A DYNAMIC SIMULATION OF A DISTILLATION COLUMN

By

JASPAL SINGH SABHARWAL

Bachelor of Engineering
University of Roorkee
Roorkee, India
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Thesis Approved:

Jan Wagner
Thesis Adviser

KAM Gasem

Ruth C Erbar

Thomas C. Collins
Dean of the Graduate College

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NOMENCLATURE

A_t = effective area of tray

E = porosity

h = time interval

h_i = specific enthalpy of liquid on stage i

H_i = specific enthalpy of vapor on stage i

h_t = crest height of liquid in weir

hf_i = specific enthalpy of feed stream to stage i

h_w = height of weir

K_i = K-value of component j on stage i

L_i = liquid molar flowrate from stage i

M_i = molar holdup on stage i

q_i = volumetric liquid flowrate on tray i

Q_i = heat loss from stage i

SL_i = liquid side draw molar flowrate from stage i

SV_i = vapor side draw molar flowrate from stage i

v_i = specific volume of liquid in weir

V_i = vapor molar flowrate from stage i

W = effective weir width

x_{ij} = liquid mole fraction of component j on stage i

y_{ij} = vapor mole fraction of component j on stage i

z_{ij} = mole fraction of component j in feed to stage i

CHAPTER I

INTRODUCTION

In recent years, process engineers have become increasingly interested in the control of industrial processes. Due to the widespread application of distillation in the process industry, the effective control of distillation columns has gained immense importance. Many advanced control strategies are available to improve the control of distillation columns, but in order to apply these control schemes properly, it is important to understand the dynamic behavior of the columns. Attempts have been made to study the unsteady state behavior of distillation columns by setting up small scale plants and developing a model based on operating data. Since plant data are often not available or expensive and difficult to obtain, it may be advantageous to perform computer simulation to predict the dynamic behavior using a reliable dynamic model. The primary objective of this study is to develop such a model and to evaluate the accuracy with available data.

The dynamic behavior of distillation columns can be rigorously described by a set of ordinary differential and algebraic equations. The distillation column is considered to consist of a known number of trays. Mass balances on each component on each tray and the overall mass and energy balances give rise to a set of differential equations which can be solved simultaneously to obtain the dynamic behavior. The correct formulation of such a system of equations was known long before digital computers came into common use. Analysis was limited to linearized models, for columns with a small number of trays, often only for binary mixtures and the computations were usually carried out on analog or hybrid computers. Not until the vast improvement in digital computer technology over the past three decades, have rigorous plate to plate calculation of distillation columns been feasible. A lot of work has been done in this field using digital computers and many models have been developed to describe the unsteady state behavior of distillation columns. The trend is towards better prediction of the dynamics. This study attempts to continue that trend.

CHAPTER II

LITERATURE REVIEW

Research on dynamic models for industrial processes dates back to 1932 when Ivanoff (16) presented a paper in which he made the first attempt at developing a mathematical model, from a strictly empirical point of view. Several other early authors (1, 29) also statistically correlated the behavior of a process with changes in independent variables and developed an approximate model of the process. Others (4, 10) approached the problem of developing a dynamic model by constructing small scale plants and then developing a dynamic model from the results obtained. Together these workers formed the foundation of modern process dynamics.

The first mathematical model of the dynamic behavior of a distillation column was proposed by Marshall and Pigford (17) in 1947. They considered the column to consist of equilibrium trays connected to each other by streams. Material balances were made on each tray for each component. The drawback of the model was that even for a simple column with a small number of trays, there were several differential equations to be solved simultaneously. Since neither digital nor analog computers were developed at the time, a rigorous solution was almost impossible. They tried to simplify the model by assuming constant molar overflow, negligible vapor holdup and a straight pseudo equilibrium curve, but these assumptions reduced the accuracy of the model.

Rose and co-workers (28) modeled a dynamic batch distillation column without the assumptions of Marshall and Pigford. Although they used a computer for simulation , there was still the drawback of excessive computer time requirement.

Voetter (33) was perhaps the first to combine experimental data with a theoretical analysis. He compared the equations of Marshall and Pigford with experimental data obtained on a sixty tray Oldershaw column. The experimental and calculated values compared excellently during the earlier portion of the transient period, but as the column approached steady-state, the values differed significantly.

Further work using a tray-by-tray model was done by Peiser and Grover (24) who simulated the dynamics of a multicomponent distillation column with flooding in trays near the bottom of the tower. Waggoner and Holland (32) developed a column model using a similar approach but assuming that plate efficiencies were known. A generalized model that takes into account the effects of the hydraulics and mixing on the trays was presented by Tetlow (31) . However the theta method of convergence used by Holland and co-workers (12) is iterative and relatively inefficient for the large number of equations present in the system. More recent work includes that of Howard (13), in which a general model was developed with the basic column equations to allow the specification of variable plate holdups, variable plate efficiencies, heat loss from the column and finite-time liquid-flow dynamics. Using the Kutta-Merson integration method, with relatively small integration steps to ensure stability, Howard (13) proceeded to solve a dynamic distillation problem involving a 14 tray column operated at total reflux with a mixture of benzene, toulene and ethyl benzene. In a subsequent study, Howard (13) compared the simulated results to the experimental data obtained from an existing column and concluded that inadequate information about the characteristics of the column caused more errors in the simulation results than the deficiencies in the generalized computer model did. The basic mathematical model used by these authors forms the basis of most models developed.

Morris and Svrcek (22), in response to the inability of conventional equilibrium models to handle absorbing and stripping problems, developed a distillation tray model based on a mass transfer approach. The model was tested with data obtained from a 75 stage industrial distillation unit, but the general application of this model to other columns still requires a prior knowledge of the mass transfer characteristics of the components.

Most published results on column simulation do not contain sufficient details to allow duplication or continued investigation. Among the exceptions are the collection of simulation results compiled by Holland and Liapis (12) and the simulation study of the extractive distillation column by Gallun (8), in which Gear's algorithm is applied with the utilization of the Kubicek algorithm for efficient solution of banded sparse matrices.

Since then, a number of different numerical methods and solution procedures have been used over the years for the solution of stiff differential equations that arise in column simulation. For stability considerations most methods are implicit and are often incorporated with some selection scheme for integration time steps for better efficiency. Among the various integration methods available the semi-implicit Runge-Kutta (SIRK) method has gained a lot of popularity over the last few years. To reduce the enormous dimensionality of the process model associated with trains of distillation columns, so that computer simulation could be possible, Cho and Joseph (5) proposed a reduced order dynamic model which approximates the composition and flow profiles in sections of a columns by polynomials. Orthogonal collation was used to approximate the partial difference equation and a semi-implicit Runge - Kutta procedure proposed by Ballard (2) was utilized to integrate the transient equations. More recently, Wong (36) used the adaptive semi-implicit Runge - Kutta (ASIRK) method proposed by Prokopakis (25) to simulate the dynamics of a hydrocarbon separator, a pilot scale water-methanol binary distillation column and an extractive distillation column.

Based on a mathematical model of a distillation column and the solution procedure of the ASIRK a computer program has been developed in this study to simulate the steady state and dynamic behavior of several distillation columns and to study the nonlinear behavior exhibited by the column. Further, the steady state results have been compared with those obtained from MAXI*SIM, which is a steady state simulator developed at the Department of Chemical Engineering, Oklahoma State University, Stillwater, Oklahoma.

In Chapter III of this study, a formal treatment of the basic model of a generalized column is given. This includes the formulation of the stage mass balances, energy balances and the tray holdup equations and a look at the special cases of trays, the reboiler and condenser.

This is followed in Chapter IV by the numerical procedures used to solve the different type of equations handled in this simulation.

In Chapter V, the application of the numerical techniques to the material and energy balance equations and the algorithm of the simulation is discussed.

Chapter VI contains the different cases considered to verify the accuracy of the model. This chapter also has a comparison with data obtained from the simulator MAXI*SIM.

The conclusions and recommendations for further study are presented in Chapter VII.

CHAPTER III

DYNAMIC MODEL OF COLUMN

Introduction

In a distillation process, liquid and vapor flowing counter-currently come into continuous contact on a series of trays. The complexity of the process can range from a simple column with a single feed and two product streams to a complex column with multiple feed streams, multiple side and product streams and with non-ideal reacting chemical species on all trays. The rigorous modeling of such a process requires simultaneous treatment of the material balance equations and the energy balance equations.

In this chapter, the modeling equations for a generalized tray are presented. These equations are easily extended for a series of trays to describe a complete distillation column. The equation can also be modified to model units such as reboilers and condensers. These equations form the basis of a dynamic simulator which can be implemented in a digital computer for simulating the dynamic behavior of distillation columns.

Model of a Tray

The distillation column is considered as a series of stages with the condenser and the reboiler as two stages with special characteristics. In this simulation, the stages are counted from top to bottom with the condenser as the first stage and the reboiler as the last one. A schematic diagram of the ith stage with its input and output streams is shown in Fig. 1. The stage receives an external feed, a vapor stream from the tray below and a liquid stream from the tray above. The streams leaving the tray are a vapor stream to the tray above, a liquid stream to the tray below, a vapor sidestream and a liquid sidestream. Apart from these material streams there is a heat loss stream on every stage. The streams are subscripted according to the tray from which they originate. For example, the vapor stream leaving tray i is named V_i. Figure 2 shows the equivalence of a distillation column to the mathematical model considered in this work.

Material Balance

The following assumptions have been made to derive a total and a component mass balance equation for a tray -

a) The mixture is not chemically reactive.

b) The liquid on the tray is perfectly mixed.

c) Material storage in the vapor and the downcomer is negligible

An overall mass balance on the tray gives -

$$dM_i/dt = F_i + V_{i+1} + L_{i-1} - (V_i + SV_i) - (L_i + SL_i) \qquad (3.1)$$

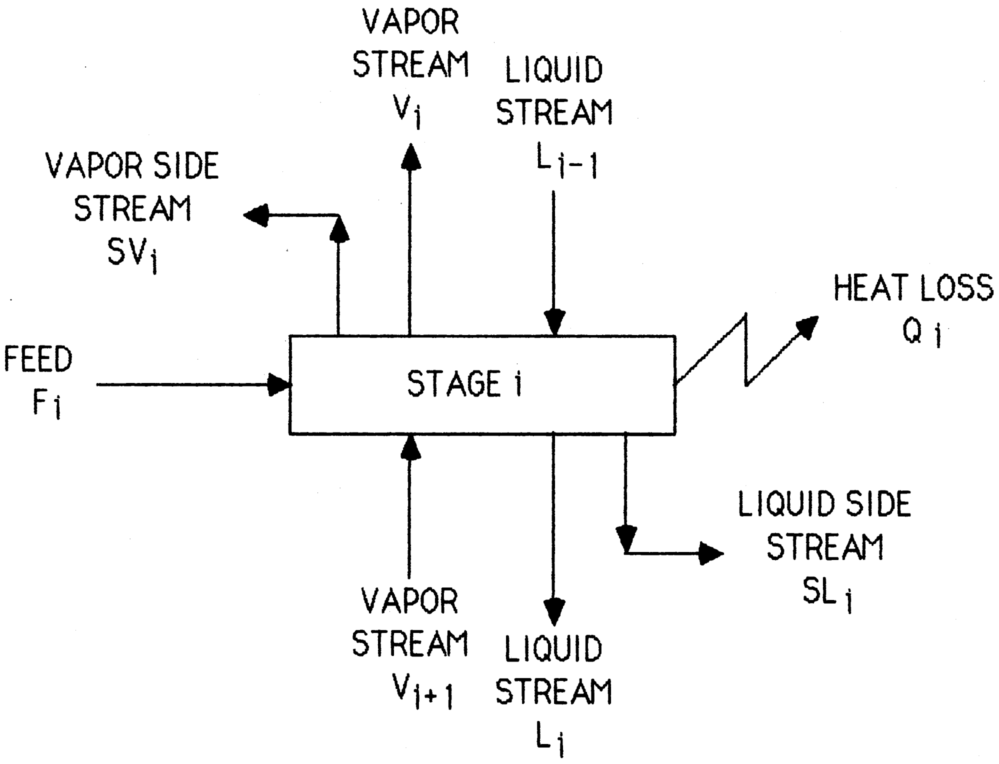


Figure 1. An Equilibrium Stage with the Incoming and Outgoing Material and Energy Streams

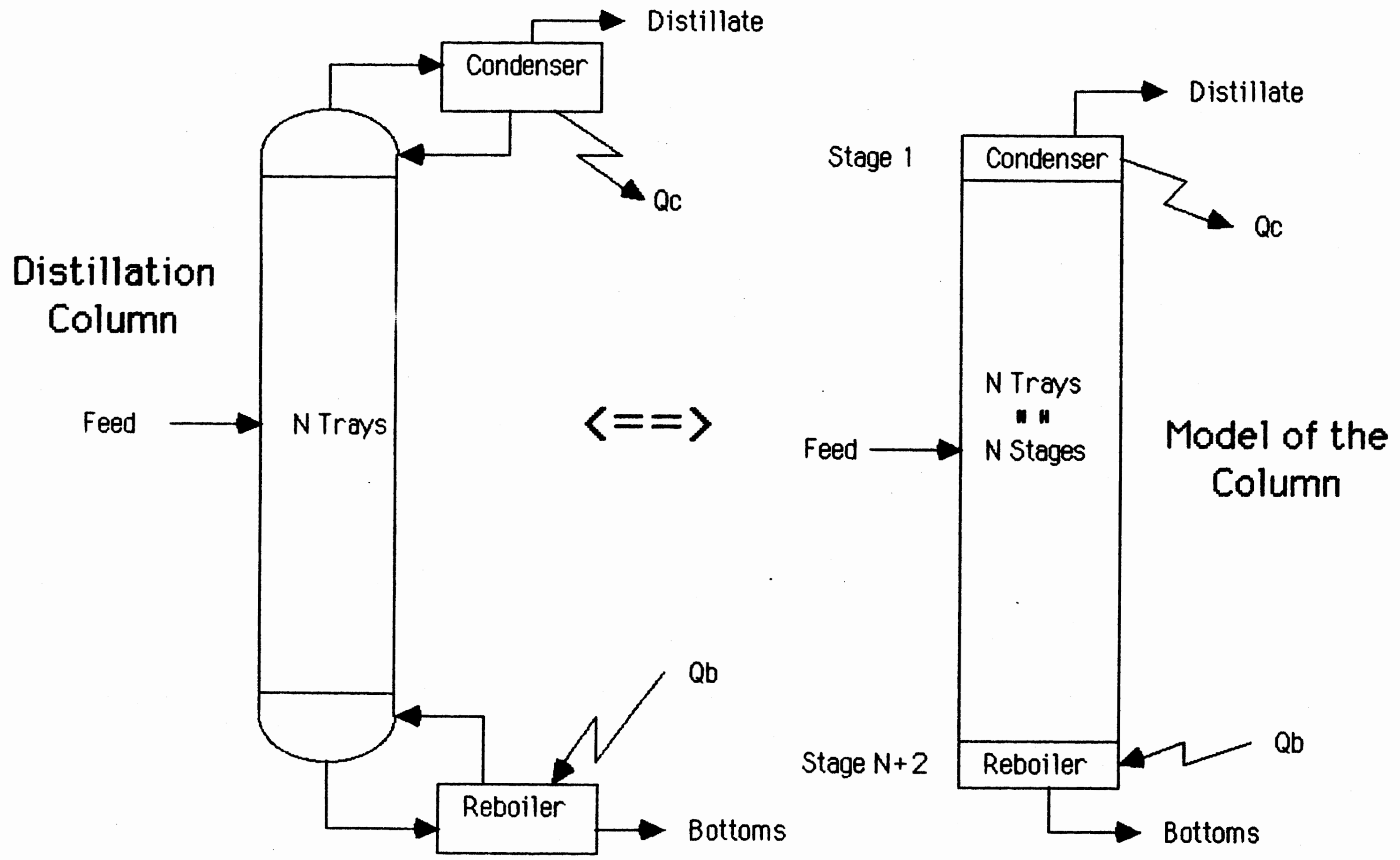


Figure 2. A Distillation Column and its Equivalent Model

A schematic diagram of a stage with the input and output material streams is shown in Figure 3. The component balance for component j is given by -

$$d(M_i x_{ij})/dt = F_i z_{ij} + V_{i+1} y_{i+1j} + L_{i-1} x_{i-1j} - (V_i + SV_i) y_{ij} - (L_i + SL_i) x_{ij} \qquad (3.2)$$

Also,

$$d(M_i x_{ij})/dt = M_i (dx_{ij}/dt) + x_{ij}(dM_i/dt) \qquad (3.3)$$

Substituting Equations (3.1) and (3.2) into Equation (3.3) and then rearranging terms results in the following form of the component material balance

$$dx_{ij}/dt = [\ F_i(z_{ij} - x_{ij}) + V_{i+1}(y_{i+1j} - x_{ij}) + L_{i-1}(x_{i-1j} - x_{ij}) - (V_i + SV_i)(y_{ij} - x_{ij})\ ]\ /\ M_i \qquad (3.4)$$

Energy Balance

Several simplifying assumptions have been made in deriving the energy balance. These are -

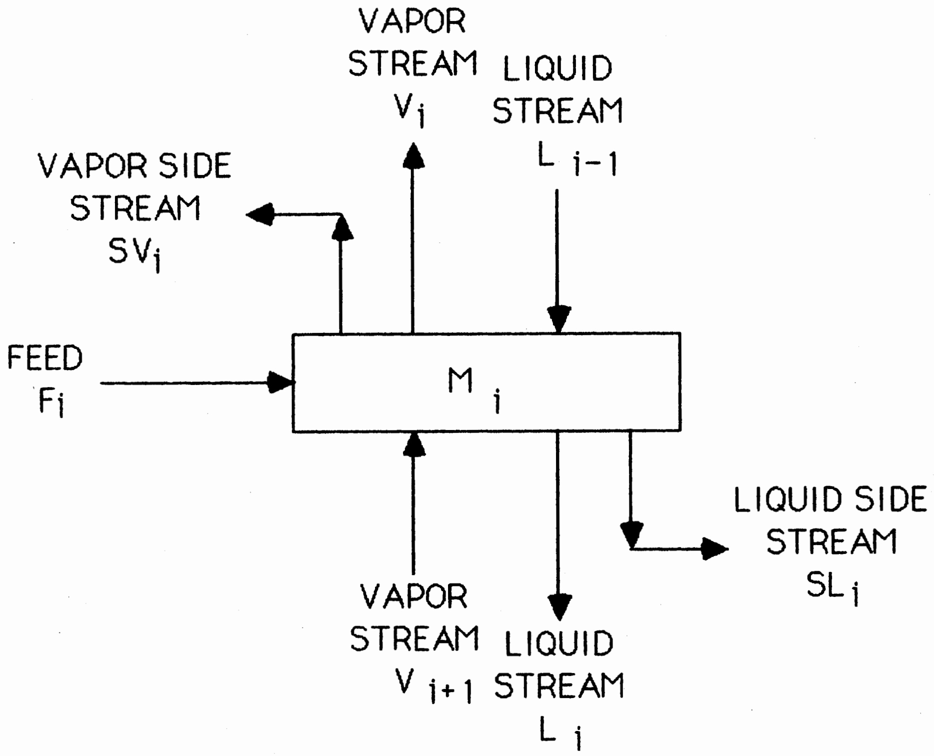
a) Energy and material accumulation in the vapor phase is negligible.

b) Energy accumulation in tray metal is negligible.

c) Energy accumulation in the downcomer is negligible.

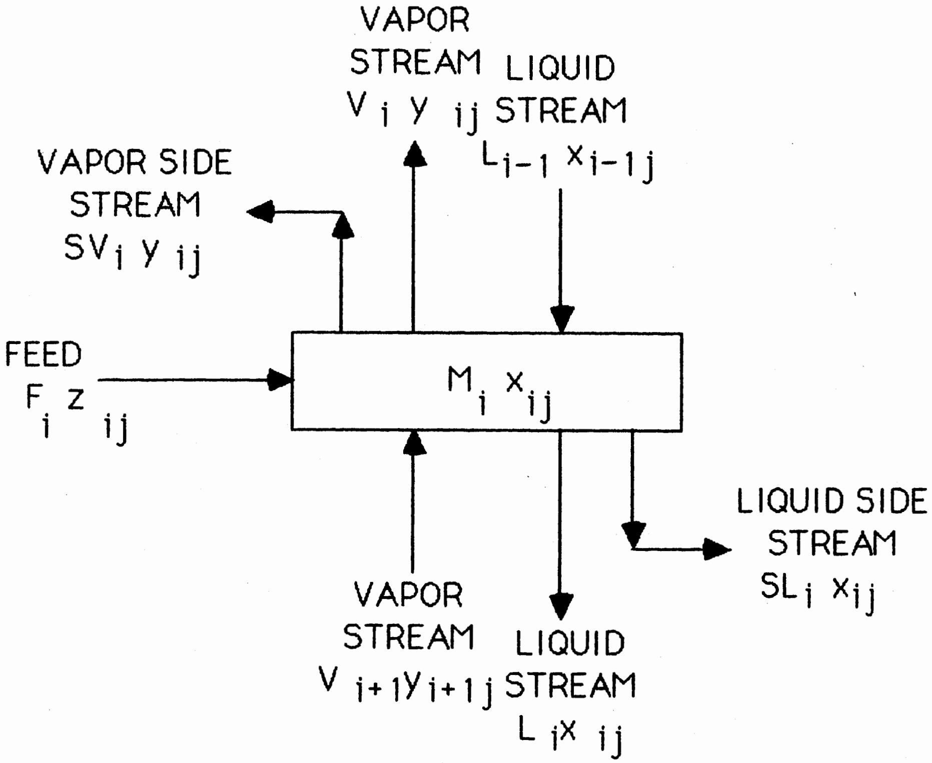
d) The heat of mixing among the chemical species is negligible.

Assumption a) is generally valid when the pressure inside the column is low and the vapor density is small.



$$\frac{dM_i}{dt} = F_i + V_{i+1} + L_{i-1} - (V_i + SV_i) - (L_i + SL_i)$$

Figure 3. Mass Balance on a stage



$$\frac{dM_i x_{ij}}{dt} = F_i z_{ij} + V_{i+1} y_{i+1j} + L_{i-1} x_{i-1j} - (V_i + SV_i) y_{ij} - (L_i + SL_i) x_{ij}$$

Figure 4. Component Mass Balance on a stage

This assumption however, must be applied with caution for simulating the behavior of high pressure systems. Assumptions b) and c) are also generally valid for low pressure columns. Assumption d) is true in most chemical systems since the dominant heat effect in distillation processes is due to the vaporization and condensation of fluids, which usually involves a much larger amount of heat exchange than the heat of mixing.

Based on these assumptions, the energy balance equation on tray i is -

$$d(M_i h_i)/dt = \{ F_i hf_i - Q_i + V_{i+1} H_{i+1} + L_{i-1} h_{i-1} - (V_i + SV_i) H_i - (L_i + SL_i) h_i \} \quad (3.5)$$

A schematic diagram of a stage with the input and output energy streams is given in Figure 5. Also,

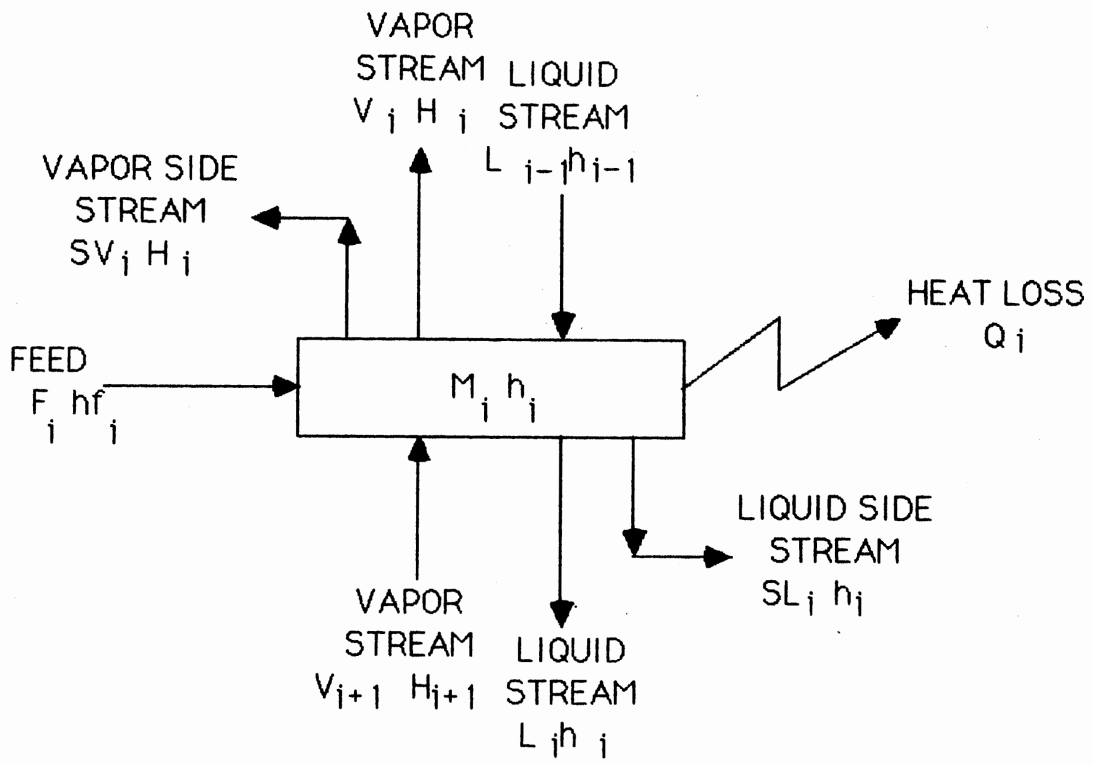
$$d(M_i h_i) = M_i (dh_i/dt) + h_i (dM_i/dt) \quad (3.6)$$

Substitution of Equations (3.1) and (3.5) in Equation (3.6) and subsequent rearrangement of terms results in the following equation.

$$dh_i/dt = \{ F_i(hf_i - h_i) - Q_i + V_i+1(H_{i+1} - h_i) + L_{i-1}(h_{i-1} - h_i) - (V_i + SV_i)(H_i - h_i) \} / M_i \quad (3.7)$$

By using properties of partial derivatives, Equation (3.7) is transformed into a linear algebraic equation of the form

$$E_i = -a_i L_{i-1} + \beta_i V_i - \Phi_i V_{i+1} \quad (3.8)$$



$$\frac{dM_i h_i}{dt} = F_i hf_i + V_{i+1} H_{i+1} + L_{i-1} h_{i-1} - (V_i + SV_i) H_i - (L_i + SL_i) - Q_i$$

Figure 5. Energy Balance on a stage

The derivation of Equation (3.8) and the definition of E_i, a_i, β_i and Φ_i are given in Appendix A.

Tray Holdup

The mass balance and the energy balance are solved simultaneously to obtain the liquid and vapor flow rates. Two different approaches can be used to calculate the tray holdup term dM_i/dt in the mass balance. These are

a) Mass balance based on constant tray holdup

b) Mass balance based on tray holdup as a function of liquid flow rates

For the first case, the mass balance becomes an an algebraic equation since the dM_i/dt term equals zero. The mass balance can be written as

$$m_i = L_{i-1} - L_i - V_i + V_{i+1} \qquad (3.9)$$

where

$$m_i = SL_i + SV_i - F_i \qquad (3.10)$$

For the second case, the Francis weir formula(24) is used to correlate the liquid flow rate with the tray holdup. The Francis weir formula(24) is given as

$$q_i / W = 1.839 (h_t)^{1.5} \qquad (3.11)$$

where q_i is the volumetric liquid flow rate on tray i in cubic meters per second, h_t is the crest height of the liquid in the weir in meters and W is defined as the width of the weir in meters. This equation is modified to calculate the liquid flow rates in the form

$$dL_i/dt = [\ F_i + V_{i+1} + L_{i-1} - (V_i + SV_i) - (L_i + SL_i)\ ]$$
$$[\ W / (\ 0.02898\ A_t\ (1 - E))\ ]$$
$$[\ W / L_i v_i\ ]^{-1/3} \qquad (3.12)$$

The liquid flow rates obtained by numerically integrating this ordinary differential equation are used to calculate the molar holdups using the following equation derived from the Francis weir formula(24) -

$$M_i = [\ 0.04347\ (\ L_i v_i\ / W)^{2/3} + hw\ ]$$
$$A_t (1 - E)\ /\ v_i \qquad (3.13)$$

The vapor profile is calculated using the energy balance equation. The derivations of all the derived equations and variables are included in Appendix B. In this study, only the case of constant molar holdup has been considered for verification.

Special Cases of The Generalized Tray Model

Condensers and reboilers can be modeled as stages with special conditions and restraints. The conditions for a partial reboiler, total condenser and a partial reboiler are listed below.

Partial Reboiler

In the case of a partial reboiler, some part of the liquid stream from the bottom tray of the distillation column is vaporized while the liquid in the reboiler, which is in equilibrium with the vapor is drawn off as the bottoms product. The bottoms product is considered as the liquid side stream from the tray. The applicable conditions to this type of reboiler are

$$V_{N+1} = 0 \tag{3.14}$$

$$L_N = 0 \tag{3.15}$$

where N is the total number of stages including the condenser and the reboiler. On applying these conditions to the generalized overall mass balance and energy balance equations, Equations (3.1) and (3.5) respectively, the resulting equations are

$$dM_N/dt = F_N + L_{N-1} - (V_N + SV_N) - SL_N \tag{3.16}$$

and

$$\begin{aligned} d(M_N h_N)/dt = \{ & F_N hf_N - Q_N + L_{N-1} h_{N-1} \\ & - (V_N + SV_N) H_N - SL_N h_N \} \end{aligned} \tag{3.17}$$

Total Condenser

In the case of a total condenser, the vapor stream from the top tray of the distillation column is condensed to a saturated or subcooled liquid. A portion of this condensed liquid is returned to the column as reflux and the rest is drawn off as the distillate product, which will be represented as the liquid side stream from tray number one. Thus,

$$L_0 = 0 \tag{3.18}$$

$$V_1 = 0 \tag{3.19}$$

It should be noted that according to one of the assumptions of the derivation of the generalized tray model, the outgoing condensed liquid streams are saturated. Although the liquid may be subcooled, the approximation is reasonable from the energy balance view point, since it is the heat of condensation of the vapor stream that contributes most to the condenser duty.

Partial Condenser

In a partial reboiler, the vapor distillate product is in equilibrium with the liquid reflux. The condition to be applied to the generalized tray model, in this case, is

$$V_0 = 0 \tag{3.20}$$

CHAPTER IV

NUMERICAL TECHNIQUES FOR THE SIMULATION

The distillation column mathematical model developed in the previous chapter involves large sets of nonlinear algebraic equations and nonlinear ordinary differential equations. For a numerical solution of these equations to be feasible in terms of the use of computing resources, it is necessary to employ efficient numerical algorithms which give reasonably accurate results. This chapter illustrates the numerical techniques used in this study.

Solution Method for a System of Linear Algebraic Equations

Large sets of algebraic equations must be solved at each time step of the simulation when implementing an integration algorithm. For a distillation column with no pumparounds, the coefficient matrix of these algebraic equations is tridiagonal in structure, and the system of equations can be solved very efficiently with the Thomas algorithm. Suppose the system of equations is

$$\mathbf{A}_{nxn} \cdot \mathbf{x}_{nx1} = \mathbf{d}_{nx1} \qquad (4.1)$$

where $\mathbf{A}$ is a tridiagonal coefficient matrix with

lower diagonal elements a_k $\quad k = 1,2,\ldots\ldots,n-1$ (4.2a)
diagonal elements b_k $\quad k = 1,2,\ldots\ldots,n$ (4.2b)
upper diagonal elements c_k $\quad k = 2,3,\ldots\ldots,n$ (4.2c)

and **x** and **d** are nx1 vectors.

According to Thomas algorithm, the equations can be solved directly as follows

$$\beta_1 = b_1 \tag{4.3a}$$

$$\phi_1 = d_1 / \beta_1 \tag{4.3b}$$

$$\beta_k = b_k - (a_k c_k - 1)/\beta_{k-1} \qquad k = 2,..,n \tag{4.3c}$$

$$\phi_k = (d_k - a_k \phi_{k-1})/\beta_k \qquad k = 2,..,n \tag{4.3d}$$

and finally,

$$x_n = \phi_n \tag{4.4a}$$

$$x_k = \phi_k - (c_k x_{k-1})/\beta_k \qquad k=n-1,..,1 \tag{4.4b}$$

Solution Method for System of Algebraic Equations

The calculation of liquid and vapor flowrates for the case of constant molar holdups involves the solution of two sets of algebraic equations, namely the mass balances and energy balance on each tray. As the coefficient matrix in this is not tridiagonal, the Thomas algorithm, described in the previous section is not applicable. For this case, the Gauss Seidel iterative method is used. This method requires reasonable initial estimates of the variables being calculated. However, this is not a problem since the values from the last time step can be used as the initial estimates. Consider a set of equations

$$f(x_1,x_2,...,x_n) = 0 \tag{4.5}$$

This set of equations can be transformed to

$$x_1 = F_1(x_2,x_3,....,x_n) \tag{4.6a}$$

$$x_2 = F_2(x_1,x_3,....,x_n) \tag{4.6b}$$

$$x_3 = F_3(x_1,x_2,x_4,....,x_n) \tag{4.6c}$$

$$\begin{array}{ccccc} \vdots & \vdots & \vdots & \vdots & \vdots \end{array}$$

$$x_n = F_n(x_1,x_2,....,x_{n-1}) \tag{4.6x}$$

Using the initial estimates of $x_2,x_3,..,x_n$, the new value of x_1 is calculated from Equation (4.6a). This value of x_1 and the initial estimates of $x_3,x_4..,x_n$ are used to calculate the new value of x_2 from Equation (3.4). This process is continued with all the equations, recursively, until the values of $x_1,x_2,...,x_n$ become constant within a specified tolerance. It is worth noting here that the latest estimates of the variables are used always.

Solution Method for System of Ordinary Differential Equations

For a system of C components, Equation (3.2) gives rise to C simultaneous nonlinear ordinary differential equations whose variable often have a large range of response times. Such a system of equations is commonly called a "stiff" system. For numerical stability the solution scheme used for this type of equations are necessarily implicit. The numerical scheme used in this study are ASIRK, the Adaptive Semi-Implicit Runge-Kutta Method developed by Prokopakis and Seider(25).

The ASIRK Integration Method

Consider the set of differential equations

$$d\mathbf{y}/d\mathbf{x} = \mathbf{f}(\mathbf{x},\mathbf{y}) \tag{4.7}$$

The solution of these equations, according to the ASIRK method is

$$\mathbf{y}^{t+h} = \mathbf{y}^{t} + w_1\mathbf{k}_1 + w_2\mathbf{k}_2 \tag{4.8}$$

where $\mathbf{y}^t$ is the value of $\mathbf{y}$ at time t and $\mathbf{y}^{t+h}$ is the value of y after the next time interval h. The rest of the variables are defined by the following equations

$$[I - haJ(\mathbf{y}^t)]\ \mathbf{k}_1 = h\ \mathbf{f}(\mathbf{x},\mathbf{y}^t) \tag{4.9a}$$

$$[I - haJ(\mathbf{y}^t)]\ \mathbf{k}_2 = h\ \mathbf{f}(\mathbf{x},\mathbf{y}^t + b\mathbf{k}_1) \tag{4.9b}$$

where

$$a = [1 + \{1 - (1 - G)/2\}^{1/2}] \ / \ (1 - G) \tag{4.10a}$$

$$b = [3(0.5 - a)]^{-1} \tag{4.10b}$$

$$w_2 = 3(0.5 - a)^2 \tag{4.10c}$$

$$w_1 = 1 - w_2 \tag{4.10d}$$

$J(\mathbf{y}^t)$ is the Jacobian Matrix at time interval t, and its elements are given by

$$J_{mn} = \partial f(x,y)_m/\partial y_n \qquad (4.11)$$

Also, at every time step, the value of G, the characteristic root of the equation when h*L tend to infinity (where L is the eigen value), is expressed in terms of the pseudo-eigenvalue of the stiffest variable, Ls. These relations are as follows

$$L_s = [1 - h\ \{f_s(x,y)/k_{1s}\}]/ha \qquad (4.12)$$

and

$$G_s = A/[B + (hL_s)2] + C/[D + hL_s] + E \qquad (4.13)$$

where

$$A = -4.9221 \qquad (4.14a)$$

$$B = 21.1642 \qquad (4.14b)$$

$$C = 0.5287 \qquad (4.14c)$$

$$D = -0.6889 \qquad (4.14d)$$

$$E = 0.0 \qquad (4.14e)$$

Prokopakis and Seider(25) also proposed a rather sophisticated step size control algorithm which requires the solution of a fourth order polynomial. In this study, a simpler approach suggested by Ballard et all(2) was employed since it has been known to give comparable results(2) and saves on computer time. The simple formula for time step control is given by

$$h^{new} = h^{old}[r/e_t]^{0.5} \qquad (4.15)$$

$$0.25 \leq h^{new}/h^{old} \leq 2.0$$

where r is the user specified error control parameter and e_t is the local truncation error.

CHAPTER V

ALGORITHM OF THE SIMULATION

The previous chapters describe the mathematical model for a distillation column and also the numerical techniques used in this study to solve the equations of the model. The proper sequence of the application of the numerical techniques, and thus the solution of the model, is described in this chapter. Figure 6 gives a conceptual depiction of the algorithm which forms the basis of this simulator.

The program starts by reading in the essential parameters of the simulation, which are, the number of trays, the number of components and the time of operation. On the basis of these parameters, the characteristics of the initial steady state which include the pressures, temperatures, feed rates, product rates, liquid and vapor flow rates, heat duties and liquid and vapor composition on each tray are read in, thus initializing all the required variables and arrays. The time at this steady state is set to zero minutes.

To calculate the liquid composition at the next time step, the integration method is applied to the component balance, Equation (3.4), in which we define

$$f(x_{ij}) = dx_{ij}/dt = [F_i(z_{ij} - x_{ij}) + V_{i+1}(y_{i+1j} - x_{ij})$$

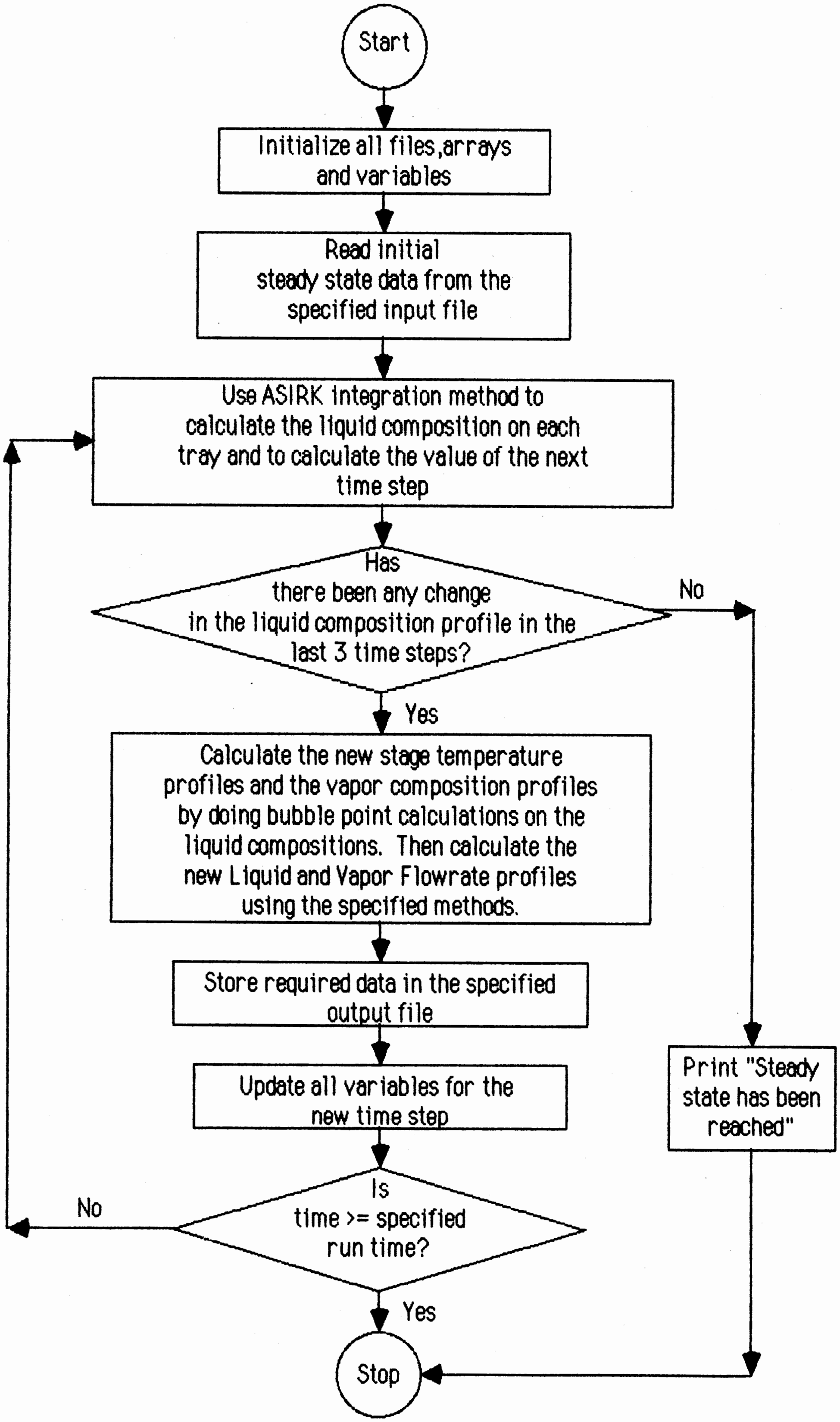


Figure 6. Flowchart of the simulation algorithm

$$+ L_{i-1j}(x_{i-1j} - x_{ij})$$
$$- (V_i + SV_i)(y_{ij} - x_{ij})]/M_i \quad (5.1)$$

When ASIRK is used as the integrator, the Jacobian matrix for the above function needs to be calculated. The Jacobian of a matrix is given by

$$J_{mn} = [\partial f(x_{mj})/\partial x_{nj}] \quad (5.2)$$

and since the compositions on the jth stage are only influenced by those of the adjacent stages, the Jacobian is a tridiagonal matrix with diagonal elements

$$J_{ii} = -[F_i + V_{i+1} + L_{i-1} + (V_i + SV_i)(K_{ij} - 1)]/M_i \quad (5.3a)$$
$$i = 1,2,....,N$$

where K_{ij} is the K-value of component j on tray i. The upper diagonal elements of the Jacobian are

$$J_{ii+1} = V_{i+1} \cdot K_{i+1j} / M_i \qquad i = 2,3,....,N \quad (5.3b)$$

and the lower diagonal elements are

$$J_{ii-1} = L_{i-1} / M_i \qquad i = 1,2,....,N-1 \quad (5.3c)$$

Due to the tridiagonal nature of the Jacobian matrix, the solution of the incremental functions, k1 and k2, involves the solution of a system of algebraic equations with a tridiagonal coefficient matrix. As mentioned before, Thomas algorithm is a very efficient method for the solution of this type of equation set.

The new liquid composition obtained from the integrators form the basis of all further calculations. A call is made to the thermodynamic package and the new liquid composition values are used to calculate the new temperatures at each tray and also the vapor compositions.

These in turn are used to calculate the values of the parameters of the algebraic form of the energy balance namely, a_i, β_i, Φ_i, E_i as defined in Appendix I.

The algebraic form of the tray energy balance rewritten here

$$E_i = -a_i L_{i-1} + \beta_i V_i - \Phi_i V_{i+1} \qquad (3.8)$$

is used with the mass balance equation to calculate the liquid and vapor flowrates. As mentioned earlier, there are two cases possible - constant tray holdup and relative tray holdup. These cases have different methods of solving for the liquid and vapor flow rates.

In the case of constant molar holdup, the mass balance, Equation (3.9), is

$$m_i = L_{i-1} - L_i - V_i + V_{i+1} \qquad (3.9)$$

Rearrangement of equations (3.8) and (3.9) gives

$$L_i = L_{i-1} - V_i + V_{i+1} - MM_i \qquad (5.4a)$$

$$V_i = (a_i L_{i-1} + \Phi_i V_{i+1} + E_i)/\beta_i \qquad (5.4b)$$

$$i = 1,2,\ldots,N$$

Applying the end conditions for the condensers and reboilers results in a set of equations which can be easily and efficiently solved by the Gauss Seidel iteration method. The vapor and liquid flowrate values of the last time step are used as the initial estimates required for this iteration method.

In the case of a relative molar holdup, the liquid rates are obtained by integrating Equation (3.12), rewritten here

$$dL/dt = [F_i + V_{i+1} + L_{i-1} - (V_i + SV_i) - (L_i + SL_i)] \\ [W/(0.02898\ A_t(1-E)][W/(L_i v_i]^{-1/3} \qquad (3.12)$$

This equation can also be solved using ASIRK, the same integration method that is used to integrate the component balance equation, Equation (3.4).

The vapor flowrates are obtained by the substitution of these liquid flow rates and the end conditions of the reboiler and condenser in the algebraic form of energy balance.

The calculation of liquid and vapor flowrates completes the calcualtion for one time step. These calculations are repeated till the convergence criteria is satisfied.

CHAPTER VI

MODEL VERIFICATION

To evaluate the performance of the model developed in the previous chapters for the simulation of the dynamic behavior of a distillation column, the model is tested with two problems. In these problems, the steady state and dynamic responses of columns are simulated using this model and then compared with verified available data. The first problem tests whether the steady state reached by the simulator after a step change in the initial conditions is the same as that predicted by a verified steady state simulator for the same final conditions. The second problem is designed to establish the accuracy of the transient response predicted by the simulator. After the accuracy of the model is tested with the two problems, it is further compared with the results of a simulation of a column predicted by Wong(36). Before going on to the problems, the property prediction package, which is a critical factor for the accuracy of a simulation, is tested.

Property Prediction Verification

Two simple examples are considered to test the accuracy of the thermodynamic property prediction package used. The property predictor has been extracted from GPA*SIM(9) simulator and is the same as that which is used in MAXI*SIM(18). This package is based on the Suave modification of the Redlich-Kwong equation of state. The thermodynamic package provides three type of data for the simulation: (1) bubble point temperatures at a given pressure and composition, (2) liquid and vapor specific enthalpies of a mixture with given composition at a given temperature and pressure and (3) K-values of the components of a mixture of given composition, pressure and temperature. These are the three property predictions tested in the two examples. Example 1 is an equilibrium mixture of 30 percent propane and 70 percent n-butane, flashed at 331.13 K and 1000 kPa. The second example is that of a bubble point mixture of 60 percent propane, 20 percent n-butane and 20 percent n-hexane at 2068 kPa (300 psi). The properties predicted by GPA*SIM(9) and by the study's thermodynamic package are compared in Table I. As can be seen the properties predicted by this work are in good agreement with those predicted by GPA*SIM(9).

Steady State Results Verification

A depropanizer is considered to test the accuracy of the predicted steady state performance for a given column configuration and set of operating parameters. Table II lists the specifications for the depropanizer. The initial steady state was simulated on MAXI*SIM(18), a rigorous tray-by-tray simulator, and then the final steady state,

TABLE I

PROPERTY PREDICTION VERIFICATION

Example 1

Specifications -

Feed Temperature : 331.13 K
Feed Pressure : 1000 kPa
Feed Composition
C_3 : 0.3
nC_4 : 0.7

Results -

		GPA*SIM(9)	This work
Liquid Enthalpy, MJ/kmol		2.674	2.673
Vapor Enthalpy, MJ/kmol		18.541	18.541
K-values	C_3	1.74352	1.74358
	nC_4	0.68132	0.68135

Example 2

Specifications -

Feed Pressure : 2068 kPa
Feed Composition
C_3 : 0.6
nC_4 : 0.2
nC_6 : 0.2

Results -

		GPA*SIM(9)	This work
Bubble Point Temperature, K		357.86	357.85
Liquid Enthalpy, MJ/kmol		6.9722	6.9721
K-values	C_3	1.38210	1.38209
	nC_4	0.67858	0.67856
	nC_6	0.17523	0.17523

TABLE II

DEPROPANIZER SPECIFICATIONS

Initial Steady State	
Number of Plates	35
Number of Components	6
Condenser	Total
Reboiler	Partial
Feed Plate	18
Column Pressure	2400 kPa
Distillate Specification	90 mole % C_3
Propane Recovery	99 %
Feed Specifications	
Temperature (Bubble Pt)	349.01 K
Composition	
CO_2	3.8 mol/s
C_2	226.1 mol/s
C_3	2100.0 mol/s
nC_4	400.0 mol/s
nC_5	200.0 mol/s
nC_6	300.0 mol/s
Step Disturbance	
Changes in Feed	
Temperature (Bubble Pt)	352.75 K
Composition	
CO_2	2.0 mol/s
C_2	208.0 mol/s
C_3	2150.0 mol/s
nC_4	350.0 mol/s
nC_5	450.0 mol/s
nC_6	250.0 mol/s

Rest of the specifications are unchanged.

after the step change, was simulated using the model developed in this study. The results obtained from the model were compared with the results from MAXI*SIM(18) for the depropanizer with the same specifications. The simulated tray temperatures, molar vapor flowrates and the mole fraction of propane in the liquid leaving each tray predicted by the two sources are compared in Table III and Figures 7 and 8.

As can be seen in Table III, there is an excellent agreement between this model and MAXI*SIM(18). The predicted tray temperatures differ by a maximum of 0.1 K, the flow rates differ by 0.5 % and the mole fractions of different components vary by 0.1 % at a maximum.

Transient Response Results Verification

An ideal test problem would be one in which the simulator results can be compared with plant operating data but unfortunately, transient operating data on simple distillation or fractionation columns is difficult to obtain. Some data is published but it is not accompanied by enough information to simulate the column on the computer. The same holds true for simulated transient response data. In this section, two simulated transient response examples are considered and the results obtained from the simulator developed in this work are compared with the published data.

The first test problem considered to verify the transient response predicted by this simulator is the solved

TABLE III

STEADY STATE RESULTS COMPARISON

Stage No.	Temperature Profile K		Vapor Flow Rate mol/s		Liquid Comp of Propane x_i*10	
	This Work	MAXI* SIM(18)	This Work	MAXI* SIM(18)	This Work	MAXI* SIM(18)
1	331.12	331.12	0000.0	0000.0	9.0000	9.0000
2	335.51	335.51	5061.2	5064.2	9.3155	9.3172
5	338.74	338.72	5067.8	5071.2	9.0981	9.1023
10	341.63	341.61	4964.9	4968.4	8.4940	8.4989
15	344.20	344.19	4868.5	4871.7	8.0313	8.0344
19	353.96	353.95	4449.7	4452.3	6.9567	6.9582
25	358.61	358.52	4624.7	4630.1	6.8959	6.9093
30	375.43	375.18	4424.8	4429.4	4.4397	4.4739
36	424.26	424.18	4643.8	4640.5	0.5023	0.5079
37	434.67	434.62	4677.8	4675.9	0.2775	0.2804

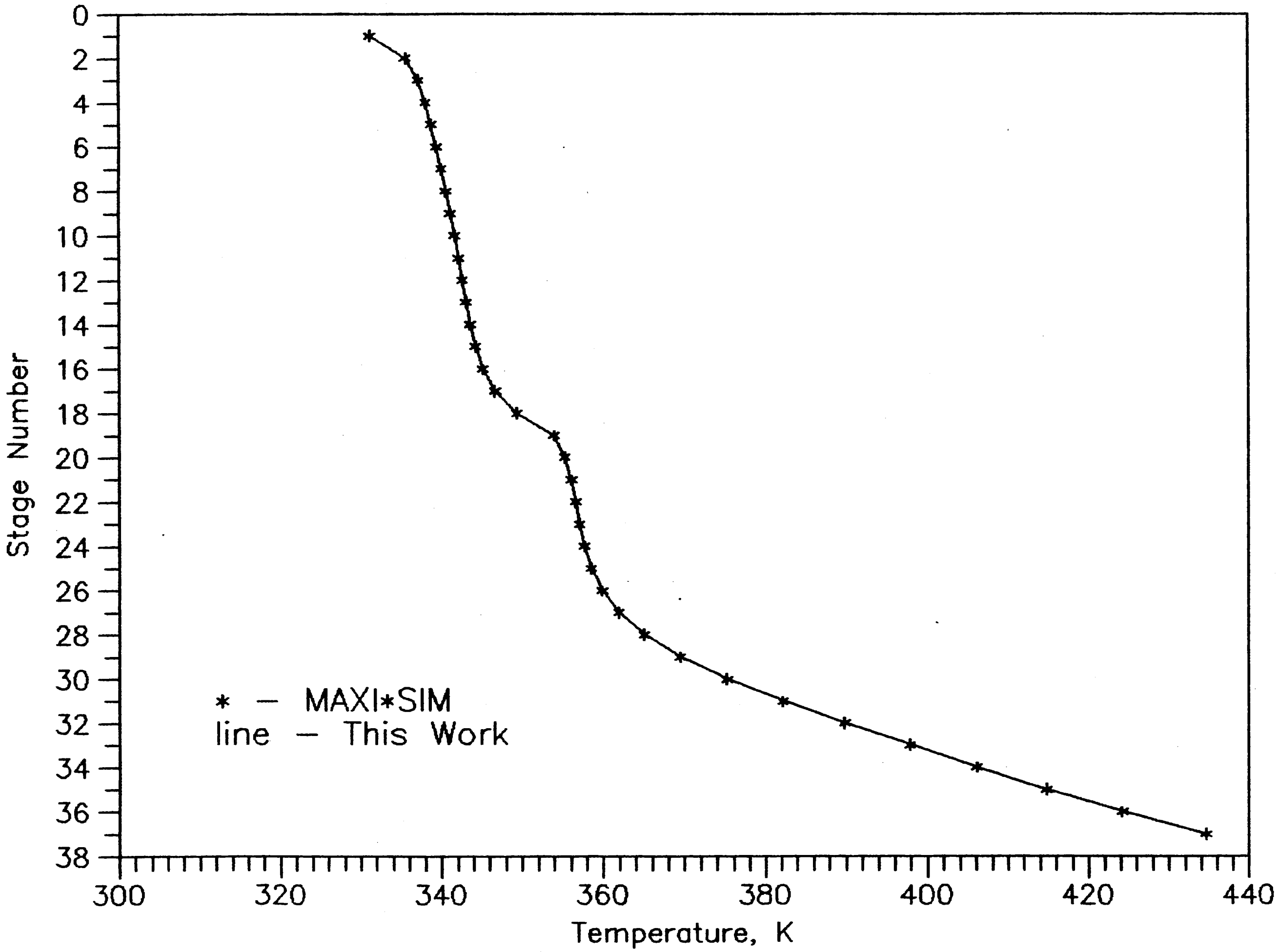


Figure 7. Depropanizer Tray Temperature Profile Comparison

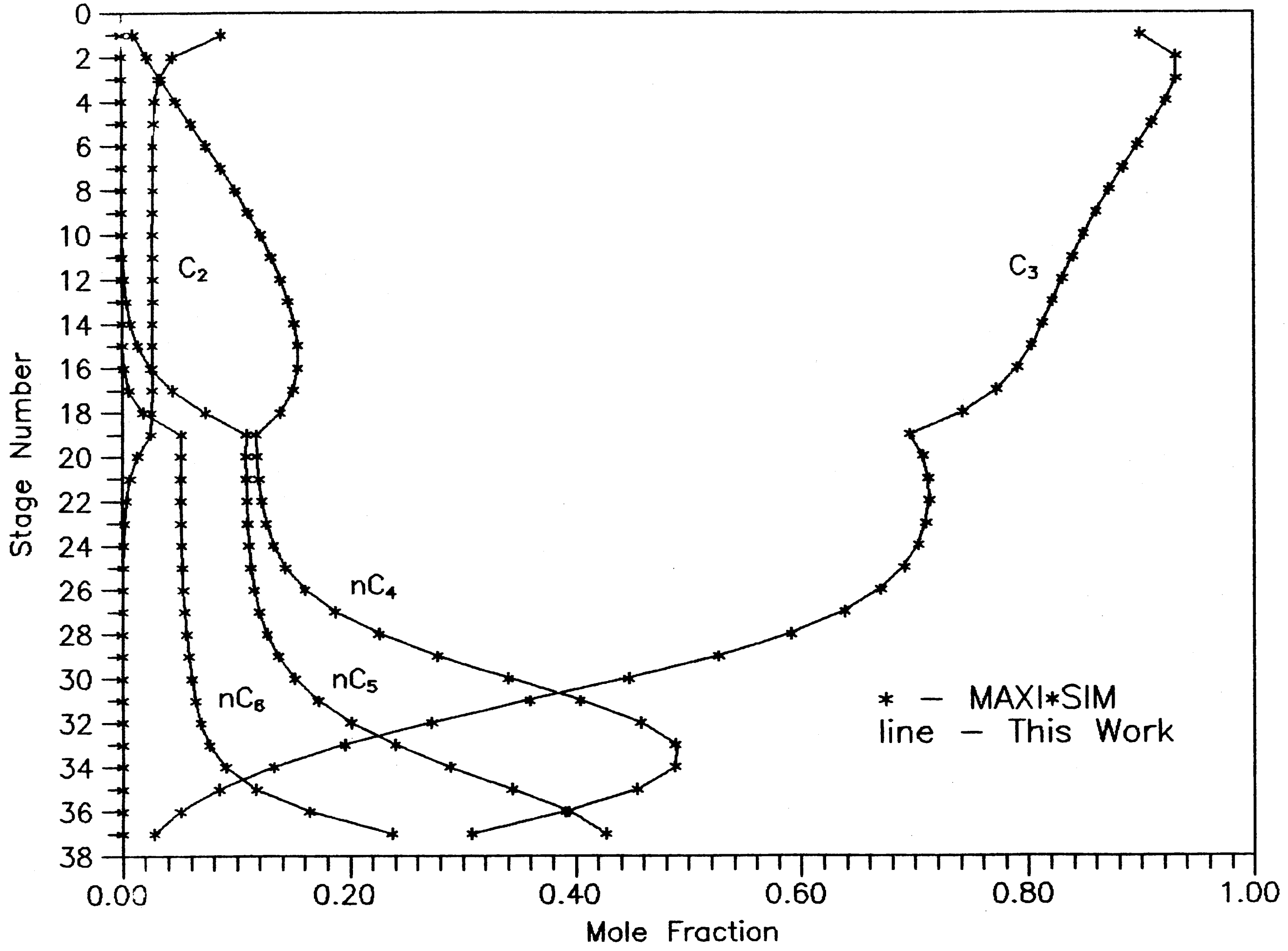


Figure 8. Depropanizer Liquid Composition Profile Comparison

Example 4.2 of Holland and Liapis(12). The column consists of 5 trays with a total condenser and a partial reboiler. The column operates at 2068 kPa (300 psi) and has one bubble point feed stream, on tray 4. The disturbance introduced to the column is a feed composition and temperature change. The temperature is the bubble point temperature at the column pressure, of the feed with the new composition. The specifications have been reproduced in Table IV. Holland and Liapis(12) used Gears algorithm as the integrating technique to simulate the final results. As the initial steady state was not defined completely, it was generated using the simulator developed in this work. The results of the initial steady state derived from the simulation are compared with the Holland and Liapis(12) data in Table V. The two sets of data show good agreement.

The transient behavior of the column after the step disturbance in feed is summarized in Figures 9 and 10. Numerical data are not compared. Since a variable time-step is used in ASIRK, the cumulative time is never the same as the transient results provided by Holland and Liapis(12). For this simulation, an initial time step of 0.1 minutes was taken. The graphs show that the simulation results compare well with the data provided by Holland and Liapis(12). Also, as shown in Figures 9 and 10 and Table VI, the final steady state results are very comparable.

The second test problem is reported by Wong(36) and was further studied by Rice(27). Wong(36) simulated a single

TABLE IV

HOLLAND AND LIAPIS(12) PROBLEM SPECIFICATIONS

<u>Initial Steady State</u>

Number of Plates	:	5
Number of Components	:	3
Condenser	:	Total
Reboiler	:	Partial
Feed Plate	:	4
Column Pressure	:	2068 kPa
Molar Holdup, mol/min	:	50 on each tray
Vapor Flow Rate from Top Tray, mol/min	:	150

Feed and Product Specifications :

	Feed	Distillate	Bottoms
Temperature, K	Bubble pt.	332.03	393.47
Component Flow Rate, mol/min			
C_3H_8	60.0000	48.3711	11.6289
nC_4H_{10}	20.0000	0.1628	18.3715
nC_6H_{14}	20.0000	43.6E-5	19.9996

<u>Step Disturbance</u>

Feed Component Flow Rates, mol/min	
C_3H_8	10.0000
nC_4H_{10}	40.0000
nC_6H_{14}	50.0000

TABLE IV (Continued)

Equilibrium Data :

$$(K_i/T)^{1/3} = a1_i + a2_i*T + a3_i*T^2 + a4_i*T^3$$

T in deg R

Component	$a1*10^2$	$a2*10^5$	$a3*10^8$	$a4*10^{12}$
C_3H_8	-14.512	53.639	-5.3052	-173.58
nC_4H_{10}	-14.181	36.866	16.521	-248.22
nC_6H_{14}	1.1507	-33.88	97.795	-542.36

Liquid Enthalpy Data :

$$(h_i)^{1/2} = c1_i + c2_i*T + c3_i*T^2$$

T in deg R

Component	c1	$c2*10$	$c3*10^5$
C_3H_8	-14.5000	1.98022	-2.90488
nC_4H_{10}	-20.2981	2.30057	-3.86634
nC_6H_{14}	-23.8704	2.67681	-4.41978

Vapor Enthalpy Data :

$$(H_i)^{1/2} = e1_i + e2_i*T + e3_i*T^2$$

T in deg R

Component	e1	$e2*10^4$	$e3*10^6$
C_3H_8	81.7959	389.819	36.4709
nC_4H_{10}	152.668	-1153.48	146.641
nC_6H_{14}	85.8349	1522.39	-34.018

TABLE V

HOLLAND AND LIAPIS(12) PROBLEM INITIAL STEADY STATE COMPARISON

Temperature and Vapor Profiles

Stage No.	Temperature K		Vapor Flowrate mol/min	
	This Work	Holland & Liapis	This Work	Holland & Liapis
1	332.21	332.03	0.00	0.00
2	334.44	334.26	150.60	150.00
3	338.02	337.83	146.83	146.32
4	343.62	343.42	141.45	141.10
5	355.19	355.00	130.93	130.98
6	366.55	366.36	123.62	123.73
7	393.66	393.47	108.92	109.10

Product Compositions

Component	Distillate mol/min		Bottoms mol/min	
	This Work	Holland & Liapis	This Work	Holland & Liapis
C_3H_8	48.372	48.371	11.6270	11.6289
nC_4H_{10}	1.6278	1.6289	18.3732	18.3715
nC_6H_{14}	43.61E-5	43.56E-5	19.9996	19.9996

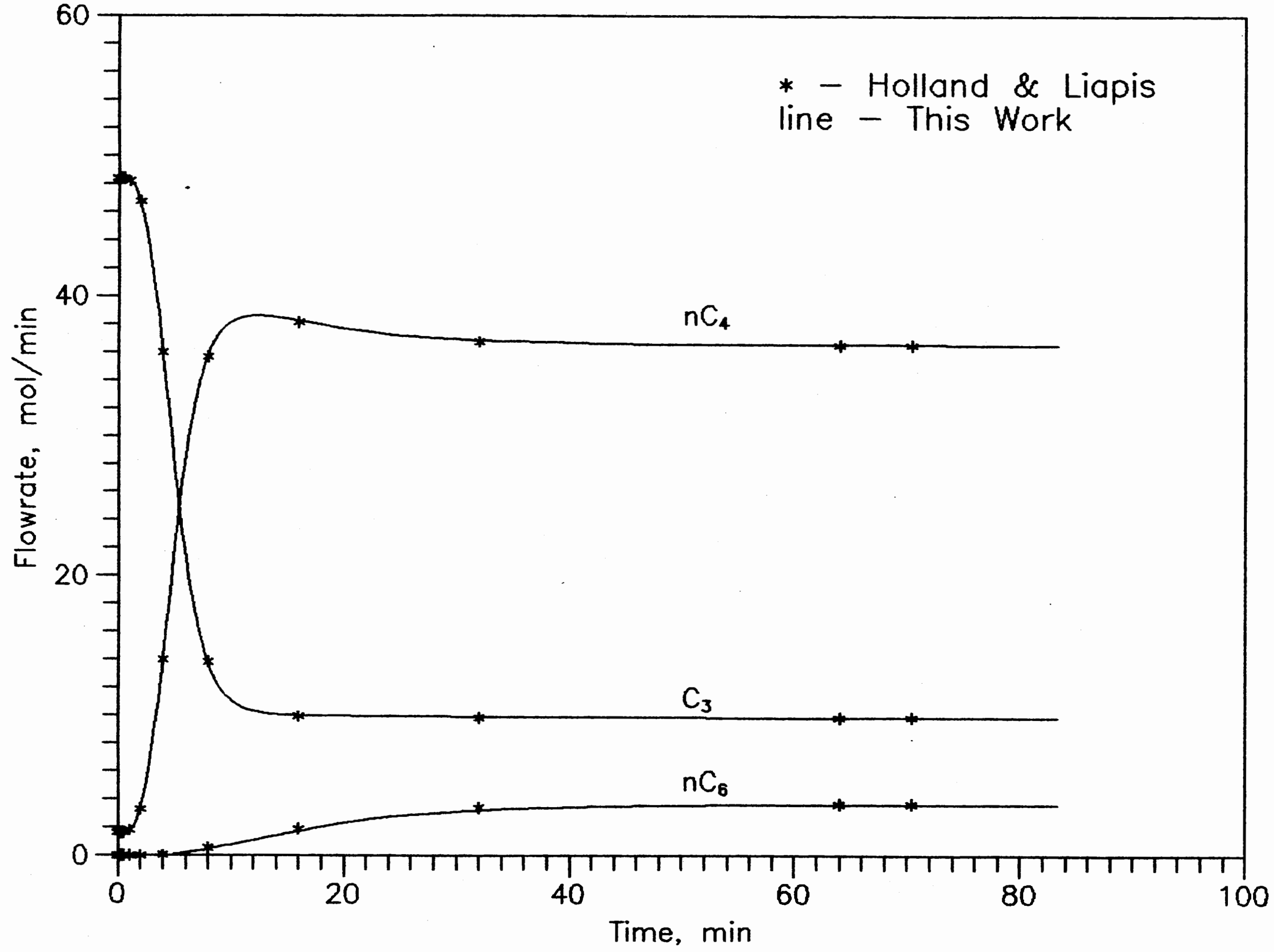


Figure 9. Component Distillate Rate Profiles

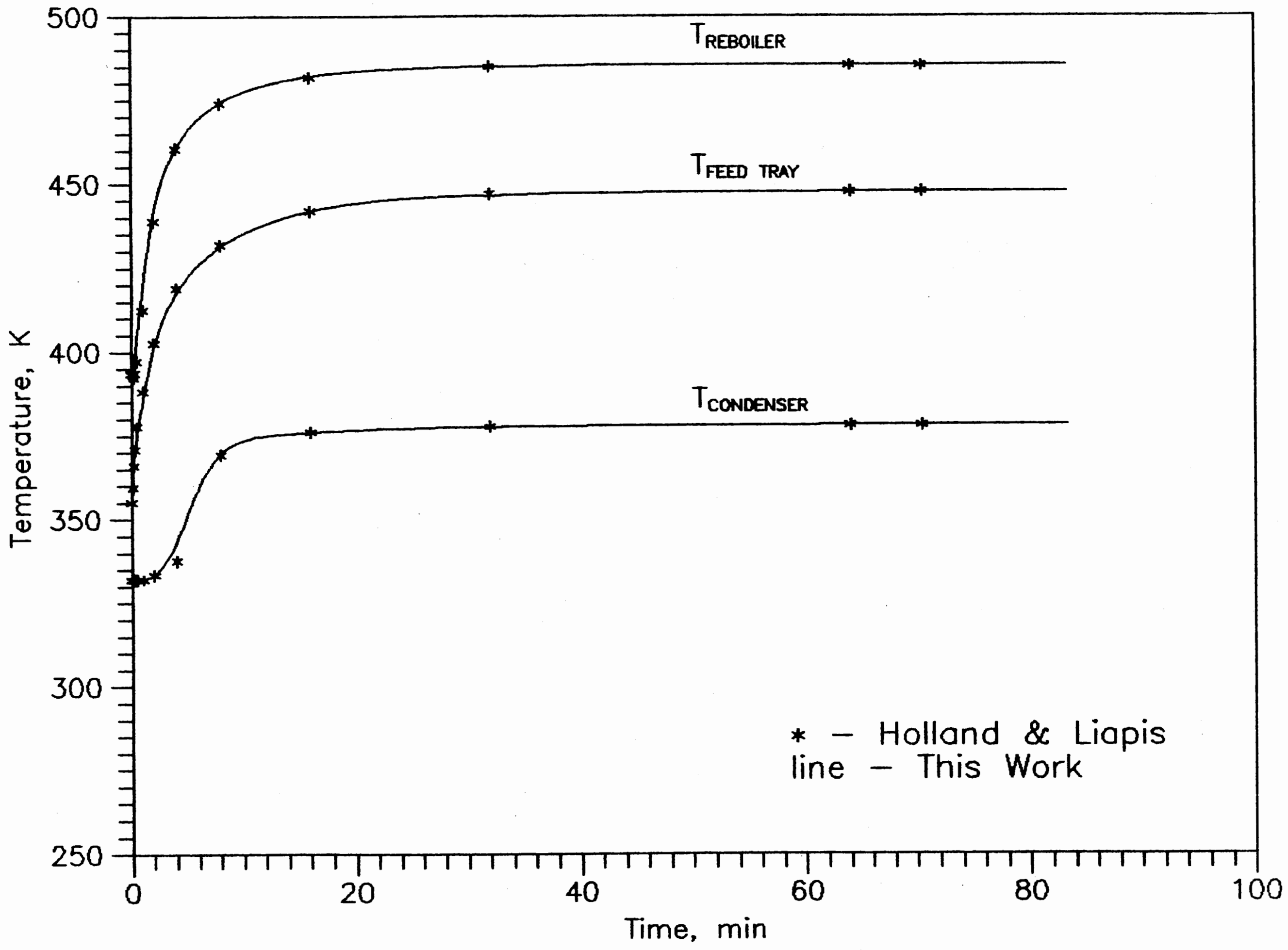


Figure 10. Temperature Profile Comparison

TABLE VI

HOLLAND AND LIAPIS(12) PROBLEM FINAL STEADY STATE COMPARISON

Temperatures in Kelvin

	This Work	Holland & Liapis
Condenser	377.98	377.92
Feed Plate	447.59	447.59
Reboiler	447.36	447.27

Component Distillate Rates in mol/min

	This Work	Holland & Liapis
C_3H_8	9.8526	9.8520
nC_4H_{10}	36.4846	36.4829
nC_6H_{14}	3.6675	3.6651

feed column equipped with 29 trays, a partial condenser and a partial reboiler. The complete column configuration is given in Table VII. Wong(36) did not provide complete details of the thermodynamic property prediction algorithm he used for the simulation and so the GPA*SIM(9) subroutines were used in this simulation. The transient response study included step changes in the feed rate, reflux rate and the reboiler duty. All these changes were studied individually, keeping the other parameters constant. These step changes have also been listed in Table VII.

The results obtained for the simulations are presented in Figures 11, 12 and 13. As can be seen, the transient behavior predicted by this study shows a similar trend to that predicted by Wong(36). This system is supposed to exhibit inverse response behavior i.e. a change in the direction of change of propane composition in the distillate. This simulation clearly shows this behavior. along with the similarities, there are obvious differences in the actual values of the composition of propane in distillate at a given time and also in the times predicted for the system to reach steady state. Due to an incomplete description of the simulation by Wong(36), it is difficult to ascertain the exact cause of the differences. The difference in behavior prediction can generally be caused by the difference in the thermodynamic packages and the difference in the integration technique. Even if the integration subroutine is the same, as it is in this case, the differences in the user specified

TABLE VII

WONG(36) PROBLEM SPECIFICATIONS

Initial Steady State

Number of Plates	29
Number of Components	5
Condenser	Partial
Reboiler	Partial
Feed Plate	12
Column Pressure	2400 kPa
Tray Holdup	14.0 kmol
Reboiler Holdup	50.0 kmol
Condenser Holdup	50.0 kmol
Tray Efficiency	100 %
Feed Composition	
C_2H_6	0.03
C_3H_6	0.40
C_3H_8	0.15
iC_4H_{10}	0.15
$c\text{-}2C_4H_8$	0.27
Feed Temperature	Bubble Point
Feed Flowrate	0.8333 kmol/s
Reflux Rate	1.5000 kmol/s
Reboiler Duty	22655 kJ

Step Disturbances

Case 1 - 10 % Decrease in Reflux Rate

Feed Flowrate	0.8333 kmol/s
Reflux Rate	1.3500 kmol/s
Reboiler Duty	22655 kJ

Case 2 - 10 % Increase in Reboiler Duty

Feed Flowrate	0.8333 kmol/s
Reflux Rate	1.5000 kmol/s
Reboiler Duty	24920 kJ

Case 3 - 10 % Decrease in Feed Flowrate

Feed Flowrate	0.7500 kmol/s
Reflux Rate	1.5000 kmol/s
Reboiler Duty	22655 kJ

TABLE VII (Continued)

Temperature and Flowrate Profiles

Tray	Temperature K	Vapor Flowrate kmol/s	Liquid Flowrate kmol/s
Condenser	330.17	0.000	1.500
1	331.20	1.972	1.504
5	333.18	1.968	1.488
10	340.99	1.873	1.364
12	347.83	1.797	2.165
15	350.27	1.811	2.171
20	359.39	1.786	2.140
25	378.41	1.799	2.177
29	389.52	1.856	2.222
Reboiler	391.39	1.861	0.000

Liquid Composition Profile

Tray	C_2H_6	C_3H_6	C_3H_8	iC_4H_{10}	$c\text{-}2C_4H_8$
Condenser	0.02782	0.69494	0.27376	0.00316	0.00032
1	0.01765	0.68467	0.29176	0.00527	0.00065
5	0.01092	0.63458	0.32135	0.02569	0.00746
10	0.01010	0.51923	0.27295	0.10440	0.09332
12	0.00957	0.44016	0.22403	0.13586	0.19038
15	0.00149	0.39234	0.25507	0.15100	0.20011
20	0.00006	0.25055	0.24449	0.24209	0.26281
25	0.00000	0.08080	0.11378	0.38358	0.42184
29	0.00000	0.01843	0.03349	0.36901	0.57907
Reboiler	0.00000	0.01148	0.02224	0.34378	0.62250

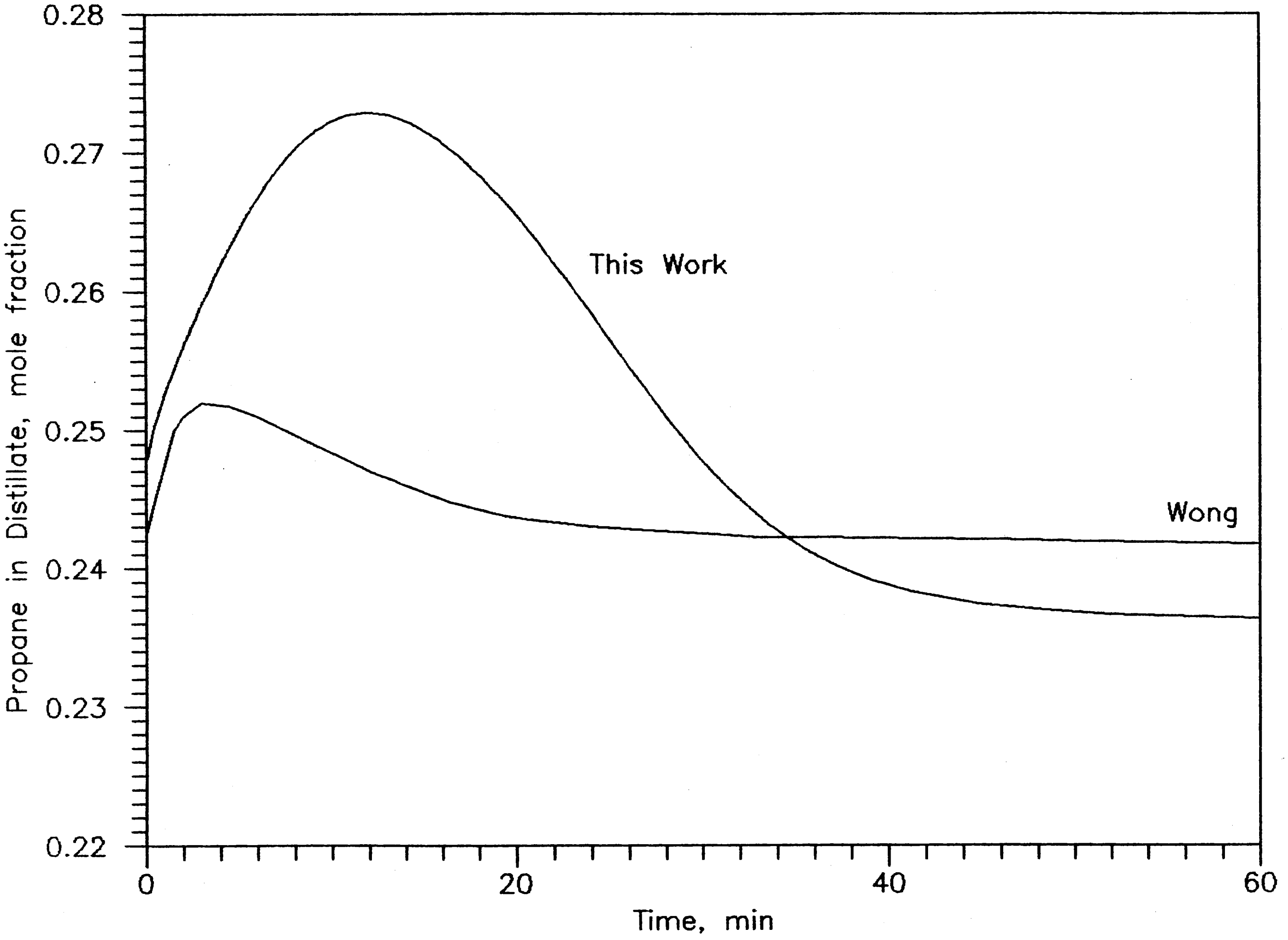


Figure 11. Response of Distillate Propane Composition to a 10 Percent Decrease in Reflux Rate

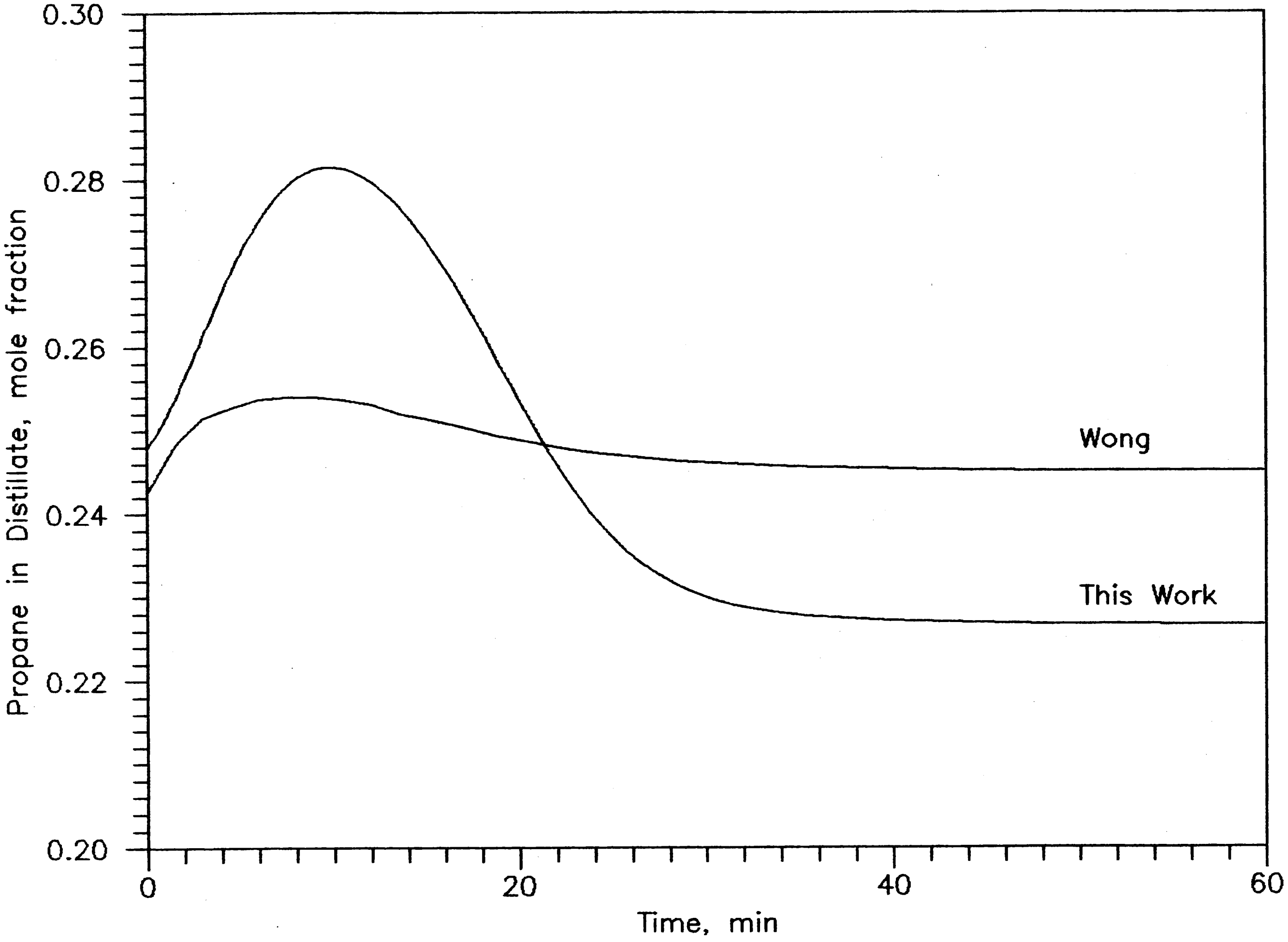


Figure 12. Response of Distillate Propane Composition to a 10 Percent Increase in Reboiler Duty

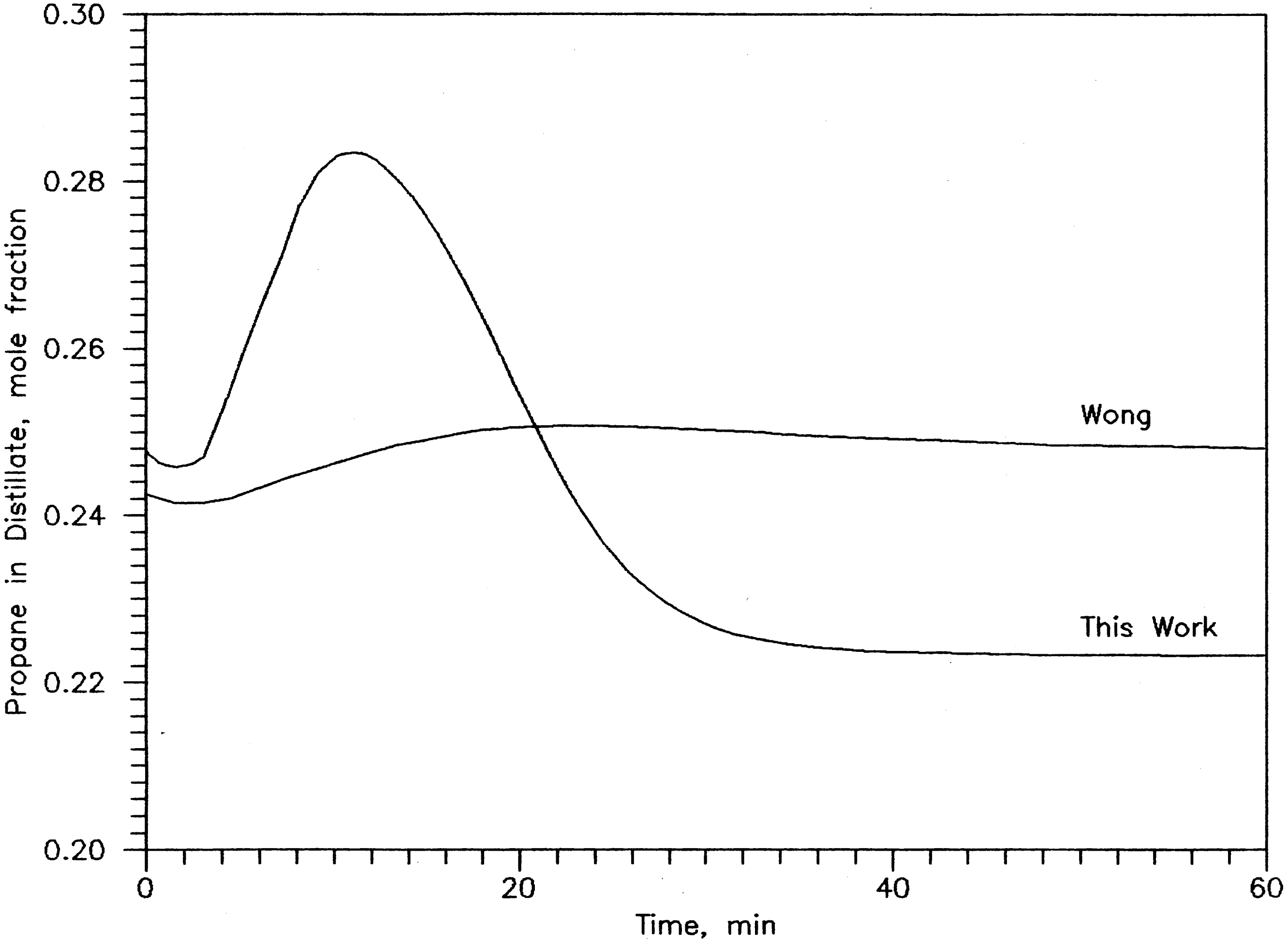


Figure 13. Response of Distillate Propane Composition to a 10 Percent Decrease in Feed Flowrate

parameters of the integration technique can lead to different results.

Computational Considerations

Apart from the accuracy aspect, an analysis of the computational efficiency of the different parts of the algorithm has been conducted. Two major efficiency considerations studied are the CPU time required by different thermodynamic property prediction packages and CPU time required by adaptive and non-adaptive integration techniques. The Holland and Liapis(12) test problem, described in Table IV, has been used for these studies. In each case, the time spent in different subroutines is profiled using the MicroSoft Source Profiler(21).

In the first case, the column is simulated using two different thermodynamic property prediction packages: 1) the subroutines taken from GPA*SIM(9) and 2) polynomial equations for the K-value and enthalpy predictions developed by Maxwell(19). The subroutines were categorized into three major categories: a) Thermo - which contains all the subroutines involved in generating thermodynamic properties, b) I/O - which includes the subroutines involved with the input and output operations of the program and c) Rest - which contain the subroutines which do not fall in the previous two categories. The results are summarized in Table VIII. Inspection of the results shows that use of the polynomial equations, to predict properties, cuts down significantly on

TABLE VIII

COMPUTATIONAL TIME COMPARISONS

Study of Thermal Property Prediction Packages

	GPA*SIM(9)	Maxwell(19)
Number of time steps in 1 hour simulation time	57	49
Run time per iteration, ms	114774	7281
Category of run time, %		
a) Thermo	96.0	34.9
b) I/O	2.1	34.1
c) Rest	1.9	31.0

Study of Integratrating Techniques

	Adaptive Time Step	Constant Time Step
Simulation 1		
Initial Time Step = 0.1 min :		
Simulation Time = 1 min -		
Number of time steps	24	10
Run Time, ms	174744	59480
Simulation Time = 35 min -		
Number of time steps	42	350
Run Time, ms	304534	2038980
Simulation 2		
Initial Time Step = 0.4 min :		
Simulation Time = 1.2 min -		
Number of time steps	6	3
Run Time, ms	43424	21321
Simulation Time = 44 min -		
Number of Time Steps	32	110
Run Time, ms	209738	666314

the run time per iteration, by about 94 %. For the cases in which such accurate polynomial equations are available, it will be worth using them and saving time.

In the second case the run times for a simulation with an adaptive time step control scheme have been compared to that with a constant time step scheme. The study has been conducted for two different initial time steps: 1) 0.1 min and 2) 0.4 min. The time steps are chosen small enough as not to loose the accuracy of the results. The results of this study are also presented in Table VIII. For the case with initial time step of 0.1 minutes, the constant time step scheme saves time initially, for around 1 minute simulation time, but after 35 minutes of simulation time, it takes 15 times more time steps than the adaptive time step scheme. And so, the run time of the constant time step scheme for 35 minutes of simulation time, is 6.7 times the run time for adaptive scheme. The second test with initial time step 0.4 minutes also shows similar results. These results prove that the adaptive control scheme is more efficient than the constant time step scheme.

CHAPTER VII

SUMMARY AND RECOMMENDATIONS

Summary

The model developed in this work to study the transient behavior of distillation columns gave excellent results when tested for its thermal property predictions, steady state predictions and transient response predictions. The study of the computational efficiencies of different parts of the program shows that the use of polynomial equations for predicting thermodynamic properties considerably reduces the run time but accuracy may suffer if the properties can not be well defined in the form of rational approximations. Also, the adaptive time step algorithm is found to be more efficient than a constant time step algorithm.

Recommendations

Unsteady State response simulators are very good tools to study the transient response of unit operations with the application of different control algorithms. Further work on this model also lies mainly in the direction of studying the controlled response of distillation columns. The model has been programmed to allow a convinient interface with a control algorithm. With such an interface the transient response to different parameters of the control system can easily be studied. The program can also be varied easily to simulate complex columns with multiple feed streams, multiple product streams and side heat exchangers.

Also, a user interface can be designed to simplify the simulation of columns on this simulator.

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APPENDIXES

APPENDIX A

DERIVATION OF ENERGY BALANCE EQUATION

The differential form of energy balance, presented in Chapter III, Equation (3.7), is

$$dh_i/dt = \{ F_i(hf_i - h_i) - Q_i + V_i+1(H_{i+1} - h_i) + L_{i-1}(h_{i-1} - h_i) - (V_i + SV_i)(H_i - h_i) \} / M_i \quad (3.7)$$

To convert this equation into an algebraic equation, the enthalpy of a stream on a tray is assumed to be a function of temperature and equilibrium composition only. The effect of pressure on enthalpy is negligible and hence is assumed to be zero. Based on these assumptions, the left hand side of Equation (3.7) can be expanded as

$$dh_i/dt = [\partial h_i/\partial T_i][dT_i/dt] + \Sigma_i[(\partial h_i/\partial x_{ij}).(dx_{ij}/dt)] \quad (AA.1)$$

Taking,

$$dT_i/dt = \Sigma_i[(\partial T_i/\partial x_{ij})(dx_{ij}/dt)] \quad (AA.2)$$

$$j = 1,\ldots,C$$

and

$$\partial h_i/\partial T_i = Cp_i \quad (AA.4)$$

where Cp_i, is the constant pressure heat capacity of the liquid stream from tray i, Equation (AA.1) is transformed to

$$\begin{aligned} dh_i/dt = \Sigma_i[Cp_i(\partial T_i/\partial x_{ij}) \\ + \partial h_i/\partial x_{ij}][dx_{ij}/dt] \end{aligned} \tag{AA.5}$$

The term $Cp_i(\partial T_i/\partial x_{ij}) + \partial h_i/\partial x_{ij}$ is defined as g_{ij} thus simplifying the equation to

$$dh_i/dt = \Sigma_i[g_{ij}][dx_{ij}/dt] \tag{AA.6}$$

The component balance equation, Equation (3.4), is

$$\begin{aligned} dx_{ij}/dt = [\ F_i(z_{ij} - x_{ij}) + V_{i+1}(y_{i+1j} - x_{ij}) \\ + L_{i-1}(x_{i-1j} - x_{ij}) \\ - (V_i + SV_i)(y_{ij} - x_{ij})\ ] / M_i \end{aligned} \tag{3.4}$$

Substitution of the term dx_{ij}/dt in equation (AA.6) by the component balance and subsequent rearrangement of terms gives

$$\begin{aligned} dh_i/dt = \{F_i\Sigma_i[g_{ij}(z_{ij}-x_{ij})] \\ + V_{i+1}\Sigma_i[g_{ij}(y_{i+1j}-x_{ij})] \\ + L_{i-1j}\Sigma_i[g_{ij}(x_{i-1j}-x_{ij})] \\ - (V_i + SV_i)\Sigma_i[g_{ij}(y_{ij}-x_{ij})\} / M_i \end{aligned} \tag{AA.7}$$

For the purpose of simplicity, the following terms without any physical interpretation are defined

$$SUM1_i = \Sigma_i[g_{ij}(z_{ij}-x_{ij}) \tag{AA.8a}$$

$$SUM2_i = \Sigma_i[g_{ij}(y_{i+1j}-x_{ij}) \tag{AA.8b}$$

$$SUM3_i = \Sigma_i[g_{ij}(x_{i-1j}-x_{ij}) \tag{AA.8c}$$

$$SUM4_i = \Sigma_i[g_{ij}(y_{ij}-x_{ij}) \qquad (AA.8d)$$

Thus Equation (AA.6) takes the form

$$dh_i/dt = \{ F_i SUM1_i + V_{+1} SUM2_i$$
$$+ L_{i-1} SUM3_i - (V_i + SV_i) SUM4_i \} / M_i \qquad (AA.9)$$

Also, the energy balance given by Equation (3.7) is

$$dh_i/dt = \{ F_i(hf_i - h_i) - Q_i + V_i+1(H_{i+1} - h_i)$$
$$+ L_{i-1}(h_{i-1} - h_i) - (V_i + SV_i)(H_i - h_i) \} / M_i \quad (3.7)$$

Elimination of the term dh_i/dt from the two equations gives

$$F_i(hf_i - h_i - SUM1_i) - Q_i - SV_i(H_i - h_i - SUM4_i)$$
$$= V_i(H_i - h_i - SUM4_i) - L_{i-1}(h_{i-1} - h_i - SUM3_i)$$
$$- V_{i+1}(H_{i+1} - h_i - SUM4_i) \qquad (AA.10)$$

Let

$$a_i = h_{i-1} - h_i - SUM3_i \qquad (AA.10a)$$
$$\beta_i = H_i - h_i - SUM4_i \qquad (AA.10b)$$
$$\Phi_i = H_{i+1} - h_i - SUM4_i \qquad (AA.10c)$$
$$E_i = F_i(hf_i - h_i - SUM1_i) - Q_i$$
$$- SV_i(H_i - h_i - SUM4_i) \qquad (AA.10d)$$

Using the above definitions, Equation (AA.9) gives the required equation

$$E_i = -a_i L_{i-1} + \beta_i V_i - \Phi_i V_{i+1} \qquad (3.8)$$

APPENDIX B

DERIVATION OF THE TRAY HOLDUP EQUATIONS

The Francis Weir formula(22) is given as

$$q_i \ / \ W = 1.839 \ (\ h_t \ ) \ ^{1.5} \qquad (3.11)$$

where q_i is the volumetric liquid flow rate on tray i in cubic meters per second and h_t is the crest height of the liquid in the weir in meters. With time units expressed in minutes, the equation is

$$q_i \ / \ W = \ 32.626 \ (\ h_t \ ) \ ^{1.5} \qquad (AB.1)$$

And since

$$q_i = L_i v_i \qquad (AB.2)$$

where v_i is the molar volume of the mixture in kmol/m^3, the following expression is obtained

$$h_t = 0.04347 \ (L_i v_i / W)^{2/3} \qquad (AB.3)$$

Further, the molar holdup can be expressed as

$$M_i = [(h_t + h_w) A_t / v_i](1 - E) \qquad (AB.4)$$

where h_w is the height of weir in meters, A_t is the effective area of the tray in m^3 and E is the porosity.

Substitution of the expression for h_t into Equation (AB.4) yields

$$M_i = [\ 0.04347\ (\ L_i v_i\ /\ W)^{2/3} + hw\ ]\ A_t(1 - E)\ /\ v_i \qquad \text{(AB.5)}$$

Differentiating L_i with respect to M_i and rearranging gives

$$dL_i/dM_i = [W/(0.02898\ A_t(1 - E))]\ [W/L_i v_i]^{-1/3} \qquad \text{(AB.6)}$$

And since

$$dL_i/dt = [dL_i/dM_i]\ [dM_i/dt] \qquad \text{(AB.7)}$$

substitution of dL_i/dM_i from Equation (AB.6) and dM_i/dt from the mass balance equation, Equation (3.1), yields

$$dL_i/dt = [\ F_i + V_{i+1} + L_{i-1} - (V_i + SV_i) - (L_i + SL_i)\ ]\ [\ W\ /\ (\ 0.02898\ A_t\ (1 - E))\ ]\ [\ W\ /\ L_i v_i\ ]^{-1/3} \qquad \text{(3.12)}$$

VITA

Jaspal Singh Sabharwal

Candidate for the Degree of

Master of Science

Thesis: A DYNAMIC SIMULATION OF A DISTILLATION COLUMN

Major Field: Chemical Engineering

Biographical:

Personal data: Born in Amritsar, India, August 8, 1968, the son of Avtar and Joginder Sabharwal.

Education: Graduated from Springdales High School, New Delhi, India, in June 1985; received Bachelor of Engineering Degree in Chemical Engineering from University of Roorkee, Roorkee, India in June 1989; Completed requirements for the Master of Science degree at Oklahoma State University in December,1991.

Professional Experience: Teaching assistant for graduate level courses of thermodynamics and stagewise unit operations at the Department of Chemical Engineering, Oklahoma State University, Stillwater, August, 1990 to May, 1991; Summer employment in the Process Development Center of Ethyl Corporation, Baton Rouge, Louisiana, May to August, 1990; Instructor at the Department of Chemical Engineering, Oklahoma State University, August, 1989 to May, 1990; Summer Intern at Process Department, Indian Oil Corporation, Mathura Refinery, India, June, 1988 to August, 1988.