the "conventional" method of manipulating reflux rate and that the composition is generally much more sensitive to changes in
product rate than to internal flow rate changes. Perhaps the most important asset claimed for the pressure control loop is that it tends to speed up the response of the control system to other variables, thus enhancing the composition control loop. The combination of material balance control and the top pressure-reboiler heat loop provide for very efficient and fast-acting distillate purity control. The overall material balance of the column was maintained by adjusting the bottoms product rate using the reboiler liquid level as the controlled variable. This control system is discussed in greater detail in Chapter 4.

The open-loop response of column pressure to various step changes in reboiler heat were recorded. The unusual responses were attributed to the natural feedback mechanisms inherent in the dynamic composition and thermal responses. The open-loop responses and closed-loop responses were examined in Chapter 5. This research was not an exhaustive study of the control system. The research program which was initiated by this work has as its ultimate goal the completion of a definitive study of this type control system in order to evaluate its advantages and disadvantages under a wide range of operating conditions. This study was considered the first step in the complete research program, laying the groundwork for future studies.
CHAPTER 1

LITERATURE REVIEW

The study of distillation dynamics and the study of distillation control are often found together in the literature. This is because the only practical application of distillation dynamics is for the purpose of automatic control. Many of the early articles appearing in the literature cover both dynamics and control in a single monograph. However, most later articles focus on just one of the two categories. Therefore, this chapter surveys the two concepts separately. The survey of articles considering distillation dynamics modeling (especially those with pressure dynamics) is covered first. Automatic distillation control (emphasizing pressure control) is then covered.

Modeling

Before the advent of analog and digital computers, there was not much need for dynamic distillation models (except for batch distillation), because these models do not lend themselves very well to hand calculation. Among the first to publish an unsteady state distillation model were Marshall and Pigford (13) in 1947. This model was very simple, assuming linear vapor-liquid equilibrium
relationships, constant liquid holdups, and constant and uniform liquid and vapor flow rates. They also assumed negligible vapor holdups and perfectly mixed liquid holdups. These latter two assumptions are fairly standard in subsequent models, but the other assumptions are found primarily in simpler linearized models.

Among the pioneers modeling more complex multicomponent distillation dynamics were Peiser and Grover (17). Other relatively rigorous models include that of Tetlow, Groves, and Holland (23). In 1973, Yu (30), produced a general, yet practical constant pressure model that was not linearized. Rademaker, Rijnsdrop, and Maarleveld (19) feature a very complete literature survey in their 1975 book.

Models which feature dynamic pressure are comparatively rare. Rademaker and Rijnsdorp (18) produced a linearized model for integration by analog computer in 1959. Aside from the linearization, their model was quite rigorous in the interest of accurate automatic control studies. Obviously, the model is only valid if the variables do not stray far from the point of linearization. Mickley, Gould, and Schwartz (15) produced a similar model focusing on bubble cap trays. Harriot (10) generalized a model in which the vapor holdups between the plates are explicitly modeled. Most models avoid this feature since the vapor dynamics are considerably faster than the liquid dynamics, making integration more difficult.
Rijnsdrop (20) proposed a model which assumed that the pressure drop between trays is negligible, which makes this model valid only for high pressure columns. Rijnsdrop formulated his model in the LaPlace domain basically because his paper featured the study of interactive control. Davison (8) produced an unusual linearized model which assumed negligible liquid holdups on the trays, negligible pressure drops across trays as well as the typical assumptions made during linearization. Buckley, Cox, and Rollins (4) included liquid aeration on perforated trays in their LaPlace domain model for the purpose of studying inverse response. In their book, Rademaker, Rijnsdrop, and Maarleveld (19) exhibited a fairly complex model which included pressure dynamics. The equations were shown in not only the LaPlace form for linear control algorithms, but, also in the electrical analog form, which is not very familiar to many chemical engineers. All models discussed above (except that of Buckley, et. al.) were explicitly for the purpose of studying automatic control strategies.

It should be noted that with the exception of the work of Yu, all of the above models were linearized. This research combined Yu's non-linearity with pressure dynamics to develop a unique model- a non-linear dynamic distillation model which includes dynamic pressure.
Control

Before computers were practical, distillation control schemes were developed on an empirical basis, heavily influenced by highly simplified analytical solutions to simple models. Of course, many of these empirical concepts are still in use today. Rather than outline all the concepts and strategies which have been suggested in distillation control, only pressure control techniques will be discussed here.

Among the first to publish column pressure control methods was Boyd (2), who addressed flooded condensers among other methods. His approach was purely empirical, yet utilized solid engineering ideas. Many of his ideas are used in subsequent articles by others. Rademaker and Rijnsdrop (18) introduced not only a fairly rigorous dynamic model, but approached the control from a more theoretical point of view, using the dynamic model to estimate the various transfer functions. Davison (8) applied Rosenbrock's modal analysis technique to his unconventional dynamic model. He compared his results with conventional control techniques using a digital computer and claimed great success. In their comprehensive book, Rademaker, Rijnsdrop, and Maarleveld (19), discussed in detail, the relative advantages and disadvantages of many various control strategies, including pressure control techniques. Naturally, the authors were slightly biased toward techniques described in their many
previous articles, but had researched the literature very thoroughly. Most of the discussion dealt with the particular situations each particular control scheme would handle well or poorly. In his very popular book, Shinskey (21) discussed control in terms of saving money, which is, of course, a significant driving force. One of the major points he emphasized was the concept of "material balance control" of product purity, which is discussed in Chapter 4 of this dissertation. In a rather general article, Lupfer (12) followed Shinskey's monetary interest with special reference to pressure control, even though he featured only one example and one control scheme. Wright and Johncock (28,29) discussed an overall control strategy developed at Amoco, which utilizes pressure to adjust reboiler heat. This strategy, using analog control, is now being successfully marketed as "Fractronic" by Transmation. Although generally successful, the techniques used are basically semi-empirical and have never been evaluated by modeling effort. Chin (6) presented a survey of twenty-one popular pressure control techniques, listing the relative advantages and disadvantages of each. Each technique examined, focused on the top of the column and the condenser/accumulator section and was primarily concerned only with how to maintain column pressure rather than with using pressure control as an integral part of an overall column control strategy to accomplish separation control.
It is very important to contrast two completely different approaches (or definitions) to pressure control. The first is the traditional approach, to keep the pressure constant to keep operations smooth. All of the above-mentioned articles and books, except those of Wright and Johncock, follow this line. The other approach, which is relatively new, uses pressure control as an important functional part of an overall control strategy. Wright and Johncock used pressure control to close the energy balance loop. It is this approach which was to be evaluated in this research.
CHAPTER 2

DYNAMIC DISTILLATION MODEL

INTRODUCTION

A dynamic mathematical model of a distillation column usually consists of a combination of differential equations and algebraic equations. In reality, a completely dynamic model would contain only differential equations. Algebraic equations are used to express relationships between variables which are assumed to happen so fast, compared to the slower controlling phenomena, that instantaneous relationships may be used to represent the more rapid phenomena.

In order to compute the algebraic variables and the derivatives of the integrated variables for a distillation column, five basic relationships can be used. These are as follows:

1. Total mole balances
2. Component mole balances
3. Enthalpy balances
4. Equilibrium relationships (bubble point, dew-point, etc.)
5. Momentum balances (vapor and liquid-phase pressure drops)
All of these relationships are used on each subsection of the column model (each ideal tray, condenser, and reboiler) to calculate all the flow rates and intensive properties (temperature, composition, etc.). There are a number of potential ways to use the relationships to compute variables. For example, whenever the liquid on each tray is considered to be at its bubble point, the bubble point relationship could be used to calculate the bubble point temperature if the pressure were independently known, or the bubble point pressure may be computed from this relationship if the temperature of the liquid has been previously computed by a heat balance. Exactly which relationship is used to calculate a particular variable depends primarily upon the assumptions and approximations that are made when the model is formulated. In models in which the pressure on each tray is considered essentially constant, the former use of the bubble point relationship is always followed. In this model, the latter use is required in order to permit calculation of dependently varying pressure on each tray.

One other important concept is that the modeling of any vapor spaces (holdups) in a column should be avoided. The obvious reason behind this is that the dynamics in vapor spaces are extremely fast because the relative sparseness of the vapor means very small molar holdups. Therefore, the numerical integration would be much slower
because of small time steps. Thus, only liquid holdups are to be modeled.

To avoid iterative calculations on each time step, the values used to calculate any given variable or its derivative should be current. That is, the computation of that variable should not involve a value of any other variable which has not yet been updated for the current time step. Otherwise, iteration on each time step would be required, resulting in more computation time. As already noted, dynamic distillation modeling involves both integrated variables and algebraic variables. To avoid iteration, the current values of the algebraic variables, which are needed to calculate the derivatives, should be calculated first. Furthermore, these algebraic relationships should be computed in proper sequence to avoid iteration. In some models the relationships are such that simultaneous solution of algebraic nonlinear equations cannot be avoided. In this model, however, it was not necessary.

**ALBEGRAIC VARIABLES**

The algebraic variables in this model are the liquid and vapor flow rates throughout the column. As previously explained, this means that the relationship establishing the flow rates are assumed to occurs instantaneously. This of course is not strictly true, but the time constants associated with these flow phenomena are probably
less than 0.01 seconds. It is considered that the use of differential equations for the relationships would in no way improve or affect the accuracy of the simulation results of interest in this study, and, of course, it would increase the computational effort and time many fold. Therefore, this choice was made. The nomenclature is presented with a schematic diagram in Figure 2-1. With the one exception of the vapor flow to the overhead condenser, all flow rates are calculated by steady state pressure drop relationships and standard correlated tray hydraulics relationships.

**Liquid Rates Over Weirs**

Liquid flow rates over weirs are computed using the Francis weir formula:

\[
Q_{ow} = (24.1206)(l_w)(h_{ow})^{3/2}
\]  

(2-1)

Where \(Q_{ow}\) is the liquid flow over the weir, in cubic feet per hour, \(l_w\) is the length of the weir in inches, and \(h_{ow}\) is the liquid crest over the weir in feet. The liquid crest is simply the difference between the liquid level on the tray and the height of the straight weir. Knowing the liquid molar density, equation (2-1) may be used to compute the molar flow rate over the weir.
Figure 2-1. Typical Column Tray
Liquid Rates From Downcomers

Liquid flow rates from the downcomers onto the trays below are also calculated from standard steady-state pressure drop equations. Using the nomenclature from Figure 2-1, the pressure drop available to cause liquid flow through the downcomer and its bottom restrictive opening is expressed by:

\[
(h_{da})_{j-1} = (h_{dc})_{j-1} - (h_w + h_{ow})_j + P_{j-1} - P_j \tag{2-2}
\]

where \((h_{da})_{j-1}\) is the pressure drop available to cause flow onto tray \(j\) in feet of liquid, \((h_{dc})_{j-1}\) is the height in feet of liquid in the downcomer \((j-1)\), \((h_w + h_{ow})_j\) is the total height of liquid on tray \(j\), and \(P_{j-1}\) and \(P_j\) are the pressures above the liquid on trays \(j-1\) and \(j\), respectively. Before equation (2-2) may be utilized, all pressures must be converted to feet of liquid to make the units consistent. Using the pressure computed by equation (2-2), the liquid flow rate through downcomer \((j-1)\) onto tray \((j)\), may be calculated by:

\[
(Q_{dc})_{j-1} = (17334)(A_{da})(h_{da})_{j-1}^{1/2} \tag{2-3}
\]

where \((Q_{dc})_{j-1}\) is the liquid flow rate onto tray \(j\) in the cubic feet per hour and \(A_{da}\) is the area of the restricted
opening under each downcomer in square feet. (This neglects the minute pressure drop due to flow through the downcomer itself.) As with equation (2-1), this volumetric flow rate can be converted to a molar density at that point in the column.

**Vapor Flow Rates**

The computations for the liquid flow rates are more or less standard for most columns, because the correlations were based on basic engineering fluid-flow fundamentals. However, relationships for calculation of the vapor flow rates from one tray to the next, based on pressure drops, depend upon the type of tray used in the column (perforated trays, bubble cap trays, or ballast valve trays). For the analysis in this model, perforated "trays" were chosen for the following reasons. First, the pressure drop relationships for perforated or sieve trays are much more straightforward and standard than for bubble cap or ballast valve trays. Ballast valve trays are generally proprietary in design, so each design has its own pressure drop relationships. Bubble cap trays have very complex pressure drop relationships based upon a number of bubble cap design parameters and are more susceptible to liquid height gradients, making tray hydraulics more involved. Second, most new columns are being built with perforated trays, making this model relevant. The weir heights are generally lower with sieve
trays, making overall column pressure drops lower than bubble cap or ballast valve trays. With rising energy costs, columns are being built with great numbers of trays to lower required reflux ratios. These larger columns make the overall pressure drop difference and the perforated trays' lower cost even more attractive. Third, it is doubtful that the study of column control for which this model was developed would be in any way substantially affected by the choice of vapor flow-pressure drop relationship. If in fact it is, this will have to be discovered by a later researcher.

Perforated trays exhibit relatively simple vapor flow pressure drop relationships. For practical purposes, the pressure drop between trays can be considered to be composed of two parts - the friction pressure drop due to vapor flowing through the perforations (holes) and the static head of liquid on the tray. (This ignores any additional resistance required to cause the vapor to flow upward through the liquid due to its buoyancy. At extremely high flow rates this would not be correct, but we are not interested in modeling the column under abnormal operating conditions.) Thus, given the current total pressure drop between two trays, and the liquid heights on those trays, the friction pressure drop available to cause flow through the tray holes may be calculated:

\[(h_f)_j = (P_j - P_{j-1}) - (h_w + h_{ow})_{j-1}\] (2-4)
where \((h_f)_j\) is the available friction pressure drop from stage \(j\) causing vapor flow through the holes in tray \((j-1)\) in feet. Using standard orifice flow relationships:

\[
(U_h)_{j+1} = (C_v) \left[ (12)(\rho_l)_j(h_f)_j / ((\rho_v)_{j+1})(0.186) \right]^{1/2} \tag{2-5}
\]

where \(C_v\) is a pressure drop coefficient based upon the tray thickness, hole diameter, and the fraction of the tray area which is holes, \((\rho_l)_j\) and \((\rho_v)_{j+1}\) are the densities of the liquid and vapor on each respective stage, and \((U_h)_{j+1}\) is the average velocity of the vapor through the holes of tray \(j\) in feet per second. Using equation (2-5), the molar vapor density, and the total hold area of the trays, the molar vapor rate from stage \((j+1)\) may next be computed.

**Top Vapor Rate**

The vapor rate from the top tray to the condenser is computed in a different fashion. This top vapor flow rate cannot be calculated as it was for all the other trays as a flow through an orifice. One of the other four basic relationships, mentioned in the introduction of this chapter, must be used instead. Using the concept of a flooded condenser, and neglecting vapor holdup, which is the situation being modeled here, it is clear that the top vapor rate must equal that rate at which vapor is being condensed by the condenser. Therefore an
energy balance can be used to compute the top vapor rate. Figure (2-2) shows the details of the condenser modeled here. Since the liquid level is purposely kept at a height which covers the lower part of the condenser tubes, the rate at which vapor condenses can be calculated by considering that only the exposed tube area extracts heat from the condensing vapor. This, of course, is a simplified model of the condenser, with the overall heat transfer coefficient of the condensing vapor section considered constant. However, even if the condensing vapor coefficient were calculated using some correlation, it would not materially affect the dynamics, since the primary controlling factor for the condensation rate is clearly the exposed area of the tubes. The higher the liquid level rises in the vertical condenser, the less area there is available for condensation, and the lower the vapor condensation rate becomes. As discussed elsewhere, used with an appropriate automatic control scheme, the vertical flooded condenser is an effective device for using the pressure in the column to adjust the vapor rate (boilup rate) in the column.

If \( h_{ct} \) is the total length of the vertical tubes which is available for heat transfer, and \( A_{htc} \) is the square feet of heat transfer area on the tubes per foot of length, the heat transfer area available is:

\[
A_{tc} = (h_{ct} - h_c)(A_{htc})
\]  \hspace{1cm} (2-6)
Figure 2-2. Flooded Condenser
The general energy balance for this simply modeled heat exchanger is:

\[ A_c = (U_c)(A_{tc}) (\Delta T_{lm}) \]  \hspace{1cm} (2-7)

where \( U_c \) is the overall heat transfer coefficient in the condensing section, and \( \Delta T_{lm} \) is the log mean average temperature difference. To simplify calculations, it was assumed that the coolant flow rate was great enough that the coolant temperature does not change appreciably. (Again this is not an important factor in the dynamics being studied here.) An alternate simplifying assumption would be to assume a fixed temperature rise in the cooling medium. Either of these assumptions merely negates the need to integrate in another spatial dimension.

Since the vapor enters at its dew point \( (T_2) \), and finally condenses at its bubble point \( (T_1) \), and these are known, \( \Delta T_{lm} \) may be computed. (Any subcooling of the condensed liquid trickling down the tubes is neglected. Clearly it is assumed that the \( T \) vs. \( Q \) curve is a straight line in order for the \( \Delta T_{lm} \) formula to apply.) This assumption is also not considered critical for the dynamics being studied:

\[ \Delta T_{lm} = \frac{T_2 - T_1}{\ln \left( \frac{(T_2 - T_c)}{(T_1 - T_c)} \right)} \]  \hspace{1cm} (2-8)
where $T_2$ is the temperature of the first tray (second stage), $T_1$ is the bubble point of the condensing vapor, and $T_C$ is the temperature of the cooling medium. The overhead vapor rate may then be computed by an energy balance:

$$V_2 = \frac{Q_c}{(\bar{\bar{H}}_v)_2 - (\bar{\bar{H}}_1)}$$

where $V_2$ is the overhead vapor rate, $(\bar{\bar{H}}_v)_2$ is the average molar enthalpy of the entering vapor at its dew point, and $(\bar{\bar{H}}_1)_1$ is the average molar enthalpy of the condensed liquid at its bubble point.

**DERIVATIVES OF INTEGRATED VARIABLES**

The integrated (dynamic) variables in the model are composition, temperature, pressure, and liquid height on each stage, as well as the liquid height in each downcomer. Note that the unique contribution of this model is the inclusion of pressure on each tray as a dynamic variable. By using the previously computed algebraic flows, the derivatives of the integrated variables may be calculated by total mole balances, component mole balances, enthalpy balances, and equilibrium relationships.

The differential equations describing the behavior of the variables on the trays are the most general in nature, and are representative of the equations for the
other stages. Derivations of the following equations may be found in Appendix A. Note that the dot (.) atop any variable indicates the time derivative of that variable.

TRAYS

Liquid Holdup

An overall material (mole) balance yields the time derivative of the total moles (M) on a tray:

\[ \dot{M}_j = V_{j+1} + (L_d)_{j-1} - V_j - L_j \]  

(2-10)

where \( \dot{M}_j \) is the time derivative of the moles on tray \( j \), \( V_{j+1} \), \( (L_d)_{j+1} \), \( V_j \), and \( L_j \) are the molar vapor rate leaving tray \( j+1 \), molar liquid flow rate leaving downcomer \( j-1 \), and molar vapor and liquid flows leaving tray \( j \), respectively. Using equation (2-10), the derivative of the liquid height on tray \( j \) may be computed:

\[ \dot{h}_j = \frac{\dot{M}_j}{(\rho_{lm})_j(A_t)} \]  

(2-11)

where \( \dot{h}_j \) is the derivative of the liquid height on tray \( j \), \( (\rho_{lm})_j \) is the liquid molar density on tray \( j \), and \( A_t \) is the active tray area.
Liquid Composition

To compute the derivatives of the mole fractions on each tray \((X_{i,j})\), component material balances are performed:

\[
\dot{X}_{i,j} = \frac{(V_{j+1})(Y_{i,j+1}) + (L_d)_{j-1}(X_{i,j-1})}{M_j}
\]

\[
-\frac{(V_j)(Y_{i,j}) - (X_{i,j})(L_j + M_j)}{M_j}
\]

where the \(X's\) and \(Y's\) are the liquid and vapor mole fractions respectively, of component \(i\) on the respective trays.

Liquid Temperature

The energy balance on each tray is used to compute the temperature derivatives:

\[
\dot{T}_j = \frac{(V_{j+1})(\bar{H}_v)_{j+1} + (L_d)_{j-1}(\bar{H}_l)_{j-1} - (V_j)(\bar{H}_v)_j}{(M)_j(C_{pl})_j}
\]

\[
-\frac{(\bar{H}_l)_j (L_j + M_j) - (M_j) \sum_{i=1}^{nc} (X_{i,j})(\bar{H}_l)_{i,j}}{(M)_j(C_{pl})_j}
\]

where \(\bar{H}_v\) and \(\bar{H}_l\) are the average molar vapor and liquid specific enthalpies for the respective trays. The terms
\((C_{pl})_j\) and \((H_{i})_{i,j}\) represent the average liquid molar heat capacity and individual component specific enthalpy (for each component \(i\)) on each tray \(j\). The index "nc" is the number of components. The relatively unfamiliar (not present in most other models) summation term in equation (2-13) represents the contribution by the composition derivative to the energy transient. It is important to note that this use of the heat balance differs substantially from most other models. In other models (where the pressure on each tray is independently known), the heat balance is used to solve for the vapor rate (assuming that any imbalance in heat results in changes in vapor generation). In this model, vapor rate leaving a tray is calculated by the previously described flow equations and the imbalance in the heat equation results in a change in the liquid temperature, and a corresponding change in pressure.

**Bubble Point Pressure**

The calculations involving the equilibrium relationships in most distillation models are usually bubble point calculations computing the bubble point temperature at the given pressure. Such calculations generally are of an iterative, or trial-and-error type. Clearly, computationally long iterative calculations need to be minimized in a computation scheme which requires many functional evaluations. In separate theses, Snyder (22)
and Tramontin (25) developed relationships in which the bubble point temperature of an equilibrium mixture is integrated at constant pressure. This concept was successfully applied by Yu (30). The main assumption in this concept, in this concept, and also for bubble-point iteration, is that the liquid on any stage is always at its bubble point. This, in turn, assumes that the equilibrium dynamics on any given stage are extremely fast compared to the other dynamics, and that each stage is perfectly mixed. These assumptions are vital to any practical dynamic distillation model. Equation (2-14), derived in Appendix A, computes the derivatives of all of the pressures except that in the condenser. (The condenser pressure is assumed to equal that of the top tray.) Equation (2-14) differs from the approach of Snyder, Tramontin, and Yu, in that the bubble-point pressure is integrated as a function of the temperature rather than vice-versa.

\[
P_j = \sum_{i=1}^{nc} (K_{i,j}) \left( \frac{\partial X_{i,j}}{\partial T} \right) (X_{i,j})(T_j) + \sum_{i=1}^{nc} \left( \frac{\partial K_{i,j}}{\partial T} \right) (X_{i,j})(T_j) \\
\sum_{i=1}^{nc} (X_{i,j})(K_{i,j})/P_j
\]

(2-14)

where \( P_j \) is the pressure derivative on each stage, \( K_{i,j} \) is the equilibrium constant of component \( i \) for stage \( j \), and
\( \left( \frac{\partial K}{\partial T} \right)_{i,j} \) is the partial derivative of \( K_{i,j} \) with respect to the temperature.

**Feed Tray**

The previous differential equations lack the provision of a feed to the stage. If a liquid feed is assumed, equation (2-10) would become equation (2-15) for the feed stage.

\[
\begin{align*}
\dot{N}_j &= V_{j+1} + (L_d)_{j-1} - V_j - L_j + F \\
\end{align*}
\]  

(2-15)

The composition derivative calculation for the feed stage simply adds to the numerator of equation (2-12) the term \((F)(X_f)_i\), where \((x_f)_i\) is the mole fraction of component \(i\) in the feed. To compute the temperature derivative of the feed stage, equation (2-13) is modified to include \((F)(\bar{H}_f)\) in the numerator, where \(\bar{H}_f\) is the average molar specific enthalpy of the feed. The equation which calculates the pressure derivative is unchanged on the feed stage.

**Reboiler Equations**

The differential equations describing the reboiler are very similar to the previous equations. The liquid exit flow, \(L_j\), in equations (2-10), (2-12), and (2-13), is replaced with the bottoms flow rate, \(W\), which is a controlled variable. Obviously, there is no vapor entering the reboiler, unlike the other stages.
The temperature derivative computation for the reboiler also involves an additional term, that of the heat added to the reboiler. Since many reboiler heating fluids are condensing vapors (often steam), the entering temperature is assumed very close to the exit temperature. That is, sensible heat changes of the steam are neglected. In this model, the reboiler is considered a perfectly-mixed vessel, so the temperature of the boiling liquid is assumed uniform. Therefore, the heat transferred to the reboiler is merely:

\[ Q_r = (U_r)(A_{tr})(T_{steam} - T_{reb}) \]  

(2-16)

where \( U_r \) is the overall heat transfer coefficient in the reboiler \( A_{tr} \) is the reboiler heat transfer area, \( T_{steam} \) is the temperature of the heating fluid, and \( T_{reb} \) is the temperature of the boiling liquid in the reboiler. The energy balance, rearranged to compute the derivative of the reboiler temperature appears as:

\[
\frac{\Delta T_{reb}}{\Delta t} = \frac{(L_{nt})(H_1)_{nt} + Q_r - (V_{nr})(\bar{H}_v)_{nr} - (\bar{H}_l)_{nr}(M+W)}{(M)_{nr}(C_{pl})_{nr}} - \sum_{i=1}^{nc} (X_{wi})(H_{lw})_{i} \]

(2-17)
where the subscripts "nt" and "nr" represent the stage numbers of the last tray and reboiler, and \((X_w)_i\) is the special designation for the composition of the reboiler contents and bottoms product. The other terms are similar to those in equation (2-13), except for \((H_{lw})_i\), which is the individual component liquid enthalpy of component \(i\) in the reboiler.

**Top Tray**

The top tray is simulated exactly like the other trays except that the reflux rate \(R\) replaces \((L_d)_{j-1}\) and \((X_d)_{j}\) represents the mole fraction of component \(i\) in the distillate and reflux. The reflux is assumed to distribute evenly over the top tray, neglecting liquid gradients and assuming complete liquid mixing.

**Condenser**

Equations (2-10) - (2-17) describe the dynamics in all the trays and the reboiler, but as previously stated, the condenser is modeled differently. First, the condenser is simulated as two separate parts - the top portion where the vapor is condensing and the bottom portion where the liquid accumulates.

The relationships in the top portion of the accumulator were previously described in the calculation of the vapor rate from the top tray. As stated, momentum balances and vapor holdup in this section were neglected.
Because the liquid running down the tubes and vapor holdups are so minute in the condensing section, overall and component balances are not practical. The energy balance was used for the vapor rate calculation, so the relationship remaining is the equilibrium relationship. This is used to compute the derivative of the bubble point temperature of the of the condensing vapor, which changes with pressure and composition. This temperature is used in the energy balance governing the top vapor rate, and affects the enthalpy of the accumulator section. The relationship which produced equation (2-14) may be used to compute the derivative of the bubble point temperature in the condenser. Since the vapor dynamics are so fast, it was assumed that the composition of the condensing liquid (which completes condensation at its bubble point) is the same as the vapor leaving the top tray at all times. Therefore, the derivatives of the composition of the condensing liquid are the same as the derivatives of the top vapor mole fractions.

\[ \dot{Y}_{i,2} = (X_{i,2}) \left[ \left( \frac{\partial k}{\partial T} \right)_{i,2} \left( \frac{\partial (T)}{\partial T} \right)_{i,2} \right] + (K_{i,1}) \left( \frac{\partial (X_{i,2})}{\partial T} \right) + (K_{i,1}) \left( \frac{\partial (X_{i,2})}{\partial T} \right) \]

(2-18)

Since the pressure in the condenser equals the pressure on the top tray, the pressure derivative is the same for each. Thus, the condenser bubble point derivative is calculated by:
\[ T_1 = \sum_{i=1}^{nc} \left( K_i \right) \left( X_i \right) - \sum_{i=1}^{nc} \left( X_i \right) \left( P_i \right) \left( P_1 \right) \]

where the subscript 1 designates the top stage, the condensing section. The accumulator (which in this model is not a separate vessel but is the lower part of the condenser which contains liquid) is among the simplest of the sections in the column simulator. The overall material balance is:

\[ \dot{M}_a = V_2 - R - D \]

where \( M_a \) is the total moles in the accumulator section of the condenser and \( R \) and \( D \) are the reflux and distillate, both controlled variables. As with the trays, knowing the molar density and the effective cross-sectional area of the condenser, equation (2-20) may be converted to a height derivative \( h_c \). The component material balances for the accumulator and distillate may be written as:

\[ \dot{(X_D)}_i = \frac{(V_2)(X_{i,2}) - (R + D + \dot{M}_a)(X_{d,i})}{M_a} \]
It is reasonable to assume that the accumulator liquid will give up a small amount of sensible heat to the cooling fluid. This is calculated as follows:

$$Q_{\text{sens}} = (U_{cl})(A_{htc})(H_c)(T_{\text{acc}} - T_{\text{cool}})$$  \hspace{1cm} (2-22)

where $U_{cl}$ is the (usually small) heat transfer coefficient for the condensate and $T_{\text{acc}}$ is the temperature of that condensate in the accumulator. The subsequent energy balance yields the derivative of $T_{\text{acc}}$:

$$T_{\text{acc}} = \frac{(V_2)(\bar{H}_1) - (R+D+\dot{M}_a)(\bar{H}_1)_{a} - Q_{\text{sens}}}{(M_a)(C_{pl})}$$

$$- \sum_{i=1}^{nc} \frac{(X_d)_i(H_i)_{i,a}}{(M_a)(C_{pl})}$$  \hspace{1cm} (2-23)

where the subscript "a" denotes the condition in the accumulator.

**Downcomers**

The downcomer dynamics should be modeled because the holdup in each downcomer is of the same order of magnitude as that on each tray. Clearly, to model the downcomer liquid as strata of liquid (i.e., plug flow), would not be accurate because the impact of the liquid from the
tray above would cause considerable backmixing. The downcomers contain only one input (liquid flow from the tray above) and one output (liquid flow to the tray below). Thus, each downcomer may be considered to be an extension which serves merely as an additional holdup. The temperature and composition in the downcomer then with little error may be assumed to be those of the tray above. At the beginning of this study, energy and individual component balances were included, modeling the liquid as perfectly mixed. Later, however, it was discovered that these balances could be excluded, saving considerable computer time with very little effect on column behavior. These studies were carried out with these simplifications. The possible effects of adding the energy and component balances on control behavior are left to be examined in later research. Therefore, the material balance is the only relationship used in the downcomers. The simple differential equations is:

\[
(M_d)_j = L_j - (L_d)_j
\]  

(2-24)

where \((M_d)_j\) is the total moles in downcomer \(j\). Using \(A_{dc}\) the cross-sectional area of the downcomer, and \((\rho_{lm})_j\) the liquid molar density of both tray \(j\) and downcomer \(j\), the derivative of the downcomer liquid height may be computed:
MANIPULATED VARIABLES

The previous equations describe the behavior of algebraic and integrated variables through the column. Also integrated are the reflux rate, distillate product takeoff rate, and bottoms product rate. These however are manipulated variables, therefore, their derivatives, once the control system is described, are functions of other derivatives, such as liquid height, temperature, and pressure. These relationships are discussed in Chapter 4.

ARRANGEMENT OF COMPUTATIONS

To recap previous statements, the model computations were ordered such that no equation needs a value which has not yet been calculated on the particular time step. First, the algebraic variables are computed using the integrated variables, which were all determined by performing a time step in the integration. Next, the algebraic variables are in turn used to compute the derivatives of the integrated variables to be used in the next integration. However, there are more subtle sequencing maneuvers required to make such that each algebraic and differential equation uses "fresh" values. For example,

\[
b_{dc} = \frac{(M_d)_j}{(\rho_{lm})_j (A_{dc})}
\]  

(2-25)
when the calculation of a derivative requires the derivative of another variable, the derivative needed should be calculated before the derivative that needs it.

Initialization Computations

Upon beginning a computer "experiment", the first step is to use a suitable steady-state solution method to compute the flows, temperatures, pressures, and compositions for the initial conditions. This is because all "experiments" begin at steady-state. The steady-state computations were made in a separate model via the method of Wang and Henke (27), which had been modified to include the tray hydraulics relationships discussed in this chapter.

Given the steady-state initial conditions, initialization is completed by the program computing physical properties and liquid heights. These heights are calculated by the reverse analogs of equations (2-1) through (2-9).

Use of Vectors for the Variable Storage

After the initialization procedure, the integration process begins. Obviously, there are a large number of differential equations in a simulated column of any realistic number of stages. It would be quite impractical to integrate and handle the variables and their derivatives in their mnemonic forms. In terms of FORTRAN
programming language, these should be placed in vector form for easy application of "DO LOOP" programming. However, a vector format alone would produce a very cryptic code when computing the flows and derivatives. In order to use the respective advantages of the mnemonic and vector notations, routines were developed to convert between the two. When the integration routine calls for the function evaluation routine, the integrated variables are transferred from the vector format to the recognizable mnemonic or "named" format. After derivatives have been computed, the integrated variables and their respective derivatives are both transferred back to the vector form before being sent back to the integration routine.

**Sequencing of Calculations in the Model**

Upon being called by the integration routine, the function evaluator first transfers the integrated variables from the vector form into mnemonic variables, then computes the physical properties - enthalpies, densities, and vapor-liquid equilibrium constants. Since the vapor mole fractions are not integrated, they are next computed by using previously computed equilibrium constants. Using equations (2-6) through (2-9), the top vapor rate is evaluated. Next the other vapor rates are computed by equations (2-4) and (2-5). Equation (2-1) is then used to calculate the liquid flow rates over the
weirs. Then equations (2-2) and (2-3) evaluate the liquid flows onto the trays from the downcomers.

After the flow rates have been computed, the derivatives are determined. First, equations (2-24) and (2-25) evaluate the derivatives of the liquid heights in the downcomers. Next, the derivatives of liquid height, composition, and temperature are evaluated for the top tray. Next, equations (2-10) - (2-13) are used to compute the height, composition, and temperature derivatives for all the other trays. Then these same derivatives are calculated for the reboiler. Subsequently, equation (2-14) computes the pressure derivative for all the trays as well as the reboiler. Using equations (2-18) and (2-19), the derivative of the bubble point temperature of the condensing top vapor is determined. Afterwards, equations (2-20) and (2-21) compute the derivatives of liquid height, composition, and temperature in the accumulator section of the condenser and for the distillate product and reflux.

After the flows and derivatives have been computed, the automatic control routine is called. This section uses the values of the variables as well as their derivatives to evaluate the derivatives of the manipulated variables (distillate and bottoms product rates, reflux rate, steam temperature, etc.). Upon the return from the "controller", the integrated variables and the derivatives
are converted back to the vector form for integration. This sequence is outlined in Table 2-1.
TABLE 2-1

SEQUENCING OF COMPUTATION IN FUNCTIONAL EVALUATION MODEL

1. Convert integrated variables from vector form to mnemonic form.
2. Compute liquid and vapor enthalpies and densities and vapor-liquid equilibrium constant on all stages.
3. Compute vapor mole fractions for all stages.
4. Compute top vapor flow rate.
5. Compute all other vapor flow rates.
6. Compute liquid flow rates over weirs.
7. Compute liquid flow rates from under downcomers.
9. Compute liquid height, temperature, and composition derivatives on trays.
10. Compute height, temperature, and composition derivatives in reboiler.
11. Compute pressure derivatives on all trays and reboiler.
12. Compute derivatives of bubble point temperature of the condensing top vapor.
15. Convert integrated variables and derivatives to vector form.
From the outset of this research, the need was seen for an extremely efficient numerical integration algorithm to avoid excessive computer time. The fact that the simulation model was quite large and was expected to be very stiff justified research on integration techniques. Stiffness is a phenomenon that occurs when a relatively large system of differential equations contains a combination of slow and fast-acting differential equations, requiring a smaller stable step size than would normally be expected. One unusual feature of stiff systems is that (contrary to many non-stiff systems) higher order integration methods show no substantial superiority over lower-order methods such as modified Euler. This concept and its application to linearized dynamic distillation models is discussed in an article by Tyreus, Luyben and Schlesser (26).

Since the evaluation of the derivatives takes the major portion of computation time, the most desirable integration method is the one which is able to handle stiff systems (i.e., use a reasonable step size) and also uses as few functional evaluations per time step as possible, for equivalent accuracy.
Among the most popular integration methods used for integrating stiff differential equations are predictor-corrector methods such as those of Adams and Moulton (7), and Milne (16). A subset of these multi-step methods are iterative methods, such as Hamming's (9). (Note that the term "multi-step" refers to predictor-corrector methods, rather than methods such as Runge-Kutta which are purely explicit in nature.) Although these techniques are fairly efficient, they all have two major drawbacks. First, they are rather complicated to program, particularly when starting the integration and changing step size. Second, these methods generally require the storage of many extra "previous" points for automatic step size computation. This drawback is particularly detrimental when the user's computer installation places a premium on core memory.

Also popular are simpler (lower order) predictor-corrector methods. These techniques have the advantages of relative programming ease and simplicity when an automatic step size regulator is employed. And it has been claimed that for stiff systems they are more efficient than the higher order methods, since the higher order methods do not achieve the expected gains in step size and require more time when step size is changed. One of the most-used algorithms is the "improved Euler" or Heun formula:
\[ Y^0_{n+1} = Y_n^1 + (h)(f(X_n, Y_n^1)) \] predictor step \hspace{1cm} (3-1)

\[ Y^1_{n+1} = \frac{Y_n^1}{2} + \frac{h}{2}(f(X_n, Y_n^1) + f(X_{n+1}, Y_{n+1}^0)) \] corrector step \hspace{1cm} (3-2)

where \( X_n \) is value of the independent variable on the "nth" time step, \( Y^0_{n+1} \) is the predicted value of the dependent variable on the "n+1th" time step, \( Y^1_{n+1} \) is the corrected value of the dependent variable, \( h \) is the step size of the independent variable and \( f \) is the derivative of \( Y \). Obviously, the algorithm employs a first-order predictor and a second-order corrector, that is, a first-order correct equation computes the first estimate of the dependent variables, while the second-order correct equations improves the estimate. An important point is that the predictor equation is explicit in \( (Y_{n+1}) \) (which makes it the "predictor") and the corrector equation is implicit in \( (Y_{n+1}) \). Thus this corrector step provides improved accuracy and stability to the numerical integration. (In normal usage, the corrector equation is applied only once, because the increased truncation accuracy is not usually merited by the extra computation time. Better results are achieved from using only one corrector application and a slightly smaller step size.)

When an algorithm consists of a predictor of one order, but a corrector of another higher order, the truncation error of the algorithm will be significantly higher
than could be achieved by using a predictor of higher order. This concept may be applied to the improved Euler technique with a second-order predictor equation:

\[ y_{n+1}^0 = y_n^1 + \frac{h}{2} (3f(X_n, y_n^1) f(X_{n+1}, y_{n+1}^1)) \]

where \( x_{n+1} \) and \( y_{n-1} \) are the values from the previous step. This second-order predictor uses no more new functional evaluations per step than its first order counterpart and adds very little numerical complexity. The only disadvantage of the second-order predictor is the requirement of the storage of the functional evaluations for one previous integration point. Unfortunately, this disadvantage becomes exacerbated when automatic step size regulation is performed. However, the complications resulting from the storing of previous points needed is much smaller than, for example, fourth-order integration methods.

The above two methods require only half the number of functional evaluations per step than the very popular fourth-order Runge-Kutta techniques, but twice as many as the simple Euler algorithm (which is not itself a predictor-corrector scheme). As previously state, when dealing with large stiff differential systems, the number of functional evaluations should be optimized. The desired product of this optimization is the minimization of computer (cpu)
time needed for a given simulation time and a given accuracy. In this thesis research, an important adjustment to any predictor-corrector algorithm has been developed which uses only one functional evaluation per step but provides truncation accuracy equivalent to that of the unchanged algorithm, which requires two functional evaluations per time step. This new method when applied to the improved Euler method achieves the same order of local error, but can run roughly twice as fast because it uses only half as many functional evaluations per integration step. This adjusted algorithm, which is temporarily and rather immodestly termed the Johnson-Stewart Modified Euler (JSME), achieves the savings by calculating derivatives (functional evaluations) only at the predicted points for each step. Although all predictor-corrector algorithms assume that on each step the latest available information (the corrected points) should be used to calculate derivatives for use in the predictor equation to provide increased accuracy, it can be shown that the predicted and corrected values of the dependent variable are so close together that the slight improvement in accuracy that results from using the corrected value instead of the predicted value to calculate the derivative is of a higher order than the accuracy of the step (See Appendix B) and therefore does not significantly lower the accuracy of the algorithm. The proposed method capitalizes on this fact by never making a functional
(derivative) evaluation using the corrected point. The new proposed JSME algorithm (which was used in this research is:

\[ Y_{n+1}^0 = Y_n^1 + \frac{h}{2}(3F(X_n, Y_n^0) - f(X_{n-1}, Y_{n-1}^0)) \]  

**second-order predictor**  

\[ Y_{n+1}^1 = H_n^1 + \frac{h}{2}(f(X_n, Y_n^0) + f(X_{n+1}, Y_{n+1}^0)) \]  

**second-order corrector**  

Equation (3-4)

Equation (3-5)

The JSME algorithm may be used for a first-order predictor equation instead of the second-order predictor equation given in equation (3-4), and the concept of calculating the function only for predicted points can be extended to any predictor-corrector algorithm.

Two major points of concern pertaining to numerical integration are stability and truncation error. Particularly when dealing with stiff differential systems, the stability of the integration algorithm is of major concern. Whenever any derivative becomes relatively high, high-frequency perturbations often become unmanageable. Also important is the local truncation error, for these errors can accumulate and leave the final value of the integrated variable a considerable distance from the "true" solution. One of the most popular criteria used in multistep integration formulas for controlling local truncation error is the absolute value of the differences
between the predicted and corrected values of the integrated variable divided by the corrected value. This equation is:

\[
\frac{Y^1_{n+1} - Y^0_{n+1}}{Y^1_{n+1}} \leq \varepsilon \tag{3-6}
\]

where \(\varepsilon\) is a small positive number.

It can be shown (5) that for a predictor-corrector algorithm, the numerator of equation (3-6), is proportional to the truncation error of the variable \(Y\) on any given step. Thus, by imposing equation (3-6) as a requirement to be met, this error, relative to the current value of \(Y\), may be kept below some small number of each integration step. The quotient in equation (3-6) is kept within present limits by adjusting the step size of the integration.

\[
\varepsilon_1 \leq \frac{Y^1_{n+1} - Y^0_{n+1}}{Y^1_{n+1}} \leq \varepsilon_2 \tag{3-7}
\]

In practice, it appears that \(\varepsilon_1\), should be roughly 1 or 2 orders of magnitude less than \(\varepsilon_2\), to avoid having the step size fluctuate unnecessarily.

This step size regulation procedure is easily applied to the integration of a single differential equation. For systems of differential equations, however, the method is modified, using only slightly more complex logic. If the quotient in equation (3-7) is greater than
the maximum limit for any of the differential equations, the step size should be decreased (normally halved). If the quotient in equation (3-7) is smaller than the minimum limit for all of the differential equations, the step size should be increased (normally doubled).

Clearly, if on any given step, the step size is increased, the integrated variables and their associated derivatives are valid since the truncation error was acceptable, and the integration may proceed. On the other hand, if the step size is decreased, then the truncation error was not acceptable, so the last computed values of the integrated variables contain too much error. Many algorithms call for the recalculation of the last point on that basis. However, intuitively, if the integration has been proceeding and the test fails, the margin of failure would likely be quite small. Tests have proven this assumption to be true. Therefore, if the maximum tolerances are chosen slightly smaller than that required for stability and accuracy, the last calculated values may be considered valid, and the integration may proceed to the next step using the new step size, saving the computer time required to re-calculate the points. This procedure was followed in this work.

Obviously, if the step size is changed on any given step, the values of $Y^n_0$, $f(x^n,Y^n_0)$, $Y^n_{n-1}$, and $f(x_{n-1},Y^n_{n-1})$ must be stored for use in equation (3-4) and (3-5) on the next integration step. This is because these equations
assume that the step sizes separating the points are equal. In such cases, the back values must be recalculated. Back-integration would prove too time consuming, so second-order (quadratic) interpolation between the calculated points is used. This is why step sizes are most often halved or doubled, as this makes the interpolation process easier. However, this does require the storage of additional previous points, which are not needed if the step size is doubled. The previously-stated concept that fourth-order multistep methods require extensive back-point storage is borne out by this analysis.

The proposed JSME integration technique has been successfully used by others (24), providing external verification of the validity of the algorithm.

To demonstrate the effectiveness of the proposed algorithm, a simple test was devised. This test was to integrate sine(x) over a range of x from zero to 314.16 (100\pi). The differential equation describing sine(x) is:

\[ y'' + y' = 0 \]  \hspace{1cm} (3-10)

which is a second-order differential equation. This can be converted into two first-order equations by substitution:

\[ y'_2 = y_1 \]  \hspace{1cm} (3-11)

If \( y_1 \) is sine(x), then \( y_2 \) is cosine(x), and the following differential equations may be written:
\[ Y_1' = Y_2 \]  
(3-12)

\[ Y_2' = -Y_1 \]  
(3-13)

where the initial conditions of \( Y_1 \) and \( Y_2 \) are zero and one respectively.

The first test was with a constant step size of \( 10^{-3} \). The comparisons among the simple Euler equation, between the improved Euler algorithm with second-order predictor are shown in Table 3-1. The values of \( Y_1 \) were compared with \( \sin(x) \) to calculate the relative error at various points. Table 3-1 shows that the relative errors of the two second-order methods are virtually the same, with substantially less error than the simple Euler equation. This graphically illustrates that second-order accuracy can be achieved with one functional evaluation per time step. Also quite evident is that the truncation error is propagated quite markedly in the case of simple Euler integration. However, both second-order methods show a decrease in error as the integration proceeds. This dramatically shows the advantages of the corrector equation.

The second test was very similar to the first, except that automatic step size adjustment was utilized and the Euler equation was not tested. (Since it is not a predictor-corrector method, the automatic step size adjustment procedure required is different from that used
The values of $e_1$ and $e_2$ for equation (3-9) were $1.0 \times 10^{-8}$ and $1.0 \times 10^{-6}$, respectively. The results, shown in Table 3-2, show substantially the same promising results as shown in Table 3-1. The average step sizes for both were approximately $2.2 \times 10^{-3}$ time units.

A number of other simple tests (employing only a few simultaneous differential equations) were also performed, all tests giving results similar to the above example. In addition, the algorithm is used in this research, in that of a Master's thesis (24) and in other research in the LSU Chemical Engineering Department. In all use to date, the basic advantage of the JSME algorithm has been realized. The equivalent accuracy of the improved Euler has been achieved with one half the functional evaluations, thus, in large models, half the computer time.
TABLE 3-1

COMPARISON OF SIMPLE EULER, IMPROVE EULER, JSME ALGORITHMS

SINE(X) WITH A CONSTANT STEP SIZE

<table>
<thead>
<tr>
<th>X</th>
<th>Improved Euler</th>
<th>JSME</th>
<th>Euler</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.559 x 10^{-3}</td>
<td>1.571 x 10^{-3}</td>
<td>1.264</td>
</tr>
<tr>
<td>50</td>
<td>1.531 x 10^{-3}</td>
<td>1.536 x 10^{-3}</td>
<td>2.538</td>
</tr>
<tr>
<td>100</td>
<td>1.416 x 10^{-3}</td>
<td>1.417 x 10^{-3}</td>
<td>5.133</td>
</tr>
<tr>
<td>150</td>
<td>1.319 x 10^{-3}</td>
<td>1.218 x 10^{-3}</td>
<td>7.794</td>
</tr>
<tr>
<td>200</td>
<td>0.925 x 10^{-3}</td>
<td>0.922 x 10^{-3}</td>
<td>10.52</td>
</tr>
<tr>
<td>250</td>
<td>0.511 x 10^{-3}</td>
<td>0.507 x 10^{-3}</td>
<td>13.32</td>
</tr>
<tr>
<td>300</td>
<td>-0.063 x 10^{-3}</td>
<td>-0.068 x 10^{-3}</td>
<td>16.18</td>
</tr>
</tbody>
</table>

Note: Both algorithms used second-order predictors, and a constant step size of 1.0 x 10^{-3}. 
TABLE 3-2

COMPARISON OF IMPROVED EULER AND JSME ALGORITHMS
INTEGRATING SINE(X) WITH VARIABLE STEP SIZE

<table>
<thead>
<tr>
<th>X</th>
<th>Improved Euler</th>
<th>JSME</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.427</td>
<td>1.424</td>
</tr>
<tr>
<td>50</td>
<td>1.251</td>
<td>1.646</td>
</tr>
<tr>
<td>100</td>
<td>1.281</td>
<td>1.277</td>
</tr>
<tr>
<td>150</td>
<td>1.044</td>
<td>1.114</td>
</tr>
<tr>
<td>200</td>
<td>0.790</td>
<td>0.900</td>
</tr>
<tr>
<td>250</td>
<td>0.437</td>
<td>0.492</td>
</tr>
<tr>
<td>300</td>
<td>-0.069</td>
<td>-0.092</td>
</tr>
</tbody>
</table>

Note: Both algorithms used second-order predictors and variable step size.
CHAPTER 4

AUTOMATIC CONTROL SYSTEM

INTRODUCTION

The control system model in this research was based on an analog control system first proposed by Wright and Johncock (28,29). A commercial version of this type of system has been marketed under the trade name "Fractronic" by Transmation, Inc. of Rochester, N. Y. The most singular feature of the Fractronic system is that reboiler heat (boilup rate) is manipulated to control the pressure at the top of the distillation column. In order to do this, it is necessary to operate with a "flooded" condenser, i.e., with the condensed distillate liquid level somewhere inside the condenser rather than in a separate accumulator. This type of control system has in recent years enjoyed increasing popularity in the field, and is apparently preferred over other control systems by many control engineers who have tried it. To date, there has been no simulation and analysis research done on this control system, presumably because of the difficulty of modeling the pressures in a column. The system which was simulated and studied in this research utilizes a flooded condenser and manipulates reboiler heat to control the column pressure, as in done in the Fractronic system.
See Figure (4-3). The purpose of this research was to investigate the utility of this particular control strategy, used in conjunction with material balance control of top product quality.

In the following sections, a discussion of distillation column control is presented to give insight into the rationale for the choice of this system for study.

In Chapter 1, it was mentioned that the reflux rate and both product rates are integrated variables. This is not exactly correct. The fractional opening of the respective valves are integrated, thus they have derivatives. The flow rates through those valves may then be computed as a function of the fraction of valve opening, valve size and characteristics, and the pressure drops across the respective valves.

Traditional Control of Product Quality

For many years, it was considered that top product quality (purity) should be controlled by manipulating R, the external reflux rate to the column and that bottoms product quality should be controlled by manipulating V, the boilup rate from the reboiler. (See Figure 4-1). The product rates are generally set by level control on each respective end of the column. In practice, the severe interactions between the two product purity control loops effectively prevented the use of two tightly tuned loops, one on each product. As a result, only one
Figure 4-1. Conventional Column Control of Distillate Product Quality
product quality can be controlled, while the other must be left essentially uncontrolled (i.e., with an extremely low gain, or manually adjusted). Accordingly to meet specifications on both products, it was found necessary to set either the reflux rate or the boilup rate at some high value manually, thereby insuring that the separation capacity of the column is kept high, then to use a tuned control loop to maintain one of the products on specification. The high separation capacity of the column insures that the other product quality is as high as possible at all times. Clearly this procedure is wasteful of energy, although it does succeed in maintaining both product qualities within specifications as long as disturbances are not too large.

Material Balance Control

Shinskey (21) and others recognized that this traditional control system is not fundamentally sound because both manipulated variables in reality adjust the same basic variable, the yield of products (D/F and W/F). When either one of the manipulated variables R or V is held constant, adjustment of the other one simply changes the product yields. But in order to change the separation capacity of a column, both of these variables must be increased or decreased together. The two fundamental variables which determine product quality of an operating column are now recognized to be product yields (D/F and
W/F) and separation capability (R/F and V/R together). The phrase "material balance control" was coined to describe a control system which manipulates product yields without affecting the separation capability of the column, and permits manipulation of separation capability of the column without affecting product yields. This is accomplished by manipulating the top (or bottom) product flow rate with one control loop while adjusting boilup rate (or reflux rate) with the other loop. (See Figure 4-2). As an example of how material balance control is useful, a steady-state analysis may be examined. Suppose that a very pure top product is required and that "X" moles of the lightest (light key) component is introduced into the feed. If more than "X" moles are drawn off as the distillate product, no amount of reflux can possibly achieve a pure product. However, if the distillate rate is decreased to "X" moles or less, a basically pure product is then possible. Even if the separation capability of the column operation is low, a pure distillate product can usually be achieved by cutting back severely on distillate yield. This of course results in an impure bottoms product and a loss of distillate into the bottoms product. In the material balance control scheme of Figure 4-2, two liquid level control loops permit a change in D to be accompanied by the necessary change in W at the bottom of the column, and correspondingly, a change in reboil rate (V) to be accompanied by the necessary change in R.
Figure 4-2. Typical Material Balance Control of Distillate Product Control
in the top of the column. Unfortunately, however, the associated changes are not accomplished without considerable lags, and in both cases, the liquid dynamics on each tray in the column are involved in the sequence, so that a very long time indeed may transpire before a step change in either manipulated variables \( D \) or \( R \) is propagated through the column and new flow conditions established.

**Floated Condenser**

The use of a floated condenser has recently become recognized as a means of eliminating both the accumulator drum and the liquid level controller on the accumulator level. Instead, the column pressure, which in other control schemes is controlled independently of the product quality control system, can be utilized to transmit information rapidly from the top of the bottom of the column, thereby speeding up substantially the operation of a material balance scheme. In Figure 4-3, the use of boilup rate to maintain column pressure, in conjunction with a material balance control loop on the distillate rate, can be seen to provide the desired advantages. Whenever the distillate rate is changed, there is no effect upon the reflux rate, which is adjusted by a separate controller. Consequently, the liquid level inside the condenser changes, causing a change in the heat removal rate (by changing the available condensation heat transfer area), which in turn causes the pressure in
Figure 4-3. Material Balance Control of Distillate Product Quality
the top of the column to change. This all happens quite fast. The pressure control loop then adjusts the column boilup rate to control the pressure (this is also very fast because vapor rates propagate up the column very swiftly) and finally the liquid level control loop at the bottom of the column adjusts the bottom product rate. Note how much faster this response can be visualized to be than the slower process of cascading liquid rates down the column, which is required by the material balance scheme without a flooded condenser. It is this speedup of column dynamics afforded by the pressure control loop which is the primary feature of the Fractronic control scheme, and which is simulated in this research. Note also that whenever the reflux rate \( R \) is changed, the pressure control loop also transmits this change to the boilup rate, causing \( V \) to change very quickly, rather than requiring the cascade of the liquid down the column to transmit the change. The pressure control feature is similar in its action to a feed forward ratio controller, as it causes \( W \) and \( V \) to respond so quickly to changes in \( D \) and \( R \), respectively. Whether or not this increase in response action rate results in improved column control is the basic justification for this research.

**PRESSURE CONTROL**

The literature concerning distillation control has produced myriad schemes to control column pressure (see
Chapter 2). Some methods use the introduction of inert gases. Others use level control on flooded condensers or vapor bypass lines. The underlying theme these methods share is manipulation of variables in the top of the column system to control the top pressure. With this tone set, why would one propose to control the column top pressure with the manipulation of the reboiler heat input at the bottom of the column? As was explained in the introduction to this chapter, the rapid propagation of vapor rate changes from the top of a column affords the possibility that use of a pressure control system of the type studied here may improve other column response dynamics substantially. Even though a pressure wave causes by a boilup change may have to pass through many trays and travel a relatively long distance to get to the top of the column, the complete column response to this adjustment may still be fast enough to provide adequate pressure control. Its use in industry at the present attests to this.

In Chapter 1, mention was made of two contrasting approaches to pressure control. One approach is simply to maintain as closely as possible a constant column top pressure by using schemes which do not communicate with the control loops which maintain product purities. The other approach (the one used in this research) is to use the column pressure as an integral part of the overall control scheme for product purity. This approach is realized
in this research by using pressure to manipulate the reboiler heat.

The Transmation control system discussed by Wright and Johncock (28,29), utilizes a fairly sophisticated network of flow pressure temperature transmitters to compute the quota of reboiler heat needed which, using feed-forward and cascade controllers, manipulates the flow of hot oil to the reboiler. (Such systems are needed when a hot oil source of heat is used because the heat transferred is not proportional to hot oil flow, and because the hot oil inlet temperatures may change). In this research, the link between the pressure transmitter and the steam control valve is a simple proportional-integral controller, shown in Figure 4-3. Again, this version of the Fractronic control scheme is simplified, but this research is interested primarily in assessing the nature of the response in the reboiler-top pressure control loop.

Note that the dot (.) atop any variable indicates the time derivative of that variable.

The differential equation describing the action of the reboiler steam controller is:

\[ \dot{f}_s = -K_s \left( \dot{P}_1 + \frac{P_1 - P_{ls}}{T_{Is}} \right) \]

where \( f_s \) is the fraction of the steam valve opening, \( K_s \) is the controller gain, \( P_{ls} \) is the set point of the top
pressure, and $T_l$ is the controller reset (integral) time. For an increase in top pressure, a decrease in reboiler heat is described to lower the pressure throughout the column, and ultimately, the top pressure. Hence, the negative sign in equation (4-1). The steam flow through the valve and the pressure and temperature of the steam are modeled by the following three equations:

$$P_{\text{steam}} = f(T_{\text{steam}})$$  \hspace{1cm} (4-2)

$$W_{\text{steam}} = (U_r)(A_{tr})(T_{\text{steam}}T_{\text{reb}})/\lambda_{\text{steam}}$$  \hspace{1cm} (4-3)

$$W_{\text{steam}} = (C_v)_s(A_s)(f_s)(P_u-P_{\text{steam}})^{1/2}$$  \hspace{1cm} (4-4)

where $P_{\text{steam}}$ is the pressure of the steam in the reboiler, $\lambda_{\text{steam}}$ is the latent heat of vaporization of the steam as a function of temperature, $W_{\text{steam}}$ is the flow rate of the steam, $(C_v)_s$ is the valve constant, $A_s$ is the maximum valve area, and $P_u$ is the steam pressure upstream of the valve. Equation (4-2) represents the vapor pressure relationship of the steam (neglecting dry superheat). Equation (4-3) is the energy balance for the condensing steam (neglecting subcooling), and equation (4-4) represents the valve pressure drop relationship. These three equations must be solved simultaneously (by the Newton-Raphson technique since they are non-linear) to compute $T_{\text{steam}}$ used in equation (2-15).
COMPOSITION CONTROL OF ONE PRODUCT

Assuming that the distillate product is the one whose quality is considered to more important, its composition is controlled by the manipulation of the distillate product rate (material balance control). (Clearly there are many cases where the bottoms product composition is to be controlled, rather than the distillate product composition. The following discussion still applies.) In general, there are two possible controlled variables available to composition control. The first is a composition itself, generally the composition of the overhead vapor. This involves expensive (and sometimes cantankerous) analyzers, but is a popular option. The second (used in this research) is inferential control by monitoring a temperature, the top tray in this research. As with the pressure control, the composition controller is a simple proportional-integral unit.

The differential equation for this valve is:

\[ f'_D = -\left( K_D \right) \left( \frac{T_2}{T_{ID}} + \frac{T_2 - T_{2s}}{T_{ID}} \right) \]  \hspace{1cm} (4-5)

where \( f_D \) is the fractional opening of the distillate product valve, \( K_D \) is the controller gain, \( T_2 \) is the temperature on the top tray, \( T_{2s} \) is the set point of that temperature and \( T_{ID} \) is the controller reset time. If the temperature of the top tray goes up (the purity of the top vapor goes down), the distillate rate must be cut
back to decrease the amount of impurities in the distillate product and reflux, and thus decrease the top tray temperature. Therefore, the negative response shown in equation (4-5). The distillate product rate through the valve is simply:

$$D = (C_v)_D(A_D)(f_D)(\Delta P_D)^{1/2}$$  \hspace{1cm} (4-6)

where \((C_v)_D\) is the valve constant, \(A_D\) is the maximum valve area, and \(\Delta P_D\) is the pressure drop across the valve.

**MAINTENANCE OF OVERALL MATERIAL BALANCE**

As with all process units, maintenance of the overall material balance is very important in the long-term stability of the distillation operation. Since the distillate product rate is under composition control, (which has been previously terms "material balance control"), the bottoms product must be manipulated to maintain the overall material balance, and this is done by controlling the liquid level in the reboiler. Clearly, a simple proportional control is in order here, since it is not important to eliminate offset in most liquid level controllers. The differential equation for this valve is:

$$\dot{f}_W = (K_w)(\dot{h}_r)$$ \hspace{1cm} (4-7)
where $f_W$ is the fraction of the maximum valve opening, $K_W$ is the controller gain, and $h_Y$ is the liquid height in the reboiler. It is clear that if the reboiler height increases, an increase in the bottoms product will be desired to bring the liquid back down. Therefore, the control action is direct, as shown in equation (4-7). The bottoms product rate is simply:

$$W = (C_v)_W(A_w)(f_w)(\Delta P_w)^{1/2}$$  \hspace{1cm} (4-8)

where $(C_v)_W$ is the valve constant, $A_w$ is the maximum valve area, and $\Delta P_w$ is the pressure drop across the valve.

**COMPOSITION CONTROL OF THE OTHER PRODUCT**

As typical of many industrial distillation systems, the reflux rate in this system is held constant by a flow controller (which can be manually adjusted) to avoid interacting with the top product quality controller. However, a ratio feed-forward controller monitoring the feed rate may in some cases be used to adjust the reflux rate. As this was not the initial thrust of this research, two product control was not studied. For future studies with this model, the control model can be easily modified to include two-product quality control and/or feed-forward control as desired.
INTRODUCTION

This research can be thought of as containing four phases. These are:

I  Problem definition and model development.
II  Programming and debugging of the model.
III  Investigation of numerical integration techniques and optimization of model efficiency.
IV  Production runs to evaluate and understand the physical system.

Phase III became more comprehensive and time consuming than originally expected, yet did not give as efficient a model as required. Therefore, Phase IV was severely limited in scope. However, a number of very interesting results were obtained, as discussed in the following sections.

DEVELOPMENT OF MODEL

Physical Properties

In Chapter 2, mention was made of various physical properties - enthalpies and densities of the liquid and
vapor as well as the vapor-liquid equilibrium relationships (K values). The data bank of this distillation model consists of the correlations for physical properties of paraffin hydrocarbons. In general, when dealing with reasonably short chain hydrocarbons, a number of simplifying assumptions can be made concerning the physical properties without materially affecting the characteristics behavior of a dynamic model such as this distillation control model. The pure component enthalpy correlations as functions of temperature and pressure were obtained from the appendix of Holland (11), based on data by Maxwell (14). In this model, ideal liquid and vapor mixing was assumed in order to compute the molar average enthalpies. Again, this was not an assumption which materially affected the dynamic behavior of the model. The vapor-liquid equilibrium constants were computed using correlations also from Holland, and were also functions of temperature and pressure.

The liquid densities were calculated as functions of temperature, using correlations of data from Maxwell. Again, ideal liquid mixtures were assumed. The vapor densities were computed using the ideal gas law. This assumption was tested using multicomponent mixing law based on the Virial equation. It was found that for the pressures and temperatures of the system studied here the ideal gas law gave excellent agreement, using far less computer time than the non-ideal relationship.
Choice of Numerical Integration Methods

It has been mentioned previously that the Johnson-Stewart Modified Euler (JSME) algorithm was used to integrate the differential equations in this research. However, many other integration techniques were also tried. In Chapter 3, it was predicted that the JSME algorithm should be twice as fast as the improved Euler method, but with equivalent accuracy. Computer experiments with the distillation model shows this to be true, eliminating the improved Euler method as the "optimum" integration method. In addition, fourth-order Runge-Kutta and Runge-Kutta-Gill techniques were also tested on the distillation model. These were found to be roughly a factor of four slower than the JSME algorithm. In his dissertation, Yu (30) also found that the Runge-Kutta methods consumed excessive computer time for his non-linear model, except that he used the simple Euler method and used constant step sizes for both cases. These results seem to confirm that the Runge-Kutta methods are not efficient for integrating the stiff equations of a non-linear dynamic distillation model. The last numerical integration algorithm tried was Hamming's fourth-order interactive method (9). Although this is a popular technique (5), particularly for stiff differential systems, it was roughly 2.5 times slower than the JSME algorithm in this application. Tyreus, Luyben, and Schlesser (26) developed an integration technique for stiff systems
which uses the Jacobian matrix of a set of linearized differential equations in the corrector step(s) of a predictor-corrector integration technique. Since the Jacobian matrix is constant for a set of linear differential equations, no special computations are required for linearized systems. However, for non-linear equations, considerable computer time must be spent in the evaluation of the Jacobian matrix. Therefore, it was felt that this method probably was not optimal for the distillation model developed in this research, and was not tried. This leaves open the question of whether use of the technique of Tyreus, et.al., could indeed have proved more efficient than the methods which were tried. These comparisons do not prove that the JSME algorithm is superior to the Runge-Kutta or Hamming methods for all systems of differential equations. However, since it was found to be the most efficient for the model used in this research, it was used throughout the simulations.

Parameters in Automatic Step Size Adjustment

The values of the convergence constants used for step size regulation were chosen by experimentation with simulation runs. Various values were chosen for the upper and lower convergence limits to compare the speed and stability of the simulation using these values. After an extensive trial-and-error search, the final values of $\varepsilon_1$ and $\varepsilon_2$ (as defined in equation (3-7)) for
the dynamic model used in this research were $1.0 \times 10^{-9}$ and $1.0 \times 10^{-8}$, respectively. The single order of magnitude difference of the two limits seemed to be the most efficient, keeping the step size from becoming too small for efficient integration, yet also avoiding unnecessary fluctuation in the step size. When the limits were set lower, the step size was kept too small for efficient integration. When the limits were set higher, the "fast" differential equations caused the numerical solution to be in error, compared to the results from runs with lower limits, and the step size fluctuated greatly. Not only were the integrated variables incorrect, but the average step size was actually smaller than when the convergence limits were set lower.

Even using these "optimal" parameters, the integration was very slow, with the average step size on the order of $10^{-7}$ hours. As a result, depending upon upsets and controller action rates, one minute of simulation time required between ten and twenty minutes of computer (cpu) time. This is certainly not a desirable ratio, as it results in a consumption of from three to seven hours of cpu time for each open-loop and closed-run, thereby severely limiting the total number of runs that could be made and obviously the extent of the evaluation study phase of the work. However, a great deal of work went into making the dynamic model run faster, increasing the
speed some hundred fold, compared to the speed when the model was initially operational.

In the course of optimizing the convergence parameters it was felt that some proof was needed that the system of differential equations was indeed stable. Any possible errors in formulation and/or programming could result in an non-stable system. Dr. A. B. Corripio of the LSU Chemical Engineering Department suggested that the Jacobian matrix of the set of differential equations be examined. The Jacobian matrix may be defined by:

\[ A \cdot X = \dot{X} \]

where \( X \) is the vector of integrated variables, \( \dot{X} \) is the vector of the derivatives of those variables and \( A \) is the Jacobian matrix where:

\[ A_{i,j} = \frac{\partial X_i}{\partial X_j} \]

and, in a set of non-linear equations, is not constant. For stability, the diagonal elements of the matrix \( A \) \((A_{i,i})\) must all be negative. That is, for stability, the change in the derivative of an integrated variable must be negative if only that variable were to increase incrementally. A special program was developed to compute
this Jacobian matrix numerically at steady-state conditions, and through this, it was shown that the diagonal elements of the Jacobian matrix were all negative, hence the system is stable. Clearly for this physical system, these diagonal elements should all be negative. Had any been found positive, this would indicate an error in formation or programming. However, the diagonal elements of this matrix varied considerably in magnitude, which indirectly indicates the stiffness of this set of differential equations.

Importance of Column Design Parameters

It was indicated by Tyreus, Luyben and Schlesser (26) that dynamic distillation model stiffness is increased by raising the purities of the components. This research discovered, qualitatively, other factors which affect the apparent stiffness of the differential equations.

As should be expected, and actual column's operation will be unmanageable if the design parameters (column diameter, weir height, hole area, etc.) are not compatible with the column throughput, pressure, and separation desired. This unmanageable behavior may take many forms - high pressure drops across trays, cyclic behavior, overlarge liquid holdups, weeping, flooding, etc. As might be expected, this phenomenon is also true for dynamic distillation simulation when the tray hydraulics are modeled rigorously, as they are in the model used in this
research. In order to avoid unmanageable "operation", which causes the simulation to use excessive computer time as also does stiffness, proper design must be implemented. For example, if the orifice pressure drop of the vapor through the trays is too small compared with the static pressure drop of the liquid head on the trays, then very small pressure fluctuations may cause the vapor rates to fluctuate greatly (by equations (2-4) and (2-5), causing unnecessary material and energy imbalances on the trays. In actual columns, this pressure drop imbalance generally causes the trays to weep or dump. As mentioned in Chapter 2, a steady-state distillation model which includes tray hydraulics was used to set up the initial conditions for the dynamic simulation. Using criteria discussed by Bolles (1), and the design parameters were chosen to promote stable operation in an actual or simulated distillation column.

**Dynamic Studies**

Table 5-1 shows the flow, component and design parameter data used for the dynamic and control studies in this research. The particular choice of physical systems was made for two reasons. First, the relatively "easy" separation, i.e., a three component light hydrocarbon mixture, made the dynamic responses more graphic for analysis. The example used in this research is typical of certain industrial separations in which material
## Table 5-1

**Physical Data Used in Dynamic Studies**

### Flow and Component Data (Steady State)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed Rate</td>
<td>600 lb.-moles/hr.</td>
</tr>
<tr>
<td>Feed Composition</td>
<td>40 mole % propane, 25% normal butane, 35% normal pentane</td>
</tr>
<tr>
<td>Feed Temperature</td>
<td>125°F (bubble point)</td>
</tr>
<tr>
<td>Distillate Rate</td>
<td>250 lb.-moles/hr.</td>
</tr>
<tr>
<td>Distillate Composition</td>
<td>95.28%, 4.71%, 0.01%</td>
</tr>
<tr>
<td>Bottoms Rate</td>
<td>350 lb.-moles/hr.</td>
</tr>
<tr>
<td>Bottoms Composition</td>
<td>0.51%, 39.49%, 60.00%</td>
</tr>
<tr>
<td>Reflux Rate</td>
<td>750 lb.-moles/hr.</td>
</tr>
<tr>
<td>Top Pressure</td>
<td>120 psia</td>
</tr>
<tr>
<td>Steam Temperature</td>
<td>281.62°F</td>
</tr>
<tr>
<td>Cooling Water Temperature</td>
<td>70°F</td>
</tr>
<tr>
<td>Accumulator Level</td>
<td>3.8 ft.</td>
</tr>
<tr>
<td>Reboiler Level</td>
<td>3.00 ft.</td>
</tr>
</tbody>
</table>

### Column Design Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Ideal Trays</td>
<td>9</td>
</tr>
<tr>
<td>Number of Feed Trays</td>
<td>5</td>
</tr>
<tr>
<td>Column I.D.</td>
<td>5.0 ft.</td>
</tr>
<tr>
<td>Weir Length</td>
<td>44.0 in.</td>
</tr>
<tr>
<td>Weir Height</td>
<td>1.8 in.</td>
</tr>
</tbody>
</table>
TABLE 5-1 (continued)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Per Cent Hole Area</td>
<td>-- 6.0%</td>
</tr>
<tr>
<td>Vapor Pressure Drop Coefficient</td>
<td>-- 0.696 (dimensionless)</td>
</tr>
<tr>
<td>Active Tray Area</td>
<td>-- 15.78 sq. ft.</td>
</tr>
<tr>
<td>Downcomer Area</td>
<td>-- 2.03 sq. ft.</td>
</tr>
<tr>
<td>Area Under Downcomer</td>
<td>-- 0.147 sq. ft.</td>
</tr>
<tr>
<td>Total Height of Condenser Tubes</td>
<td>-- 10.0 ft.</td>
</tr>
<tr>
<td>Square Feet of Heat Transfer Area per Foot of Condenser Height</td>
<td>-- 375 sq. ft./ft.</td>
</tr>
<tr>
<td>Overall Condensing Heat Transfer Coefficient</td>
<td>-- 200 BTU/(sq. ft. hr. °F)</td>
</tr>
<tr>
<td>Condensate Heat Transfer Coefficient</td>
<td>-- 0.0</td>
</tr>
<tr>
<td>Effective Cross-Sectional Area in Accumulator</td>
<td>-- 10.0 sq. ft.</td>
</tr>
<tr>
<td>Heat Transfer Area in Reboiler</td>
<td>-- 500 sq. ft.</td>
</tr>
<tr>
<td>Overall Reboiler Heat Transfer Coefficient</td>
<td>-- 200 BTU/(sq. ft. hr. °F)</td>
</tr>
<tr>
<td>Effective Cross-Sectional Area in Reboiler</td>
<td>-- 10.0 sq. ft.</td>
</tr>
<tr>
<td>Control Parameters</td>
<td></td>
</tr>
<tr>
<td>Distillate Rate Coefficient ($C_v D A_D$)</td>
<td>-- 100 lb. moles/(hr.)(psia)</td>
</tr>
<tr>
<td>Pressure Drop Across Distillate Valve</td>
<td>-- 25.0 psia</td>
</tr>
<tr>
<td>Distillate Controller Gain</td>
<td>-- 0.005 °F⁻¹</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td><strong>TABLE 5-1 (Continued)</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Distillate Controller</strong></td>
<td>-- 0.0</td>
</tr>
<tr>
<td><strong>Integral Time</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Bottoms Rate Valve</strong></td>
<td>-- 140 lb. moles/(hr.)(psia)</td>
</tr>
<tr>
<td>Coefficient ( C_v ) ( W(A_W) )</td>
<td></td>
</tr>
<tr>
<td><strong>Bottoms Controller</strong></td>
<td>-- 1.0 ft.(^{-1})</td>
</tr>
<tr>
<td><strong>Gain</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Pressure Drop Across</strong></td>
<td>-- 25.0 psia</td>
</tr>
<tr>
<td><strong>Bottoms Valve</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Steam Valve</strong></td>
<td>-- 2500 lb./(hr.)(psia)</td>
</tr>
<tr>
<td>Coefficient ( C_v ) ( S(A_S) )</td>
<td></td>
</tr>
<tr>
<td><strong>Steam Pressure</strong></td>
<td>-- 100.0 psia</td>
</tr>
<tr>
<td><strong>Upstream of Valve</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Steam Controller</strong></td>
<td>-- 0.25 psia(^{-1})</td>
</tr>
<tr>
<td><strong>Gain</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Steam Controller</strong></td>
<td>-- 0.0</td>
</tr>
<tr>
<td><strong>Integral Time</strong></td>
<td></td>
</tr>
</tbody>
</table>
balance control is used to shift the separation capability of the column towards one of the products. In this case, the excess distillate product rate results in a relatively impure distillate product, but a pure bottoms product. This type of separation shows the non-linearity of the system much better than a separation where the top temperature can change in only one direction because of the relative closeness of the bubble point and dewpoint of the distillate product. The second reason was mentioned earlier in this chapter. The easier separation made the differential equations less stiff, increasing the speed of the simulations. This was very important considering the fact that the IBM 370/3033 computer used for the simulations was usually over-utilized, and that the model required copious cpu time, both making computer job turnaround very slow on average.

In order to learn how the column responds to the proposed manipulated variables and to various disturbance variables, a series of open-loop response runs were made. Only one control loop, the liquid level controller in the reboiler, was in operation in these runs. Clearly this loop is necessary in order for the system to be self-restoring to a steady state condition. The results of these studies are described in the following sections. First the response to the steam valve in the reboiler was examined, since this is the manipulated variable of primary interest. Then the open-loop (uncontrolled) response
to a number of loads (disturbances) was determined; cooling water temperature, feed composition, feed temperature, feed rate, and distillate product rate. Of course, the latter may also be thought of as a manipulated variable, since it is used to control the distillate composition inferentially through the top tray temperature.

It is important to recognize that these particular open-loop runs themselves are unique, having never before been investigated by computer simulation. In this column, since the column pressure is not maintained by an external pressure control system, but is dictated by the operation of the flooded condenser, any change in a manipulated or load variable will result in changes not only in flows, compositions, and temperatures, but also in pressures throughout the column. This is clearly evident in the results of the runs described below.

**Open-Loop Response to Reboiler Heat Change**

As previously discussed, a primary emphasis in this study was the control of column pressure with reboiler heat input. In order to better understand the dynamic response to the manipulated variable, reboiler heat, an open-loop response "experiment" was undertaken. As already explained the only functioning control loop was the reboiler level-bottoms product loop, which of course had to be tuned and implemented first before any other
studies could be made. (Tuning of this loop consisted simply of choosing a proportional gain which resulted in full-open to full-closed valve operation for a change in reboiler level of 1.0 ft., which is 16.7% of full reboiler level range. This is typical for an industrial reboiler level controller, and of course, no integral control action was used.) All other external values, including those for both the distillate product rate and the reflux rate, were held constant. A 10% step increase was imposed on the reboiler inlet steam valve opening, and the resulting column behavior was observed. The primary variable of interest was the top pressure, since this was to be controlled by manipulating reboiler heat. Certainly, the expected response is that the increased reboiler heat should result in an increase in column pressure. However, since both D and R were maintained constant, the level of condensate in the overhead condenser must rise so that when a new steady state is reached, both the rate of condensation and the rate of boilup have returned to their original values, but at a higher column pressure.

The unanticipated results are shown in Figure 5-1. The usual expected open-loop response of complex physical systems may certainly be more complicated than a first-order lag, but it is at least most often monotonic. (Sometimes a slight initial inverse action is observed, which, when it does occur, degrades the tuned control
Figure 5-1. Open-Loop Pressure Response to a Step Increase in Steam Valve Position
loop behavior substantially). In this case, a much more complex response was observed.

Figure 5-1 shows that the top pressure first increased very quickly from 120.0 psia to about 121 psia, then fell to about 116 psia during the next seven minutes. It then rose slowly, and appeared to be lining out at about 127 psia after about 40 minutes. This behavior was a double reverse action occurring over a substantial period of time. The implications of such a response upon the pressure control behavior of the column (using the steam flow valve as the manipulated variable) are both staggering and unpredictable (particularly when it is also considered likely that the non-linearity of the system may well result in substantial changes in this observed response to the steam valve when other valves are manipulated simultaneously). The top tray temperature response curve (not shown) looked quite similar to Figure 5-1, having a sharp increase, a sharp decrease, then a slow increase. Clearly an interpretation of the observed response is needed. A suggested interpretation of the behavior is given in the following paragraphs.

Obviously, a column has a natural internal feedback mechanism involving many variables. There are two major natural feedback mechanisms, known as inherent-regulation mechanisms, in this case. When the heat input to the reboiler is suddenly increased, this increases the vaporization rate from the reboiler, which, in turn causes
increased vapor rates and an accompanying increased pressure wave to propagate up through the column. This raises the bubble point temperatures throughout the column as well. After a short period of time (apparently about one minute in this case), the resulting decreased temperature driving force in the reboiler causes a reduction in boilup rate from the peak rate reached immediately after the valve was opened, while the increased temperature driving force in the condenser due to the increased pressure increases the condensation rate. This reduction in boilup combined with the increase in overhead condensation causes the pressure to drop back from its initial peak. As mentioned above, the final steady state conditions must be such that both boilup rate and condensation rate return to their original values, since the product and reflux rates are held constant. Therefore, since the steam valve is open wider, the column pressure must be higher so that the temperature driving force in the reboiler remains unchanged. At the top, the areas for heat transfer must decrease to counteract the increased temperature driving force which results from the higher pressure and corresponding higher top temperature. However, as evidenced in Figure 5-1, reaching new steady-state conditions apparently takes a very long time and is not a simple monotonic response.

The second phenomenon which contributes to the unusual response is that when the boilup rate increases
initially, a heavier-than-normal vapor is sent toward the top of the column. With the reflux rate held constant, as is the case here, the contents of each tray in the column gradually become heavier (more higher-boiling components). The heavier composition on the trays eventually causes a substantial drop in bubble point pressures, which apparently accounts for the dropping of top column pressure below the initial value of 120 psia until finally, compositions return to their original values, raising the pressures back up. This double reverse phenomenon was mentioned also by Rademaker, Rijnsdrop, and Maarleveld, who noted that it has been reported by several experimenters. They indicated that this behavior may be expected for flooded condenser operation whenever a relatively large upset occurs in the energy balance, whether in the reboiler, or in the condenser, or in the feed temperature. The latter two examples are examined in the following sections.

To compare with the response shown in Figure 5-1, another experiment was undertaken to measure the response of the top pressure to a 10% decrease in the steam valve opening. Figure 5-2 shows this response is qualitatively a mirror image of Figure 5-1. The pressure underwent a sharp decline, then rose to a peak at about 10 minutes, then steadily decreased. Because of the high degree of non-linearity, it would not be reasonable to expect that the two response curves would be exact mirror images,
Figure 5-2. Open-Loop Pressure Response to a Step Decrease in Steam Valve Position
even though the response were caused by the same physical phenomena.

**Open-Loop Response to Cooling Water Temperature**

Next, an experiment was run to measure the effect of a change in a load, or disturbance variable. Figure 5-3 shows the open-loop (uncontrolled) response of the top pressure to a step increase in cooling water temperature. The temperature was increased from 70°F to 71°F, lowering the log mean temperature driving force in the condenser instantaneously by about 6.7%. As with the reboiler heat change, the final steady state conditions in this case must be such that all vapor and liquid rates are essentially the same as before, since D, R, and W were maintained constant. The reduction in temperature driving force in the condenser initially caused an abrupt decrease in the rate of overhead vapor condensed by the condenser, quickly raising the top tray temperature and pressure and also gradually lowering the liquid level in the condenser. This pressure increase of course propagated down the column very quickly, raising all the pressures sharply and cutting back on vapor rates. This phenomenon of pressure and temperature increases slowed down and began to reverse about one minute because more heat transfer area was uncovered in the condenser (the reflux and distillate product rates were held constant while the overhead vapor rate decreased), which caused
Figure 5-3. Open-Loop Pressure Response to a Step Increase in Cooling Water Temperature
the top vapor condensation rate to begin to increase. As described in the previous section, a second phenomenon which helped cause the top temperatures to reverse and begin to decrease was that when the overhead vapor rate was cut back, it gradually became much lighter in impurities, causing the bubble point temperatures to decrease. Eventually the top pressure was brought back down. In this case, the temperatures and pressures must eventually go back essentially to their original values after the column lines out, because the original overall flow rates, including the reflux rate, were maintained constant and the steam valve opening was not changed. The only difference between the "before" and "after" conditions should be that the condenser liquid level be lower than its original value to expose more heat transfer area to make up for the lowered temperature driving force in the condenser. The reboiler would have to be at essentially the same pressure as before in order to generate the same vapor rate, since its value opening did not change. Notice that the response here is apparently not a double reverse as the previous examples were.

Open-Loop Response to Feed Temperature

Figure 5-4 shows the open-loop response of the column top pressure to a step decrease in the feed temperature. As in the previous examples, the product and reflux rates were held constant. The feed temperature,
Figure 5-4. Open-Loop Pressure Response to a Step Decrease in Feed Temperature
originally at its bubble point (125°F), underwent a step decrease to 115°F. The resulting response to top pressure is very similar to Figure 5-2, the response due to a decrease in the steam valve opening. However, the absolute response was smaller in magnitude (note the scales on the respective figures). The magnitude of the response curve 5-4 is smaller because the thermal upset is merely a sensible heat change in the feed. The pressure dropped off sharply (because of the cooling effect of the feed enthalpy), then rose sharply due to the higher temperature differential in the reboiler causing an increase in boilup from the reboiler. The pressure peaked at about 121 psia, then fell due to reduced temperature differentials in the condenser and reboiler as well as the increased impurities in the top of the column. In essence, the response curve shape is due to the same negative feedback discussed in the earlier examples. When the system finally reaches steady state, the pressures in the column must be slightly lower, as explained in the following steady state analysis. Because the enthalpy of the feed is lowered, and both the product and reflux rates are held constant, more heat input from the reboiler will be needed. Since the steam valve opening is held constant, the increased temperature driving force required must come from a lowered bottoms product temperature. Since the material balance is held constant, the only
way the temperature can be lowered is by lowering the pressures.

Open-Loop Response to Feed Composition

As shown in Table 5-1, the initial steady-state feed composition was 40 mole % propane, 25% normal butane, and 35% normal pentane. The feed composition underwent a step change to 35%, 27.5%, and 37.5%, respectively. The response of the top pressure, top tray temperature, and condensing temperature are shown in Figure 5-5, 5-6, and 5-7, respectively. Since both the reflux and distillate product rates were held constant, the response of the top tray temperature shown in Figure 5-6 would be expected—a monotonic increase due to the increase in the higher-boiling components in the column.

But why did the top pressure decrease as shown in Figure 5-5? The answer is that the increased butane and pentane content also affected the bottom of the column by initially increasing the bottoms temperature. This lowered the temperature driving force in the reboiler, temporarily decreasing the boilup rate. This in turn lowered the top pressure as discussed in previous examples. To reach steady state again, the bottoms temperature must resume its original value, which is accomplished by a reduction in overall column pressure which exactly counteracts the temperature rise which would have
Figure 5-5. Open-Loop Pressure Response to a Step Change in Feed Composition
Figure 5-6. Open-Loop Top Tray Temperature Response to a Step Change in Feed Composition
Figure 5-7. Open-Loop Condensing Temperature Response to a Step Change in Feed Composition
otherwise occurred because of the increased heavies concentrations.

The bubble point temperature of the condensing vapor also went down, even though its dew point temperature (the top tray temperature) went up. As the purity of a single component product decreases, the difference between its bubble point and dew point increases. If the pressure had been held constant, both temperatures would have gone up. In this case, the relatively large pressure decrease opposed both temperature increases, actually lowering the condensing temperature, even though the condensing vapor was higher in impurities (15%, up from 5%).

Open-Loop Response to Feed Rate

The open-loop response to a change in feed rate was examined by imposing a 5% step increase to the feed rate, from 600 to 630 lb-moles per hour. The feed composition and temperature were held constant, as were the reboiler steam valve and distillate rate. As before, in order to maintain the overall column material balance, the reboiler level controller was functional. The response of the column top pressure, top tray temperature, and condensing temperature are shown in Figures 5-8, 5-9, and 5-10, respectively. Because the distillate rate was held constant, the distillate composition became more pure. Before the upset, there were 240 moles of propane fed to
Figure 5-8. Open-Loop Pressure Response to a Step Increase in Feed Rate
Figure 5-9. Open-Loop Top Tray Temperature Response to a Step Increase in Feed Rate
5-10. Open-Loop Condensing Temperature Response to a Step Increase in Feed Rate
the column and 250 moles of distillate product, so a pure distillate product was prevented by material balance considerations. With the additional feed, 252 moles of propane were fed, making a very pure distillate product feasible. This can be clearly seen in Figure 5-9 and 5-10. These represent the dew point and bubble point, respectively, of the vapor going overhead to the condenser. Clearly, as the purity of a single component product (such as propane) increases, its dew point and bubble point will converge. This is what these two figures show. The difference between the two temperatures started at about 4°F and converged to within 1.5°F as the distillate purity rose from about 95.3% to about 98.4%. During the dynamic period (about 20 minutes), the reboiler also went through transition. During this transition period, the reboiler contents also became lighter as the bottoms product rate increased to accommodate the additional feed. This caused the reboiler temperature driving force to increase, which caused an increased boilup rate. This, in turn, instigated a vapor rate-pressure wave, increasing all of the pressures until, as in previous examples, the vapor rates later returned to those necessary to supply the overall product and reflux rates, which had not been changed. (See Figure 5-8). By this time, the bottoms product had lined out to 380 moles per hour as it should, so the material and energy balances steady after about 20 minutes, with all temperatures,
pressures, and compositions at new steady-state values. Since this particular run reached new steady state conditions, the results were compared to a steady state model's results. The two were very close, verifying the capability of the model to reach new valid steady state conditions after a dynamic upset period.

Open-Loop Response to Distillate Product Rate

Figures 5-11, 5-12, and 5-13 show the response of the column top pressure, top tray temperature, and condensation temperature, respectively, to a 10% step increase in the distillate product rate. The response of the top tray temperature is shown in Figure 5-12, a monotonic increase to the new steady state. However, the top pressure and the bubble point of the condensing vapor did not behave as one might expect. Ordinarily, the assumption might be made that the condensation temperature would also increase, with an essentially constant pressure. The reason that the pressure dropped initially was that the sudden increase in distillate rate caused the flooded condenser level to drop, "pulling" more vapor overhead, lowering the pressure in the process, as explained in previous examples. This in turn lowered the bubble point temperature of the condensate. The explanations for this behavior are the same as in the previous examples. It is interesting that this example, the response to feed composition, and the response to feed rate
Figure 5-11. Open-Loop Pressure Response to a Step Increase in Distillate Product Rate
Figure 5-12. Open-Loop Top Tray Temperature Response to a Step Increase in Distillate Product Rate
Figure 5-13. Open-Loop Condensing Temperature Response to a Step Increase in Distillate Product Rate
exhibited similar behavior as a result of upsets in the material balance, unlike the response to the thermal upsets of the other open-loop examples. That is, the response to material balance upsets are monotonic, and appeared approximately first order. These material balance upsets did not cause instantaneous thermal imbalances, as did the previous examples.

To summarize the above results of open-loop tests, it must be noted that although final steady state responses can be predicted, the unusual dynamic responses would not be predictable by a control engineer. As explained in the above examples, the unusual responses were due to a series of rather complex dynamic relationships. Because of the complexity of the system, when simultaneous changes are made, the responses observed here may not at all be superpositioned on each other, but may generate completely different behavior due to the high non-linearity of the system. These results show that the model developed in this research provides the ability to examine complex responses which previously could have been studied at most only in actual columns.
CONTROL STUDIES

Reboiler Level Control

As mentioned in Chapter 4, the reboiler level controller is a simple proportional unit, and the gain theoretically can be as high as possible. As with most level controllers, the gain was chosen high enough to maintain the level without having the valve bounce unnecessarily. The gain chosen is such that the valve changes from full-open to full-closed by a 1.0 ft. change in the reboiler level which is 16.7% of full scale.

Pressure Control

The obvious controller tuning sequence was to set first the reboiler level controller, then the pressure controller, then the top tray temperature (distillate purity) controller. As mentioned in the previous paragraph, the reboiler level controller was tuned without any problems. However, the pressure control loop tuning later proved to be more complex because of unforeseen interaction between the pressure control loop and the top tray temperature.

The pressure control loop was tuned initially by computer "experiments" in which the cooling water temperature was upset. The objective was to determine the ultimate gain of the loop and the ultimate period, from which reasonable controller settings could be chosen by
the Ziegler-Nichols closed-loop procedure. However, the characteristic response expected from linear analysis were not obtained. The unimodal response curves necessary for open-loop controller tuning were not present. In fact, the closed-loop response contained reversals and other non-linear behavior which made trial-and-error the only feasible controller tuning method. After making several runs, it was found, as can be seen in Figure 5-14, that a proportional-only controller with a gain of 10.0 (see equation 4-1) performed extremely well in response to an increase in the cooling water temperature. This was the same upset that caused the open-loop response of Figure 5-3, yet the controller kept the pressure within .015 psi of the target pressure. This gain was tentatively chosen as a good parameter setting, based on this performance, and clearly no integral control was needed to give acceptable control. Note that even though the pressure control was quite fast and with little deviation, total settling down of unit, as evidenced by top tray temperature (see Figure 5-15), was much longer. (This temperature was not controlled in this case.)

Why did the top tray temperature go down while the pressure above it was held constant? The pressure controller cut back on the boilup rate, causing a buildup of material in the reboiler, since the feed and reflux were held constant. Also the decreased vapor rate throughout the column caused every tray and the reboiler to increase
Figure 5-14. Closed-Loop Pressure Response to a Step Change in Cooling Water Temperature with Excessive Pressure Controller Gain.
Figure 5-15. Open-Loop Temperature Response to a Step Change in Cooling Water Temperature With Excessive Pressure Controller Gain
in more volatile component concentrations. This meant, as column operators say, the column began to "lighten up". That is, the condenser, reboiler, and each tray contained more of the lighter components than before. (The heavy components were exiting the column via the increased bottoms product flow rate). Because of the much lighter reboiler contents (the pentane content dropped from 60 mole % to 46.7%), the bottom temperature decreased from about 203°F to about 172°F. The top tray temperature dropped and leveled out at about 81°F. This is because the distillate product purity increased from about 95% to about 99.5%, and the temperature could not fall below the boiling point of propane at 120 psia. The time scale of Figures 5-14 and 5-15 is relatively short and steady state was not reached in this run. As mentioned in the previous section concerning the open-loop response to an upset in cooling water temperature, the column should line out eventually back at its initial conditions, with the exception that the liquid height in the flooded condenser would be lower to provide more heat transfer area to accomodate the lowered temperature difference in the condenser.

Later, during the temperature control loop tuning, it became apparent that the high gain of 10.0 on the pressure controller adversely affected the performance of the temperature controller as well as other variables. This is discussed in later paragraphs. A much lower
pressure controller gain (0.25) was chosen to minimize these adverse interactions, while still providing acceptable pressure control. Notice this new gain was a factor of 40 lower than the gain obtained by the previous tests. Even though the new gain necessarily could not maintain the pressure as tightly as the much larger gain could, the controlled response was still acceptable. (Maximum deviations of less than 0.5 psi were usually achieved.)

Figure 5-16 shows the response of the top pressure to a step change in the pressure set point from 120 psia to 125 psia with a gain of 0.25. The distillate product and reflux rates were held constant, but the reboiler level controller was functional. Figure 5-17 shows the response of the reboiler steam flow to effect the pressure response shown in Figure 5-16. The steam valve opening initially jumped from about 51% open to full open, immediately raising the steam flow from about 8600 lb./hr. This had an immediate effect on the top pressure, which almost instantaneously rose from 120 psia to 124.5 psia. Unfortunately, the pressure then dropped very sharply to about 109 psia in about 1.6 minutes, then rose rapidly to 124 psia in about six minutes. The pressure then asymptotically approach the set point of 125 psia within ten minutes of elapsed time. During the period of pressure descent, because of the proportional action of the pressure controller, the steam flow increased markedly (after a very sharp decrease) to about
Figure 5-16. Response of Pressure to a Step Change in Pressure Set Point
Figure 5-17. Response of Manipulated Steam Flow to a Step Change in Pressure Set Point
15000 lb. hr. As the pressure rose again, the steam flow began to decrease, and as the pressure approached the set point, the steam flow also began to level out at near its original value (as it must in order to complete the overall column energy balance). With proportional-only control, some offset would naturally result at steady state, but the gain was large enough for this to be acceptable.

A look at the overall pressure response reveal three important things. First, the pressure reached its set point initially extremely quickly, as predicted in Chapter 4. Second, the pressure eventually appeared to be lining out very close to the set point, certainly a criterion for a good control loop. However, between the quick initial response and the smooth final approach to set point, the drastic drop and subsequent recovery in pressure occurred. The reason for this drop can be traced to phenomena discussed in relation to Figures 5-1 and 5-2. That is, the changes in the heat exchanger temperature driving forces and compositions caused the reversal, just as seen in the step changes in reboiler heat. As before, once the severe upset in composition was over, then the pressure control loop was able to do its job.

In a second test of the pressure control system, an experiment was undertaken in which the feed rate underwent a step increase of 5%, while the reflux and distillate product rates were held constant and the reboiler
level was controlled. In essence, these was the same
experiment that produced the open-loop responses of
Figures 5-8 - 5-10. The controlled response of the top
pressure is shown in Figure 5-18. While the uncontrolled
pressure (Figure 5-18) reached a peak of 120.5 psia after
10 minutes, then declined and seemed to line out at about
120.2 psia, certainly within reasonable limits. Figure
5-19 shows the response of the manipulated variable,
steam flow to the reboiler, which behaved, as would be
expected, in an inverse manner to the pressure. One
interesting point is that although the pressure rose only
a maximum of 0.5 psia, or about 0.42%, the steam flow
decreased about 1000 lb./hr, or about 11.6%, due to the
proportional gain action. Figure 5-20 shows that the top
tray temperature decreased in a similar manner as it did
in the completely open-loop case, shown in Figure 5-9.
The differences in the responses were that in the present
case, the temperature decreased more quickly at first,
and lined out at about 81°F, the boiling point of propane
at 120 psia when the top composition became almost pure
propane. The condensing temperature response (not shown)
looks very much like Figure 5-20, decreasing from its
initial value of 82.9°F to its boiling point of 81°F.
Although the pressure response shown in Figure 5-18
appears immoderate, the pressure was well controlled.
(Note the expanded scale on the pressure axis.)
Figure 5-18. Closed-Loop Pressure Response to a Step Increase in Feed Rate With Pressure Control Only.
Figure 5-19. Response of Manipulated Steam Flow to a Step Increase in Feed Rate With Pressure Control Only
Figure 5-20. Open-Loop Temperature Response to a Step Increase in Feed Rate With Pressure Control Only
Temperature Control

In order to study the response of the temperature control loop, the first order of business was to tune the loop. In the first phase of tuning, the pressure controller gain was set at 10.0, based on the excellent performance shown in Figure 5-14. The temperature loop tuning was initially tried by the two classical methods. The first method was by open-loop response, based on the Ziegler-Nichols open-loop criteria. In this experiment, the distillate rate valve opening was increased 5% to yield a step increase of the distillate rate from 250 lb.-moles/hr. to 252.6 lb.-moles/hr. In theory, the top tray temperature response should be a monotonic increase to some new steady state. However, the actual result, shown in Figure 5-21, is not at all monotonic and does not appear to be even close to reaching steady state after about eight minutes. After a dead time of three minutes, the top tray temperature rose extremely quickly to about 130°F, then curiously decreased and increased again, followed by another decrease. The response curve of the overhead vapor condensation temperature (not shown) looked very much like Figure 5-21, except for a smaller temperature range. To better understand this highly unusual behavior, the response curves of the column top pressure (Figure 5-22) and the steam flow to the reboiler (Figure 5-23) must be examined. The pressure remained constant at 120 psia for five minutes, then took a sharp
Figure 5-21. Temperature Response During Open-Loop Tuning With Excessive Pressure Controller Gain
Figure 5-22. Closed-Loop Pressure Response During Open-Loop Tuning With Excessive Pressure Controller Gain.
Figure 5-23. Response of Manipulated Steam Flow During Open-Loop Tuning With Excessive Pressure Controller Gain
drop to 108 psia, and rebounded back to 120 psia and remained essentially constant for the following minute. The steam flow rose slowly for about three minutes from about 8600 lb./hr. to about 16000 lb./hr., almost doubling. Note that this sharp increase corresponds chronologically to the sharp temperature increase shown in Figure 5-21. The steam flow then dropped sharply, then moderately, then sharply again.

This experiment was very similar to that which produced Figures 5-11 - 5-13, except that in the present case, the upset was only half as large, and, more importantly, the pressure controller was operational (with an excessive gain, however). The completely open-loop experiment produced very smooth monotonic (although unexpected in direction) curves which appeared first order. Clearly, then, the cause for the eccentric behavior produced in this semi-open-loop case must be the pressure control loop. In the completely open-loop case, the pressure decreased (see Figure 5-11). Therefore, the pressure control loop must increase the steam flow rate in order to maintain the pressure at 120 psia, and was doing quite well for the first three minutes. However, the high gain in the pressure controller caused the steam flow to greatly increase, creating a much larger boilup. This heavies-laden boilup caused the purity in the top of the column to plummet, which drove the top tray temperature up sharply (see Figure 5-21). The much higher
top temperatures created a very large temperature driving force in the condenser, "pulling" more vapor overhead and the pressure dropped extremely quickly. This in turn brought the top tray temperature down slightly. The pressure then began to rise as the column began to return to normal, and appeared to level out at about 120 psia. This brought the top tray temperature up to an even higher level. As the steam flow dropped to accommodate the return of the pressure to the set point, the temperatures began to fall again at the end of the experiment.

In terms of the original purpose of this experiment, tuning the temperature controller, this particular run was obviously useless. However, it did serve to show the severe non-linear interactions throughout the column and to show the impositions on the rest of the system caused by the overactive pressure control loop.

The other popular tuning method is to use the closed-loop response to an upset to the system to finding the ultimate gain, which is the gain which causes the response of the controlled variable to be stable oscillations. Then, by using Ziegler-Nichols closed-loop criteria or some other suitable method, estimates of the optimum controller constants may be computed.

The upset which was chosen was to make a 5% step increase in the feed rate, the same upset which provided the response curves shown in Figures 5-8 - 5-10 and 5-18 - 5-20. In the present case, all control loops were
functional. The search for the ultimate gain is necessarily trial-and-error with a complex system such as a distillation column. Considering that the pressure control gain was much too high, this particular search proved fruitless. However, the results were enlightening, as shown in the results of the following typical example.

In this trial, the temperature controller gain was set at 0.5, as defined by equation (4-5). Figure 5-24 shows the response of the top tray temperature, which very much resembles the response curve of the previous example (see Figure 5-21) except that the apparent dead time in this case was about eight minutes. The response of the manipulated variable, the distillate product rate, appears to be an under-damped sine wave, as shown in Figure 5-25. The curves of the pressure response (Figure 5-26) and manipulated steam flow (Figure 5-27) are very similar to their counterparts in the previous semi-open-loop example, except for the even more drastic drop in pressure in this case, and the aforementioned increase in the apparent dead time to about eight minutes.

As shown in Figure 5-20, the tendency of the top tray temperature is to monotonically drop to about 81°F, the boiling point of pure propane at 120 psia. Therefore, after a short dead time of approximately one minute, the distillate rate rose to about 340 lb.-moles/hr., then fell to about 45 lb.-moles/hr., rose again to about 675
Figure 5-24. Temperature Response During Closed-Loop Tuning With Excessive Pressure Controller Gain
Figure 5-25. Response of Manipulated Distillate Product Rate During Closed-Loop Tuning With Excessive Pressure Controller Gain
Figure 5-26. Closed-Loop Pressure Response During Closed-Loop Tuning With Excessive Pressure Controller Gain
Figure 5-27. Response of Manipulated Steam Flow During Closed-Loop Tuning With Excessive Pressure Controller Gain
lb.-moles/hr., then abruptly dropped to zero. Note that this immoderate manipulation was in response to very small fluctuations in the top tray temperature. Clearly then, the temperature controller gain was far too high. The other responses, which were due to the last peak of the distillate rate, appear to be very similar to those in the previous example. Even though they appear to be lining out at the end of the run, because the distillate rate had bottomed out, there is no assurance that they would line out. In essence, this behavior was caused by the same phenomena discussed in the previous example. Much lower gains for the temperature were tried, but because of the excessive gain in the pressure controller, acceptable response could not be achieved.

Clearly, these open-loop and closed-loop tuning runs suggest that the pressure controller gain of 10.0 was far too high for acceptable response of the other variables. As mentioned in the previous section, a much lower gain of 0.25 was chosen by trial-and-error. The criteria used for this search was to find the lowest possible pressure controller gain (to minimize interactions with the rest of the column) that would give acceptable pressure control. It was hoped that with this new, much lower gain, the temperature control loop could be tuned much more easily.

First, the open-loop tuning method was re-tried, since it is not a trial-and-error method, and should thus
be a quicker route to the proper controller constants. However, as can be seen in Figure 5-28, the temperature gain responded in an unusable manner. Although the response was not as choppy as that with the pressure controller gain of 10.0 (Figure 5-21), it was nonetheless very similar in its general behavior. The closed-loop pressure response, shown in Figure 5-29, is very similar to that in the previous open-loop test (See Figure 5-22), except that it is a little smoother in the transition areas. Accordingly, the manipulated response of the steam flow (not shown) is similar to that shown in Figure 5-23, except that is smoother. This particular run seems to indicate that although the much lower pressure controller gain gives a slightly smoother response, the pressure control mechanism itself causes this tuning method to be unusable. That is, the step change in the distillate product rate causes the pressure controller to act in an unacceptable manner, creating not only poor pressure control, but also unpredictable behavior in other variables.

After the above disappointing but informative experiment, the closed-loop tuning method was tried. Initially, the search was for the ultimate gain in order to estimate the optimum controller constants. This, however, also proved fruitless because of the severe interactions discussed previously, even with the much lower pressure controller gain. It as then decided to try a proportional-only temperature controller that would provide, if not
Figure 5-28. Temperature Response During Open-Loop Tuning With Moderate Pressure Controller Gain
Figure 5-29. Closed-Loop Pressure Response During Open-Loop Tuning With Moderate Pressure Controller Gain
good control, at least reasonably steady behavior after a reasonable length of time.

After a number of trials, the temperature controller gain was set to 0.010. Using the same upset as before (a 5% increase in the feed rate), a closed-loop experiment was performed. As shown in Figure 5-30, the top tray temperature did not remain at the set point (87.2°F), but slowly reached a new pseudo-steady state of 81.5-82.0°F. Then after about 24 minutes, the temperature rose extremely quickly to about 124.7°F, then dropped slightly as the pressure dropped, then rose again. The distillate product rate, manipulated in response to the top tray temperature, rose to about 278 lb.-moles/hr. and seemed to be reasonably steady until the temperature shot up, then tracked the temperature in an inverse fashion, as it should until it bottomed out. The pressure, shown in Figure 5-32, remained about 120 psia until the top tray temperature rose, at which point it plummeted to about 97.4 psia, then rose again in response to the increased steam flow, shown in Figure 5-33.

Perhaps the most unusual feature shown in these response curves is that both the controlled variables and the manipulated variables seemed to have settled for some time, yet each deviated very sharply at the end of the run. For the 5% feed rate change, the distillate rate should have also risen 5% (in the steady state). Instead, it rose some 15% and stayed there. Although the top tray
Figure 5-30. Temperature Response During Closed-Loop Tuning
With Temperature Controller Gain of 0.010
Figure 5-31. Response of Manipulated Distillate Product Rate During Closed-Loop Tuning With Temperature Controller Gain of 0.010
Figure 5-32. Closed-Loop Pressure Response During Closed-Loop Tuning
With Temperature Controller Gain of 0.010
Figure 5-33. Response of Manipulated Steam Flow During Closed-Loop Tuning With Temperature Controller Gain of 0.010
temperature and pressure appeared to have lined out, the rest of the column was still changing. Because the top tray temperature was essentially at the boiling point of pure propane (the distillate purity at this point was about 99.5%), the temperature did not move much. The reason that the distillate product became so pure is that the overhead vapor rate dropped by about 7%, which naturally meant that less impurities reached the top of the column. The overhead vapor rate dropped because the steam flow rate to the reboiler decreased, since the top pressure's natural tendency is to rise slightly with an increase in feed rate (see Figure 5-8). When the top vapor finally rate rose to accommodate the increased distillate product rate, the previous behavior had temporarily decreased the propane concentrations on the other stages from their steady state values (more propane was leaving with the distillate product than was being fed to the column). Therefore, the increased overhead vapor rate was considerably less pure than usual, causing the top purity to decrease rapidly, bringing up the top tray temperature. The greatly increased temperature driving force "pulled" even more vapor overhead, which caused the top pressure to drop. This in turn brought the steam flow rate up, which aggravated the situation seriously. This extremely high steam flow rate caused the reboiler to run dry, despite that the bottoms product rate had been shut off by the rapidly decreasing reboiler
liquid level. It is this problem which caused the final departure for each of the variables, since the model was unable to deal with the dry reboiler.

This experiment having failed to help tune the temperature control loop, it was decided to try one more temperature controller gain half the previous one, or 0.005. The responses of top tray temperature, distillate product rate, top pressure, and steam flow to the reboiler are shown in Figures 5-34, 5-35, 5-36, and 5-37, respectively. These response curves show much more moderate action than in the previous test, although the temperature controller did not hold the top tray temperature as well. Although the pressure response looks bad, the scale has been greatly expanded, as was the case for the other figures as well. One interesting point is that the distillate rate rose to about 265 lb.-moles/hr., which is very close to the steady state value desired (262.5). As in the previous example, although the variables appear to have lined out, they began to deviate at the end. In fact, each began paths which look very much like those in the previous example when they began to deviate from their pseudo-steady states. Of interest is that the lower gain did not prevent the "disaster" encountered in the previous run, but merely delayed it a few minutes. Of course, it cannot be stated with certainty that this particular run would have the same unfortunate results as the previous run, but the derivatives of
Figure 5-34. Temperature Response During Closed-Loop Tuning
With Temperature Controller Gain of 0.005
Figure 5-35. Response of Manipulated Distillate Product Rate During Closed-Loop Tuning With Temperature Controller Gain of 0.005
Figure 5-36. Closed-Loop Pressure Response During Closed-Loop Tuning With Temperature Controller Gain of 0.005
Figure 5-37. Response of Manipulated Steam Flow During Closed-Loop Tuning With Temperature Controller Gain of 0.005
the variables at the end of this run are very similar to those of the previous run when the sharp deviations took place. This finding coincides with previous runs, including those not presented in this dissertation. That is, lower temperature gains do not prevent any calamities experienced with higher gains, but they simply delay them.

After failing to find a well-behaved temperature response, even a low proportional gain, an experiment was run to determine the closed-loop column response when the feed composition was upset. The feed composition underwent a step change to 35 mole % propane, 27.5% butane, and 37.5% pentane, which was the same upset that produced the open-loop response curves of Figures 5-6 -5-8. The pressure controller gain was kept at 0.25. Figure 5-38 shows the response of the top tray temperature. This response was very similar to those produced in previous unrelated runs, such as those shown in Figure 5-24 and 5-28. The manipulation of the distillate product rate in response to the top tray temperature is shown in Figure 5-39. In this case, the results suggests that the temperature controller gain is still much too high. The response of the top pressure and its manipulated variable, the steam flow to the reboiler, are shown in Figures 5-40 and 5-41, respectively. Again, this behavior was seen in previous examples. Clearly, the same forces which produced those previous responses caused the unusual
Figure 5-38. Closed-Loop Temperature Response to a Step Change in Feed Composition
Figure 5-39. Response of Manipulated Distillate Product Rate to a Step Change in Feed Composition
Figure 5-40. Closed-Loop Pressure Response to a Step Change in Feed Composition
Figure 5-41. Response of Manipulated Steam Flow to a Step Change in Feed Composition
Figure 5-42. Closed-Loop Temperature Response to a Step Change in Temperature Set Point
Figure 5-43. Response of Manipulated Distillate Product Rate to a Step Change in Temperature Set Point
Figure 5-44. Closed-Loop Pressure Response to a Step Change in Temperature Set Point
Figure 5-45. Response of Manipulated Steam Flow to a
Step Change in Temperature Set Point
behavior of the column in this example. The only unique feature in this example is that the apparent dead time is much shorter than in previous runs. This is because the dynamics were slowed in the previous runs (responses to increased feed rate) by the hydraulic lags necessary to effect the internal flow and composition changes.

A final experiment was run to determine the controlled response to a step change in the top tray temperature set point from 87.2°F to 84.0°F. The response of the top tray temperature, shown in Figure 5-42, shows tendencies very similar to those in the last tuning run (See Figure 5-34). That is, it reached a pseudo-steady state (although not at the new setpoint), then began to wander upward, perhaps to similar disaster. The very interesting manipulated response of the distillate product rate is shown in Figure 5-43. At first, the distillate was cut back from 250 lb.-moles/hr. to about 242 lb.-moles/hr. in response to the step increase in the temperature set point. It then curiously rose above the previous steady state and remained there for a while, then decreased in response to the climbing top tray temperature. The responses of the top pressure and the steam flow are shown in Figures 5-44 and 5-45, respectively. The pressure, while relatively constant at 120 psia, began a rather steep descent toward the end of the run, much like it did in the final tuning run (see Figure 5-36). The steam flow decreased by about 1000 lb./hr. because of the
lower initial distillate product rate. As discussed previously, this meant that the lowered overhead vapor was much more propane-pure than in the steady state. The produced the very unusual situation of drawing more distillate product than initially, while the distillate was purer than initially. Clearly, this situation was necessarily temporary, lasting until the diminished propane concentrations throughout the column could no longer support this condition. At that point (about 25 minutes of elapsed time), the temperatures rose, the top pressure dropped, and the manipulated variables began to stray. This situation was then exactly like that discussed previously in the tuning runs.

**SUMMARY OF RESULTS**

A number of unusual and very interesting results were obtained using the dynamic model to produce both open-loop and closed-loop responses. The extensive inverse response shown in the open-loop behavior of the system surfaced to disrupt the closed-loop behavior using the topical control system. Now that the behavior has been examined and speculated upon, it can be said with some confidence that the depth of the inverse response behavior was due in a large part to the particular distillation system chosen. Whenever the ratio of the key components (propane and butane) changed on any given stage, this had a profound effect on the bubble-point
pressure of that stage. In fact, it is conceivable that this effect may be greater than that of the vapor rates which are indirectly used to control the pressures in this control scheme. Thus, in a distillation system which had much lower relative volatilities, the separation of isomers, for example, this internal feedback behavior would probably be considerably lower than experienced in this example system.

Because of the very long cpu time presently required for each run, the total number of runs was severely limited. Therefore, the development of the control system was likewise limited. Had this not been the case, more appropriate control parameters (including more complex control schemes) would have been developed in order to better control this particular distillation system. Also of interest would be to determine how much more controllable a distillation system of closer-boiling components would be.
The primary purpose of this research was to develop and use a new distillation model which would permit investigation of a distillation control system which uses reboiler heat to control column pressure. A non-linear dynamic distillation model was built which included pressure dynamics and a dynamic model of both the condenser and reboiler. To more efficiently integrate the model's stiff differential equations, a new numerical integration algorithm was devised. In order to begin to understand the column dynamic response mechanisms, dynamic studies were made of open-loop responses to not only the manipulated variables, but a number of loads (upsets) as well. Next, dynamic studies of the column equipped with the subject control system were made to determine the closed-loop behavior of the system. These different aspects of the research were by necessity sequentially handled, rather than examined in parallel. Below are summaries of each of the aspects studied, as well as recommendations for future research.

**Numerical Integration Technique**

It was shown in Chapter 3 that the proposed JSME algorithm should be equal to in accuracy to the improved
Euler method using only half the functional evaluations. This result was confirmed in the integration of the dynamic distillation model developed in this research and through use by other researchers. These successes do not prove that the JSME algorithm is the best of all methods for the integration of any possible set of differential equations, but it does indicate a decided advantage over the improved Euler technique and should give equivalent advantage when used with a predictor-corrector scheme of any order.

**Dynamic Distillation Model**

As mentioned, the model developed and utilized in this research is absolutely unique to the literature. With this type of model, many previously impossible simulation projects (such as the automatic control scheme discussed in this research) may now be performed. The non-linear dynamics, including the pressure dynamics, included in the model must be considered more comprehensive than in previously published dynamic models. Clearly, a model of the complexity of this one is not needed in all situations. However, for simulating systems in which pressure dynamics and monitoring need to be studied over a wide range of operation, the model presented in this research would be very valuable. The dynamic studies done in Chapter 5 reveal that the model simulates actual column operations very well in that dynamic behavior
previously found in actual columns was reproduced here in addition to results previously unreported anywhere. However, the amount of cpu time required for integration of the differential equations for this model is quite large, severely limiting the number of investigative computer runs which could be made.

**Open-Loop Behavior**

The dynamic studies investigated the open-loop responses of the column (e.g., pressure and the top temperatures) to step changes in both the manipulated variables (reboiler heat input and distillate product rate) as well as a number of typical column disturbances, or loads. The responses to changes in the reboiler heat level were very unusual and highly non-linear, exhibiting severe inverse response characteristics, apparently due to internal feedback mechanisms inside the column. Other thermal upsets caused similarly complex responses. Responses to material balance upsets were approximately first-order and more linear in nature with minor inverse response, but material balance and thermal imbalances both produced some unusual responses. Because of the non-linearity of the system, responses to the various loads and manipulated variables should not be considered superimposable, and therefore the prediction of controlled behavior is very difficult. The relatively large periods of negative (inverse) response would appear to indicate
that the implementation of the particular pressure control strategy studied here might prove difficult.

Closed-Loop Behavior With Control System

The inverse and highly non-linear responses shown in the open-loop response curves foreboded the possible problems that might be encountered when the particular control system studied here is implemented. In fact, the inverse behavior did surface when control runs were made. The control algorithms studied here were, in fact, very simple feedback loops. Certainly it is conceivable that a more complicated control system involving feed-forward loops, cascade loops and/or non-linear control algorithms with the same general relationships (material balance purity control and pressure control via reboiler heat) might prove more successful in dealing with the highly non-linear behavior of the system.

In retrospect, it is now believed that a major factor contributing to the unusual open-loop response and the relatively poor controlled behavior of the system studied was the interaction between changes in the composition of the vapor and liquid streams with the bubble and dew point pressures of the streams. In the system studied here, as the propane-butane ratio changed, the effect on column pressures was greater than the effect of changing the vapor rate itself. Had the column been separating two key components with closer boiling points, such as
isomers, this effect of composition on bubble point would have been much less, and the pressure control loop might have been less interacting with the composition control loop.

Recommendations for Future Research

Because of the difficulties encountered in getting the dynamic model to run at speeds anywhere close to that desired, and because of the length of time consumed in making runs, the studies presented here represent only a small part of those needed to accomplish a definitive study which would evaluate comprehensively this control system. Future work needed to complete this study are:

(1) Continued attempts at improving the efficiency of integrating the stiff system equations (perhaps involving the use of the Jacobian matrix as suggested by some authors). No further significant studies should be made without first achieving this.

(2) Assuming goal (1) above is reached, then completion of the studies started here to find out what controller settings (including possible integral action) results in best performance for the system, and to define under what conditions the system will work well and what conditions will cause it to work poorly, can then be done to provide a definitive evaluation of this control system. From that point, the need for more complex control action (feed-forward, cascade, and/or non-linear logic) should
be evaluated to further define the control system's capabilities.
NOTE: The dot (.) atop a variable indicates the time derivative of that variable.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_D$</td>
<td>Maximum flow area of distillate product valve</td>
</tr>
<tr>
<td>$A_{da}$</td>
<td>Area of restricted opening under each downcomer in square feet.</td>
</tr>
<tr>
<td>$A_{dc}$</td>
<td>Cross-sectional area of the downcomer</td>
</tr>
<tr>
<td>$A_{htc}$</td>
<td>Square feet of heat transfer area on the condenser tubes per foot of length</td>
</tr>
<tr>
<td>$A_s$</td>
<td>Maximum flow area of steam valve</td>
</tr>
<tr>
<td>$A_t$</td>
<td>Active tray area</td>
</tr>
<tr>
<td>$A_{tr}$</td>
<td>Reboiler heat transfer area</td>
</tr>
<tr>
<td>$A_W$</td>
<td>Maximum flow area of bottoms product valve</td>
</tr>
<tr>
<td>$(C)_{pl}$</td>
<td>Average liquid molar heat capacity on each tray</td>
</tr>
<tr>
<td>$C_v$</td>
<td>Pressure drop coefficient for the vapor flowing through the holes in the column trays</td>
</tr>
<tr>
<td>$(C_v)_D$</td>
<td>Distillate product valve constant</td>
</tr>
<tr>
<td>$(C_v)_R$</td>
<td>Reflux rate valve constant</td>
</tr>
<tr>
<td>$(C_v)_S$</td>
<td>Steam valve constant</td>
</tr>
<tr>
<td>$(C_v)_W$</td>
<td>Bottoms product valve constant</td>
</tr>
<tr>
<td>$D$</td>
<td>Distillate product rate</td>
</tr>
<tr>
<td>$F$</td>
<td>Feed rate to column</td>
</tr>
<tr>
<td>$f_D$</td>
<td>Fractional distillate product valve opening</td>
</tr>
<tr>
<td>$f_R$</td>
<td>Fractional reflux valve opening</td>
</tr>
<tr>
<td>$f_S$</td>
<td>Fractional steam valve opening</td>
</tr>
<tr>
<td>$f_W$</td>
<td>Fractional bottoms product valve opening</td>
</tr>
</tbody>
</table>
\( g \) Acceleration due to gravity

\( \bar{H}_f \) Average molar specific enthalpy of the feed

\( (\bar{H}_{1w})_i \) Individual component liquid enthalpy of component 
\( i \) in the reboiler

\( \bar{H}_v \) Average molar vapor specific enthalpies

\( \bar{H}_l \) Average liquid specific enthalpies

\( (\bar{H}_l)_{i,j} \) Individual component specific enthalpy for each 
component on each tray \( j \)

\( h_{ct} \) Total length of the vertical tubes which is 
available for heat transfer

\( h_{da} \) Pressure drop available to cause flow onto tray 
in feet of liquid

\( h_{dc} \) Height in feet of liquid in downcomer

\( h_j \) Liquid height on tray \( j \)

\( h_{ow} \) Liquid crest over a straight weir in feet

\( K_{i,j} \) Equilibrium constant of component \( i \) for stage \( j \)

\( K_d \) Feedback controller gain for distillate product 
valve

\( K_s \) Feedback controller gain for steam flow valve

\( K_w \) Feedback controller gain for bottoms product valve

\( L_d \) Molar liquid flow rate leaving downcomer

\( L_j \) Liquid flow rate over weir of tray \( j \)

\( l_w \) Length of weir in inches

\( M_a \) Total moles in the accumulator section of the 
condenser

\( (M_d)_{j} \) Total moles in downcomer \( j \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_j$</td>
<td>Total moles on tray $j$</td>
</tr>
<tr>
<td>$n_c$</td>
<td>Number of components</td>
</tr>
<tr>
<td>$n_r$</td>
<td>Stage number of the last reboiler</td>
</tr>
<tr>
<td>$n_t$</td>
<td>Stage number of the last tray</td>
</tr>
<tr>
<td>$P_j$</td>
<td>Pressure above the liquid on tray $j$</td>
</tr>
<tr>
<td>$P_s(T)_i$</td>
<td>Vapor pressure of component $i$ as a function of temperature</td>
</tr>
<tr>
<td>$P_{steam}$</td>
<td>Pressure of steam in reboiler</td>
</tr>
<tr>
<td>$P_u$</td>
<td>Steam pressure upstream of the control valve</td>
</tr>
<tr>
<td>$P_{ls}$</td>
<td>Set point of the top pressure</td>
</tr>
<tr>
<td>$Q_{dc}$</td>
<td>Liquid flow rate onto tray in cubic feet per hour</td>
</tr>
<tr>
<td>$Q_{ow}$</td>
<td>Liquid flow over the weir in cubic feet per hour</td>
</tr>
<tr>
<td>$q$</td>
<td>Liquid flow rate in cubic feet per second</td>
</tr>
<tr>
<td>$q'$</td>
<td>Volumetric flow rate of liquid in gallons per minute</td>
</tr>
<tr>
<td>$R$</td>
<td>Reflux rate</td>
</tr>
<tr>
<td>$T_{acc}$</td>
<td>Temperature of the condensate in accumulator</td>
</tr>
<tr>
<td>$T_C$</td>
<td>Temperature of the cooling medium in the condenser</td>
</tr>
<tr>
<td>$T_{ID}$</td>
<td>Integral time in distillate product controller</td>
</tr>
<tr>
<td>$T_{is}$</td>
<td>Integral time in steam controller</td>
</tr>
<tr>
<td>$T_{reb}$</td>
<td>Temperature of the boiling liquid in the reboiler</td>
</tr>
<tr>
<td>$T_1$</td>
<td>Bubble point of the vapor in the condenser</td>
</tr>
<tr>
<td>$T_2$</td>
<td>Temperature of the first tray (second stage)</td>
</tr>
<tr>
<td>$T_{2s}$</td>
<td>Set point of temperature of the first tray</td>
</tr>
<tr>
<td>$U_c$</td>
<td>Overall heat transfer coefficient in the condensing section</td>
</tr>
</tbody>
</table>
Average velocity of the vapor through the holes of the tray in feet per second

Overall heat transfer coefficient in the reboiler

Molar vapor rate leaving tray j

Bottoms product flow rate

Flow rate of steam through valve

Mole fraction component i in the distillate and reflux

Mole fraction of component i in the feed

Liquid mole fraction of component i on tray j

Liquid mole fraction of component i in the reboiler and in the bottom product

Vapor mole fraction of component i

Pressure drop distillate product valve

Pressure drop across bottoms product valve

Log mean average temperature difference

Partial derivative of $K_{i,j}$ with respect to temperature

Latent heat of vaporization of steam

Density of the liquid on each respective stage

Liquid molar density of both tray j and downcomer j

Density of vapor on each respective stage
REFERENCES


Notes: The dot (.) atop any variable denotes the
time derivative of that variable. A capital "T"
denotes temperature and a small "t" represents time.

Equation (2-1) Francis weir formula for liquid
flow from a tray

Bolles (1) gives the Francis weir formula as:

\[ H_{ow} = 0.48 \left( \frac{q'}{l_w} \right)^{2/3} \]

where \( H_{ow} \) is the liquid crest over a straight weir in
inches, \( q' \) is the volumetric flow rate of liquid in
gallons per minute, and \( l_w \) is the length of the weir in
inches. By converting units and algebraically moving the
flow rate to the left side of the equation, equation
(2-1) may be formulated.
Equation (2-3)  Liquid flow from a downcomer

Bolles (1) presents the empirical relationship for the flow under a downcomer apron as:

\[ q = 0.6 \ A_{da} \ (2g(h_{da}))^{1/2} \]  \hspace{1cm} (A-2)

where \( q \) is the liquid flow rate in cubic feet per second, and \( g \) is the acceleration due to gravity. Assuming \( g \) equal to \( G_c \) (32.2 ft/sec\(^2\)) and by converting units, equation (2-3) may be derived.

Equation (2-12)  Time derivative of liquid mole fractions

An unsteady-state component balance for component "i" on tray "j" would appear as:

\[ (V_{j+1})(Y_{i,j+1}) + (L_d)_{j-1}(X_{i,j-1}) - (V_j)(Y_{i,j}) - (X_{i,j})(L_j) \]

\[ = \frac{d}{dt} \left[ (M_j)(X_{i,j}) \right] \]  \hspace{1cm} (A-3)

The right-hand side of equation (A-3) may be expanded by the product law:
\[
\frac{d}{dt} [M_j(X_{i,j})] = (M)(X_{i,j}) + (M)(X_{i,j}) \quad (A-4)
\]

By substituting equation (A-4) for the right-hand side of equation (A-3) and manipulating algebraically, equation (2-12) may be derived.

**Equation (2-13)**

**Temperature derivative of liquid on a tray**

A dynamic energy balance on tray "j" may be written as:

\[
(V_{j+1})(\bar{H}_v)_{j+1} + (L_d)_{j-1}(\bar{H}_l)_{j-1} - (V_j)(\bar{H}_v)_j - (L_j)(\bar{H}_l)_j
\]

\[
= \frac{d}{dt} [M_j(\bar{H}_l)_{j}]
\quad (A-5)
\]

The right-hand side of equation (A-5) is expanded to:

\[
(M)(\bar{H}_l)_j + (M) \left( \frac{dH_l}{dT} \right)_j (T) + \sum_{i=1}^{nc} (\frac{dH_l}{dX})_{i,j} (X)_{i,j}
\]

\[
= \frac{d}{dt} [M_j(\bar{H}_l)_j]
\quad (A-6)
\]
The \( \left( \frac{\partial H}{\partial t} \right)_j \) is the average heat capacity on tray \( j \) \( ((C_p)_j) \) and the term \( \left( \frac{\partial H}{\partial t} \right)_{i,j} \) may be assumed to be \( (H_i)_i,j \) if ideal liquid mixtures are assumed. Combination of equation (A-5) and equation (A-6), equation (2-13) may be derived using algebraic machinery.

**Equation (2-14) Pressure derivative above a tray**

When a liquid is at its bubble point, not only do the liquid mole fractions add to one, but the vapor mole fractions do, also. (Note: In this derivation, the stage subscript "\( j \)" will be omitted for clarity).

\[
\sum_{i=1}^{nc} Y_i = 1 \quad \text{(A-7)}
\]

If equation (A-7) is true, it can be proved that:

\[
\sum_{i=1}^{nc} Y_i = 0 \quad \text{(A-8)}
\]

Using the definition of the equilibrium constant, then:

\[
Y_i = (K_i)(X_i) \quad \text{(A-9)}
\]
thus

\[ \dot{y}_i = (K_i)(x_i) + (x_i) \frac{dK}{dT}_i \left( \frac{dT}{dt} \right) + \frac{dK}{dP_i} \left( \frac{dP}{dt} \right) \]  \hspace{1cm} (A-10)

The term \((K_i)(x_i)\) may be expanded using the chain rule and again assuming ideality:

\[ \dot{y}_i = (K_i)(x_i) + (x_i) \left( \frac{dK}{dT}_i \left( \frac{dT}{dt} \right) + \frac{dK}{dP_i} \left( \frac{dP}{dt} \right) \right) \]  \hspace{1cm} (A-11)

Since the equilibrium constant \(K\) is usually an explicit function of the temperature \(\frac{dK}{dT}_i\) is usually no real problem to compute. The term \(\frac{dK}{dP_i}\) may be estimated by assuming an Antoine relationship. That is:

\[ K_i = \frac{(P_s(T))_i}{P} \]  \hspace{1cm} (A-12)

where \((P_s(T))_i\) is the vapor pressure of component \(i\) as a function of temperature. Differentiation of equation (A-12) with respect to pressure yields:

\[ \frac{dK}{dP}_i = \frac{-(P_s(T))}{P^2} \]  \hspace{1cm} (A-13)

which, using equation (A-10), may be simplified to:
By substituting equation (A-14) into equation (A-11), which is in turn substituted into equation (A-8) we get:

\[ \sum_{i=1}^{nc} (K_i) \dot{x}_i + (x_i) \left[ \frac{dK}{dT}_i (T) - \frac{(K)(P)}{(P)} \right] = 0 \]  

(A-15)

Rearrangement of equation (A-15) with the re-addition of the "j" subscripts yields equation (2-14).

Equation 2-19) Bubble point temperature derivative in condenser

The derivatives of the top vapor mole fractions (equal to the derivatives of the respective liquid mole fractions condensing in the condenser) use the same basic relationship as equation (2-14). Thus by substituting equation (A-14) into equation (2-12), equation (2-19) may be obtained for the top tray.
Equation (2-20)  Liquid molar holdup in condenser

The summation term, equation (A-15) may also be manipulated to obtain equation (2-20). Inherent in equation (2-20) is the assumption that since $P_1$ is set to $P_2$ at all times, $P_1$ equals $P_2$. 
TRUNCATION ERROR ANALYSIS FOR THE JSME ALGORITHM

If \( Y_n \) represents the "true" value of the integrated variable at \( X_n \), then it can be shown (7) that the equation for the integrated variable integrated by the improved Euler algorithm may be written as:

\[
y_{n+1}^c = Y_n + (h/2)(f_n^c + f_{n+1}^c) + O(h^3)
\]  \( (B-1) \)

where \( y_{n+1}^c \) is the converged value of the numerically integrated variable at the time step "n+1", i.e., the value after many applications of the corrector step (equation 3-3). The variable \( h \) is the step size of the integration, and \( f_n \) is the true time derivative of \( Y \) at step \( n \) and \( f_{n+1}^c \) is the time derivative at step \( n+1 \) using \( y_{n+1}^c \). The truncation error on this step is known to be of the order of the step size cubed, represented by \( O(h^3) \). It can also be shown (7) that the accumulated error for converged integration by improved Euler is "n" times "\( O(h^3) \)" (where \( n = (X_{\text{final}} - X_{\text{initial}})/h \)) and is therefore equal to \( O_A(h^2) \), where \( O_A(h^2) \) represents the accumulated truncation error of the order of the step size squared. If this is substituted into equation (B-1), there are then two error terms, an accumulated error \( O_A \) and the error introduced on the
present time step \( (O) \). Now we wish to use the derivative associated with the converted solution \( Y_n \) instead of the true solution \( Y_n \) to examine the error in this derivative. If a simple linear differential equation is assumed,

\[
f_n = (A)(Y_n)
\]

then the error of the derivatives associated with the accumulated error in the integrated variables is:

\[
\text{Error} = (A)(Y_n - Y_n^c) = O_A(h^2)
\]

The converged corrected value of the integrated variable then may be written as:

\[
Y_n^{c} = Y_n^{c} + O_A(h^2) + (h/2)(f_n^c + f_{n+1}^c) + O_A(h^2) + O(h^3)
\]

When the accumulated error inside the parenthesis is multiplied by the step size, the resulting error term is of the order of the step size cubed, which is the same as the overall step. It can also be shown (7) that the predicted value of the integrated variable may be written as:

\[
Y_{n+1}^{p} = Y_n + (h/2)(3f_n^c - f_{n-1}^c) + O(h^3)
\]
which has the same order truncation error as the corrector equation although the coefficient of the error is larger for the predictor step. Following the previous logic, equation (B-5) may be written in terms of the converged variable:

\[ y_{n+1}^p = y_n^c + O_A(h^2) - (h/2)(3 \frac{f_n^c}{n} - \frac{f_{n-1}^c}{n-1}) + O(h^3) \]  

(B-6)

Of interest here is the fact that the orders of both the local and accumulated truncation error are the same in the corrector equation (equation B-4) and the predictor equation (equation (B-6)). As mentioned in Chapter 3, the corrector equation in the improved Euler algorithm is usually applied only once per time step. However, the local truncation error for a single corrector step is of the same order as when the corrector is applied many times. Even though the coefficient is slightly larger for the single-corrector case, the truncation error cannot be appreciably decreased by multiple corrector steps. Therefore, equations (B-4) and (B-6) still are valid for a single application of the corrector equation.

The basis for the JSME algorithm, as explained in Chapter 3, is that it offers the same order truncation error as the improved Euler method using only half the functional evaluations. If the previously calculated predicted values are substituted for the corrected values
in equation (B-5), then the error accrued in using the predicted value rather than the "true" solution in the functional evaluation, again assuming a linear differential equation is still the same order as before:

$$\text{Error} = A(Y_n - \bar{Y}_n) = o(h^2) \quad (B-7)$$

Substituting this result in equation (B-5) and using the JSME procedure:

$$Y_{n+1}^c = Y_n^c + o_A(h^2) + (h/2)(f_{n}^P + f_{n+1}^P + o_A(h^2)) + o(h^3) \quad (B-9)$$

Again, the error term in the parenthesis, when multiplied by the step size, is of the same order as the error of the overall step. Therefore, the order of the error is not increased by using the predicted values to obtain the time derivatives. These latter two equations not only sustain the assumption made for equation (B-7), but, also show that the local and accumulated errors are of the same order as for the improved Euler algorithm.
VITA

William Bell Stewart, Jr. was born April 29, 1953 in Minden, Louisiana. He attended the public schools in Winnfield, Louisiana, graduating from Winnfield Senior High School in May 1971.

He then enrolled in Louisiana State University, where he received the degree of Bachelor of Science in Chemical Engineering in December 1975. He became a member of Tau Beta Phi honorary engineering fraternity and Delta Tau Delta social fraternity. In August 1974, he married the former Bess Castille.

In December 1977, he received the degree of Master of Science in Chemical Engineering. During the summers of his undergraduate and graduate studies, he worked for Ethyl Corporation, Ludwig Consulting Engineers, and Energy Coordination at LSU, all in Baton Rouge. He also spent one year as half-time Instructor in the Chemical Engineering Department at LSU. During his graduate work, he was admitted to Phi Lambda Upsilon honorary chemical fraternity.

He is a present a candidate for the degree of Doctor of Philosophy, also in chemical engineering.
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Major Field: Chemical Engineering

Title of Thesis: Simulation and Evaluation of Distillation Control Systems Which Control Pressure With Reboiler Heat

Approved:

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James E. Irwin
Dean of the Graduate School

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Date of Examination:

February 11, 1981