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STEADY-STATE ANALYSIS FOR THE CONTROL OF A BENZENE-TOLUENE-*o*-XYLENE DISTILLATION COLUMN WITH A SIDE STREAM

A Thesis

Presented for the

Master of Science

Degree

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Clemence Marie Noakes

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To Mom and Dad
Thanks for everything

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Above all I want to thank the Chief Educator and Master of Distillation, Almighty God, who exhorts all to "Take instruction, and not silver / And knowledge rather than choicest gold. / For wisdom is better than jewels; / And all desirable things can not compare with her," for He Himself daily distills the dew.

ABSTRACT

The objective of this thesis is to present a steady-state analysis of the first-level structure of a control system for a benzene-toluene-*o*-xylene distillation column. This analysis uses Singular Value Decomposition as well as the Relative Gain Array and is based entirely on composition as a controlled variable. The analysis assumes that composition can be measured at selected points in the column as well as on the three product streams.

Presented in this work are new analysis procedures to determine where the analyzers should be placed and which are the most important components to analyze. Included in this procedure is also the possibility to present either composition or component ratios to the first-level control system.

The analysis of the benzene-toluene-*o*-xylene column strongly favors two first-level steady-state control structures. The first is an LQS control structure which controls the liquid compositions of benzene at tray 40, *o*-xylene at tray 24, and toluene at tray 13. The other is also an LQS control structure which controls the liquid component ratios of toluene/benzene at tray 40, toluene/benzene at tray 24, and the component *o*-xylene at tray 13.

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"To that great and benevolent Being, who, during the preparation of this work, has sustained a feeble constitution, amidst obstacles and toils, disappointments, infirmities and depression; who has . . . given me strength and resolution to bring the work to a close, I would present the tribute of my most grateful acknowledgements. And if the talent which he entrusted to my care, has not been put to the most profitable use in his service, I hope it has not been 'kept laid up in a napkin,' and that any misapplication of it may be graciously forgiven."

Noah Webster, upon completion of the *American Dictionary of the English Language,* New Haven, Connecticut, 1828.

CHAPTER 1

INTRODUCTION

The goal of distillation is to fractionate a given feedstock by application of heat into components which are more valuable. The value of these products depends entirely on their quality, making quality control a paramount objective in operating a column. However, the heat consumed by distillation columns accounts for about three percent of the total energy consumed in the United States.[6] As a result distillation is singled out as the largest energy user in both the chemical and petroleum industries and a major consumer of profit.[13] Consequentially, as the need for energy efficiency escalates, refineries are combining two and three columns into a single multiple-product column with sidestream products in an effort to eliminate some of the reboilers and condensers.

The control of a distillation column must therefore not only address quality specifications, but also its operation must be profitable and meet whatever production objectives are set for it. To better understand the relationships of quality, profit, and production and the role of the control system in meeting these three objectives, a benzene-toluene-*o*-xylene distillation column with a sidestream from the petroleum industry is selected for detailed analysis.

This detailed analysis incorporates an introduction to the need for enhanced control in Chapter 1, background assessments in Chapter 2, one controlled variable and multiple controlled variables studies in Chapter 3, control analyses in Chapter 4, and recommendations and conclusions in Chapter 5.

1.1 DESCRIPTION OF THE PROCESS

The most economical configuration for the benzene-toluene-*o*-xylene separation is shown in Figure 1.1.[3] This configuration has 600 lbmoles/hr of liquid feed containing 10% benzene, 45% toluene, and 45% *o*-xylene introduced onto tray 20 of a 40-tray column. A

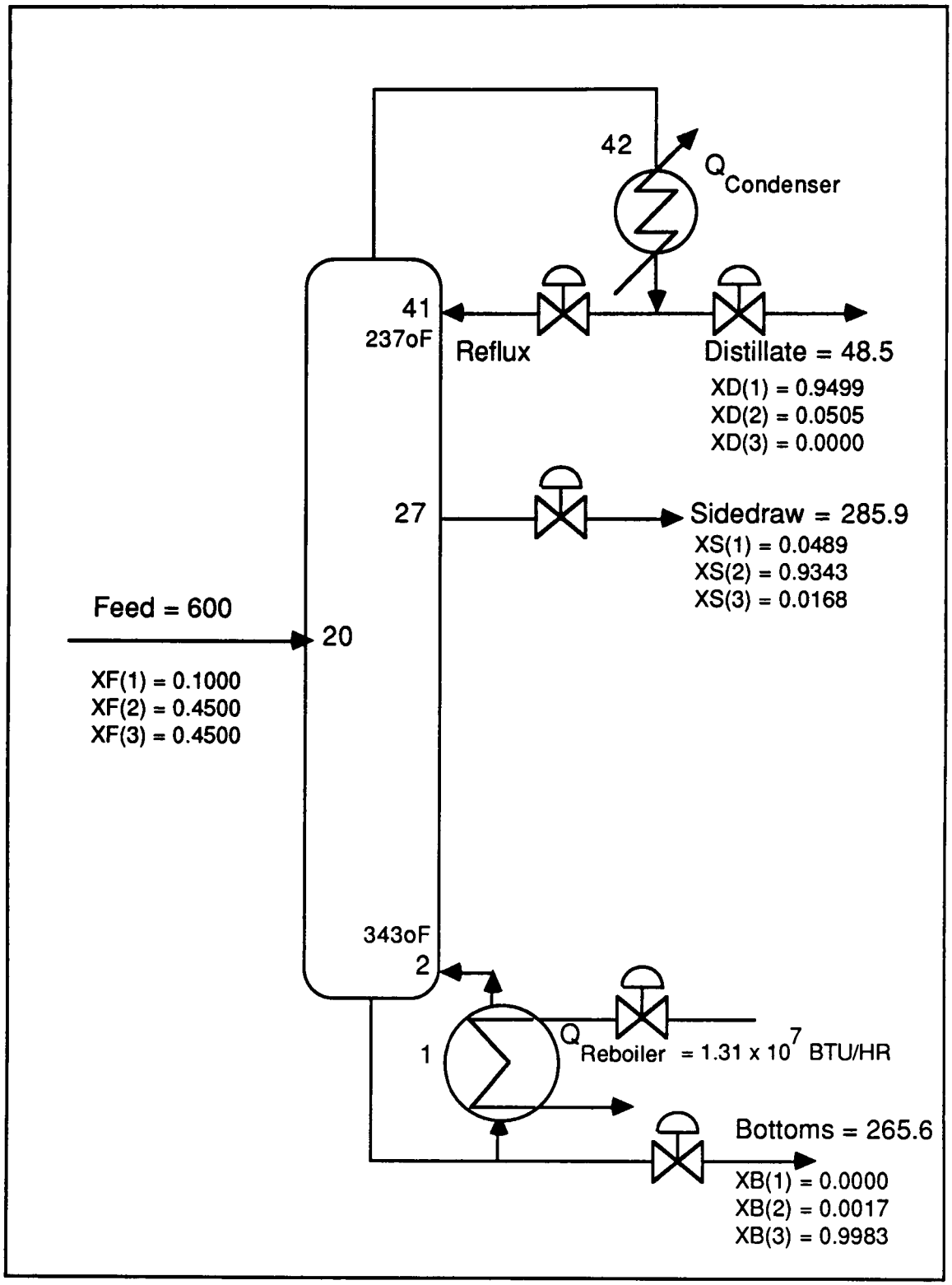

Figure 1-1. Benzene-Toluene-*o*-Xylene Column. (All flow rates are in lbmol/hr.)

liquid sidestream product consisting of 93.43% toluene, 4.89% benzene, and 1.68% *o*-xylene is withdrawn from tray 27. The internal diameter of the column is 100 inches. The tray liquid molar holdup ranges from 5.0 to 7.0 moles as the a tray weir height is 1.5 inches. Holdups in the column base and in the reflux drum are 78.2 and 93.3 moles, respectively. The small distillate flow rate of 48.5 lbmoles/hr requires a reflux ratio of 20. A partial reboiler,100% tray efficiency, a total condenser, and saturated liquid feed at a temperature of 118°F[5] and reflux are assumed. The top and bottom temperatures are 237°F and 346°F, respectively. The column operates with a linear pressure profile extending over the range of 760 torr at the top and 880 torr at the bottom. The column specifications are shown in Table 1.1. For the simulation the condenser and the reboiler are each considered a stage.

1.2 CONTROL OBJECTIVES

As previously stated there are three firmly interlocked objectives in column control: quality, profit, and production. To meet these goals product specifications and quality variations, product recovery, and the cost of cooling and heating must be taken into account.

Table 1-1. Operating Conditions of the Benzene-Toluene-*o*-Xylene Column

Stream ID	Flow lbmol/hr	Press. torr.	Temp. °F	Composition		
				Benzene	Toluene	o-Xylene
Distillate	48.5	760.0	237.0	0.9499	0.0505	0.0000
Feed	600.0	823.0	244.4	0.1000	0.4500	0.4500
Sidedraw	285.9	1020	247.4	0.0489	0.9343	0.0168
Bottoms	265.6	1520	342.6	0.0000	0.0017	0.9983

1.2.1 Product Specifications and Quality Variations

The primary focus of the benzene-toluene-*o*-xylene column study is composition control for highly purified products that can either be sold as final goods or be used directly as components for a final commodity. In either of these two cases the output of the column must meet certain minimum product specifications as agreed between customer and dealer. The product, whether intermediate or final, failing to meet such specifications is refused, unless the agreement is negotiable. Intelligent business practice therefore stipulates that violation of product specification never occurs, essentially with disregard for the expense. This establishes an arbitrary but very real economic constraint on a chemical or petroleum plant.

Figure 1.2 depicts the economic difficulty associated with the manufacture of products with a guaranteed grade.[13] As long as the required impurity is at or below the specification limit, the product mandates a monetary value established by the market for its quality.

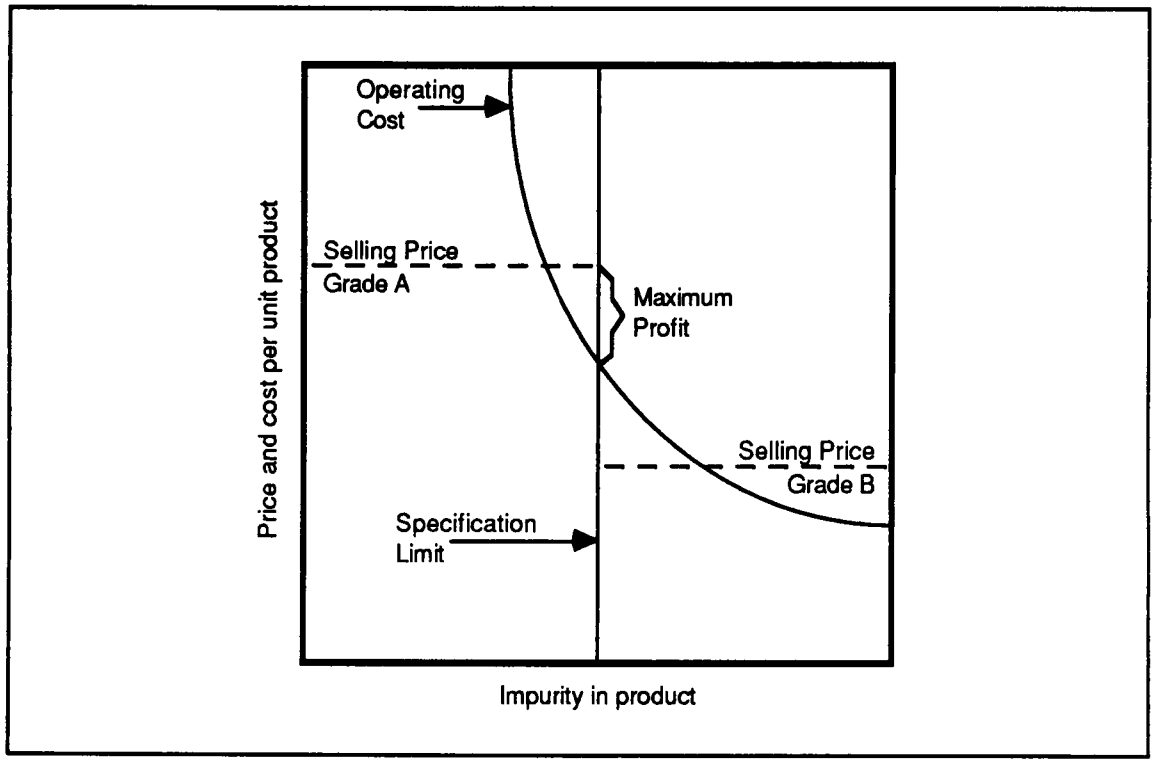

Figure 1-2. Economics vs. Impurity[13]

[13]Shinskey, F. G., *Distillation Control for Productivity and Energy Conservation*, Second Edition, McGraw-Hill, New York, 1984.

Attenuating the impurity below the constraint has absolutely no influence on the selling price. However, the operating process expense is inextricably linked with the amount of impurity, along a smooth curve which is a mathematical function of energy, capital, labor, and the process itself. Maximum profit is attained at the point where selling price surpasses operating cost by the largest margin.

Inability to achieve the specification limit alters the economic picture entirely. The selling price decreases stepwise to a lower worth corresponding to the market for the inferior quality product, assuming that a market and price exist for the lower-quality product. However, at the point of transition between high- and low-grade products, the operating cost is fundamentally as high as required to manufacture the higher-grade product. This reflects an extremely adverse operating point of either minimum profit or possibly even loss.

1.2.2 Product Recovery

Improved recovery of the more valuable product is the principal economic benefit of enhanced column control. However, recovery and purity vary inversely with each other, making the cost of increased quality frequently a reduced quantity. In other words, improved recovery is realizable by operating nearer to quality specifications.

When a product leaves the column unrecovered, its value is reduced to that of the other stream. A second penalty may occur in that the unrecovered product may lower the worth of the stream.

The cost of the unrecovered product can be stated mathematically as

$$\$_D = \Delta v(D_S - D) \qquad (1.1)$$

where D_S is the product flow attained if specifications are exactly met, and Δv is the difference in worth between product D and the presence of its principal component in the other stream. Typically, application of advanced control systems saves 50 to 80 percent of this loss.[13]

1.2.3 The Costs of Cooling and Heating

As previously stated distillation accounts for about 3 percent of the total United States energy consumption. Retrofitting instrumentation and controls is listed first among the options recommended to reduce everyday consumption.[6]

One of the primary reasons that the distillation process is so energy-intensive is because the prerequisite of superior recovery is a maximum rate of energy input to the operation. Minimizing the amount of energy consumed requires that recovery be downgraded to some adequate minimum value.

Energy consumption can be reduced by operating the column more efficiently for any given set of compositions. This requires different strategies such as increasing the relative volatility of the components, adding more trays to the tower, improving tray efficiency, using a feed preheater, or relocating the feed to a more optimum tray. Of these strategies improving relative volatility via minimum-pressure technique is the method most readily implemented by controls and can be applied to all separations. Energy consumption can be reduced as much as 5 percent at evening and as much as 25 percent during colder months by using atmospheric cooling to minimize column pressure.

Equation 1.2 gives the relationship between recovery and purity,

$$R_i = 1/y_i \tag{1.2}$$

where R_i is the recovery of component i, and y_i is the specification purity. Because recovery cannot exceed the reciprocal of purity, the relationship of energy consumption, recovery, and purity is asymptotic. Attempting to attain a high recovery and a high grade simultaneously can be very expensive in terms of energy consumption. Because of the nonlinearity of this relationship, cycling about a set point consumes more energy than operating at a steady-state at the set point. The ability of advanced control strategies to operate at a steady-state at the set point significantly reduces this costly waste of energy.

CHAPTER 2

BACKGROUND

Processes with multivariable control loops have a high probability of interactions among their loops, with these interactions most likely generating aberrant results. For example, when two controllers manipulate two valves, two ways of associating those single loops exist, one of which could be better behaved than the other. If one pairing controls nearly independent of the other and, hence, has very little interaction, the reverse pairing will be par. If neither valve holds a dominant influence over the controlled variables, either pairing will yield virtually parallel outcomes but with maximum interaction, and, as a consequence, destabilization will occur when both controllers operate automatically.

Typical distillation columns employ as many as four to six controlled and manipulated variables, giving the tally of achievable configurations of single control loops increasing factorially with the quantity of variables. If all the conceivable ratios are considered, the total of possible control-loop configurations is a permutation of the system's degrees of freedom. In the case of the benzene-toluene-*o*-xylene column, which has three degrees of freedom, there are 79,506 possible configurations. This abundance of possibilities is the primary cause of difficulty in designing control systems for distillation columns. Cantor[2] eliminates many superfluous alternatives and provides for the summary in Tables 2-1 and 2-2. The variables in Table 2-2 must be associated judiciously as they are not necessarily independent.

Two numerical algorithms well-suited for evaluating control loop interaction, stability, and sensitivity are the Singular Value Decomposition (SVD) and the Relative Gain Array (RGA). These two algorithms can be employed to evaluate steady-state simulations and models of either new or existing fractionation units in an attempt to filter out inadequate control schemes and further investigate possible control strategies to implement in the design phase or to retrofit inferior strategies in existing columns.

Table 2-1. Manipulated Variable Schemes

Manipulated Variables	Abbreviation
Reflux Rate, Steam Rate, Sidedraw Rate	LQS
Distillate Rate, Steam Rate, Sidedraw Rate	DQS
Reflux Rate, Bottoms Rate, Sidedraw Rate	LBS
Reflux Ratio, Steam Rate, Sidedraw Rate	RQS
Reflux Ratio, Bottoms Rate, Sidedraw Rate	RBS

Table 2-2. Controlled Variable Abbreviations for a BTX Column

Controlled Variables	Abbreviation
Temperature	T
Benzene Liquid	X(1)
Benzene Vapor	Y(1)
Toluene Liquid	X(2)
Toluene Vapor	Y(2)
o-Xylene Liquid	X(3)
o-Xylene Vapor	Y(3)

2.1 SINGULAR VALUE DECOMPOSITION

Quantitative data about controller pairing, sensor placement, and controllability as well as supplying a structure for a steady-state decoupler can be obtained from the numerical algorithm Singular Value Decomposition (SVD).

Daniel and Nobel[10] describe SVD as a linear transformation of a matrix obtained by introducing arbitrary orthonormal bases for both the range space and domain space of the matrix. A very simple representation, namely a diagonal, can be found. Klema and Laub[4] state that it is usually recognized that the SVD is the only generally dependable procedure of evaluating the rank of a matrix numerically.

Moore[7,8] and Noble and Daniel[10] state that the SVD of a matrix **K** results in three component matrices as follows:

$$\mathbf{K} = \mathbf{U}\Sigma\mathbf{V}^T \tag{2.1}$$

where:

K is an n x m gain matrix which demonstrates the steady-state association between the manipulated variables and the different process sensors. The elements of **K** should be physically adjusted to be characteristic of what the control system will really see and should incorporate the range and span of the valves and sensors. Each element of **K** is ascertained experimentally or by a detailed simulation and is specified as follows:[1]

$$k_{ij} = \partial x_i/\partial m_j \mid \partial m_K = 0 \text{ when } k=j \tag{2.2}$$

where **X** is an 'n' dimension vector of sensor variables and **M** is an "m" dimension vector of manipulated variables.A convenient rationale for physical scaling is in terms of percent deviations such that the units of kij will be approximately

(% of sensor span) / (% of range of manipulator) (2.3)

U is an n x n arbitrary orthonormal set of vectors used as a basis for the range space of **K**, the columns of which are call the "left singular vectors". It is a suitable coordinate system for picturing the sensors aligned in such a fashion that the first column vector, $\mathbf{U_1}$, targets the direction of the most responsive combinations of sensors. The second column vector, $\mathbf{U_2}$, targets the direction of the next most responsive combination of sensors, and so on.

V is an m x m arbitrary orthonormal set of vectors used as a basis for the domain space of **K**, the columns of which are called the "right singular vectors". It is a coordinate system for picturing the manipulated variables aligned in such a fashion that the first column vector, $\mathbf{V_1}$, targets the combination of control actions which has the largest result on the sensors. The second column vector, $\mathbf{V_2}$, targets the combination which has the next largest result on the sensors, and so on.

Σ is an n x m diagonal matrix of positive square root scalars σ_i of the nonzero eigenvalues of $\mathbf{K}^H\mathbf{K}$ arranged in descending order such that $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \ldots \geq \sigma_k \geq 0$. In terms of the multivariable control problem, the singular values delineate the "decoupled" open loop gains of the multivariable system. The number of nonzero singular values of **K** establishes its rank.

CN is the "condition number", defined as σ_1/σ_k, and is another powerful parameter which can be assessed from the singular value decomposition. It is the ratio of the largest singular value to the smallest nonzero singular value and is a clue to the difficulty of the "k x k" multivariable control problem. The larger the condition number, the more challenging if not impossible it will be to control all "k" variables. An ideally conditioned system has a condition number equal to unity.

Any multivariable system with "n" manipulated variables and "n" sensors can be observed as illustrated by Moore[8] in Figure 2.1, View A. By reason of the SVD relationship $\mathbf{K} = \mathbf{U}\Sigma\mathbf{V}^T$, View A can be illustrated as in Figure 2.1, View B. The orthonormal property $\mathbf{ß}^T\mathbf{ß} = \mathbf{ß}\mathbf{ß}^T = \mathbf{I}$ allows all but the diagonal matrix of singular values to be eliminated:

$$\mathbf{U}^T(\mathbf{U}\Sigma\mathbf{V}^T)\mathbf{V} = \Sigma \tag{2.4}$$

Expressed in block diagram form as in Figure 2.1, View C, it is clear that the blocks which enclose the $\mathbf{U}^T$ and the **V** functions construct successful and facile valve and sensor decouplers. In this array the control system detects and manipulates the structured variables (X' and M') instead of the authentic variables (X and M). From this "structured" mode the artificial process that the control system observes is "n" independent, non-interacting control loops, as seen in Figure 2.1, View D.

The "valve-decoupler" is described by Moore[8] as coordinate rotation which adjusts the structured manipulated variables with the directions of the capabilities and limitations of the

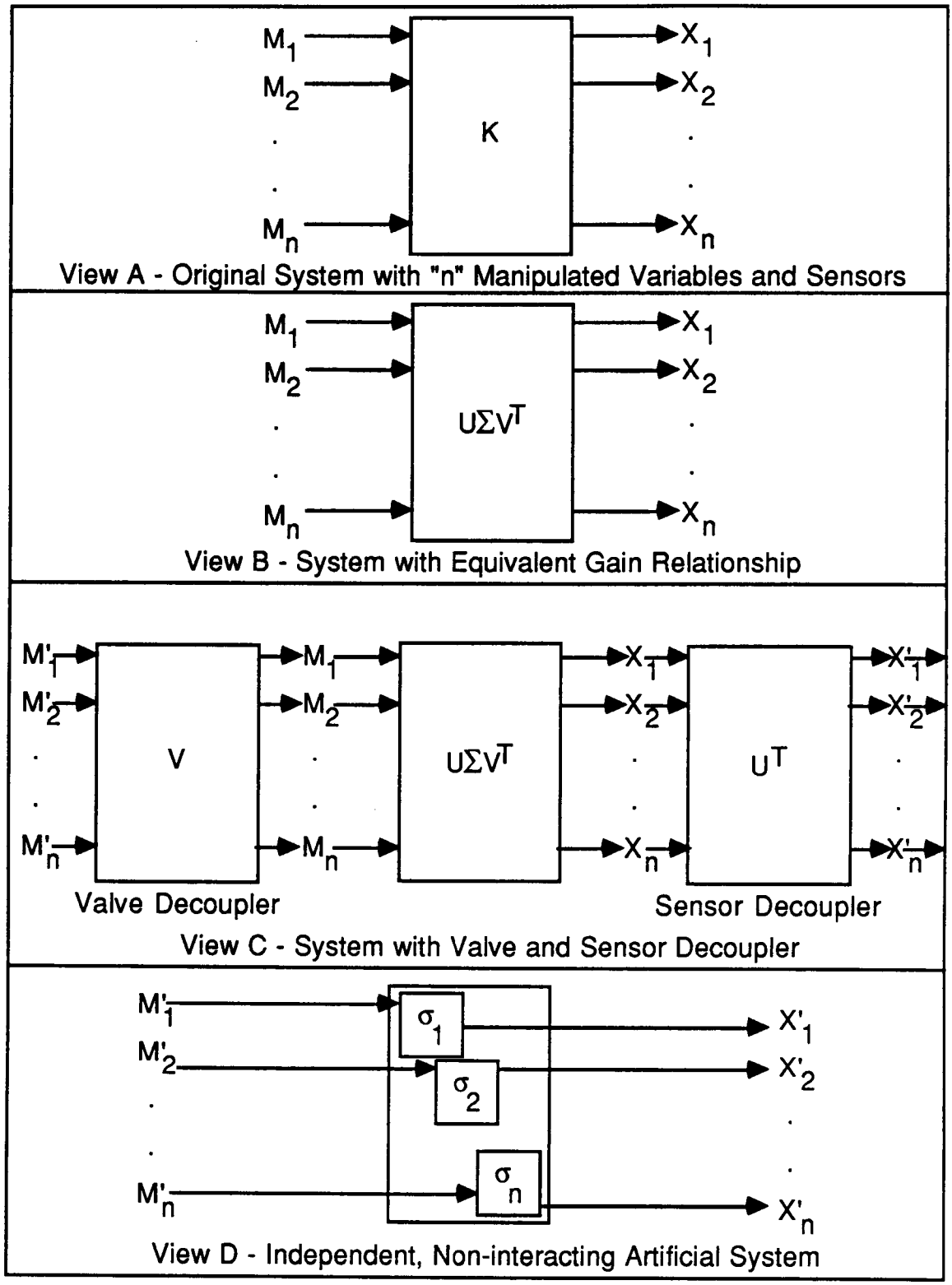

Figure 2-1. SVD Decoupler Block Diagrams for a Multivariable Process[8]

[8]Moore, C. F., *Multivariable Control Methods*, To be published by ISA Publications, Research Triangle, NC.

manipulated variables. The "sensor-decoupler" is a coordinate rotation which adjusts the structured control variables with the directions of the relative capabilities and limitations of the sensors.

The decision about sensor location is crucial to the achievement or downfall of any multivariable control system. If sensor locations are not selected with regard to sensitivity and a low degree of interaction, the control system is ill-fated from its inception. SVD is an exceptional method to use in making a quality decision on the balance which frequently must be made between these two often diametric objectives.

One direct method that works reliably in most cases utilizing data from an SVD analysis is the principle component method described by Cantor[2]. This technique supports the selection of the placement on the principle components in the left singular vectors, the **U** matrix. Recalling that each column in **U** is an orthonormal vector whose coordinate directions are detailed by each one of the process sensors, the $\mathbf{U}_1$ vector targets the most sensitive direction of the column, $\mathbf{U}_2$ targets the next most sensitive direction which is normal to the dominant direction of sensitivity, and so on. It makes sense that the location of the principle component of each vector would be desirable preferences for sensor locations which are relatively sensitive but also relatively independent.

The principal component method is direct and performs dependably as a rule. It is founded on the conjecture that the entire **U** vector can be fairly well estimated by a considerably smaller vector consisting of only those stages in which a sensor is actually present. This assumption may not always be valid. It is necessary to understand that the control system will really encounter only that portion of the overall system. After the sensor locations have been chosen, which can be done by applying the principal component technique, it is necessary in every instance verify the SVD evaluation of the partial system to check if the condition numbers and the singular values are reasonable.

Moore[8] explains that the singular values of the partial analysis are almost always less than the singular values for the complete system. The condition number for the partial system, however, can be better or worse than forecasted by the overall analysis, contingent on the relative shifts in each of the singular values. An enhanced condition number most often indicates a greater penalty in sensitivity in the first singular value than in the smallest. A

condition number which is larger implies that the greater loss in sensitivity is in the smallest singular value. From the perspective of a control system design, the overall assessment is pertinent in measuring the scope of the control problem and in establishing desirable sensor locations. The partial analysis, however, is the most expedient to employ for a more detailed level of the control system strategy. In terms of the challenge of specifying sensor locations, if the condition number confirmed by the partial analysis is nearly the same as (or better than) the overall analysis, then the placement of the sensors found by the principal component method is most likely a good decision. However, if the condition number from the partial analysis is significantly larger, then recourse to a more detailed evaluation of the proposed strategy may be in order.

2.2 THE RELATIVE GAIN CONCEPT

The relative gain concept was first introduced by E. H. Bristol[1] in 1966 as "control-loop interaction," with the measure of this interaction proposed as "relative gain" by F. G. Shinskey[14] in 1967. Because of the inherently multivariable nature of distillation, the relative gain concept has its prime potential in the fractionation process.

Every controlled variable in an interacting system is vulnerable to influence by every manipulated variable. In a process encompassing n pairs of variables, there are n^2 open-loop gains yielding n^2 relative gains. The relative gain for a designated combination of variables c_i and m_j is defined:

$$\lambda_{ij} \equiv \frac{dc_i}{dm_j}\bigg|_m \Big/ \frac{dc_i}{dm_j}\bigg|_c \qquad (2.5)$$

The relative gains for a group of manipulated and controlled variables are arrayed in a square matrix as illustrated in Figure 2-2. The array has the very useful quality of having the numbers in every row and column totaling to 1.0. This is a notable asset in a two-loop system as only one relative gain term requires estimation. An additional practical aspect of the concept is that it is not affected by scaling. Due to the process gain being, in essence, divided by itself under equivalent conditions, this factor vanishes. In general, relative gains

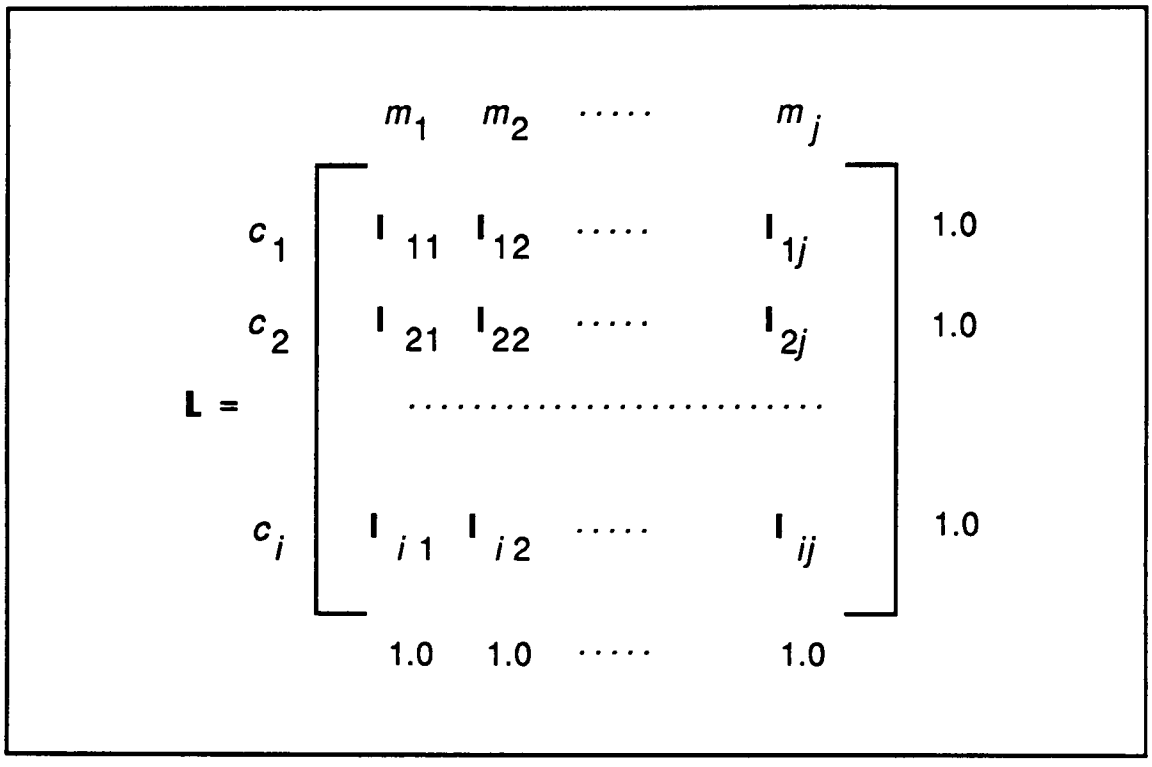

Figure 2-2. The Typical Relative Gain Array

approaching 1.0 display minimal interaction; these loops are the optimum selections for closure. When the relative gain nears infinity, the denominator in Eq. 2.5 is zero, implying failure of c_i to respond to m_j when other loops are closed. As a consequence, c_i is controlled by other manipulated variables other than m_j and therefore is not successfully controlled independently. This is the case of a superfluous control loop. A summary of relative gain properties is given in Table 2-3.

Shinskey[13] relates that the relative gain array can be determined for any quantity of variables using vector-matrix notation:

$$\mathbf{c} = \mathbf{K} \cdot \mathbf{m} \qquad 2.6$$

where matrix **c** represents the controlled variables, matrix **m** represents the manipulated variables, and matrix **K** is a square matrix of gains. Another manner of depicting the same process would be to declare the manipulated variables in terms of the controlled variables:

$$\mathbf{m} = \mathbf{H} \cdot \mathbf{c} \qquad 2.7$$

Table 2-3. A Summary of Relative Gain Properties

l_{ij}	Significance
< 0	Conditionally stable - do not close loop
0	Control depends on other loop(s)
0 - 1	Interaction extends period and raises gain
1.0	No interaction with other loops
> 1	Interaction reduces control effectiveness
∞	Loops are completely dependent

Equation 2.7 is the inverse of equation 2.6, so that $H = K^{-1}$. The relative gain matrix R can easily be calculated, then, by developing a square matrix of the gains at the most sensitive locations and employing equation 2.8:

$$R = K \cdot INV(K)^T \qquad 2.8$$

2.3 SVD VS. RGA

Normally the SVD pairing methodology yields solutions parallel with Bristol's Relative Gain Array. However, in some instances the resolutions of the SVD and the RGA techniques are quite disparate. Moore[8] details how in those instances, the optimal decision rests on circumstantial justification. In view of this, it is an intelligent routine to always weigh together the RGA and SVD analyses when the final choice is executed regarding controller pairing. The following discussion includes the points in which results of the RGA and SVD are occasionally in dissension.

Commonly systems with large condition numbers for the SVD pairing are incongruous with those suggested by an RGA examination. Moreover, for large condition numbers, the realization of a multivariable control system is extremely remote despite the analytical technique employed whether it is controller pairing, decoupling, or any other multivariable strategy. Controller pairing should not be performed without some referral to the sensitivity and the condition of the multivariable system. The RGA evaluation does not solely signal poor conditions. The SVD assessment plainly indicates such obstacles, and the controller pairing in such circumstances can be judged as the prime systematic approach to extenuate the control objectives to an acceptable level.

The SVD technique addresses exclusively the open loop character of the system, advising controller pairing which produces a control system with the greatest open loop enhancement in terms of the compromise between interaction and sensitivity. SVD does not consider the problem of disengaging an on-line controller while Bristol's RGA method does. The RGA alerts with negative numbers controller associations which would invert sign if another controller were decommissioned. This is a challenging industrial situation where controllers are repeatedly switched between manual and automatic. Correction for the dilemma is achievable with a feedforward adjustment in controller gains. This should, however, be bypassed unless the more conservative association suggested by the RGA develops in an unsatisfactory fully-automatic control performance.

CHAPTER 3

OPERATIONAL STUDIES

3.1 ONE CONTROLLED VARIABLE STUDIES

With the column's simulated operation at the conditions described in Chapter 1, characteristics of a single variable that changes stagewise can be determined. Temperature or a single component in a single phase are readily incorporated into currently available software, described in Appendix A. A summary of these studies is available in Appendix E.

Temperature is currently the most common measurement used for composition control because of the relationship existing between composition, temperature, and total pressure.[13] Because temperature is being used as an indirect method of controlling composition, the stagewise temperature is maintained constant and the heat to the reboiler is manipulated until the desired steady-state is achieved. Of the manipulated variable schemes listed in Table 2-1, the DQS strategy produced process gains that represent the most manageable system.

Each of the three components was controlled using each of the five schemes in Table 2-1. Two studies, the SVD and the partial SVD, were necessary to determine the optimal control strategy. The DQS design to control toluene liquid proved to be the best conditioned system. Appendix C contains the distillation simulation output for this control strategy.

3.2 MULTIPLE CONTROLLED VARIABLES STUDIES

Historically, the compositions of the distillate and the bottoms are not controlled variables. Cantor[2] relates the trend of controlling the condenser level with the distillate flow rate, the reboiler level with the bottoms flow rate, and the endpoint compositions with the steam and reflux flow rates, stating that this is functional for most columns, but with the price tag of high energy costs. The alternative to this approach is manipulating the set points of the optimal first-level control strategy to hold the product specifications to the desired value.

Two new concepts initiated by C. F. Moore and developed in this study for establishing the optimal first-level control strategy for total composition control are the stacked matrix method and the ratio-gain method.

3.2.1 The Stacked Matrix Method

The objective of the Stacked Matrix analysis is to determine a total composition profile of the column which would differentiate which of the three components, whether individually or in combination, affords the most sensitive measurement as well as the choice location of sensors and manipulated variable scheme.

For each of the five manipulated variable schemes listed in Table 2-1, the original gain matrix of the liquid phase analysis for each component was "stacked" on top of each other resulting in a 126 x 3 matrix where rows 1 through 42 represented benzene, rows 43 through 84 represented toluene, and rows 85 through 126 represented *o*-xylene. An SVD analysis of these stacked matrices was then executed.

Using the LQS manipulated variable data, given in Appendix D, as an example, the total composition profiled by the **U** matrix plot is illustrated in Figure 3-1. Further inquiry into the **U** matrix analysis can be accomplished by separately plotting the columns of the matrix, isolating each component's effect by feigning rows 1 through 42 (benzene), rows 43 through 84 (toluene), and rows 85 through 126 (*o*-xylene) to be independent vectors. The $\mathbf{U_1}$ plot in Figure 3-2 indicates that the most sensitive measurement is obtained from toluene and *o*-xylene at tray 13. A good assessment of benzene and toluene is available at tray 40 The $\mathbf{U_2}$ plot in Figure 3-3 confirms measuring toluene and *o*-xylene at tray 13, benzene and toluene at tray 40, and augments measuring toluene at tray 2. The $\mathbf{U_3}$ plot in Figure 3-4 supports measuring toluene at tray 2, benzene and toluene at tray 40, and supplements measuring toluene and *o*-xylene at tray 24 as well as at tray 13.

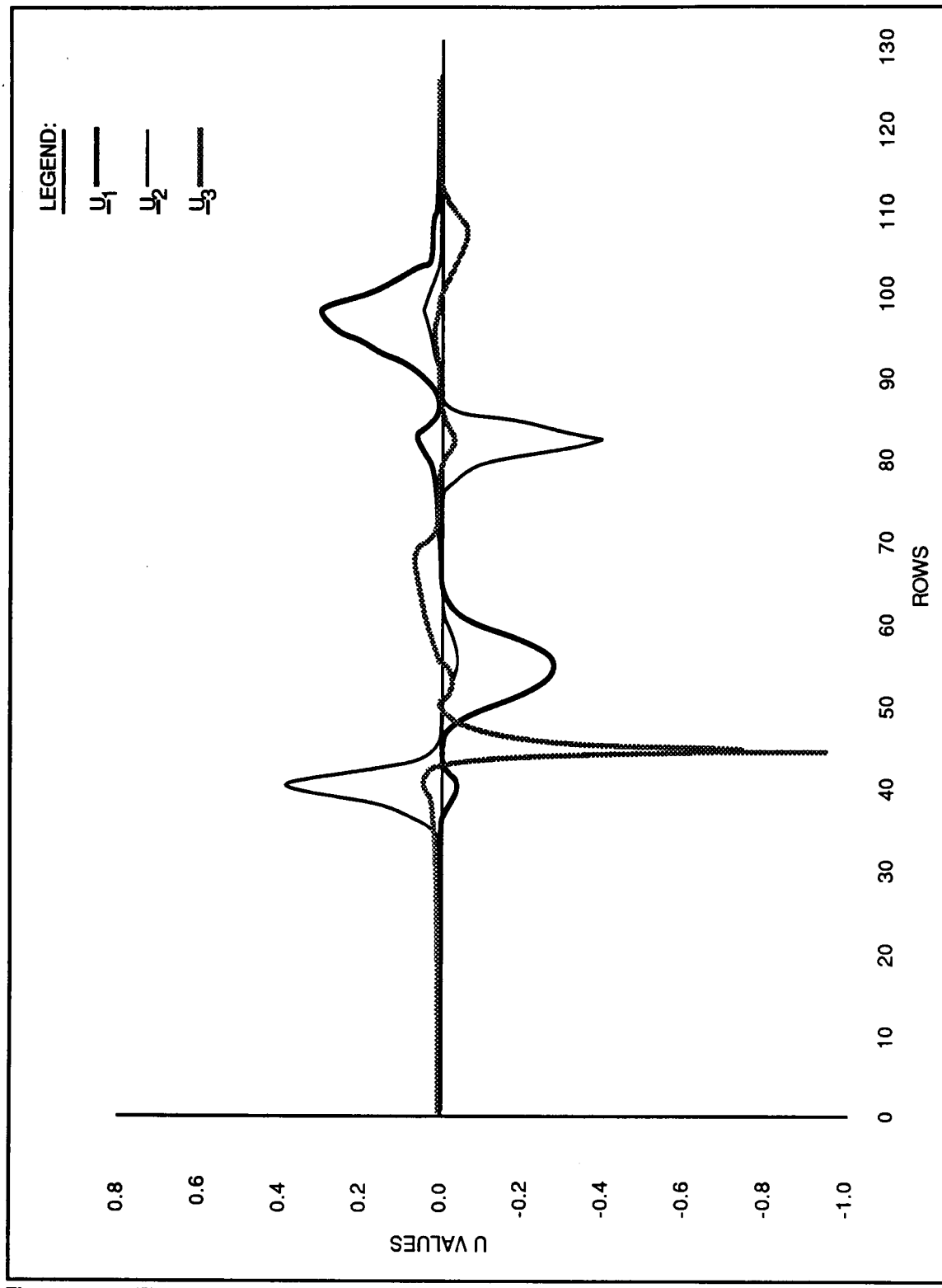

Figure 3-1. The Original $\underline{U}$ Matrix Plot for the LQS Analysis of a BTX Column Determined Via the Stacked Matrix Approach

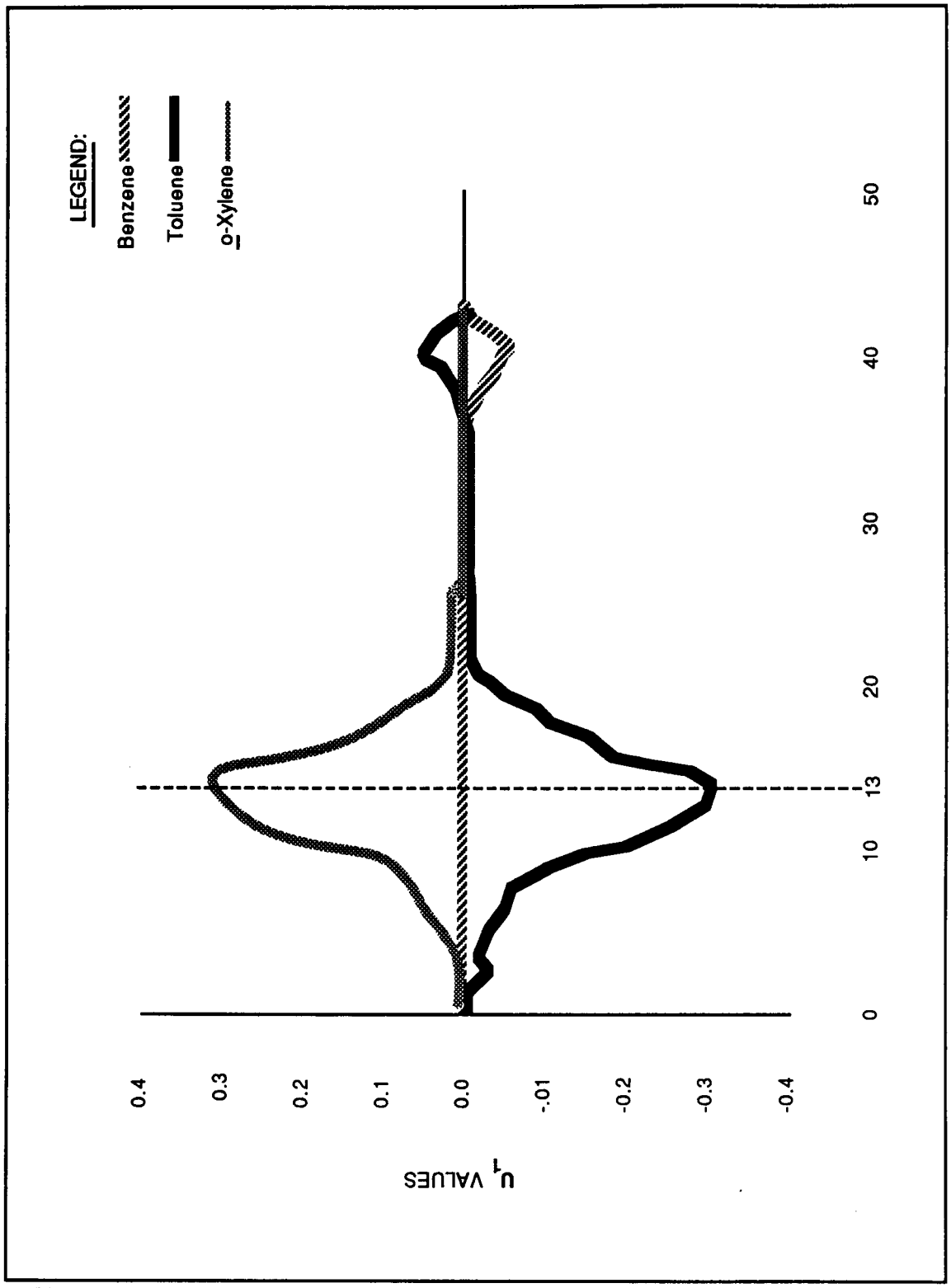

Figure 3-2. The $\underline{U}_1$ Plot of the LQS Analysis of a BTX Column Determined Via the Stacked Matrix Approach

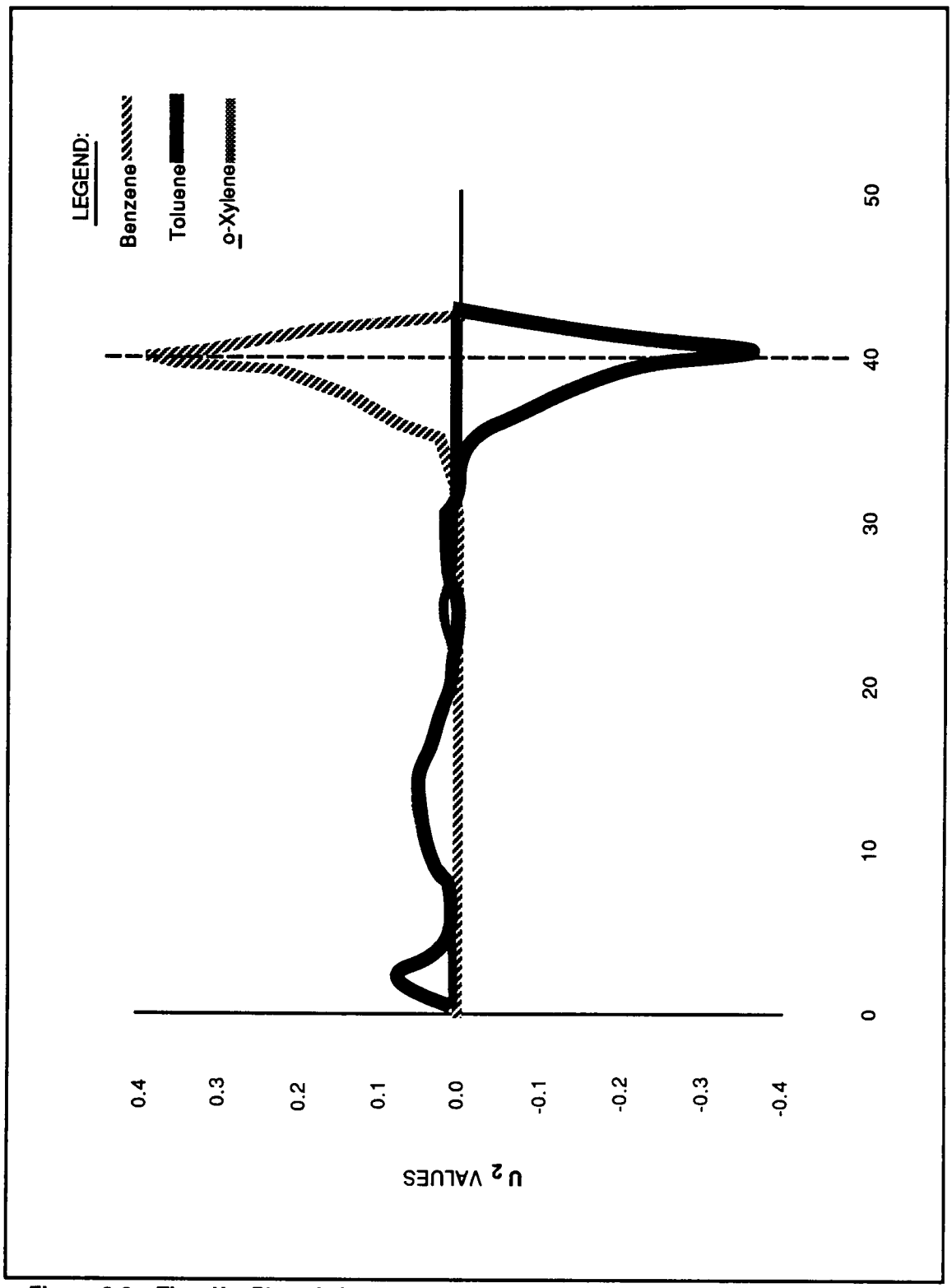

Figure 3-3. The U_2 Plot of the LQS Analysis of a BTX Column Determined Via the Stacked Matrix Approach

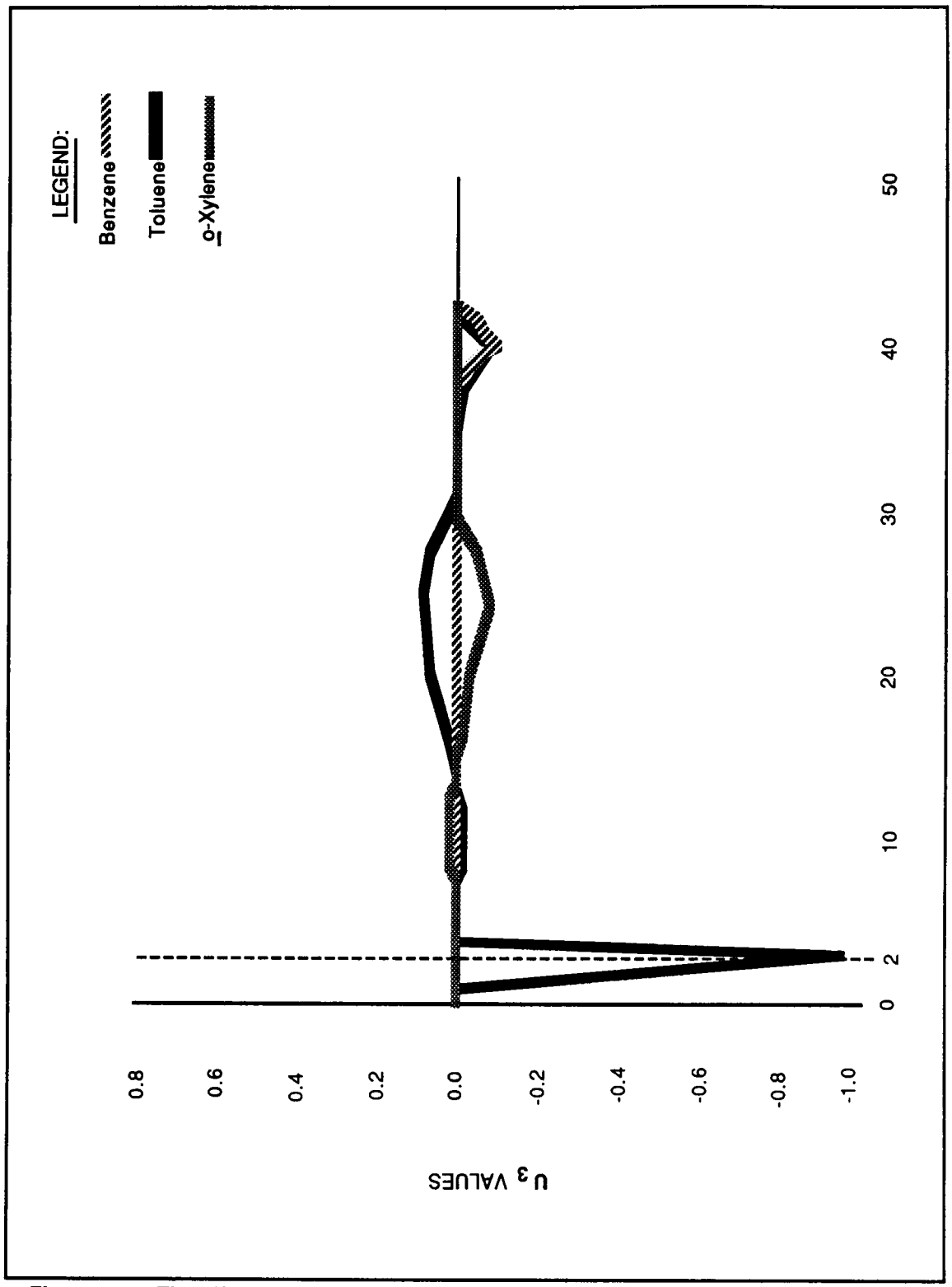

Figure 3-4. The $\underline{U}_3$ Plot of the LQS Analysis of a BTX Column Determined Via the Stacked Matrix Approach

3.2.2 The Ratio-Gain Matrix Method

The goal of the ratio-gain matrix analysis is to determine specific component ratios and placement of sensors in a distillation column. This examination of the column's total composition is achieved through differentiation of the mole fractions and their respective gains using Equation 3.1:

$$d\left(\frac{x}{y}\right) = \frac{ydx - xdy}{y^2} \tag{3.1}$$

to develop the ratio-gain matrix Equation 3.2

$$R_{ij} = \frac{(x_{ci})(a_{ij}) - (x_{ai})(c_{ij})}{(x_{ci})^2} \tag{3.2}$$

where:

R_{ij} is an i x j matrix.

x_{ci} is the liquid mole fraction of component c at tray i.

x_{ai} is the liquid mole fraction of component a at tray i.

a_{ij} is the ijth element of the gain matrix for component a.

c_{ij} is the ijth element of the gain matrix for component c.

Only a partial SVD is practical in this procedure as mole fractions approaching zero completely mask the benefit of other measurements at strategic points in the column. Recalling that the stacked matrix analysis strongly indicate that the most beneficial ratios to measure were toluene to benzene and toluene to *o*-xylene at trays 13, 24, and 40 using an LQS manipulated variable scheme, partial SVD analyses were established for three ratios, two ratios and a single component, one ratio with two single components, and three single components.

CHAPTER 4

CONTROL ANALYSIS

The primary objective in determining a control scheme for a distillation column is evaluating the sensitivity of the column to the manipulated variables. This evaluation was executed for both approaches: the one controlled variable involving temperature and a single component in a single phase and the multiple controlled variables studies for total composition.

4.1 ONE CONTROLLED VARIABLE STUDIES

For the control of temperature in the BTX distillation column, the first-level manipulated variables and corresponding condition numbers and relative gain array controller pairing numbers are listed in Table 4-1. While DQS has the best SVD analysis, its RGA evaluation reveals two fairly interactive loops. The RQS system for controlling temperature has a higher condition number but two independent loops and only one moderately interactive loop.

The optimal single component system described in Appendix E is the DQS manipulated variable scheme controlling toluene liquid. To demonstrate how SVD can be applied to this problem, the steady-state gain matrix for this single component base case at normal operating conditions is shown in Table 4-2. With no specification on the placement of the control sensors, the steady-state gain matrix is a 42 x 3 array of constraints depicting the toluene liquid concentration sensitivity on each stage with respect to each of the three manipulated variables. The simplification of the gain matrix results in a 42 x 3 **U** matrix, as shown in Table 4-3, and a 3 x 3 **V** matrix, three singular values, and a condition number, as shown in Figure 4-1.

In the BTX case the largest element in U_1 (0.43173) occurs on stage 12, the largest element in U_2 (-0.55655) occurs on stage 40, and the largest element in U_3 (0.45428) occurs on stage 24. The **V** matrix, read by rows, shows the largest value to be S (-0.97958), the next

Table 4-1. Summary of Manipulated Variable Schemes Controlling Temperature in a BTX Column

Control Strategy	Condition Number	Partial Condition Number	Singular Values			Relative Gain Array Controller Pairing		
			σ_1	σ_2	σ_3	γ_1	γ_2	γ_3
DQS	119.5906	117.7150	50.414	2.4419	0.42155	1.0332	0.5788	0.5936
LBS	146.5506	147.2064	55.727	10.790	0.38026	0.5552	0.6945	0.9468
RQS	159.5239	155.88577	52.386	2.33287	0.32839	1.0618	1.0275	0.6242
RBS	181.0963	213.6145	86.718	5.5061	0.47885	1.0722	0.4405	0.7383
LQS	259.1187	250.3553	74.649	8.1400	0.28809	1.3014	0.4133	0.7870

Table 4-2. BTX Column's Original Gain Matrix for Controlling X(2) with a DQS Scheme

Stage Number	∂X(2)/∂D	∂X(2)/∂Q	∂X(2)/∂S
42	2.02660E-02	-5.17283E-03	3.71465E-03
41	3.53790E-02	-8.97334E-03	6.49851E-03
40	4.52223E-02	-1.13478E-02	8.33590E-03
39	4.12161E-02	-1.01696E-02	7.63897E-03
38	2.85047E-02	-6.83188E-03	5.33134E-03
37	1.65032E-02	-3.74136E-03	3.13781E-03
36	8.66622E-03	-1.74529E-03	1.69953E-03
35	4.33600E-03	-6.51362E-04	9.00965E-04
34	2.12227E-03	-9.50873E-05	4.87307E-04
33	1.02849E-03	1.80845E-04	2.70461E-04
32	4.91434E-04	3.22323E-04	1.31518E-04
31	2.16112E-04	4.13826E-04	-2.48546E-05
30	4.13097E-05	5.16865E-04	-3.35723E-04
29	-1.50688E-04	7.19564E-04	-1.09760E-03
28	-5.09581E-04	1.20116E-03	-3.00582E-03
27	-1.29185E-03	2.32668E-03	-7.52314E-03
26	-2.28735E-03	3.57911E-03	-1.33528E-02
25	-3.33776E-03	4.59856E-03	-1.95298E-02
24	-4.14147E-03	4.90792E-03	-2.42712E-02
23	-4.41704E-03	4.22403E-03	-2.59164E-02
22	-4.10575E-03	2.70008E-03	-2.41132E-02
21	-3.39213E-03	8.05293E-04	-1.99403E-02
20	-5.97327E-03	-1.01045E-03	-3.51287E-02
19	-1.02514E-02	-3.96957E-03	-6.03035E-02
18	-1.70916E-02	-8.69097E-03	-0.10056
17	-2.74907E-02	-1.58977E-02	-0.16175
16	-4.20728E-02	-2.60741E-02	-0.24756
15	-6.00337E-02	-3.87320E-02	-0.35325
14	-7.79785E-02	-5.15773E-02	-0.45885
13	-9.02611E-02	-6.06885E-02	-0.53114
12	-9.20813E-02	-6.26316E-02	-0.54185
11	-8.30815E-02	-5.70045E-02	-0.48890
10	-6.73726E-02	-4.65510E-02	-0.39646
9	-5.02115E-02	-3.49003E-02	-0.29548
8	-3.51642E-02	-2.45703E-02	-0.20693
7	-2.35659E-02	-1.65452E-02	-0.13868
6	-1.53105E-02	-1.07970E-02	-9.00978E-02
5	-9.71767E-03	-6.88110E-03	-5.71857E-02
4	-1.53225E-08	-4.29549E-03	-3.55633E-02
3	-5.13521E-09	-2.62040E-03	-2.16217E-02
2	-1.68934E-09	-1.54754E-03	-1.27330E-02
1	-5.30028E-10	-8.64912E-04	-7.10274E-03

Table 4-3. $\underline{U}$ Matrix for a BTX Column Controlling X(2) with a DQS Scheme

Stage Number	U_1	U_2	U_3
42	-5.04507E-03	-0.24976	6.04570E-03
41	-8.82277E-03	-0.43579	1.38049E-02
40	-1.13105E-03	-0.55655	1.46043E-02
39	-1.03552E-02	-0.50654	3.22804E-02
38	-7.21593E-03	-0.34951	3.37976E-02
37	-4.23539E-03	-0.20149	3.17693E-02
36	-2.28269E-03	-0.10493	2.91940E-02
35	-1.20002E-03	-5.16079E-02	2.72763E-02
34	-6.42133E-04	-2.43700E-02	2.61719E-02
33	-3.57054E-04	-1.09277E-02	2.58107E-02
32	-1.92816E-04	-4.35530E-03	2.63325E-02
31	-4.51014E-05	-1.05469E-03	2.85025E-02
30	2.06529E-04	8.70134E-04	3.46087E-02
29	7.96592E-04	2.64349E-03	5.06866E-02
28	2.26076E-03	5.56456E-03	9.15071E-02
27	5.71935E-03	1.16397E-02	0.18844
26	1.01982E-02	1.85860E-02	0.30190
25	1.49699E-02	2.47724E-02	0.40396
24	1.86732E-02	2.77647E-02	0.45428
23	2.00263E-02	2.58776E-02	0.42487
22	1.87388E-02	1.95430E-02	0.32242
21	1.56191E-02	1.09164E-02	0.18202
20	2.77260E-02	1.03383E-02	0.17663
19	4.77888E-02	9.56309E-03	0.17070
18	7.98660E-02	8.35882E-03	0.16181
17	0.12864	6.42196E-03	0.14658
16	0.19703	3.44731E-03	0.12104
15	0.28128	-6.69413E-04	8.22503E-02
14	0.36548	-5.50965E-03	3.17291E-02
13	0.42313	-9.99020E-03	-2.17493E-02
12	0.43173	-1.28241E-02	-6.47976E-02
11	0.38958	-1.33799E-02	-8.77483E-02
10	0.31595	-1.20387E-02	-9.03961E-02
9	0.23549	-9.72896E-03	-7.96197E-02
8	0.16493	-7.28503E-03	-6.33932E-02
7	0.11054	-5.17138E-03	-4.71649E-02
6	7.18204E-02	-3.53434E-03	-3.34678E-02
5	4.55873E-02	-2.34653E-03	-2.29136E-02
4	2.83517E-02	-1.51858E-03	-1.52096E-02
3	1.72380E-02	-9.55643E-04	-9.77122E-03
2	1.01518E-02	-5.78796E-04	-6.01355E-03
1	5.66305E-03	-3.28978E-04	-3.45344E-03

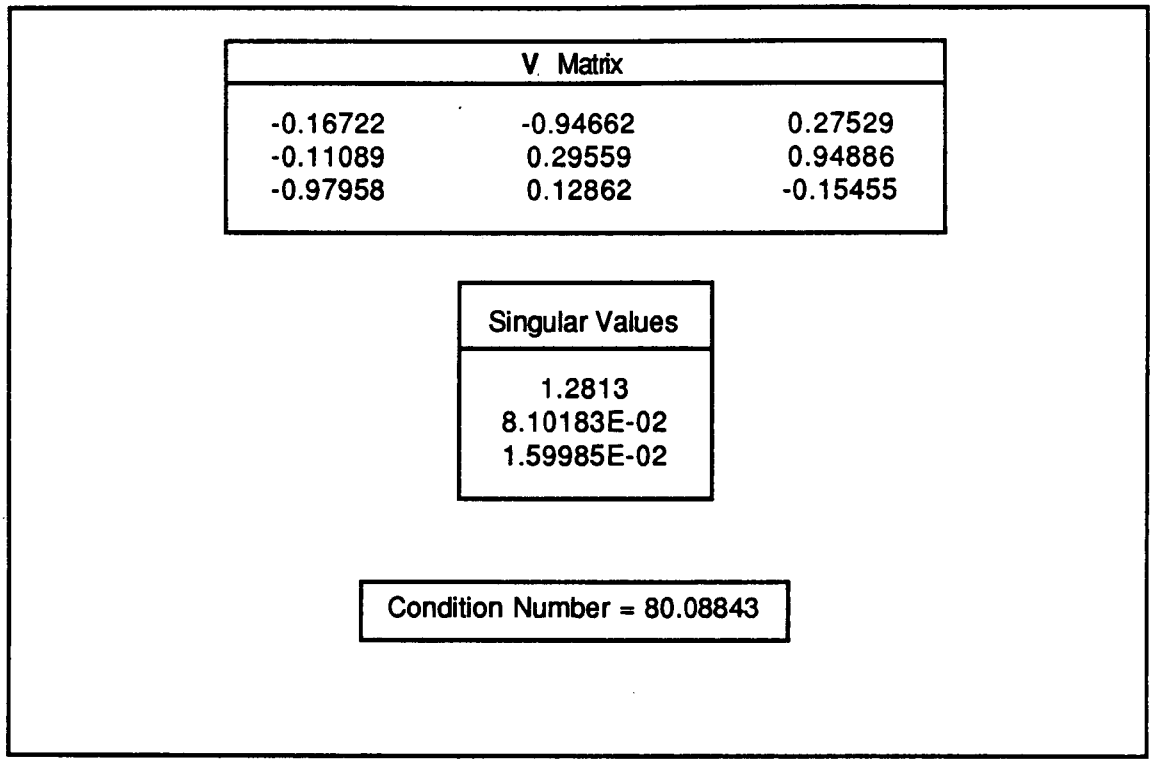

Figure 4-1. $\underline{V}$ Matrix, Singular Values, and Condition Number for a BTX Column Controlling X(2) with a DQS Scheme

largest value to be Q (0.94886), and finally D (-0.94662). The controller pairing would then be as shown in Table 4-4.

The RGA analysis for the DQS scheme controlling X(2), given in Table 4-4, exposes two moderately interactive loops, however. Data available in Appendix E indicates that the next best choices would be the RQS and LBS schemes. Table 4-5 compares the SVD and RGA analyses of these two designs. While the LBS scheme has a lower condition number, it has two moderately interactive loops. The RQS scheme has only a slightly higher condition number and one moderately interactive loop.

If only a two sensor/two valve control system is considered, there are ten possible ways to control the toluene liquid, as shown in Table 4-6. The RS, DQ, DS, and RQ strategies seem to be very well conditioned and should be reviewed as reasonable alternatives for additional analyses.

Table 4-4. Controlled/Manipulated Variable Pairing With Open Loop Gains and RGA Analysis for a BTX Column Using a DQS Scheme to Control X(2)

Sensor Location (**U** Matrix)	Manipulated Variable (**V** Matrix)	Open Loop Gain (σ_i values)	Relative Gain Array Controller Pairing
Tray 12	S	1.2813	γ_3 = 0.5181
Tray 40	Q	8.10183E-02	γ_1 = 1.0330
Tray 24	D	1.59985E-02	γ_2 = 0.6367

Table 4-5. Comparison of LBS and RQS Schemes to Control X(2) on a BTX Column

	Condition Number	Relative Gain Array		
		γ_1	γ_2	γ_3
LBS	100.4147	0.9455	0.7604	0.7604
RQS	106.7123	1.0276	0.5414	0.9168

Table 4-6. Comparison of Two-Parameter Strategies for Controlling X(2) in a BTX Column

First Level Scheme	Condition Number	Overall SVD Analysis	
		σ_1	σ_2
LQ	168.4132	0.37717	2.23957E-03
LS	74.58906	0.24679	3.30863E-03
QS	88.16980	0.28556	3.23878E-03
DQ	24.27958	7.98046E-02	3.28690E-03
DS	29.31978	7.89518E-02	2.69278E-03
LB	137.3886	0.40104	2.91903E-03
BS	321.8230	0.57822	1.79669E-03
RQ	32.01587	7.99745E-02	2.4979E-03
RS	21.59514	6.03393E-02	2.79412E-03
RB	86.73897	0.31866	3.67373E-03

4.2 MULTIPLE CONTROLLED VARIABLES STUDIES

Two innovative approaches, the stacked matrix method and the ratio-gain method, provided a good deal of information on the benzene-toluene-*o*-xylene column.

The stacked matrix approach was executed on the manipulated variables listed in Table 2-1. The condition numbers of the five analyses are listed in Table 4-7, with the LQS manipulated variable scheme having the lowest condition number. The partial SVD analysis of the stacked LQS matrix was determined by using gains for toluene at tray 13 (row 55), benzene at tray 40 (row 40), and *o*-xylene at tray 24 (row 108). This decomposition gave a partial condition number of 4.5295.

The Ratio-Gain Matrix Method was used to examined a total of 92 arrangements, finding 21 designs having condition numbers less than 200. These results are given in Table 4-8, with the analysis giving the system measuring toluene/benzene at tray 40, toluene/benzene at tray 24, and *o*-xylene at tray 13 as the most stable, its partial condition number being 6.6134.

A comparison of the stacked matrix method and the ratio-gain matrix method was desired to decide between their close partial condition numbers. This was accomplished by determining the relative gain for both systems, as illustrated in Table 4-9. This analysis using the stacked matrix method showed that the system measuring X(1) at tray 40 (γ_1 = 0.9764), X(3) at tray 24 (γ_2 = 0.9639), and X(2) at tray 13 (γ_3 = 0.9836) to have three virtually non-interactive loops. The system monitoring the ratio X(2)/X(1) at tray 40 (γ_1 = 1.0204), the ratio X(2)/X(1) at tray 24 (γ_2 = 0.9789), and the component X(3) at tray 13 (γ_3 = 0.6704) had two relatively independent loops and one moderately interactive loop.

Table 4-7. Manipulated Variable Schemes and Condition Numbers for a BTX Column Determined With the Stacked Matrix Approach

Manipulated Variable Scheme	Condition Number
LQS	47.63
DQS	81.82
LBS	101.90
RQS	108.3
RBS	124.23

Table 4-8. Partial SVD Analysis of the Ratio-Gain Matrix Analysis for a BTX Column Using an LQS Manipulated Variable Scheme

Tray 40	Tray 24	Tray 13	Partial Condition Number
Toluene/Benzene	Toluene/Benzene	o-Xylene	6.6134
Toluene/Benzene	Toluene/o-Xylene	Toluene/o-Xylene	7.2286
Toluene/Benzene	Toluene/Benzene	Toluene	7.6682
Toluene/Benzene	Toluene/o-Xylene	Benzene	7.6682
Toluene	Toluene/Benzene	Toluene	8.7188
Benzene	Toluene/Benzene	o-Xylene	8.7204
Toluene	Toluene/Benzene	o-Xylene	8.7204
Benzene	Toluene/Benzene	Toluene/o-Xylene	17.6261
Toluene	Toluene/Benzene	Toluene/o-Xylene	17.6251
Toluene/Benzene	Toluene/o-Xylene	Toluene	18.6338
Benzene	Toluene/o-Xylene	o-Xylene	18.7798
Toluene	Toluene/o-Xylene	o-Xylene	18.7798
Benzene	Toluene/o-Xylene	Toluene	18.7816
Toluene	Toluene/o-Xylene	Toluene	18.782
Benzene	Toluene/o-Xylene	Toluene/o-Xylene	23.4516
Toluene	Toluene/o-Xylene	Toluene/o-Xylene	23.4516
Benzene	o-Xylene	Toluene	178.0245
Toluene/Benzene	Toluene	o-Xylene	195.9577
Toluene/Benzene	Toluene	Toluene	196.2020
Toluene/Benzene	o-Xylene	Toluene	199.3836
Toluene/Benzene	o-Xylene	o-Xylene	199.3998

Table 4-9. Comparison of the RGA Analysis for the Stacked Matrix Method and the Ratio-Gain Matrix Method Using an LQS Scheme in a BTX Column

Relative Gain	Stacked Matrix Method (Partial Condition Number: 4.5295)	Ratio-Gain Matrix Method (Partial Condition Number: 6.6134)
γ_1	0.9764	1.0204
γ_2	0.9639	0.9789
γ_3	0.9836	0.6704

CHAPTER 5

RECOMMENDATIONS AND CONCLUSIONS

The primary attention given to the benzene-toluene-*o*-xylene column is in the area of composition control with the Singular Value Decomposition and Relative Gain Array being the applied analyses.

The SVD furnishes a clear approach for contrasting the steady-state behavior of alternate first-level control strategies. The condition number and singular values can be used as a quantitative indicator of the multivariable complications of interaction and sensitivity of each first-level strategy regarded. If only a single component is to be monitored and controlled, the behavior of each of the five 3 X 3 first-level strategies indicates that controlling toluene liquid in the BTX column is most reasonable. Temperature control was more poorly conditioned than the proposed single component composition scheme. The stacked matrix approach and the ratio-gain matrix method provided good possibilities on using multiple composition measurement, as presented in Tables 4-8 and 4-10.

The analysis of the benzene-toluene-*o*-xylene column strongly favors two first-level steady-state control structures. The first is an LQS control structure which controls the liquid compositions of benzene at tray 40, *o*-xylene at tray 24, and toluene at tray 13. The other is also an LQS control structure which controls the liquid component ratios of toluene/benzene at tray 40, toluene/benzene at tray 24, and the component *o*-xylene at tray 13.

Because the Singular Value Decomposition and the Relative Gain Array evaluations are only steady-state analyses, recommendations for further examination include assessments that include dynamics, either by computer simulation or on an actual column. The strategy's performance under dynamic conditions will ultimately determine the optimal control methodology.

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APPENDIXES

APPENDIX A

SOFTWARE

A.1 THE DISTILLATION COLUMN SIMULATOR

The hardware utilized in this analysis is the DEC VAX cluster accessible at the University of Tennessee, Knoxville. The FORTRAN program applied to investigate alternate control strategies for the BTX column is a thorough stage-to-stage steady-state simulation. The steady-state process gains that are prerequisite to calculating the SVD and RGA evaluations are evaluated with this software.

The computer simulation applies the Naphtali-Sandholm[9] convergence routine, a constrained variation of Newton's procedure, to establish the stage-to-stage steady-state profile of the column. Unlike simplified simplified methods, this simulation possesses the majority of the nonlinearities inherently in industrial columns. The main simplification is that no dynamics in the form of hydraulics are used in the calculations; the pressure profile is assumed linear throughout the column.

The program provides steady-state gains for a multicomponent, multistage distillation column accommodating a maximum of 10 components, 100 trays aside from the reboiler, 10 feed streams, and 9 sidedraws. Efficiency and heat constraints are capable of being stipulated. The simulation needs the column operating parameters given in Table A.1 as partial input requirements.

Supplemental to the data in Table A.1, a considerable inventory of physical property and vapor-liquid equilibrium (VLE) data is mandatory for performing the steady-state distillation simulation. While certain physical properties are constants such as molecular weight and molar volume, the majority of data is described via polynomial equations of second, third, or forth order with temperature being the independent variable. Vapor pressure calculations require Antoine constants.

The VLE characteristics of the BTX mixture can be estimated from several diverse equations. Liquid activity coefficients can be characterized from the Wilson, NRTL, or Scatchard-Hildebrand equation or deemed ideal. Moreover, the fugacity can be computed from the Redlich-Kwong state equation, the Vapor Phase Association model, or regarded ideal. The advantage of selecting Wilson's equation is that it may be extended to as many

Table A-1. Necessary Parameters for Distillation Simulation

Feeds	Sidedraws	Distillate	Bottom	Reflux	Top
Number Location Flow rate Comp. Temp. Pressure Phase	Number Location Flow rate Comp. Temp. Phase	Flow rate	Temp. Pressure	Ratio Temp.	Temp. Pressure

components as preferred without auxiliary assumptions and without introducing any constants other than those obtained form binary data.[11] The Redlich-Kwong equation of state is used because, in general, it is the most reliable model for mixtures of nonpolar components remote from critical conditions.[11]

The Naphtali-Sandholm procedure also requires a top- and bottom-stage stipulation. Common top-stage specifications are reflux ration, reflux rate, and distillate rate. Bottom-stage prerequisites comprise the bottom flow rate and the reboiler duty.

A.2 THE SAS/IML INTERACTIVE MATRIX LANGUAGE

The SAS/IML Interactive Matrix Language Software is an indispensable instrument in the Stacked Matrix Approach, the Ratio-Gain Matrix Method, and the Relative Gain Array. Available on the University of Tennessee, Knoxville, VAX cluster, this software is an interactive programming language that features applications on complete matrices and emulates matrix

algebra notation. The essential data entity is a two-dimensional (row by column) numeric or character matrix. Elements in numeric matrices are stored as real, double-precision, floating-point values. Elements in character matrices are stored as character strings with equal lengths from 1 to 32767 characters long. The SAS/IML software was used both in its collect and immediate modes. In immediate mode, the statements are executed as soon as they are entered. In the collect mode, the statements are collected and then executed later as a module.[12]

Figure A-1 is a SAS listing for the interactive VAX/VMS operating system to find the SVD analysis using the stacked matrix approach for the RBS control strategy to control toluene liquid. Figure A-2 is a SAS listing to print out the results from Figure A-1 and is written for the collect mode of the VAX VMS operating system. Figure A-3, written for the interactive mode, determines the relative gain array for a BTX Column Controlling X(2) with a DQS Scheme. The results of this program is displayed in Figure A-4. Figures A-5 and A-6 were also determined using this listing.

The SAS/IML SVD subroutine is based on the works of Wilkinson and Reinsch.[15] The module decomposes a real m x n matrix **A** into the form

$$\mathbf{A} = \mathbf{U}*\mathrm{DIAG}(\mathbf{Q})\mathbf{IV}' \qquad \text{A.1}$$

where **Q** is a vector of singular values in descending order. if m >= n, then

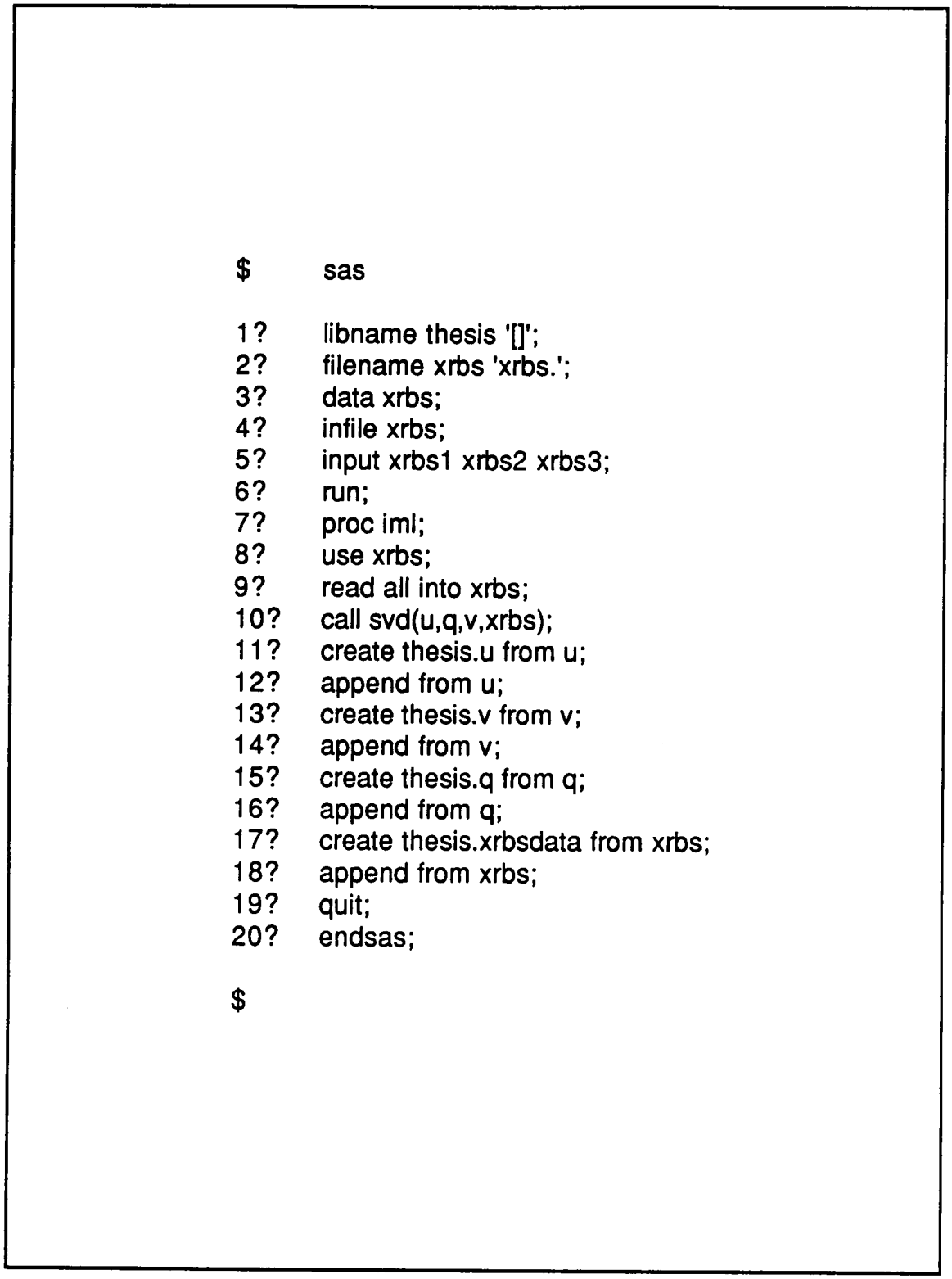
$$\mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{V}\mathbf{V}' = \mathbf{I}_n \qquad \text{A.2}$$

U is m x n, **Q** is n x 1, and **V** is n x n.

If m < n, then

$$\mathbf{U}'\mathbf{U} = \mathbf{U}\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_m. \qquad \text{A.3}$$

when m >= n, **U** consists of the orthonormal eigenvectors of **AA'**, and **V** consists of the eigenvectors **A'A**. Except for some zeros, **Q** contains the square roots of the eigenvalues of **A'A** and **AA'**.



```
$       sas

1?      libname thesis '[]';
2?      filename xrbs 'xrbs.';
3?      data xrbs;
4?      infile xrbs;
5?      input xrbs1 xrbs2 xrbs3;
6?      run;
7?      proc iml;
8?      use xrbs;
9?      read all into xrbs;
10?     call svd(u,q,v,xrbs);
11?     create thesis.u from u;
12?     append from u;
13?     create thesis.v from v;
14?     append from v;
15?     create thesis.q from q;
16?     append from q;
17?     create thesis.xrbsdata from xrbs;
18?     append from xrbs;
19?     quit;
20?     endsas;

$
```

Figure A-1. Typical SAS Listing for the Stacked Matrix Approach

```
options nocenter;
libname thesis'[]';
proc print data=thesis.xrbsdata;
title 'This is the data used in the RBS SVD Analysis.';
proc print data=thesis.u;
title 'This is the RBS Matrix U Output.';
proc print data=thesis.v;
title'This is the RBS Matrix V Output.';
proc print data=thesis.q;
title 'This is the RBS Matrix Q Output.';
data utemp;
set thesis.u;
x=_n_;
proc plot data=utemp;
plot col1*x='1' col2*x='2' col3*x='3' /overlay;
title 'This is the RBS Matrix U Plot.';
```

Figure A-2. Typical SAS Listing for Printing Stacked Matrix SVD Analysis

```
$       sas

1?      proc iml;
2?      K = {0.452223 -0.011348 0.0083349,
3?      -0.004141 -0.0049079 0.024271,
4?      -0.092081 -0.062632 0.54185};
5?      H = inv(K);
6?      HTRANS = H`;
7?      R = K # HTRANS;
8?      quit;
9?      endsas;

$
```

Figure A-3. Typical SAS Listing to Determine the Relative Gain Array

The Original Partial Gain Matrix

	dX(2)/dD	dX(2)/dQ	dX(2)/dS
Tray 40	0.452223	-0.011348	0.0083349
Tray 24	-0.004141	-0.0049079	0.024271
Tray 13	-0.092081	-0.062632	0.54185

The Inverse of the Partial Gain Matrix

22.8421	36.4583	-1.2817
0.0499081	129.7243	-5.81
-3.8875	-21.19	-0.956154

The Transpose of the Inverse

22.8421	0.0499081	-3.8875
36.4583	129.7243	-21.19
-1.2817	-5.81	-0.956154

The Relative Gain Array

1.0330	-5.5E-04	-0.032404
-0.150974	0.6367	0.5143
0.1180	0.3639	0.5181

Figure A-4. The Relative Gain Array for a BTX Column Controlling X(2) with a DQS Scheme

The Original Partial Gain Matrix			
	dX/dL	dX/dQ	dX(2)/dS
Row 40	-0.06047	-.3888	0.04602
Row 55	-0.30272	-0.046411	-0.00602
Row 108	0.01484	0.01196	-0.086395

The Inverse of the Partial Gain Matrix		
-0.385578	-3.2254	0.0193609
2.4790	0.429003	1.3504
0.2770	-0.613415	-11.384

The Transpose of the Inverse		
-0.385578	2.4790	0.2270
-3.2254	-0.429003	-0.613415
0.0193609	1.3504	-11.384

The Relative Gain Array		
0.0233159	0.9639	0.0127454
0.9764	0.0199105	0.0036928
2.9E-04	0.0161508	0.9836

Figure A-5. The Relative Gain Array for a BTX Column Controlling the Total Composition with an LQS Scheme Using the Stacked Matrix Approach

The Original Partial Gain Matrix			
	dX/dL	dX/dQ	dX/dS
Toluene/Benzene, Tray 40	-0.44444	0.4127	0.0168924
Toluene/Benzene, Tray 24	0.1570	0.0043511	-0.270127
o-Xylene, Tray 13	-0.33254	0.4764	0.5740

The Inverse of the Partial Gain Matrix		
-2.296	4.0052	1.9524
0.005075	4.3666	2.0548
-1.3344	-1.3038	1.1679

The Transpose of the Inverse		
-2.296	0.005075	-1.3344
4.0052	4.3666	-1.3038
1.9524	2.0548	1.1679

The Relative Gain Array		
1.0204	0.0020945	-0.022541
0.6288	0.0189996	0.3522
-0.649265	0.9789	0.6704

Figure A-6. The Relative Gain Array for a BTX Column Controlling the Total Composition with an LQS Scheme using the Ratio-Gain Matrix Approach

A.3 VLE COMPUTER CALCULATIONS

The vapor-liquid equilibrium parameters for the Distillation Simulator were optionally based on the Wilson equation. The binary parameters were found by inputting temperature, pressure, and mole fraction data into a program written by committee member Dr. C. H. Byers on ASPEN software and run on an IBM personal computer, both licensed to Martin Marietta Energy Systems, Oak Ridge, TN. These binary parameters were then checked for thermodynamic consistency using the Gibbs-Duhem equation programmed into Lotus® Symphony® software, also licensed to Martin Marietta Energy Systems. Equilibrium data for the *o*-xylene-toluene and *o*-xylene-benzene systems were not available, and the isomers *m*-xylene and *p*-xylene were substituted. Appropriate unit conversions were necessary before including the binary Wilson parameters into the simulation data base.The program listings, the binary parameters, and the consistency tests are given in Figures A-7 through A-25.

```
NEW DRS
TITLE 'The Noakes Problem'
DESCRIPTION "                    '***
       THIS PROBLEM TESTS THE DRS SYSTEM.  UNARY PARAMETERS
       ARE TESTED USING THE EXTENDED ANTOINE EQUATION.
       BINARY PARAMETERS ARE TESTED BY THE WILSON ACTIVITY
       COEFFICIENT EQUATION. "
;
COMPONENTS C1 BENZENE / C2 TOLUENE  ;****
IN-UNITS  TEMP=C PRES=TORR
OUT-UNITS TEMP=C PRES=TORR
HISTORY MSG-LEVEL PROPERTIES=2
;
;          THE ANTOINE AND WILSON EQUATIONS ARE USED BY SYSOP8.
;          ONLY FIT THE FIRST, SECOND, AND FORTH ANTOINE COEFFICIENTS
;          AND THE SECOND WILSON PARAMETER (GMWSNB). THE OTHER ANTOINE
;          COEFFICIENTS ARE SET TO ZERO BY THE PROP-DATA PARAGRAPH WHILE
;          THE SYSTEM DEFAULTS GMWSNA TO ZERO.
;
PROPERTIES SYSOP8
PARAMETERS
 BIPARAMETER 1 GMWSNB C1 C2 1 0.      -10000.  10000. 1.
 BIPARAMETER 2 GMWSNB C2 C1 1 0.      -10000.  10000. 1.
;
;          ACETONE-BENZENE VAPOR-LIQUID EQUILIBRIUM DATA
;           DATA-GROUP VLE1 HAS A FULL SET OF STATE VARIABLES (TPXY),
;           WHILE DATA-GROUP VLE2 HAS ONLY TPX DATA.
;
DATA-GROUP VLE1
 SYSTEM-DEF TPXY C1 C2
 PHASE-EQ VL C1 C2
 STD-DEV 1 0.1   -1.0    0.001   0.01
 DATA     1 120.0 1132.0 0.1170 0.2200 /  ;***
          2 120.0 1324.0 0.2560 0.4220/   ;***
          3 120.0 1330.0 0.2580 0.4250/
          4 120.0 1324.0 0.2640 0.4530/
          5 120.0 1515.0 0.4400 0.6390/
          6 120.0 1868.0 0.6820 0.8240/
          7 105.3 760.0 0.1000 0.2080/
          8 101.5 760.0 0.2000 0.3720/
          9 98.00 760.0 0.3000 0.5070/
         10 95.05 760.0 0.4000 0.6190/
         11 92.30 760.0 0.5000 0.7130/
         12 89.74 760.0 0.6000 0.7910  ;***
;          THE PARAMETERS ARE REGRESSED IN THREE SEPARATE CASES.
;          THE RESULTS OF THE ANTOINE CASES ARE USED IN THE WILSON CASE
;          BECAUSE THE RESULTS OF A REGRESSION ARE STORED FOR USE BY
;          LATER CASES.
;
CASE VLE
 PARAMETERS BINARY=1 2
 DATA-GROUPS VLE1
 PROPERTIES SYSOP8
```

Figure A-7. ASPEN Main Calling Program Determining Wilson Binary Parameters

```
ASPEN/SP Run on 09/29/87 by Martin Marietta Energy Systems        Page    I
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986
                              The Noakes Problem
                                  DESCRIPTION

      THIS PROBLEM USES THE DRS SYSTEM TO PREDICT BINARY PARAMETERS
      FOR THE WILSON ACTIVITY COEFFICIENT EQUATION. BINARY MIXTURES
      OF BENZENE AND TOLUENE ARE USED.


                            RUN CONTROL INFORMATION

TYPE OF RUN: NEW

INPUT FILE NAME: CNDRS

INPUT PROBLEM DATA FILE NAME: CNDR     UPDATE  NO.   0

MAIN CALLING PROGRAM NAME: CNDR

DRS ONLY RUN



ASPEN/SP Run on 09/29/87 by Martin Marietta Energy Systems        Page   II
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986
                              The Noakes Problem
                               TABLE OF CONTENTS

              PHYSICAL PROPERTIES SECTION...................  1
                   COMPONENTS...............................  1
                   OPTION SETS..............................  1

              DATA REGRESSION SECTION.......................  2
                   SUBSECTION: CASE VLE.....................  2
```

Figure A-8. Benzene-Toluene Data Input Program Determining Wilson Binary Parameters, page 1

```
ASPEN/SP Run on 09/29/87 by Martin Marietta Energy Systems        Page    1
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986

                              The Noakes Problem
                          PHYSICAL PROPERTIES SECTION

COMPONENTS

 ID        TYPE  FORMULA         DATABANK REFERENCE                ALIAS
 C1         C     C6H6            BENZENE                          C6H6
 C2         C     C7H8            TOLUENE                          C7H8

OPTION SETS

  SYSOP0

  MAJOR PROPERTY  PHILMX    HVMX      HLMX      GVMX      GLMX      SVMX
  ROUTE ID        PHILMX00  HVMX00    HLMX00    GVMX00    GLMX00    SVMX00
                  --------------------------------------------------------
                  SLMX      VVMX      VLMX      MUVMX     MULMX     KVMX
                  SLMX00    VVMX00    VLMX01    MUVMX01   MULMX01   KVMX01
                  --------------------------------------------------------
                  KLMX      DVMX      DLMX      SIGLMX    PHIV      PHIL
                  KLMX01    DVMX01    DLMX01    SIGLMX01  PHIV01    PHIL00
                  --------------------------------------------------------
                  HV        HL        GV        GL        SV        SL
                  HV00      HL00      GV00      GL00      SV00      SL00
                  --------------------------------------------------------
                  VV        VL        KS        VS        PHISMX    HSMX
                  VV00      VL01      KS01      VS01      PHISMX02  HSMX02
                  --------------------------------------------------------
                  GSMX      SSMX      VSMX      KSMX      PHIS      HS
                  GSMX02    SSMX01    VSMX02    KSMX01    PHIS02    HS02
                  --------------------------------------------------------
                  GS        SS
                  GS02      SS02

  SYSOP8

  MAJOR PROPERTY  PHIVMX    PHILMX    HVMX      HLMX      GVMX      GLMX
  ROUTE ID        PHIVMX01  PHILMX08  HVMX01    HLMX08    GVMX01    GLMX01
                  --------------------------------------------------------
                  SVMX      SLMX      VVMX      VLMX      MUVMX     MULMX
                  SVMX01    SLMX08    VVMX01    VLMX01    MUVMX02   MULMX02
                  --------------------------------------------------------
                  KVMX      KLMX      DVMX      DLMX      SIGLMX    PHIV
                  KVMX02    KLMX01    DVMX02    DLMX01    SIGLMX01  PHIV04
                  --------------------------------------------------------
                  PHIL      HV        HL        GV        GL        SV
                  PHIL04    HV01      HL02      GV01      GL01      SV01
                  --------------------------------------------------------
                  SL        VV        VL
                  SL02      VV01      VL01
```

Figure A-9. Benzene-Toluene Data Input Program Determining Wilson Binary Parameters, Page 2.

```
ASPEN/SP Run on 09/29/87 by Martin Marietta Energy Systems        Page    2
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986

                              The Noakes Problem
                          DATA REGRESSION SECTION

SUBSECTION: CASE VLE


 PARAMETER    ELEMENT      COMPONENT              PARAMETER       STANDARD
  NAME         NUMBER       OR PAIR               ESTIMATE        DEVIATION

 GMWSNB         1           C1        C2          -277.0932        141.4038
 GMWSNB         1           C2        C1           189.7269        74.77671

 NUMBER OF ITERATIONS   17


 DATA-GROUP VLE1       VARIABLE: TEMPERATURE
                       UNITS   : C

   MEASURED        ESTIMATED       STD-DEVIATION  ADJUSTMENTS  % ADJUSTMENTS
     120.0000        119.9799          .10000       -.20142E-01  -.16785E-01
     120.0000        120.0127          .10000        .12688E-01   .10573E-01
     120.0000        120.0189          .10000        .18936E-01   .15780E-01
     120.0000        119.9926          .10000       -.73896E-02  -.61580E-02
     120.0000        119.9550          .10000       -.45040E-01  -.37534E-01
     120.0000        120.0320          .10000        .32013E-01   .26678E-01
     105.3000        105.3428          .10000        .42824E-01   .40669E-01
     101.5000        101.5259          .10000        .25900E-01   .25517E-01
     98.00000        98.02216          .10000        .22163E-01   .22615E-01
     95.05000        95.05186          .10000        .18569E-02   .19536E-02
     92.30000        92.28603          .10000       -.13971E-01  -.15137E-01
     89.74000        89.71202          .10000       -.27976E-01  -.31174E-01

    ROOT MEAN SQUARES DEVIATION =  .2583684E-01
    AVERAGE ABSOLUTE DEVIATION  =  .2257494E-01
    MAXIMUM DEVIATION           = -.4504050E-01
```

Figure A-10. Benzene-Toluene Data Output Program Determining Wilson Binary Parameters, page 1

The Noakes Problem
DATA REGRESSION SECTION

SUBSECTION: CASE VLE (CONTINUED)

DATA-GROUP VLE1 VARIABLE: PRESSURE
UNITS : TORR

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
1132.000	1141.026	11.320	9.0260	.79735
1324.000	1317.902	13.240	-6.0980	-.46058
1330.000	1320.630	13.300	-9.3701	-.70452
1324.000	1327.371	13.240	3.3708	.25459
1515.000	1541.981	15.150	26.981	1.7809
1868.000	1843.597	18.680	-24.403	-1.3064
760.0000	748.8002	7.6000	-11.200	-1.4737
760.0000	753.2543	7.6000	-6.7457	-.88760
760.0000	754.1783	7.6000	-5.8217	-.76601
760.0000	759.3824	7.6000	-.61762	-.81266E-01
760.0000	763.4406	7.6000	3.4406	.45271
760.0000	767.0599	7.6000	7.0599	.92893

ROOT MEAN SQUARES DEVIATION = 12.27529
AVERAGE ABSOLUTE DEVIATION = 9.511189
MAXIMUM DEVIATION = 26.98097

DATA-GROUP VLE1 VARIABLE: COMPOSITION LIQUID C1
UNITS : MOL-FR

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
.1170000	.1167187	.10000E-02	-.28132E-03	-.24045
.2560000	.2559153	.10000E-02	-.84735E-04	-.33100E-01
.2580000	.2579445	.10000E-02	-.55498E-04	-.21511E-01
.2640000	.2641054	.10000E-02	.10536E-03	.39907E-01
.4400000	.4399476	.10000E-02	-.52449E-04	-.11920E-01
.6820000	.6821123	.10000E-02	.11235E-03	.16473E-01
.1000000	.1001176	.10000E-02	.11763E-03	.11763
.2000000	.2000709	.10000E-02	.70881E-04	.35441E-01
.3000000	.3001014	.10000E-02	.10141E-03	.33804E-01
.4000000	.4000631	.10000E-02	.63060E-04	.15765E-01
.5000000	.5000279	.10000E-02	.27916E-04	.55831E-02
.6000000	.5999822	.10000E-02	-.17775E-04	-.29624E-02

ROOT MEAN SQUARES DEVIATION = .1118379E-03
AVERAGE ABSOLUTE DEVIATION = .9086499E-04
MAXIMUM DEVIATION = -.2813241E-03

Figure A-11. Benzene-Toluene Data Output Programs Determining Wilson Binary Parameters, page 2

The Noakes Problem
DATA REGRESSION SECTION

SUBSECTION: CASE VLE (CONTINUED)

DATA-GROUP VLE1 VARIABLE: COMPOSITION VAPOR C1
UNITS : MOL-FR

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
.2200000	.2321289	.10000E-01	.12129E-01	5.5131
.4220000	.4324044	.10000E-01	.10404E-01	2.4655
.4250000	.4349199	.10000E-01	.99199E-02	2.3341
.4530000	.4425375	.10000E-01	-.10463E-01	-2.3096
.6390000	.6293572	.10000E-01	-.96428E-02	-1.5090
.8240000	.8203922	.10000E-01	-.36078E-02	-.43784
.2080000	.2118251	.10000E-01	.38251E-02	1.8390
.3720000	.3738267	.10000E-01	.18267E-02	.49106
.5070000	.5047232	.10000E-01	-.22768E-02	-.44907
.6190000	.6131900	.10000E-01	-.58100E-02	-.93860
.7130000	.7048164	.10000E-01	-.81836E-02	-1.1478
.7910000	.7829229	.10000E-01	-.80771E-02	-1.0211

ROOT MEAN SQUARES DEVIATION = .7949575E-02
AVERAGE ABSOLUTE DEVIATION = .7180469E-02
MAXIMUM DEVIATION = .1212888E-01

PARAMETER CORRELATION MATRIX

1.0000000
-.9981143 1.0000000

Figure A-12. Benzene-Toluene Data Output Program Determining Wilson Binary Parameters, page 3

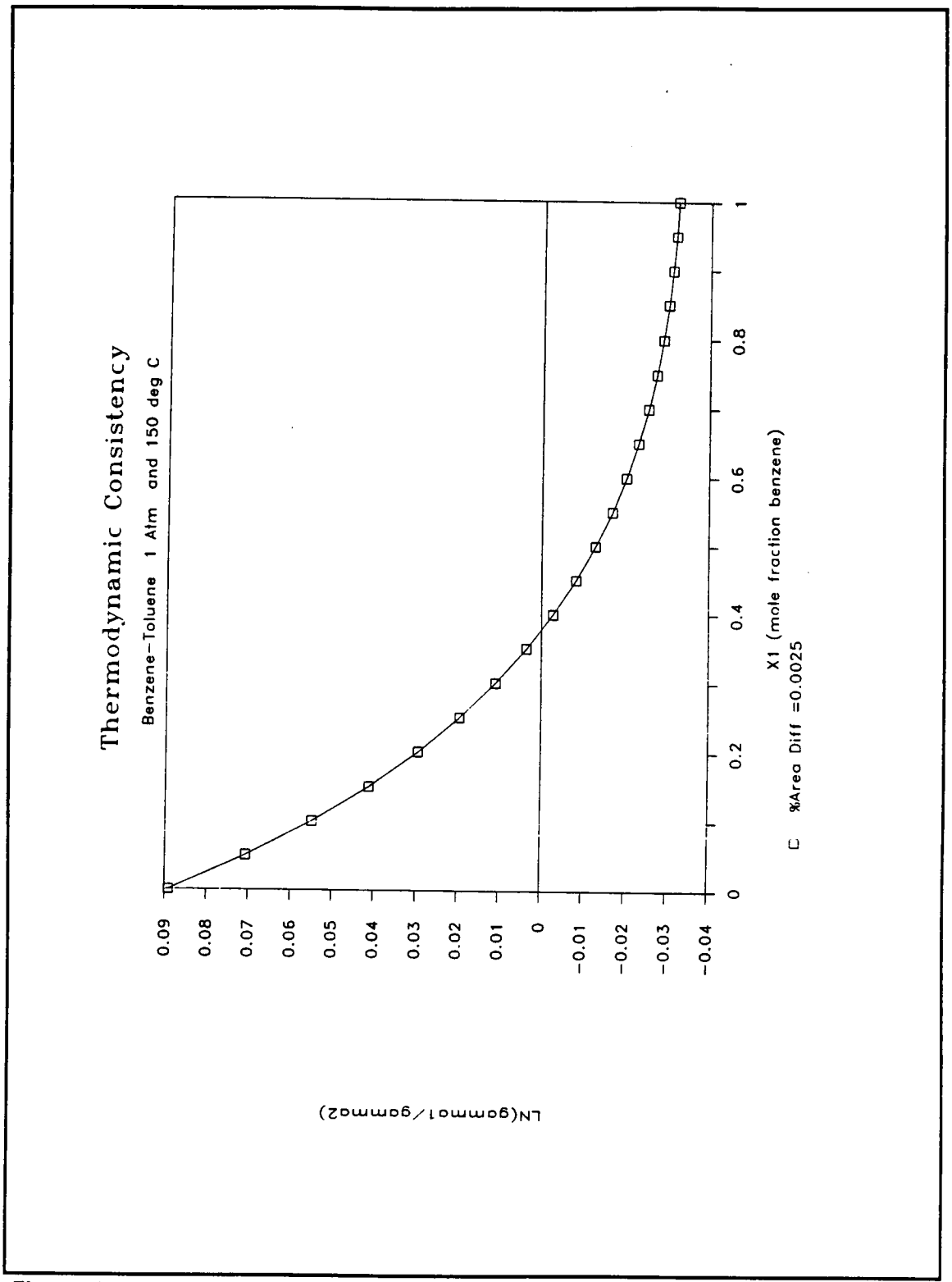


Figure A-13. Gibbs-Duhem Thermodynamic Consistency Test for Benzene-Toluene Wilson Binary Parameters

```
ASPEN/SP Run on 10/06/87 by Martin Marietta Energy Systems        Page    I
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986
                Wilson Parameter Evaluation Aromatic Systems
                            DESCRIPTION

      This program is used to evaluate the Wilson parameters for the
      two components, C1 and C2, which are based on a DRS run using x-y
      data found in the literature. For the system Benzene - M-Xylene
      the data are those of Ref. 109 in Vapor-Liquid Equilibrium Data,
      by Chu, Wang, Levy, and Paul, copyright 1956 by J. W. Edwards,
      Ann Arbor, Michigan.


                            RUN CONTROL INFORMATION

TYPE OF RUN: NEW

INPUT FILE NAME: B-X1

INPUT PROBLEM DATA FILE NAME: B-X1     UPDATE  NO.   0

MAIN CALLING PROGRAM NAME: B-X1

DRS ONLY RUN
```

```
ASPEN/SP Run on 10/06/87 by Martin Marietta Energy Systems        Page   II
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986
                Wilson Parameter Evaluation Aromatic Systems
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               PHYSICAL PROPERTIES SECTION.....................  1
                    COMPONENTS.................................  1
                    OPTION SETS................................  1

               DATA REGRESSION SECTION.........................  2
                    SUBSECTION: CASE VLE.......................  2

```

Figure A-14. Benzene-*m*-Xylene Data Input Program Determining Wilson Binary Parameters, page 1

```
ASPEN/SP Run on 10/06/87 by Martin Marietta Energy Systems        Page    1
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986
                Wilson Parameter Evaluation Aromatic Systems
                        PHYSICAL PROPERTIES SECTION

COMPONENTS

 ID        TYPE  FORMULA         DATABANK REFERENCE              ALIAS
  C1        C     C6H6            BENZENE                         C6H6
  C2        C     C8H10-2         M-XYLENE                        C8H10-2

OPTION SETS

  SYSOP0

  MAJOR PROPERTY  PHILMX    HVMX     HLMX     GVMX     GLMX     SVMX
  ROUTE ID        PHILMX00  HVMX00   HLMX00   GVMX00   GLMX00   SVMX00
                  ------------------------------------------------------
                  SLMX      VVMX     VLMX     MUVMX    MULMX    KVMX
                  SLMX00    VVMX00   VLMX01   MUVMX01  MULMX01  KVMX01
                  ------------------------------------------------------
                  KLMX      DVMX     DLMX     SIGLMX   PHIV     PHIL
                  KLMX01    DVMX01   DLMX01   SIGLMX01 PHIV01   PHIL00
                  ------------------------------------------------------
                  HV        HL       GV       GL       SV       SL
                  HV00      HL00     GV00     GL00     SV00     SL00
                  ------------------------------------------------------
                  VV        VL       KS       VS       PHISMX   HSMX
                  VV00      VL01     KS01     VS01     PHISMX02 HSMX02
                  ------------------------------------------------------
                  GSMX      SSMX     VSMX     KSMX     PHIS     HS
                  GSMX02    SSMX01   VSMX02   KSMX01   PHIS02   HS02
                  ------------------------------------------------------
                  GS        SS
                  GS02      SS02

  SYSOP8

  MAJOR PROPERTY  PHIVMX    PHILMX   HVMX     HLMX     GVMX     GLMX
  ROUTE ID        PHIVMX01  PHILMX08 HVMX01   HLMX08   GVMX01   GLMX01
                  ------------------------------------------------------
                  SVMX      SLMX     VVMX     VLMX     MUVMX    MULMX
                  SVMX01    SLMX08   VVMX01   VLMX01   MUVMX02  MULMX02
                  ------------------------------------------------------
                  KVMX      KLMX     DVMX     DLMX     SIGLMX   PHIV
                  KVMX02    KLMX01   DVMX02   DLMX01   SIGLMX01 PHIV04
                  ------------------------------------------------------
                  PHIL      HV       HL       GV       GL       SV
                  PHIL04    HV01     HL02     GV01     GL01     SV01
                  ------------------------------------------------------
                  SL        VV       VL
                  SL02      VV01     VL01
```

Figure A-15. Benzene-m-Xylene Data Input Program Determining Wilson Binary Parameters, page 2

```
ASPEN/SP Run on 10/06/87 by Martin Marietta Energy Systems        Page    2
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on September 30,
1986
                Wilson Parameter Evaluation Aromatic Systems
                        DATA REGRESSION SECTION

SUBSECTION: CASE VLE


 PARAMETER    ELEMENT      COMPONENT            PARAMETER       STANDARD
  NAME         NUMBER       OR PAIR              ESTIMATE        DEVIATION

 GMWSNB         1           C1        C2          254.6705        218.8151
 GMWSNB         1           C2        C1         -623.5297        719.4391

 NUMBER OF ITERATIONS   10


 DATA-GROUP VLE1       VARIABLE: TEMPERATURE
                       UNITS   : C

   MEASURED       ESTIMATED      STD-DEVIATION  ADJUSTMENTS  % ADJUSTMENTS
     120.0000       120.0984        .10000        .98370E-01   .81975E-01
     120.0000       120.1005        .10000        .10045       .83712E-01
     120.0000       120.0877        .10000        .87741E-01   .73118E-01
     120.0000       120.0793        .10000        .79314E-01   .66095E-01
     120.0000       120.0729        .10000        .72856E-01   .60714E-01
     120.0000       120.0617        .10000        .61716E-01   .51430E-01
     120.0000       120.0717        .10000        .71663E-01   .59719E-01
     120.0000       120.0773        .10000        .77270E-01   .64391E-01
     120.0000       120.0974        .10000        .97393E-01   .81161E-01
     140.0000       141.5126        .10000       1.5126        1.0804
     140.0000       140.0835        .10000        .83489E-01   .59635E-01
     140.0000       140.0451        .10000        .45124E-01   .32231E-01
     140.0000       140.0138        .10000        .13753E-01   .98232E-02
     140.0000       140.0242        .10000        .24246E-01   .17319E-01
     140.0000       140.0364        .10000        .36368E-01   .25977E-01
     140.0000       140.0285        .10000        .28462E-01   .20330E-01
     140.0000       140.0238        .10000        .23773E-01   .16981E-01
     140.0000       140.0437        .10000        .43718E-01   .31227E-01
     140.0000       140.0575        .10000        .57452E-01   .41037E-01
     140.0000       140.0755        .10000        .75452E-01   .53894E-01

   ROOT MEAN SQUARES DEVIATION =   .3445787
   AVERAGE ABSOLUTE DEVIATION  =   .1345587
   MAXIMUM DEVIATION           =  1.512560
```

Figure A-16. Benzene-*m*-Xylene Data Output Program Determining Wilson Binary Parameters, page 1

ASPEN/SP Run on 10/06/87 by Martin Marietta Energy Systems Page 3
ASPEN/SP Version 1.5 Released by JSD, INC., Denver, Colorado on September 30, 1986

Wilson Parameter Evaluation Aromatic Systems
DATA REGRESSION SECTION

SUBSECTION: CASE VLE (CONTINUED)

DATA-GROUP VLE1 VARIABLE: PRESSURE
UNITS : TORR

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
880.0000	854.9910	8.8000	-25.009	-2.8419
1095.000	1062.492	10.950	-32.508	-2.9688
1300.000	1265.310	13.000	-34.690	-2.6684
1500.000	1461.114	15.000	-38.886	-2.5924
1690.000	1646.299	16.900	-43.701	-2.5858
1860.000	1816.979	18.600	-43.021	-2.3130
2030.000	1972.074	20.300	-57.926	-2.8535
2180.000	2111.357	21.800	-68.643	-3.1487
2340.000	2246.829	23.400	-93.171	-3.9816
1430.000	809.6259	14.300	-620.37	-43.383
1130.000	1096.697	11.300	-33.303	-2.9472
1430.000	1413.155	14.300	-16.845	-1.1780
1725.000	1728.360	17.250	3.3603	.19480
2050.000	2039.911	20.500	-10.089	-.49212
2370.000	2339.569	23.700	-30.431	-1.2840
2650.000	2620.766	26.500	-29.234	-1.1032
2910.000	2880.468	29.100	-29.532	-1.0149
3180.000	3116.974	31.800	-63.026	-1.9819
3420.000	3329.968	34.200	-90.032	-2.6325
3660.000	3533.358	36.600	-126.64	-3.4602

ROOT MEAN SQUARES DEVIATION = 148.6683
AVERAGE ABSOLUTE DEVIATION = 74.52110
MAXIMUM DEVIATION = -620.3741

Figure A-17. Benzene-m-Xylene Data Output Program Determining Wilson Binary Parameters, page 2

Wilson Parameter Evaluation Aromatic Systems
DATA REGRESSION SECTION

SUBSECTION: CASE VLE (CONTINUED)

DATA-GROUP VLE1 VARIABLE: COMPOSITION LIQUID C1
UNITS : MOL-FR

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
.2000000	.1987575	.10000E-02	-.12425E-02	-.62123
.3000000	.2991132	.10000E-02	-.88677E-03	-.29559
.4000000	.3993928	.10000E-02	-.60725E-03	-.15181
.5000000	.4996779	.10000E-02	-.32211E-03	-.64422E-01
.6000000	.5998989	.10000E-02	-.10108E-03	-.16846E-01
.7000000	.6999865	.10000E-02	-.13487E-04	-.19268E-02
.8000000	.8001252	.10000E-02	.12521E-03	.15651E-01
.9000000	.9001899	.10000E-02	.18995E-03	.21106E-01
1.000000	1.000000	.00000E+00	.00000E+00	.00000E+00
.0000000E+00	.0000000E+00	.00000E+00	.00000E+00	
.1000000	.9924128E-01	.10000E-02	-.75872E-03	-.75872
.2000000	.1986379	.10000E-02	-.13621E-02	-.68103
.3000000	.2986975	.10000E-02	-.13025E-02	-.43416
.4000000	.3993277	.10000E-02	-.67234E-03	-.16809
.5000000	.4997749	.10000E-02	-.22507E-03	-.45015E-01
.6000000	.5999173	.10000E-02	-.82651E-04	-.13775E-01
.7000000	.7000100	.10000E-02	.10023E-04	.14318E-02
.8000000	.8001240	.10000E-02	.12398E-03	.15498E-01
.9000000	.9001766	.10000E-02	.17663E-03	.19626E-01
1.000000	1.000000	.00000E+00	.00000E+00	.00000E+00

ROOT MEAN SQUARES DEVIATION = .6663423E-03
AVERAGE ABSOLUTE DEVIATION = .4824853E-03
MAXIMUM DEVIATION = -.1362057E-02

Figure A-18. Benzene-*m*-Xylene Data Output Program Determining Wilson Binary Parameters, page 3

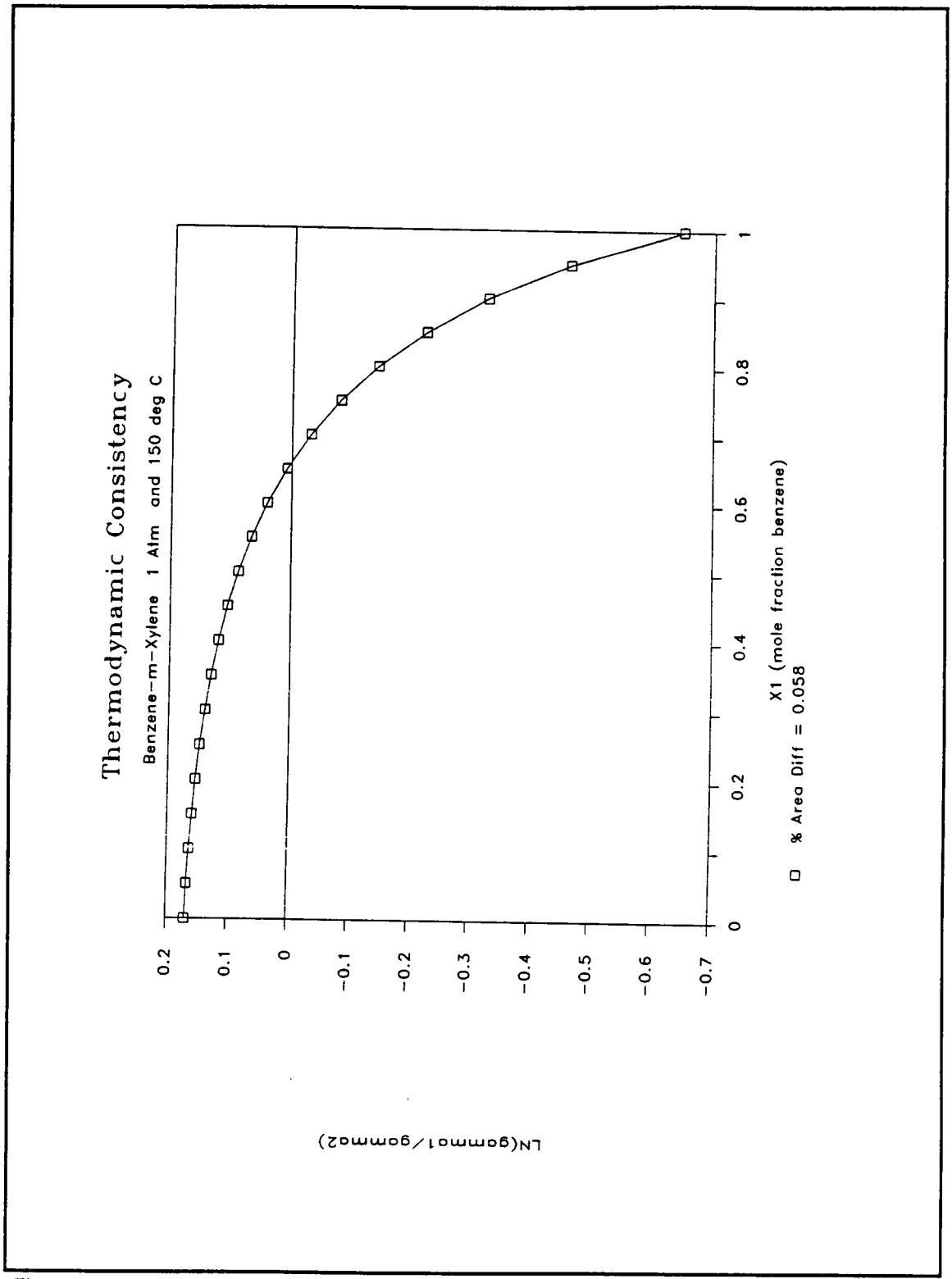

Figure A-19 Gibbs-Duhem Thermodynamic Consistency Test for Benzene-*m*-Xylene Wilson Binary Parameters

```
ASPEN/SP Run on 10/08/87 by Martin Marietta Energy Systems        Page    I
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on Sept. 30, 1986

                Wilson Parameter Evaluation Aromatic Systems
                            DESCRIPTION

      This program is used to evaluate the Wilson parameters for the
      two components, C1 and C2, which are based on a DRS run using x-y
      data found in the literature. For the system Toluene - P-Xylene
      the data are those of the Collection of Czechoslovak Chemical
      Communications by I. Wichterle, pg. 3391, copyright 1965.
      Pressures are based on an ideal gas law computation.


                          RUN CONTROL INFORMATION

TYPE OF RUN: NEW

INPUT FILE NAME: t-x2

INPUT PROBLEM DATA FILE NAME: t-x2     UPDATE  NO.   0

MAIN CALLING PROGRAM NAME: t-x2

DRS ONLY RUN
```

```
ASPEN/SP Run on 10/08/87 by Martin Marietta Energy Systems        Page   II
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on Sept. 30, 1986

                Wilson Parameter Evaluation Aromatic Systems
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          PHYSICAL PROPERTIES SECTION.....................  1
               COMPONENTS.................................  1
               OPTION SETS................................  1

          DATA REGRESSION SECTION.........................  2
               SUBSECTION: CASE VLE.......................  2

```

Figure A-20. Toluene-*p*-Xylene Data Input Program Determining Wilson Binary Parameters, page 1

```
ASPEN/SP Run on 10/08/87 by Martin Marietta Energy Systems        Page    1
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on Sept. 30, 1986

                Wilson Parameter Evaluation Aromatic Systems
                        PHYSICAL PROPERTIES SECTION

COMPONENTS

 ID        TYPE  FORMULA         DATABANK REFERENCE                ALIAS
  C1         C    C7H8             TOLUENE                         C7H8
  C2         C    C8H10-3          P-XYLENE                        C8H10-3

OPTION SETS

  SYSOP0

  MAJOR PROPERTY  PHILMX   HVMX     HLMX     GVMX     GLMX     SVMX
  ROUTE ID        PHILMX00 HVMX00   HLMX00   GVMX00   GLMX00   SVMX00
                  ---------------------------------------------------
                  SLMX     VVMX     VLMX     MUVMX    MULMX    KVMX
                  SLMX00   VVMX00   VLMX01   MUVMX01  MULMX01  KVMX01
                  ---------------------------------------------------
                  KLMX     DVMX     DLMX     SIGLMX   PHIV     PHIL
                  KLMX01   DVMX01   DLMX01   SIGLMX01 PHIV01   PHIL00
                  ---------------------------------------------------
                  HV       HL       GV       GL       SV       SL
                  HV00     HL00     GV00     GL00     SV00     SL00
                  ---------------------------------------------------
                  VV       VL       KS       VS       PHISMX   HSMX
                  VV00     VL01     KS01     VS01     PHISMX02 HSMX02
                  ---------------------------------------------------
                  GSMX     SSMX     VSMX     KSMX     PHIS     HS
                  GSMX02   SSMX01   VSMX02   KSMX01   PHIS02   HS02
                  ---------------------------------------------------
                  GS       SS
                  GS02     SS02

  SYSOP8

  MAJOR PROPERTY  PHIVMX   PHILMX   HVMX     HLMX     GVMX     GLMX
  ROUTE ID        PHIVMX01 PHILMX08 HVMX01   HLMX08   GVMX01   GLMX01
                  ---------------------------------------------------
                  SVMX     SLMX     VVMX     VLMX     MUVMX    MULMX
                  SVMX01   SLMX08   VVMX01   VLMX01   MUVMX02  MULMX02
                  ---------------------------------------------------
                  KVMX     KLMX     DVMX     DLMX     SIGLMX   PHIV
                  KVMX02   KLMX01   DVMX02   DLMX01   SIGLMX01 PHIV04
                  ---------------------------------------------------
                  PHIL     HV       HL       GV       GL       SV
                  PHIL04   HV01     HL02     GV01     GL01     SV01
                  ---------------------------------------------------
                  SL       VV       VL
                  SL02     VV01     VL01
```

Figure A-21 Toluene-*p*-Xylene Data Input Program Determining Wilson Binary Parameters, page 2

ASPEN/SP Run on 10/08/87 by Martin Marietta Energy Systems Page 2
ASPEN/SP Version 1.5 Released by JSD, INC., Denver, Colorado on Sept. 30, 1986

Wilson Parameter Evaluation Aromatic Systems
DATA REGRESSION SECTION

SUBSECTION: CASE VLE

PARAMETER NAME	ELEMENT NUMBER	COMPONENT OR PAIR		PARAMETER ESTIMATE	STANDARD DEVIATION
GMWSNB	1	C1	C2	-483.7691	136.2830
GMWSNB	1	C2	C1	266.9901	41.73022

NUMBER OF ITERATIONS 20

DATA-GROUP VLE1 VARIABLE: TEMPERATURE
UNITS : C

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
90.00000	89.94365	.10000	-.56350E-01	-.62611E-01
90.00000	89.99772	.10000	-.22812E-02	-.25346E-02
90.00000	90.04499	.10000	.44990E-01	.49989E-01
90.00000	89.92063	.10000	-.79371E-01	-.88190E-01
90.00000	90.06772	.10000	.67724E-01	.75249E-01
90.00000	90.06247	.10000	.62469E-01	.69410E-01
90.00000	90.04442	.10000	.44420E-01	.49355E-01
90.00000	89.94819	.10000	-.51810E-01	-.57566E-01
90.00000	90.03611	.10000	.36115E-01	.40127E-01
90.00000	90.01871	.10000	.18710E-01	.20788E-01
90.00000	89.98889	.10000	-.11115E-01	-.12350E-01
90.00000	90.01015	.10000	.10153E-01	.11281E-01
90.00000	89.98880	.10000	-.11197E-01	-.12441E-01

ROOT MEAN SQUARES DEVIATION = .4528283E-01
AVERAGE ABSOLUTE DEVIATION = .3820794E-01
MAXIMUM DEVIATION = -.7937110E-01

Figure A-22. Toluene-*p*-Xylene Data Output Program Determining Wilson Binary Parameters, page 1

Wilson Parameter Evaluation Aromatic Systems
DATA REGRESSION SECTION

SUBSECTION: CASE VLE (CONTINUED)

DATA-GROUP VLE1 VARIABLE: PRESSURE
UNITS : TORR

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
209.2700	212.6767	2.0927	3.4067	1.6279
217.5000	217.6894	2.1750	.18943	.87095E-01
224.5000	221.7032	2.2450	-2.7968	-1.2458
236.5000	241.9050	2.3650	5.4050	2.2854
251.1000	246.2877	2.5110	-4.8123	-1.9165
252.5000	248.0266	2.5250	-4.4734	-1.7717
264.9000	261.5130	2.6490	-3.3870	-1.2786
286.9000	291.2208	2.8690	4.3208	1.5060
303.4000	300.1711	3.0340	-3.2289	-1.0642
313.6000	311.8417	3.1360	-1.7583	-.56069
323.6000	324.6375	3.2360	1.0375	.32062
333.2000	332.1752	3.3320	-1.0248	-.30757
355.9000	357.0997	3.5590	1.1997	.33709

ROOT MEAN SQUARES DEVIATION = 3.270764
AVERAGE ABSOLUTE DEVIATION = 2.849292
MAXIMUM DEVIATION = 5.405042

DATA-GROUP VLE1 VARIABLE: COMPOSITION LIQUID C1
UNITS : MOL-FR

MEASURED	ESTIMATED	STD-DEVIATION	ADJUSTMENTS	% ADJUSTMENTS
.1670000	.1667230	.10000E-02	-.27696E-03	-.16585
.1870000	.1868468	.10000E-02	-.15317E-03	-.81912E-01
.2030000	.2029384	.10000E-02	-.61568E-04	-.30329E-01
.2980000	.2979370	.10000E-02	-.63013E-04	-.21145E-01
.3120000	.3120634	.10000E-02	.63378E-04	.20314E-01
.3200000	.3200631	.10000E-02	.63098E-04	.19718E-01
.3810000	.3810718	.10000E-02	.71789E-04	.18842E-01
.5160000	.5160155	.10000E-02	.15500E-04	.30040E-02
.5510000	.5510641	.10000E-02	.64139E-04	.11640E-01
.6020000	.6020484	.10000E-02	.48400E-04	.80399E-02
.6580000	.6580242	.10000E-02	.24167E-04	.36728E-02
.6890000	.6890266	.10000E-02	.26628E-04	.38647E-02
.7950000	.7949975	.10000E-02	-.25432E-05	-.31989E-03

ROOT MEAN SQUARES DEVIATION = .9964607E-04
AVERAGE ABSOLUTE DEVIATION = .7187413E-04

MAXIMUM DEVIATION = -.2769650E-03

Figure A-23. Toluene-*p*-Xylene Data Output Program Determining Wilson Binary Parameters, page 2

```
ASPEN/SP Run on 10/08/87 by Martin Marietta Energy Systems        Page    4
ASPEN/SP Version  1.5 Released by JSD, INC., Denver, Colorado on Sept. 30, 1986

                Wilson Parameter Evaluation Aromatic Systems
                        DATA REGRESSION SECTION

SUBSECTION: CASE VLE (CONTINUED)


 DATA-GROUP VLE1        VARIABLE: COMPOSITION VAPOR   C1
                        UNITS   : MOL-FR

   MEASURED        ESTIMATED       STD-DEVIATION  ADJUSTMENTS  % ADJUSTMENTS
     .3230000        .3303108         .10000E-01    .73108E-02    2.2634
     .3480000        .3586953         .10000E-01    .10695E-01    3.0734
     .3660000        .3805213         .10000E-01    .14521E-01    3.9676
     .5100000        .4973167         .10000E-01   -.12683E-01   -2.4869
     .5030000        .5130305         .10000E-01    .10030E-01    1.9941
     .5130000        .5218576         .10000E-01    .88576E-02    1.7266
     .5820000        .5858228         .10000E-01    .38228E-02    .65683
     .7260000        .7090357         .10000E-01   -.16964E-01   -2.3367
     .7350000        .7373016         .10000E-01    .23016E-02    .31314
     .7770000        .7761353         .10000E-01   -.86472E-03   -.11129
     .8230000        .8156922         .10000E-01   -.73078E-02   -.88795
     .8370000        .8362707         .10000E-01   -.72935E-03   -.87138E-01
     .9040000        .9002504         .10000E-01   -.37496E-02   -.41478

   ROOT MEAN SQUARES DEVIATION =  .9178066E-02
   AVERAGE ABSOLUTE DEVIATION  =  .7679912E-02
   MAXIMUM DEVIATION           = -.1696427E-01


PARAMETER CORRELATION MATRIX

    1.0000000
   -.9913067 1.0000000
```

Figure A-24. Toluene-*p*-Xylene Data Output Program Determining Wilson Binary Parameters, page 3

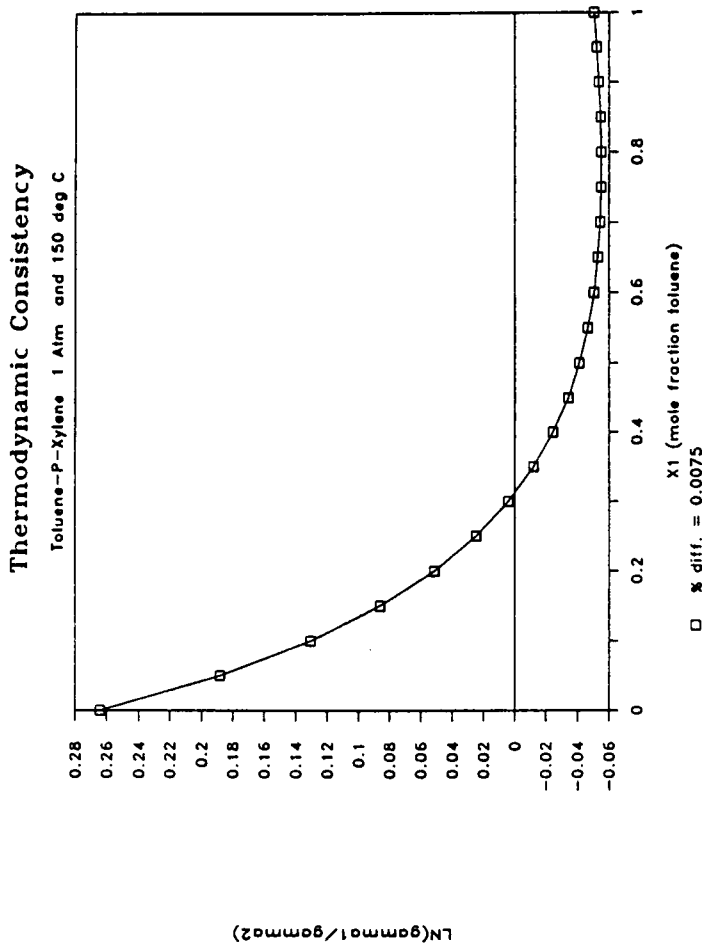


Figure A-25. Gibbs-Duhem Thermodynamic Consistency Test for Toluene-*p*-Xylene Wilson Binary Parameters

APPENDIX B

DISTILLATION SIMULATION INPUT

LISTING OF INPUT DATA

NCOMP	NTRAY	NOFEED	NOSIDE	IWILS	IGAMMA	IFE	INILE	INILQ
3	42	1	1	0	1	1	0	1

IBUG	IOUTOP	KMAX	JMAXT	JMAXV	BMETH	TMETH	IOPT	KTMAX	ICTYPE
0	1	99	99	99	1	3	1	99	1

EPS1	EPS2	EPS3	ATEMP	AVAP
0.10E-09	0.10E-03	0.00E+00	0.10E+00	0.50E-01

DISTILLATE MOLES/HR	REFLUX RATIO	PTOP TORR	PBOT TORR	TTOP DEG C	TBOT DEG C	TREF DEG C	EFF
0.48300E+02	20.000	760.00	1520.00	113.89	174.44	113.89	1.00

FEED DATA

J	N(J) (NN)	JTYPE	F(NN) MOLES/HR	TF(J) DEG C	PF(J) TORR	MOLE FRACTION(Z(I,NN)) I 1	2	3
1	21	L	0.60000E+03	118.00	823.00	0.10000	0.45000	0.45000

LIQUID SIDE DRAW LOCATED ON TRAY 28

COMPONENT DATA

NAME	XMW	AVP	BVP	CVP	AH	BH	CH	DH	AV	BV
BENZENE	78.11	15.900000	-2789.00	220.80	0.3920	8.00E-04	0.00E+00	0.00E+00	203.40	-3.60E-01
TOLUENE	92.14	16.010000	-3097.00	219.50	0.3840	8.00E-04	0.00E+00	0.00E+00	189.00	-3.00E-01
XYLENE	106.20	16.120000	-3396.00	213.50	0.4000	6.00E-04	0.00E+00	0.00E+00	180.00	-3.42E-01

NAME	DV	VOL	CV
BENZENE	0.00E+00	89.41	0.00E+00
TOLUENE	0.00E+00	106.80	0.00E+00
XYLENE	0.00E+00	121.20	0.00E+00

DENSITY PARAMETERS

VISCOSITY PARAMETERS

NAME	AD	BD	CD	AMU	BMU	CMU
BENZENE	0.577500E+02	-.780400E-01	0.000000E+00	0.00000E+00	0.00000E+00	0.00000E+00
TOLUENE	0.571200E+02	0.624300E-01	0.000000E+00	0.00000E+00	0.00000E+00	0.00000E+00
XYLENE	0.561900E+02	0.572300E-01	0.000000E+00	0.00000E+00	0.00000E+00	0.00000E+00

SURFACE TENSION PARAMETERS

NAME	ASURFT	BSURFT
BENZENE	0.00000E+00	0.00000E+00
TOLUENE	0.00000E+00	0.00000E+00
XYLENE	0.00000E+00	0.00000E+00

BINARY DATA FOR WILSON EQ,DLAM(I,J)

		I		
J		1	2	3
1	DLAM	0.00000E+00	-0.35500E+03	0.51150E+01
2	DLAM	0.37800E+03	0.00000E+00	0.11870E+03
3	DLAM	-0.39900E-01	-0.12060E+03	0.00000E+00

DATA FOR VAPOR FUGACITY COEFFICIENTS REDLICH-KWONG EQN

		I					
	1	2	3	4	5	6	7
CRIT TEMP(C)	288.90	318.60	343.90				
CRIT P(ATM)	48.34	40.55	35.62				

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

BOTTOM SPECIFICATION: REBOILER DUTY = 0.13100E+08

TOP SPECIFICATION: DISTILLATE RATE = 48.30000

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

BOTTOM SPECIFICATION: REBOILER DUTY = 0.13100E+08

TOP SPECIFICATION: REFLUX RATE -- DETERMINED USING R*D

APPENDIX C

DISTILLATION SIMULATION OUTPUT FOR A DQS SCHEME CONTROLLING TOLUENE LIQUID

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

RESULTS OF THE DISTILLATION PROGRAM

REFLUX RATIO = 20.019 REBOILER DUTY = 1.31000E+07 Btu/hr

CONDENSER DUTY = 1.17269E+07 Btu/hr NUMBER OF STAGES = 42

OVERHEAD

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
113.89 Deg. C	760.00 Torr	7058.60 Btu/mole	78.7715
237.00 Deg. F	14.70 Psia	89.6085 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr	Lbs/hr
BENZENE	0.952851	0.944849	46.0227	3594.83
TOLUENE	4.714888E-02	5.515063E-02	2.27729	209.830
XYLENE	1.873880E-10	2.526371E-10	9.050839E-09	9.611991E-07
Total	1.000000	1.000000	48.3000	3804.66

Component Name	Percent Recovery
BENZENE	0.7670
TOLUENE	8.4344E-03
XYLENE	3.3522E-11
Total	---

BOTTOMS

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
172.54 Deg. C	1520.00 Torr	14896.6 Btu/mole	106.171
342.58 Deg. F	29.39 Psia	140.308 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr	Lbs/hr
BENZENE	2.687921E-10	1.977508E-10	7.144493E-08	5.580564E-06
TOLUENE	2.079813E-03	1.804960E-03	0.552814	50.9363
XYLENE	0.997920	0.998195	265.247	28169.3
Total	1.000000	1.000000	265.800	28220.2

Component Name	Percent Recovery
BENZENE	1.1907E-09
TOLUENE	2.0475E-03
XYLENE	0.9824
Total	---

LIQUID FEED LOCATED ON TRAY 21

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
118.00 Deg. C	823.00 Torr	8945.69 Btu/mole	97.0640
244.40 Deg. F	15.91 Psia	92.1628 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr	Lbs/hr
BENZENE	0.100000	8.047268E-02	60.0000	4686.60
TOLUENE	0.450000	0.427172	270.000	24877.8
XYLENE	0.450000	0.492356	270.000	28674.0
Total	1.000000	1.000000	600.000	58238.4

LIQUID SIDE DRAW LOCATED ON TRAY 28

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
119.63 Deg. C	1019.51 Torr	8534.73 Btu/mole	91.6878
247.34 Deg. F	19.71 Psia	93.0846 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr	Lbs/hr
BENZENE	4.888874E-02	4.164893E-02	13.9773	1091.77
TOLUENE	0.934487	0.939096	267.170	24617.0
XYLENE	1.662404E-02	1.925527E-02	4.75281	504.749
Total	1.000000	1.000000	285.900	26213.5

Component Name	Percent Recovery
BENZENE	0.2330
TOLUENE	0.9895
XYLENE	1.7603E-02
Total	---

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- ENERGY BALANCE

Stage No.	Temperature Deg. C	Pressure Torr	Feed Btu/hr	Vapor Btu/hr	Liquid Btu/hr	Heat Added Btu/hr
42	82.55	760.00	--	18610.	5020.9	--
41	86.23	778.54	--	18894.	5363.4	--
40	91.72	797.07	--	19387.	5890.7	--
39	98.24	815.61	--	20074.	6527.5	--
38	104.17	834.15	--	20790.	7109.9	--
37	108.51	852.68	--	21357.	7534.5	--
36	111.35	871.22	--	21727.	7807.6	--
35	113.20	889.76	--	21946.	7979.3	--
34	114.49	908.29	--	22076.	8094.0	--
33	115.49	926.83	--	22159.	8179.2	--
32	116.34	945.37	--	22217.	8249.8	--
31	117.13	963.90	--	22265.	8313.8	--
30	117.90	982.44	--	22308.	8376.9	--
29	118.70	1000.98	--	22353.	8445.9	--
28	119.63	1019.51	--	22409.	8534.7	--
27	120.95	1038.05	--	22497.	8675.9	--
26	122.59	1056.59	--	22613.	8863.3	--
25	124.65	1075.12	--	22767.	9107.1	--
24	127.10	1093.66	--	22962.	9405.8	--
23	129.83	1112.20	--	23187.	9740.3	--
22	132.58	1130.73	--	23422.	10079.	--

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- ENERGY BALANCE

Stage No.	Temperature Deg. C	Pressure Torr	Feed Btu/hr	Vapor Btu/hr	Liquid Btu/hr
21	135.16	1149.27	8945.7	23650.	10395.
20	137.09	1167.80	--	23918.	10598.
19	138.58	1186.34	--	24094.	10754.
18	139.94	1204.88	--	24234.	10901.
17	141.43	1223.41	--	24375.	11070.
16	143.25	1241.95	--	24546.	11285.
15	145.55	1260.49	--	24772.	11568.
14	148.43	1279.02	--	25068.	11930.
13	151.78	1297.56	--	25432.	12357.
12	155.35	1316.10	--	25838.	12814.
11	158.78	1334.63	--	26244.	13253.
10	161.78	1353.17	--	26608.	13635.
9	164.23	1371.71	--	26907.	13945.
8	166.16	1390.24	--	27136.	14183.
7	167.66	1408.78	--	27307.	14364.
6	168.84	1427.32	--	27432.	14501.
5	169.79	1445.85	--	27525.	14609.
4	170.60	1464.39	--	27596.	14697.
3	171.31	1482.93	--	27654.	14772.
2	171.96	1501.46	--	27701.	14838.
1	172.56	1520.00	--	27743.	14899.

Stage No.	Stage Eff.	Heat Added Btu/hr
42	1.000	--
41	1.000	--
39	1.000	--
38	1.000	--
37	1.000	--
36	1.000	--
35	1.000	--
34	1.000	--
33	1.000	--
32	1.000	--
31	1.000	--
30	1.000	--
29	1.000	--
28	1.000	--
27	1.000	--
26	1.000	--
25	1.000	--
24	1.000	--
23	1.000	--
22	1.000	--
21	1.000	--
20	1.000	--
19	1.000	--
18	1.000	--
17	1.000	--
16	1.000	--
15	1.000	--
14	1.000	--
13	1.000	--
12	1.000	--
11	1.000	--
10	1.000	--
9	1.000	--
8	1.000	--
7	1.000	--
6	1.000	--
5	1.000	--
4	1.000	--
3	1.000	--
2	1.000	--
1	1.000	1.31000E+07

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- MATERIAL BALANCE

No.	Deg. C	Torr	Moles/hr	Moles/hr	Moles/hr	Moles/hr
42	82.55	760.00	1015.2	804.09	--	--
41	86.23	778.54	852.39	793.73	--	--
40	91.72	797.07	842.03	782.46	--	--
39	98.24	815.61	830.76	775.69	--	--
38	104.17	834.15	823.99	774.61	--	--
37	108.51	852.68	822.91	776.37	--	--
36	111.35	871.22	824.67	778.56	--	--
35	113.20	889.76	826.86	780.42	--	--
34	114.49	908.29	828.72	781.93	--	--
33	115.49	926.83	830.23	783.21	--	--
32	116.34	945.37	831.51	784.34	--	--
31	117.13	963.90	832.64	785.36	--	--
30	117.90	982.44	833.66	786.21	--	--
29	118.70	1000.98	834.51	786.74	--	--
28	119.63	1019.51	835.04	500.62	--	285.90
27	120.95	1038.05	834.82	498.70	--	--
26	122.59	1056.59	832.90	496.18	--	--
25	124.65	1075.12	830.38	493.28	--	--
24	127.10	1093.66	827.48	490.46	--	--
23	129.83	1112.20	824.66	488.24	--	--
22	132.58	1130.73	822.44	486.88	--	--

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- MATERIAL BALANCE

Stage No.	Temperature Deg. C	Pressure Torr	Vapor Rate Moles/hr	Liquid Rate Moles/hr	Feed Rate Moles/hr	Liquid Sid Moles/hr
21	135.12	1149.27	821.08	1146.0	600.00	--
20	137.02	1167.80	880.24	1151.7	--	--
19	138.45	1186.34	885.95	1155.9	--	--
18	139.74	1204.88	890.08	1159.2	--	--
17	141.10	1223.41	893.39	1162.2	--	--
16	142.74	1241.95	896.40	1165.4	--	--
15	144.82	1260.49	899.63	1169.5	--	--
14	147.46	1279.02	903.75	1175.5	--	--
13	150.64	1297.56	909.69	1184.1	--	--
12	154.16	1316.10	918.34	1195.7	--	--
11	157.68	1334.63	929.92	1209.3	--	--
10	160.87	1353.17	943.54	1223.3	--	--
9	163.55	1371.71	957.54	1236.1	--	--
8	165.68	1390.24	970.33	1246.9	--	--
7	167.33	1408.78	981.10	1255.5	--	--
6	168.62	1427.32	989.73	1262.4	--	--
5	169.66	1445.85	996.55	1267.8	--	--
4	170.52	1464.39	1002.0	1272.3	--	--
3	171.26	1482.93	1006.5	1276.1	--	--
2	171.93	1501.46	1010.3	1279.5	--	--
1	172.54	1520.00	1013.7	265.80	--	--

Stage No.	Vapor Rate Moles/hr
42	--
41	--
40	--
39	--
38	--
37	--
36	--
35	--
34	--
33	--
32	--
31	--
30	--
29	--
28	--
27	--
26	--
25	--
24	--
23	--
22	--
21	--
20	--
19	--
18	--
17	--
16	--
15	--
14	--
13	--
12	--
11	--
10	--
9	--
8	--
7	--
6	--
5	--
4	--
3	--
2	--
1	--

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 1 BENZENE

Stage No.	Mole Fractions		K Value	Activity Coefficient	Fugacity Coefficient
	Feed	Liquid	Vapor			
42	--	0.88691	0.95285	1.0743	1.0011	1.0022
41	--	0.76355	0.89065	1.1665	1.0001	1.0049
40	--	0.58385	0.77441	1.3264	0.99739	1.0098
39	--	0.39314	0.60530	1.5396	0.99335	1.0161
38	--	0.24362	0.42595	1.7485	0.98976	1.0225
37	--	0.14995	0.28524	1.9022	0.98759	1.0273
36	--	9.88081E-02	0.19698	1.9935	0.98657	1.0304
35	--	7.28801E-02	0.14870	2.0403	0.98619	1.0323
34	--	6.02340E-02	0.12417	2.0614	0.98613	1.0334
33	--	5.42023E-02	0.11216	2.0693	0.98620	1.0342
32	--	5.13788E-02	0.10640	2.0709	0.98633	1.0348
31	--	5.00872E-02	0.10367	2.0698	0.98648	1.0353
30	--	4.95057E-02	0.10239	2.0683	0.98660	1.0359
29	--	4.92048E-02	0.10179	2.0687	0.98663	1.0364
28	--	4.88887E-02	0.10147	2.0756	0.98642	1.0372
27	--	4.81997E-02	0.10119	2.0994	0.98567	1.0385
26	--	4.71813E-02	0.10090	2.1385	0.98454	1.0404
25	--	4.57198E-02	0.10045	2.1970	0.98310	1.0430
24	--	4.38401E-02	9.97639E-02	2.2756	0.98147	1.0462
23	--	4.17206E-02	9.88307E-02	2.3689	0.97986	1.0500
22	--	3.96296E-02	9.77209E-02	2.4659	0.97841	1.0540

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 1 BENZENE

Stage No.	Mole Fractions Feed	Mole Fractions Liquid	Mole Fractions Vapor	K Value	Activity Coefficient	Fugacity Coefficient
21	0.10000	3.78042E-02	9.65738E-02	2.5546	0.97721	1.0577
20	--	1.88491E-02	4.92196E-02	2.6112	0.97620	1.0606
19	--	9.26443E-03	2.45041E-02	2.6450	0.97564	1.0626
18	--	4.50317E-03	1.20310E-02	2.6717	0.97524	1.0644
17	--	2.16166E-03	5.84295E-03	2.7030	0.97483	1.0663
16	--	1.01960E-03	2.80264E-03	2.7488	0.97428	1.0688
15	--	4.68712E-04	1.32085E-03	2.8180	0.97348	1.0722
14	--	2.07906E-04	6.06564E-04	2.9175	0.97237	1.0768
13	--	8.81523E-05	2.68654E-04	3.0476	0.97097	1.0826
12	--	3.55324E-05	1.13667E-04	3.1990	0.96937	1.0892
11	--	1.36245E-05	4.56886E-05	3.3534	0.96773	1.0962
10	--	5.00104E-06	1.74625E-05	3.4918	0.96624	1.1027
9	--	1.77394E-06	6.38919E-06	3.6017	0.96502	1.1082
8	--	6.14023E-07	2.25980E-06	3.6803	0.96409	1.1126
7	--	2.09117E-07	7.80303E-07	3.7314	0.96344	1.1160
6	--	7.05079E-08	2.65205E-07	3.7614	0.96299	1.1186
5	--	2.36318E-08	8.92421E-08	3.7764	0.96270	1.1206
4	--	7.88857E-09	2.98293E-08	3.7813	0.96251	1.1222
3	--	2.61939E-09	9.90087E-09	3.7798	0.96238	1.1236
2	--	8.57861E-10	3.23780E-09	3.7743	0.96230	1.1247
1	--	2.68792E-10	1.01232E-09	3.7662	0.96225	1.1258

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 2 TOLUENE

Stage No.	Mole Fractions		K Value	Activity Coefficient	Fugacity Coefficient
	Feed	Liquid	Vapor			
42	--	0.11309	4.71489E-02	0.41693	0.98011	0.97849
41	--	0.23645	0.10935	0.46246	0.98598	0.98006
40	--	0.41615	0.22559	0.54209	0.99276	0.98305
39	--	0.60686	0.39470	0.65040	0.99773	0.98712
38	--	0.75638	0.57405	0.75894	1.0001	0.99111
37	--	0.85005	0.71476	0.84085	1.0009	0.99408
36	--	0.90119	0.80302	0.89107	1.0011	0.99589
35	--	0.92710	0.85130	0.91824	1.0012	0.99686
34	--	0.93972	0.87582	0.93200	1.0012	0.99734
33	--	0.94567	0.88779	0.93880	1.0012	0.99757
32	--	0.94828	0.89348	0.94221	1.0012	0.99766
31	--	0.94900	0.89601	0.94416	1.0013	0.99770
30	--	0.94808	0.89675	0.94586	1.0013	0.99774
29	--	0.94442	0.89593	0.94866	1.0013	0.99782
28	--	0.93449	0.89252	0.95509	1.0013	0.99806
27	--	0.90955	0.88315	0.97097	1.0012	0.99872
26	--	0.87218	0.86810	0.99533	1.0010	0.99976
25	--	0.82079	0.84564	1.0303	1.0004	1.0013
24	--	0.75733	0.81492	1.0760	0.99919	1.0034
23	--	0.68796	0.77715	1.1296	0.99745	1.0058
22	--	0.62096	0.73603	1.1853	0.99540	1.0084

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 2 TOLUENE

Stage No.	Mole Fractions Feed	Liquid	Vapor	K Value	Activity Coefficient	Fugacity Coefficient
21	0.45000	0.56315	0.69638	1.2366	0.99337	1.0109
20	--	0.57560	0.73257	1.2727	0.99330	1.0126
19	--	0.57718	0.74766	1.2954	0.99309	1.0138
18	--	0.57011	0.74892	1.3137	0.99271	1.0148
17	--	0.55393	0.73910	1.3343	0.99206	1.0159
16	--	0.52648	0.71756	1.3629	0.99101	1.0175
15	--	0.48508	0.68142	1.4048	0.98939	1.0197
14	--	0.42843	0.62713	1.4638	0.98705	1.0228
13	--	0.35896	0.55301	1.5406	0.98401	1.0267
12	--	0.28357	0.46226	1.6301	0.98052	1.0314
11	--	0.21134	0.36403	1.7225	0.97701	1.0363
10	--	0.14963	0.27029	1.8064	0.97392	1.0408
9	--	0.10166	0.19058	1.8747	0.97148	1.0447
8	--	6.69826E-02	0.12894	1.9250	0.96969	1.0477
7	--	4.31590E-02	8.45661E-02	1.9594	0.96847	1.0500
6	--	2.73501E-02	5.41911E-02	1.9814	0.96767	1.0517
5	--	1.70920E-02	3.40902E-02	1.9945	0.96716	1.0529
4	--	1.05286E-02	2.10743E-02	2.0016	0.96685	1.0539
3	--	6.36443E-03	1.27598E-02	2.0049	0.96666	1.0546
2	--	3.73539E-03	7.49166E-03	2.0056	0.96656	1.0553
1	--	2.07981E-03	4.16950E-03	2.0047	0.96651	1.0558

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 3 XYLENE

Stage No.	Feed	Mole Fractions Liquid	Mole Fractions Vapor	K Value	Activity Coefficient	Fugacity Coefficient
42	--	1.37833E-09	1.87388E-10	0.13595	0.95094	0.96165
41	--	8.62038E-09	1.31084E-09	0.15206	0.94713	0.96232
40	--	4.49537E-08	8.13665E-09	0.18100	0.94311	0.96394
39	--	1.90452E-07	4.23511E-08	0.22237	0.94161	0.96623
38	--	6.73326E-07	1.79299E-07	0.26629	0.94320	0.96843
37	--	2.10397E-06	6.33817E-07	0.30125	0.94580	0.96994
36	--	6.11760E-06	1.98075E-06	0.32378	0.94786	0.97070
35	--	1.71074E-05	5.76026E-06	0.33671	0.94914	0.97093
34	--	4.68471E-05	1.61103E-05	0.34389	0.94985	0.97085
33	--	1.26776E-04	4.41217E-05	0.34803	0.95026	0.97061
32	--	3.40530E-04	1.19412E-04	0.35067	0.95053	0.97029
31	--	9.09602E-04	3.20777E-04	0.35266	0.95077	0.96993
30	--	2.41678E-03	8.56901E-04	0.35456	0.95109	0.96958
29	--	6.37702E-03	2.27690E-03	0.35705	0.95171	0.96927
28	--	1.66240E-02	6.00817E-03	0.36141	0.95314	0.96906
27	--	4.22500E-02	1.56622E-02	0.37070	0.95645	0.96915
26	--	8.06426E-02	3.10036E-02	0.38446	0.96105	0.96951
25	--	0.13349	5.39104E-02	0.40386	0.96677	0.97021
24	--	0.19883	8.53199E-02	0.42911	0.97298	0.97128
23	--	0.27032	0.12402	0.45877	0.97883	0.97262
22	--	0.33941	0.16625	0.48984	0.98364	0.97405

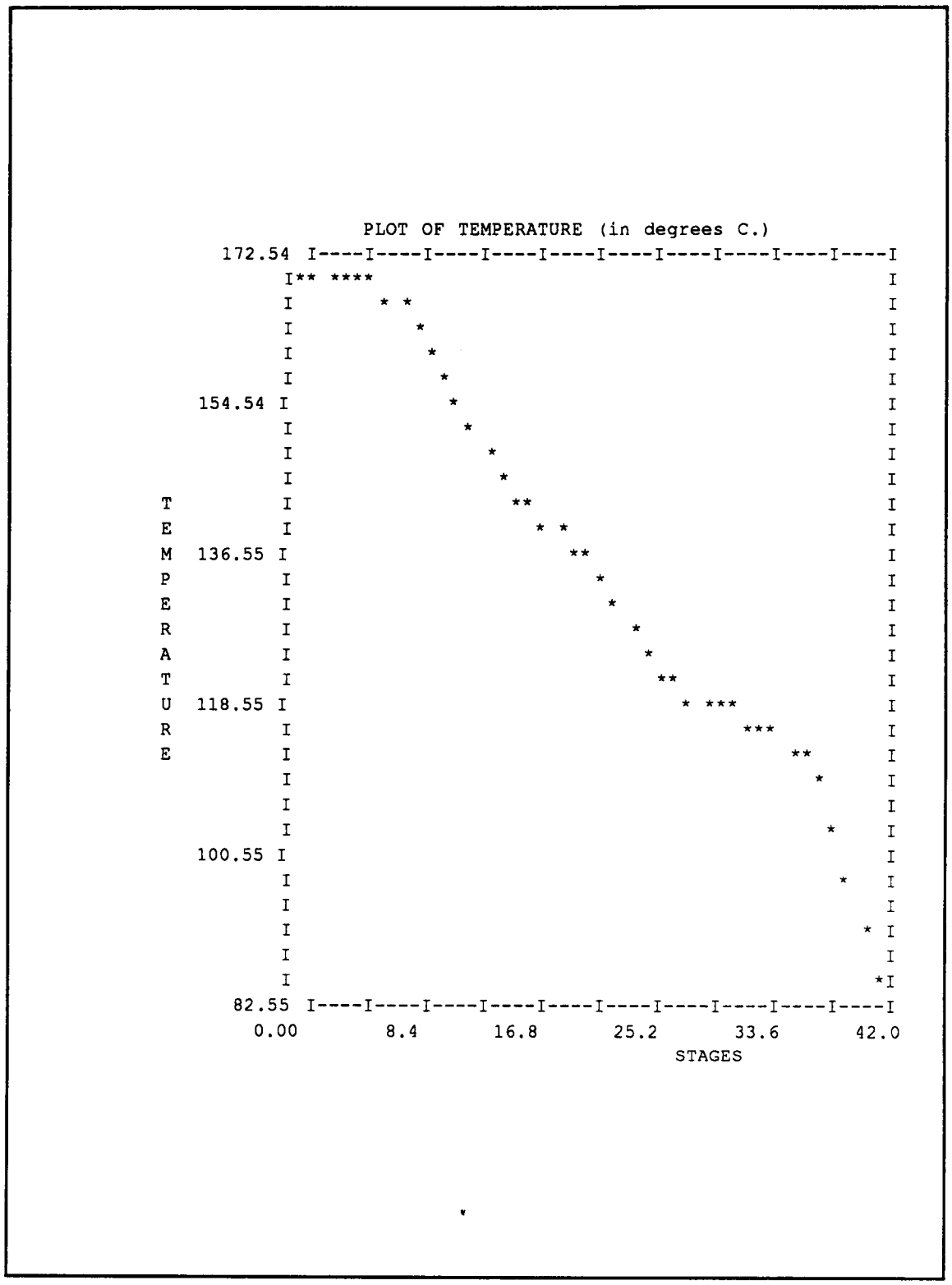
MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); D, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 3 XYLENE

Stage No.	Mole Fractions Feed	Liquid	Vapor	K Value	Activity Coefficient	Fugacity Coefficient
21	0.45000	0.39905	0.20705	0.51886	0.98720	0.97537
20	--	0.40555	0.21821	0.53806	0.98750	0.97617
19	--	0.41355	0.22783	0.55092	0.98790	0.97661
18	--	0.42539	0.23904	0.56194	0.98850	0.97696
17	--	0.44391	0.25505	0.57456	0.98941	0.97740
16	--	0.47250	0.27964	0.59183	0.99073	0.97814
15	--	0.51445	0.31726	0.61669	0.99250	0.97932
14	--	0.57136	0.37226	0.65154	0.99458	0.98110
13	--	0.64095	0.44673	0.69698	0.99669	0.98350
12	--	0.71639	0.53763	0.75046	0.99847	0.98637
11	--	0.78864	0.63592	0.80635	0.99971	0.98937
10	--	0.85037	0.72969	0.85809	1.0004	0.99216
9	--	0.89833	0.80941	0.90101	1.0008	0.99448
8	--	0.93302	0.87106	0.93359	1.0010	0.99625
7	--	0.95684	0.91543	0.95672	1.0011	0.99751
6	--	0.97265	0.94581	0.97240	1.0011	0.99838
5	--	0.98291	0.96591	0.98271	1.0011	0.99895
4	--	0.98947	0.97893	0.98934	1.0011	0.99932
3	--	0.99364	0.98724	0.99356	1.0011	0.99956
2	--	0.99626	0.99251	0.99623	1.0011	0.99971
1	--	0.99792	0.99583	0.99791	1.0011	0.99981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136.55
118.55
100.55
82.55
TEMPERATURE
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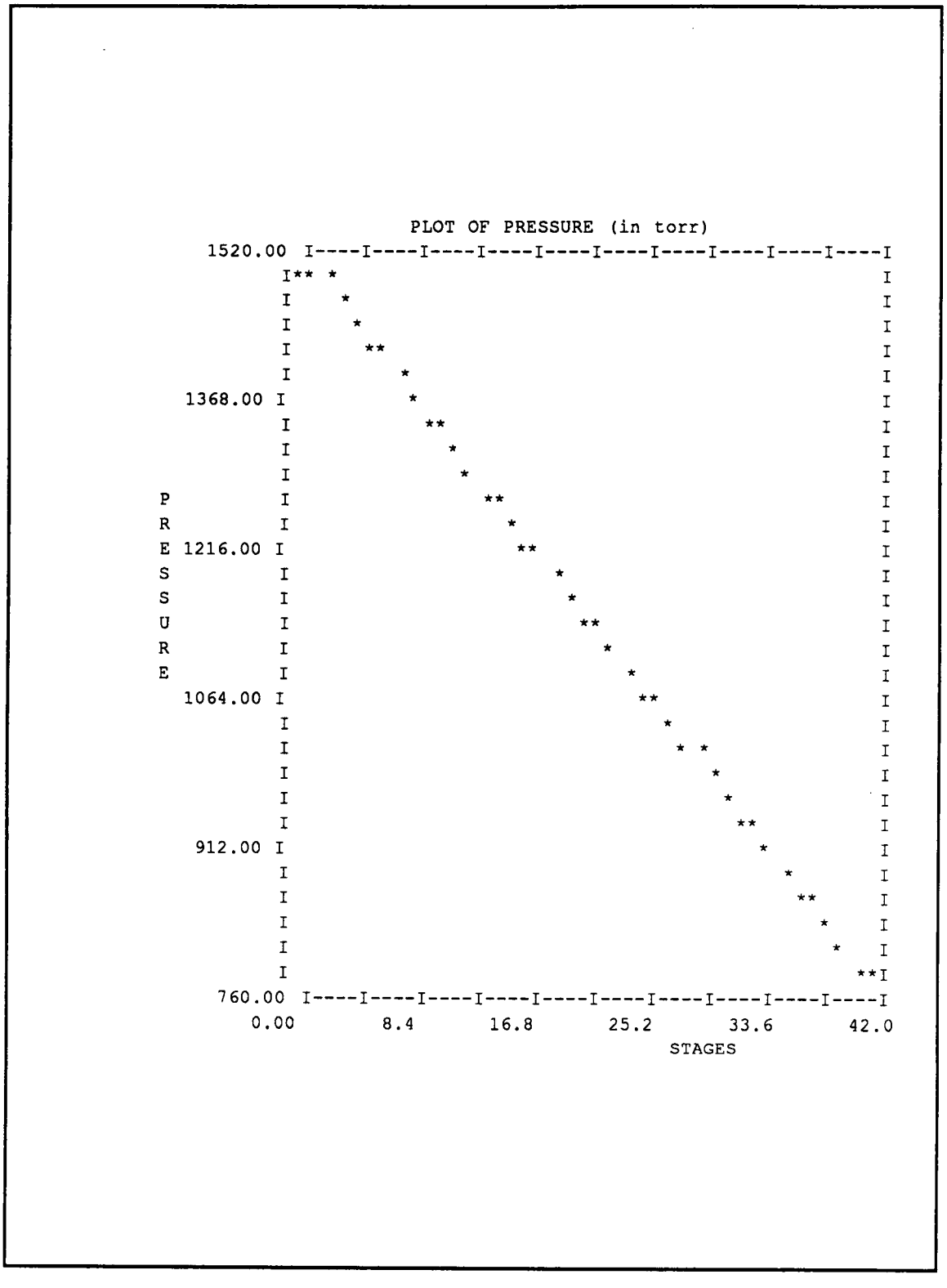
8.4
16.8
25.2
33.6
42.0
STAGES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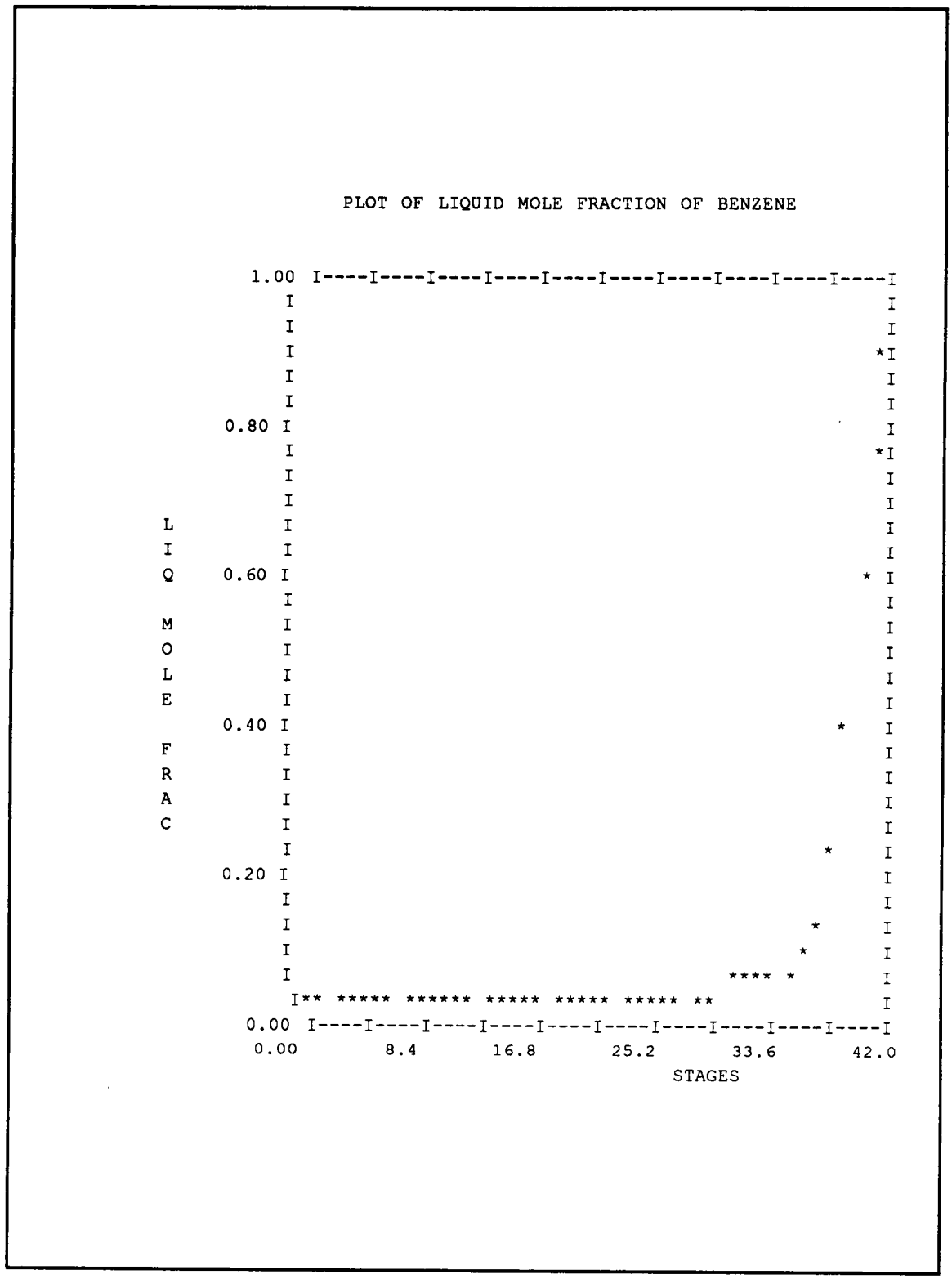
1520.00
1368.00
1216.00
1064.00
912.00
760.00
PRESSURE
0.00
8.4
16.8
25.2
33.6
42.0
STAGES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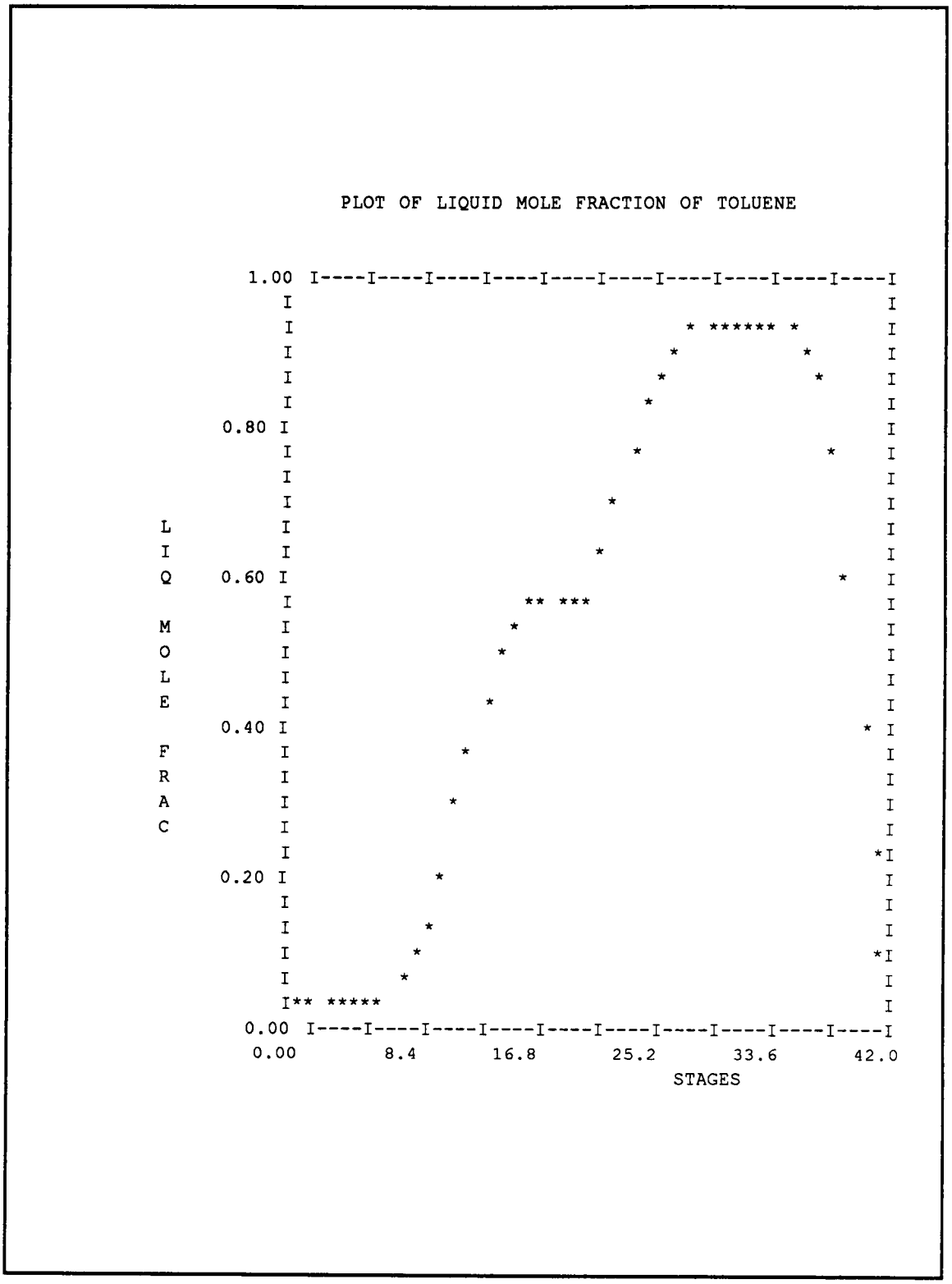
1.00
0.80
0.60
0.40
0.20
0.00
LIQ MOLE FRAC
0.00
8.4
16.8
25.2
33.6
42.0
STAGES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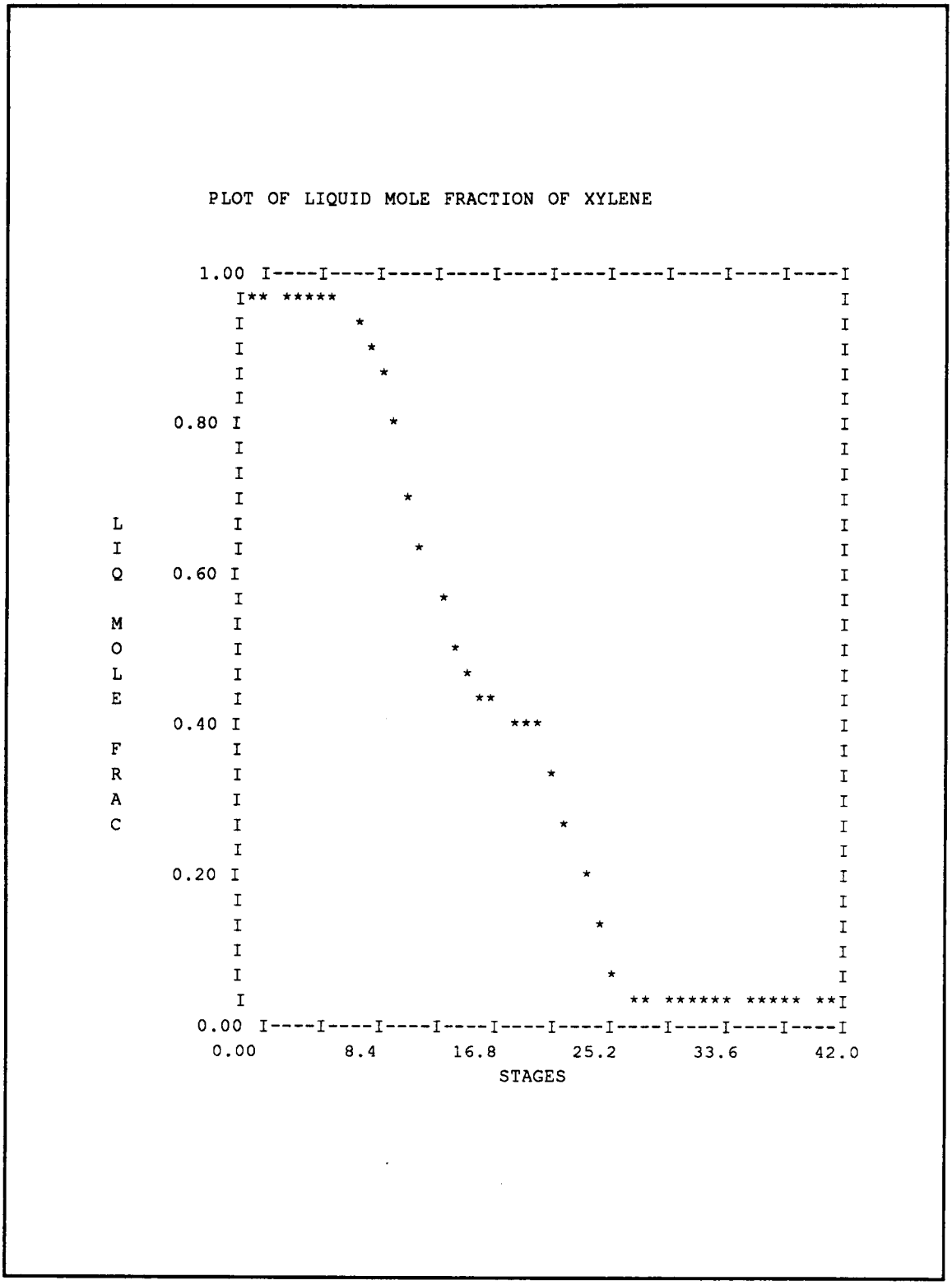
0.60
0.40
0.20
0.00
LIQUID MOLE FRACTION
0.00
8.4
16.8
25.2
33.6
42.0
STAGES


PLOT OF LIQUID MOLE FRACTION OF XYLENE
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0.80
0.60
0.40
0.20
0.00
LIQUID MOLE FRACTION
0.00
8.4
16.8
25.2
33.6
42.0
STAGES

APPENDIX D

DISTILLATION SIMULATION OUTPUT FOR A DQS SCHEME CONTROLLING TOLUENE LIQUID

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

RESULTS OF THE DISTILLATION PROGRAM

REFLUX RATIO = 19.937 REBOILER DUTY = 1.31000E+07 Btu/hr

CONDENSER DUTY = 1.17271E+07 Btu/hr NUMBER OF STAGES = 42

OVERHEAD

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
113.89 Deg. C	760.00 Torr	7061.82 Btu/mole	78.8122
237.00 Deg. F	14.70 Psia	89.6030 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr
BENZENE	0.949947	0.941482	46.0277
TOLUENE	5.005325E-02	5.851764E-02	2.42522
XYLENE	2.033571E-10	2.740250E-10	9.853237E-09
Total	1.000000	1.000000	48.4529

Component Name	Lbs/hr	Percent Recovery
BENZENE	3595.22	0.7671
TOLUENE	223.460	8.9823E-03
XYLENE	1.046414E-06	3.6493E-11
Total	3818.68	---

BOTTOMS

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
172.56 Deg. C	1520.00 Torr	14898.9 Btu/mole	106.176
342.61 Deg. F	29.39 Psia	140.323 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr
BENZENE	2.264010E-10	1.665556E-10	6.014277E-08
TOLUENE	1.719497E-03	1.492190E-03	0.456779
XYLENE	0.998281	0.998508	265.190
Total	1.000000	1.000000	265.647

Component Name	Lbs/hr	Percent Recovery
BENZENE	4.697752E-06	1.0024E-09
TOLUENE	42.0877	1.6918E-03
XYLENE	28163.2	0.9822
Total	28205.3	---

RESULTS OF THE DISTILLATION PROGRAM

LIQUID FEED LOCATED ON TRAY 21

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
118.00 Deg. C	823.00 Torr	8945.69 Btu/mole	97.0640
244.40 Deg. F	15.91 Psia	92.1628 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr
BENZENE	0.100000	8.047268E-02	60.0000
TOLUENE	0.450000	0.427172	270.000
XYLENE	0.450000	0.492356	270.000
Total	1.000000	1.000000	600.000

Component Name	Lbs/hr
BENZENE	4686.60
TOLUENE	24877.8
XYLENE	28674.0
Total	58238.4

LIQUID SIDE DRAW LOCATED ON TRAY 28

Temperature	Pressure	Enthalpy	Avg.Mol.Weight
119.64 Deg. C	1019.51 Torr	8535.45 Btu/mole	91.6909
247.35 Deg. F	19.71 Psia	93.0895 Btu/lb	

RATES

Component Name	Mole Fraction	Weight Fraction	Moles/hr
BENZENE	4.887144E-02	4.163281E-02	13.9723
TOLUENE	0.934306	0.938882	267.118
XYLENE	1.682288E-02	1.948492E-02	4.80966
Total	1.000000	1.000000	285.900

Component Name	Lbs/hr	Percent Recovery
BENZENE	1091.38	0.2329
TOLUENE	24612.3	0.9893
XYLENE	510.786	1.7814E-02
Total	26214.4	---

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- ENERGY BALANCE

Stage No.	Temperature Deg. C	Pressure Torr	Feed Btu/hr	Vapor Btu/hr	Liquid Btu/hr
42	82.70	760.00	--	18622.	5035.2
41	86.50	778.54	--	18919.	5390.5
40	92.11	797.07	--	19429.	5930.1
39	98.65	815.61	--	20125.	6568.9
38	104.48	834.15	--	20835.	7142.1
37	108.71	852.68	--	21388.	7554.8
36	111.46	871.22	--	21745.	7818.7
35	113.25	889.76	--	21956.	7985.0
34	114.52	908.29	--	22081.	8096.9
33	115.50	926.83	--	22161.	8180.6
32	116.35	945.37	--	22218.	8250.5
31	117.13	963.90	--	22265.	8314.2
30	117.90	982.44	--	22308.	8377.2
29	118.70	1000.98	--	22353.	8446.2
28	119.64	1019.51	--	22410.	8535.5
27	120.96	1038.05	--	22498.	8677.6
26	122.61	1056.59	--	22615.	8866.3
25	124.68	1075.12	--	22770.	9111.6
24	127.15	1093.66	--	22966.	9411.6
23	129.87	1112.20	--	23191.	9746.9
22	132.62	1130.73	--	23427.	10085.

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- ENERGY BALANCE

Stage No.	Temperature Deg. C	Pressure Torr	Feed Btu/hr	Vapor Btu/hr	Liquid Btu/hr
21	135.16	1149.27	8945.7	23650.	10395.
20	137.09	1167.80	--	23918.	10598.
19	138.58	1186.34	--	24094.	10754.
18	139.94	1204.88	--	24234.	10901.
17	141.43	1223.41	--	24375.	11070.
16	143.25	1241.95	--	24546.	11285.
15	145.55	1260.49	--	24772.	11568.
14	148.43	1279.02	--	25068.	11930.
13	151.78	1297.56	--	25432.	12357.
12	155.35	1316.10	--	25838.	12814.
11	158.78	1334.63	--	26244.	13253.
10	161.78	1353.17	--	26608.	13635.
9	164.23	1371.71	--	26907.	13945.
8	166.16	1390.24	--	27136.	14183.
7	167.66	1408.78	--	27307.	14364.
6	168.84	1427.32	--	27432.	14501.
5	169.79	1445.85	--	27525.	14609.
4	170.60	1464.39	--	27596.	14697.
3	171.31	1482.93	--	27654.	14772.
2	171.96	1501.46	--	27701.	14838.
1	172.56	1520.00	--	27743.	14899.

Stage No.	Heat Added Btu/hr
42	--
41	--
40	--
39	--
38	--
37	--
36	--
35	--
34	--
33	--
32	--
31	--
30	--
29	--
28	--
27	--
26	--
25	--
24	--
23	--
22	--
21	--
20	--
19	--
18	--
17	--
16	--
15	--
14	--
13	--
12	--
11	--
10	--
9	--
8	--
7	--
6	--
5	--
4	--
3	--
2	--
1	1.31000E+07

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- MATERIAL BALANCE

Stage No.	Temperature Deg. C	Pressure Torr	Vapor Rate Moles/hr	Liquid Rate Moles/hr	Feed Rate Moles/hr
42	82.70	760.00	1014.5	803.28	--
41	86.50	778.54	851.74	792.69	--
40	92.11	797.07	841.14	781.57	--
39	98.65	815.61	830.02	775.23	--
38	104.48	834.15	823.68	774.47	--
37	108.71	852.68	822.92	776.31	--
36	111.46	871.22	824.77	778.50	--
35	113.25	889.76	826.95	780.33	--
34	114.52	908.29	828.78	781.82	--
33	115.50	926.83	830.27	783.08	--
32	116.35	945.37	831.53	784.21	--
31	117.13	963.90	832.66	785.22	--
30	117.90	982.44	833.67	786.07	--
29	118.70	1000.98	834.52	786.59	--
28	119.64	1019.51	835.04	500.45	--
27	120.96	1038.05	834.80	498.52	--
26	122.61	1056.59	832.87	495.99	--
25	124.68	1075.12	830.34	493.07	--
24	127.15	1093.66	827.43	490.26	--
23	129.87	1112.20	824.61	488.05	--
22	132.62	1130.73	822.41	486.71	--

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES -- MATERIAL BALANCE

Stage No.	Temperature Deg. C	Pressure Torr	Vapor Rate Moles/hr	Liquid Rate Moles/hr	Feed Rate Moles/hr
21	135.16	1149.27	821.07	1145.9	600.00
20	137.09	1167.80	880.23	1151.6	--
19	138.58	1186.34	885.94	1155.7	--
18	139.94	1204.88	890.09	1159.1	--
17	141.43	1223.41	893.44	1162.2	--
16	143.25	1241.95	896.58	1165.8	--
15	145.55	1260.49	900.13	1170.5	--
14	148.43	1279.02	904.87	1177.5	--
13	151.78	1297.56	911.81	1187.3	--
12	155.35	1316.10	921.66	1199.9	--
11	158.78	1334.63	934.21	1213.8	--
10	161.78	1353.17	948.17	1227.5	--
9	164.23	1371.71	961.82	1239.5	--
8	166.16	1390.24	973.84	1249.4	--
7	167.66	1408.78	983.71	1257.2	--
6	168.84	1427.32	991.56	1263.4	--
5	169.79	1445.85	997.77	1268.4	--
4	170.60	1464.39	1002.8	1272.6	--
3	171.31	1482.93	1007.0	1276.2	--
2	171.96	1501.46	1010.6	1279.5	--
1	172.56	1520.00	1013.9	265.65	--

Stage No.	Liquid Side Moles/hr	Vapor Rate Moles/hr
42	--	--
41	--	--
40	--	--
39	--	--
38	--	--
37	--	--
36	--	--
35	--	--
34	--	--
33	--	--
32	--	--
31	--	--
30	--	--
29	--	--
28	285.90	--
27	--	--
26	--	--
25	--	--
24	--	--
23	--	--
22	--	--
21	--	--
20	--	--
19	--	--
18	--	--
17	--	--
16	--	--
15	--	--
14	--	--
13	--	--
12	--	--
11	--	--
10	--	--
9	--	--
8	--	--
7	--	--
6	--	--
5	--	--
4	--	--
3	--	--
2	--	--
1	--	--

Stage No.	dX 2/ /d L	dX 2/ /d Q	dX 2/ /d S(1)
42	-6.74169E-02	7.76926E-02	2.54104E-03
41	-0.11562	0.13331	4.37188E-03
40	-0.14436	0.16656	5.48736E-03
39	-0.12865	0.14861	4.93102E-03
38	-8.75541E-02	0.10134	3.40287E-03
37	-5.02131E-02	5.83338E-02	2.00116E-03
36	-2.62381E-02	3.07006E-02	1.09565E-03
35	-1.30968E-02	1.55457E-02	5.95258E-04
34	-6.40337E-03	7.82390E-03	3.33948E-04
33	-3.09959E-03	4.01326E-03	1.89527E-04
32	-1.47175E-03	2.14101E-03	7.78827E-05
31	-6.19131E-04	1.17534E-03	-8.63606E-05
30	-3.24104E-05	5.47119E-04	-4.56508E-04
29	7.01352E-04	-1.72407E-04	-1.39099E-03
28	2.17287E-03	-1.54858E-03	-3.74405E-03
27	5.44522E-03	-4.56204E-03	-9.31433E-03
26	9.64290E-03	-8.63144E-03	-1.65335E-02
25	1.40998E-02	-1.32797E-02	-2.42227E-02
24	1.75499E-02	-1.73806E-02	-3.01901E-02
23	1.88091E-02	-1.97056E-02	-3.23875E-02
22	1.76215E-02	-1.97616E-02	-3.03668E-02
21	1.47452E-02	-1.80317E-02	-2.54291E-02
20	2.61031E-02	-3.43806E-02	-4.50324E-02
19	4.47444E-02	-6.11680E-02	-7.72069E-02
18	7.40683E-02	-0.10330	-0.12782
17	0.11746	-0.16569	-0.20271
16	0.17568	-0.24950	-0.30321
15	0.24251	-0.34584	-0.41855
14	0.30175	-0.43149	-0.52082
13	0.33247	-0.47628	-0.57383
12	0.32263	-0.46281	-0.55685
11	0.27830	-0.39964	-0.48034
10	0.21760	-0.31276	-0.37559
9	0.15783	-0.22702	-0.27242
8	0.10845	-0.15610	-0.18719
7	7.17606E-02	-0.10335	-0.12386
6	4.62381E-02	-6.66342E-02	-7.98090E-02
5	2.91954E-02	-4.20970E-02	-5.03927E-02
4	1.80982E-02	-2.61092E-02	-3.12384E-02
3	1.09821E-02	-1.58505E-02	-1.89557E-02
2	6.46006E-03	-9.32746E-03	-1.11505E-02
1	3.60134E-03	-5.20123E-03	-6.21615E-03

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 1 BENZENE

Stage No.	Mole Fractions Feed	Mole Fractions Liquid	Mole Fractions Vapor	K Value	Activity Coefficient	Fugacity Coefficient
42	--	0.88055	0.94995	1.0788	1.0011	1.0023
41	--	0.75254	0.88450	1.1753	0.99994	1.0052
40	--	0.56995	0.76392	1.3403	0.99713	1.0102
39	--	0.38061	0.59213	1.5557	0.99305	1.0166
38	--	0.23502	0.41410	1.7620	0.98954	1.0228
37	--	0.14500	0.27711	1.9111	0.98747	1.0275
36	--	9.62132E-02	0.19229	1.9986	0.98651	1.0305
35	--	7.15831E-02	0.14624	2.0429	0.98617	1.0323
34	--	5.95990E-02	0.12293	2.0627	0.98611	1.0335
33	--	5.38933E-02	0.11156	2.0700	0.98619	1.0342
32	--	5.12279E-02	0.10611	2.0712	0.98633	1.0348
31	--	5.00124E-02	0.10352	2.0700	0.98648	1.0354
30	--	4.94670E-02	0.10232	2.0684	0.98660	1.0359
29	--	4.91825E-02	0.10175	2.0688	0.98663	1.0364
28	--	4.88714E-02	0.10145	2.0758	0.98641	1.0372
27	--	4.81783E-02	0.10117	2.0999	0.98565	1.0386
26	--	4.71502E-02	0.10088	2.1395	0.98452	1.0405
25	--	4.56770E-02	0.10042	2.1986	0.98306	1.0430
24	--	4.37876E-02	9.97335E-02	2.2777	0.98143	1.0463
23	--	4.16641E-02	9.87947E-02	2.3712	0.97982	1.0501
22	--	3.95760E-02	9.76820E-02	2.4682	0.97838	1.0541

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 1 BENZENE

Stage No.	Mole Fractions Feed	Liquid	Vapor	K Value	Activity Coefficient	Fugacity Coefficient
21	0.10000	3.77583E-02	9.65356E-02	2.5567	0.97719	1.0578
20	--	1.87971E-02	4.91536E-02	2.6150	0.97616	1.0607
19	--	9.21573E-03	2.44334E-02	2.6513	0.97556	1.0628
18	--	4.46141E-03	1.19662E-02	2.6821	0.97511	1.0647
17	--	2.12798E-03	5.78792E-03	2.7199	0.97463	1.0669
16	--	9.94040E-04	2.75847E-03	2.7750	0.97398	1.0698
15	--	4.50710E-04	1.28740E-03	2.8564	0.97306	1.0736
14	--	1.96368E-04	5.83027E-04	2.9691	0.97183	1.0787
13	--	8.15390E-05	2.53578E-04	3.1099	0.97033	1.0849
12	--	3.21673E-05	1.05041E-04	3.2655	0.96869	1.0917
11	--	1.20943E-05	4.13142E-05	3.4160	0.96710	1.0986
10	--	4.36839E-06	1.54827E-05	3.5443	0.96571	1.1047
9	--	1.53082E-06	5.57485E-06	3.6417	0.96461	1.1098
8	--	5.25333E-07	1.94834E-06	3.7088	0.96380	1.1138
7	--	1.77873E-07	6.67135E-07	3.7506	0.96324	1.1168
6	--	5.97441E-08	2.25466E-07	3.7739	0.96286	1.1191
5	--	1.99748E-08	7.55902E-08	3.7843	0.96262	1.1210
4	--	6.65735E-09	2.52063E-08	3.7862	0.96246	1.1224
3	--	2.20838E-09	8.35389E-09	3.7828	0.96235	1.1237
2	--	7.22817E-10	2.72937E-09	3.7760	0.96229	1.1248
1	--	2.26401E-10	8.52886E-10	3.7671	0.96224	1.1258

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 2 TOLUENE

Stage No.	Mole Fractions Feed	Liquid	Vapor	K Value	Activity Coefficient	Fugacity Coefficient
42	--	0.11945	5.00533E-02	0.41904	0.98043	0.97858
41	--	0.24746	0.11550	0.46674	0.98644	0.98024
40	--	0.43005	0.23608	0.54896	0.99319	0.98333
39	--	0.61939	0.40787	0.65851	0.99797	0.98743
38	--	0.76498	0.58590	0.76590	1.0002	0.99138
37	--	0.85500	0.72289	0.84548	1.0009	0.99426
36	--	0.90378	0.80771	0.89370	1.0011	0.99599
35	--	0.92840	0.85376	0.91960	1.0012	0.99691
34	--	0.94035	0.87705	0.93268	1.0012	0.99737
33	--	0.94598	0.88840	0.93913	1.0012	0.99758
32	--	0.94843	0.89377	0.94237	1.0012	0.99767
31	--	0.94907	0.89615	0.94424	1.0013	0.99771
30	--	0.94809	0.89682	0.94592	1.0013	0.99774
29	--	0.94436	0.89595	0.94873	1.0013	0.99782
28	--	0.93431	0.89247	0.95522	1.0013	0.99807
27	--	0.90909	0.88298	0.97128	1.0012	0.99873
26	--	0.87137	0.86777	0.99588	1.0010	0.99979
25	--	0.81961	0.84511	1.0311	1.0003	1.0013
24	--	0.75586	0.81418	1.0772	0.99915	1.0034
23	--	0.68639	0.77626	1.1309	0.99741	1.0059
22	--	0.61949	0.73508	1.1866	0.99535	1.0085
21	0.45000	0.56193	0.69551	1.2377	0.99332	1.0109

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 2 TOLUENE

Stage No.	Mole Fractions Feed	Liquid	Vapor	K Value	Activity Coefficient	Fugacity Coefficient
21	0.45000	0.56193	0.69551	1.2377	0.99332	1.0109
20	--	0.57344	0.73099	1.2748	0.99322	1.0127
19	--	0.57348	0.74487	1.2989	0.99296	1.0139
18	--	0.56396	0.74413	1.3195	0.99249	1.0150
17	--	0.54410	0.73113	1.3437	0.99170	1.0164
16	--	0.51162	0.70481	1.3776	0.99044	1.0182
15	--	0.46422	0.66210	1.4263	0.98854	1.0207
14	--	0.40191	0.60000	1.4928	0.98590	1.0241
13	--	0.32902	0.51851	1.5759	0.98263	1.0284
12	--	0.25378	0.42336	1.6682	0.97908	1.0332
11	--	0.18506	0.32546	1.7586	0.97569	1.0380
10	--	0.12870	0.23643	1.8370	0.97285	1.0423
9	--	8.62781E-02	0.16377	1.8982	0.97067	1.0458
8	--	5.63099E-02	0.10934	1.9418	0.96913	1.0485
7	--	3.60519E-02	7.10517E-02	1.9708	0.96809	1.0505
6	--	2.27518E-02	4.52498E-02	1.9888	0.96742	1.0520
5	--	1.41810E-02	2.83514E-02	1.9992	0.96700	1.0532
4	--	8.72114E-03	1.74822E-02	2.0046	0.96675	1.0540
3	--	5.26662E-03	1.05682E-02	2.0066	0.96661	1.0547
2	--	3.08926E-03	6.19902E-03	2.0066	0.96653	1.0553
1	--	1.71950E-03	3.44816E-03	2.0053	0.96649	1.0558

MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 3 XYLENE

Stage No.	Mole Fractions Feed	Liquid	Vapor	K Value	Activity Coefficient	Fugacity Coefficient
42	--	1.48799E-09	2.03357E-10	0.13667	0.95073	0.96171
41	--	9.21459E-09	1.41491E-09	0.15355	0.94683	0.96245
40	--	4.73845E-08	8.69551E-09	0.18351	0.94289	0.96413
39	--	1.97907E-07	4.46302E-08	0.22551	0.94164	0.96644
38	--	6.92157E-07	1.86278E-07	0.26913	0.94338	0.96860
37	--	2.14840E-06	6.51416E-07	0.30321	0.94598	0.97005
36	--	6.22374E-06	2.02220E-06	0.32492	0.94798	0.97077
35	--	1.73700E-05	5.85908E-06	0.33731	0.94920	0.97096
34	--	4.75154E-05	1.63545E-05	0.34419	0.94988	0.97087
33	--	1.28505E-04	4.47426E-05	0.34818	0.95028	0.97061
32	--	3.45034E-04	1.21017E-04	0.35074	0.95054	0.97029
31	--	9.21351E-04	3.24957E-04	0.35270	0.95077	0.96994
30	--	2.44733E-03	8.67802E-04	0.35459	0.95109	0.96958
29	--	6.45577E-03	2.30524E-03	0.35708	0.95172	0.96927
28	--	1.68229E-02	6.08118E-03	0.36148	0.95317	0.96907
27	--	4.27287E-02	1.58465E-02	0.37086	0.95651	0.96916
26	--	8.14834E-02	3.13503E-02	0.38474	0.96114	0.96953
25	--	0.13472	5.44649E-02	0.40430	0.96689	0.97024
24	--	0.20035	8.60912E-02	0.42970	0.97312	0.97131
23	--	0.27195	0.12495	0.45946	0.97895	0.97265
22	--	0.34093	0.16724	0.49053	0.98374	0.97409
21	0.45000	0.40032	0.20795	0.51948	0.98727	0.97541

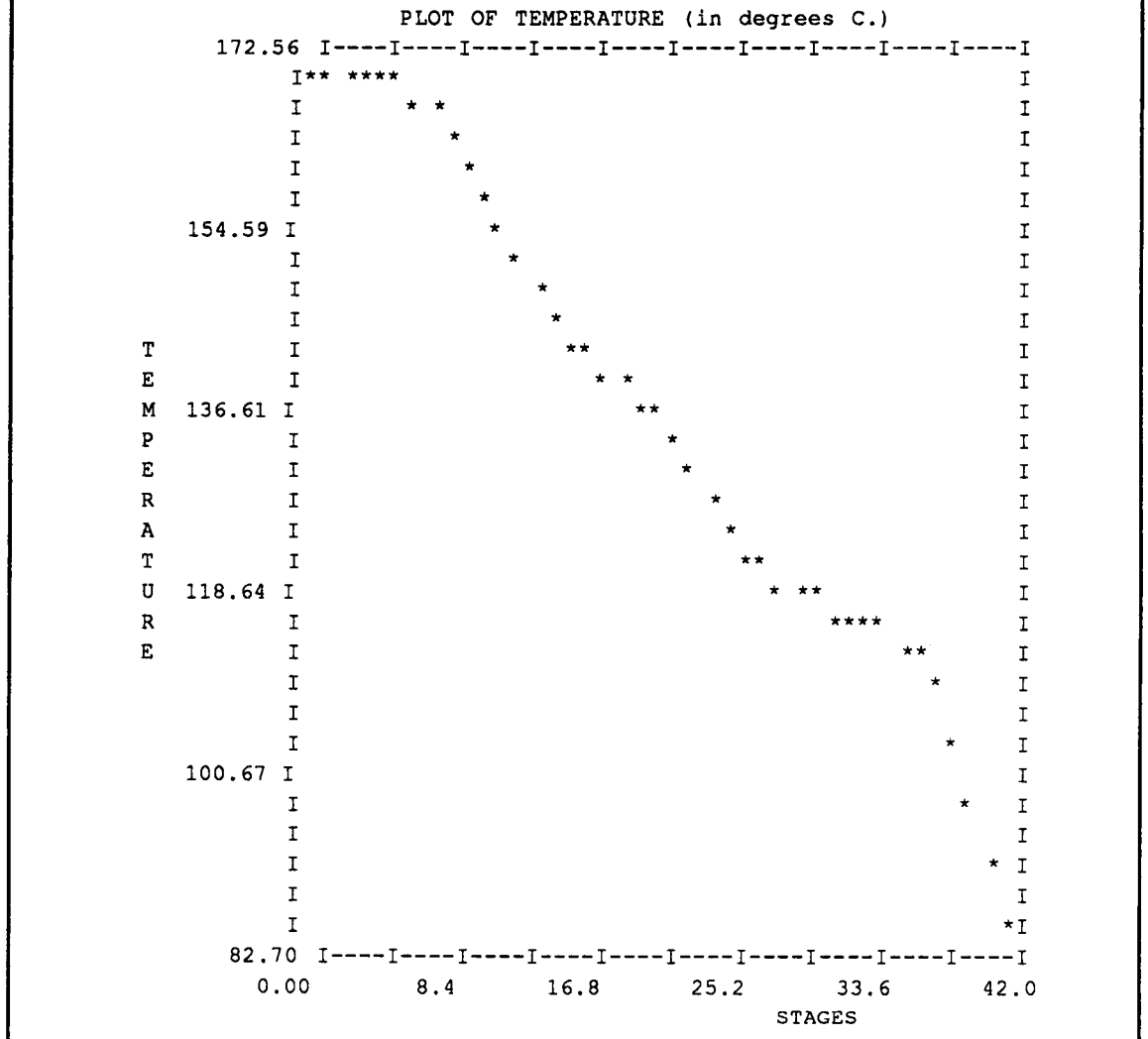
MULTICOMPONENT,MULTISTAGE DISTILLATION PROGRAM

Luyben Base Case; X(2); L, Q, S

One feed, one sidedraw, total condenser

STAGE PROFILES FOR COMPONENT NO. 3 XYLENE

Stage No.	Mole Fractions Feed	Liquid	Vapor	K Value	Activity Coefficient	Fugacity Coefficient
21	0.45000	0.40032	0.20795	0.51948	0.98727	0.97541
20	--	0.40776	0.21985	0.53917	0.98761	0.97623
19	--	0.41730	0.23070	0.55283	0.98809	0.97672
18	--	0.43158	0.24391	0.56515	0.98880	0.97714
17	--	0.45377	0.26309	0.57978	0.98987	0.97771
16	--	0.48739	0.29243	0.60001	0.99138	0.97861
15	--	0.53533	0.33661	0.62879	0.99330	0.98002
14	--	0.59789	0.39942	0.66805	0.99544	0.98205
13	--	0.67090	0.48124	0.71731	0.99746	0.98466
12	--	0.74619	0.57654	0.77264	0.99903	0.98761
11	--	0.81493	0.67450	0.82769	1.0001	0.99057
10	--	0.87129	0.76356	0.87635	1.0006	0.99318
9	--	0.91372	0.83622	0.91518	1.0009	0.99527
8	--	0.94369	0.89065	0.94380	1.0010	0.99682
7	--	0.96395	0.92895	0.96369	1.0011	0.99791
6	--	0.97725	0.95475	0.97698	1.0011	0.99864
5	--	0.98582	0.97165	0.98563	1.0011	0.99912
4	--	0.99128	0.98252	0.99116	1.0011	0.99943
3	--	0.99473	0.98943	0.99467	1.0011	0.99962
2	--	0.99691	0.99380	0.99688	1.0011	0.99975
1	--	0.99828	0.99655	0.99827	1.0011	0.99983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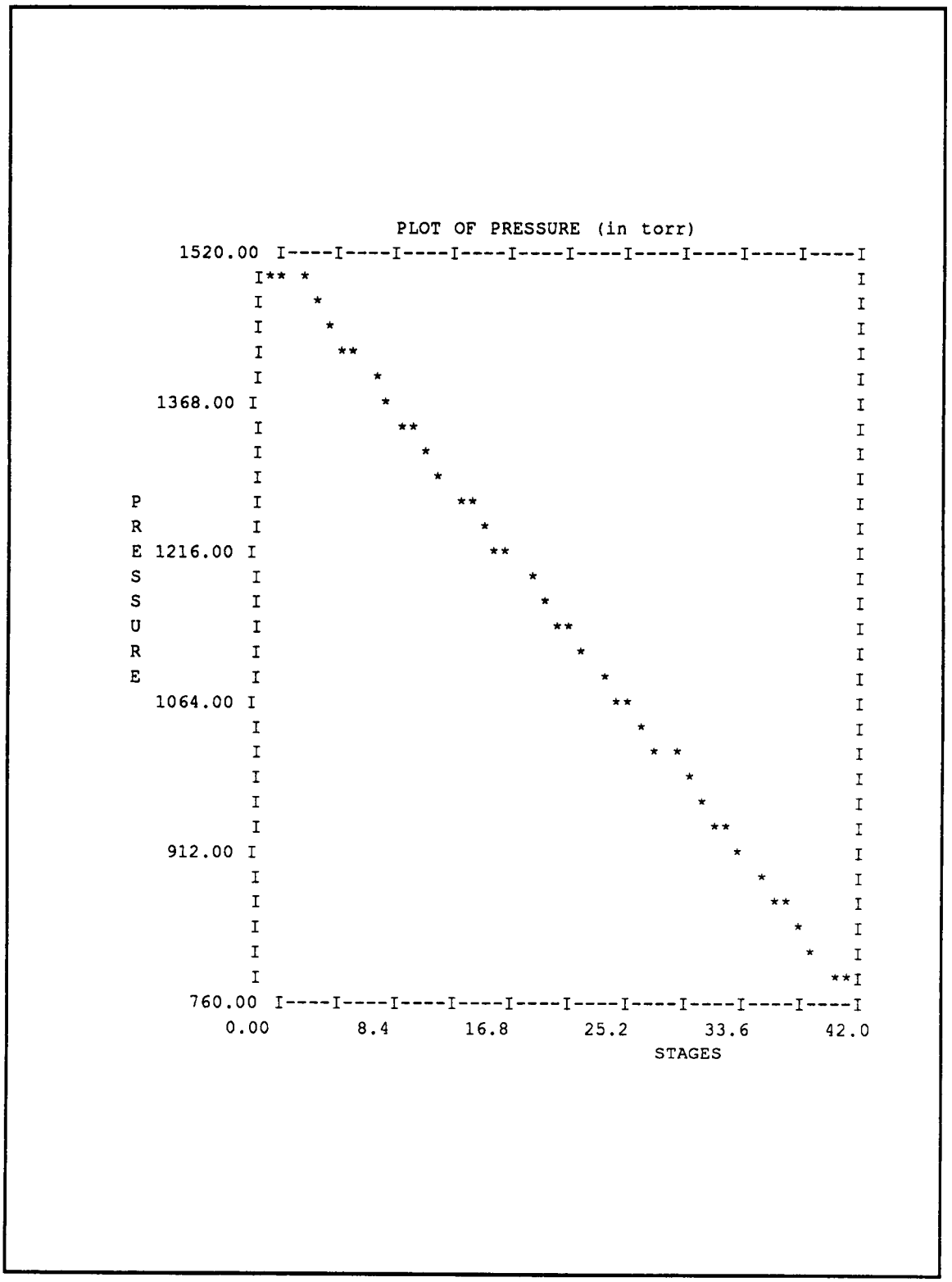
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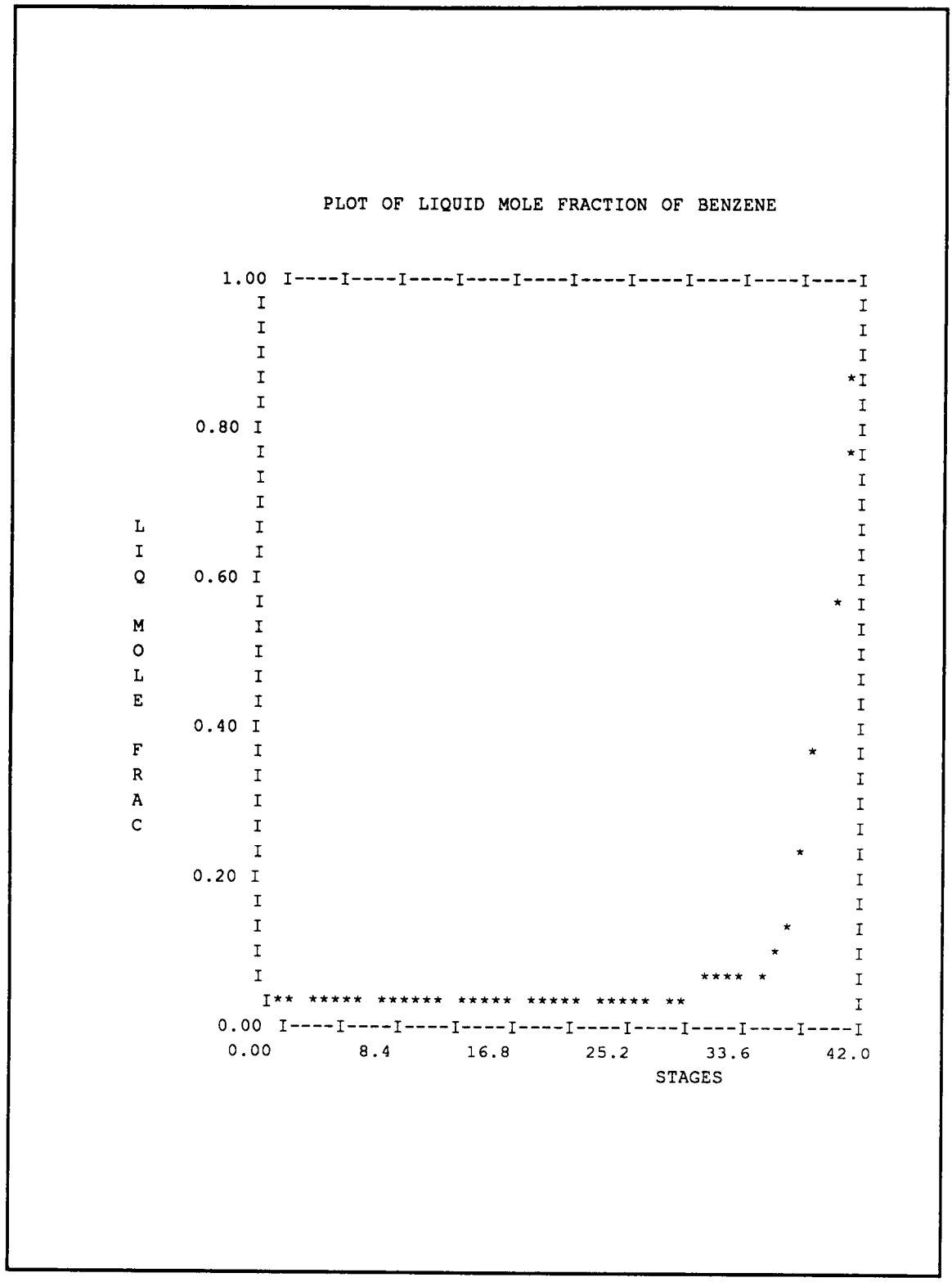
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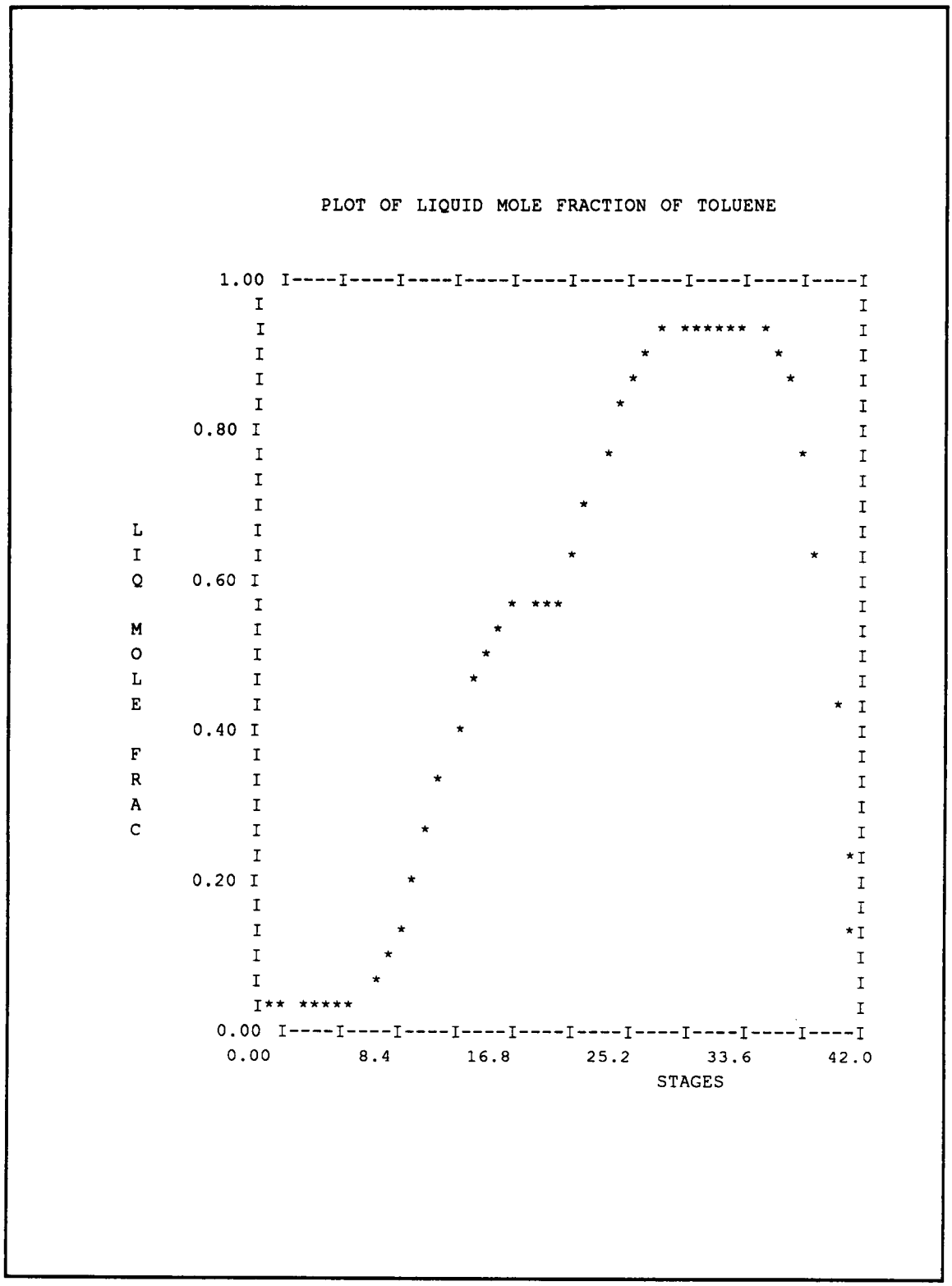
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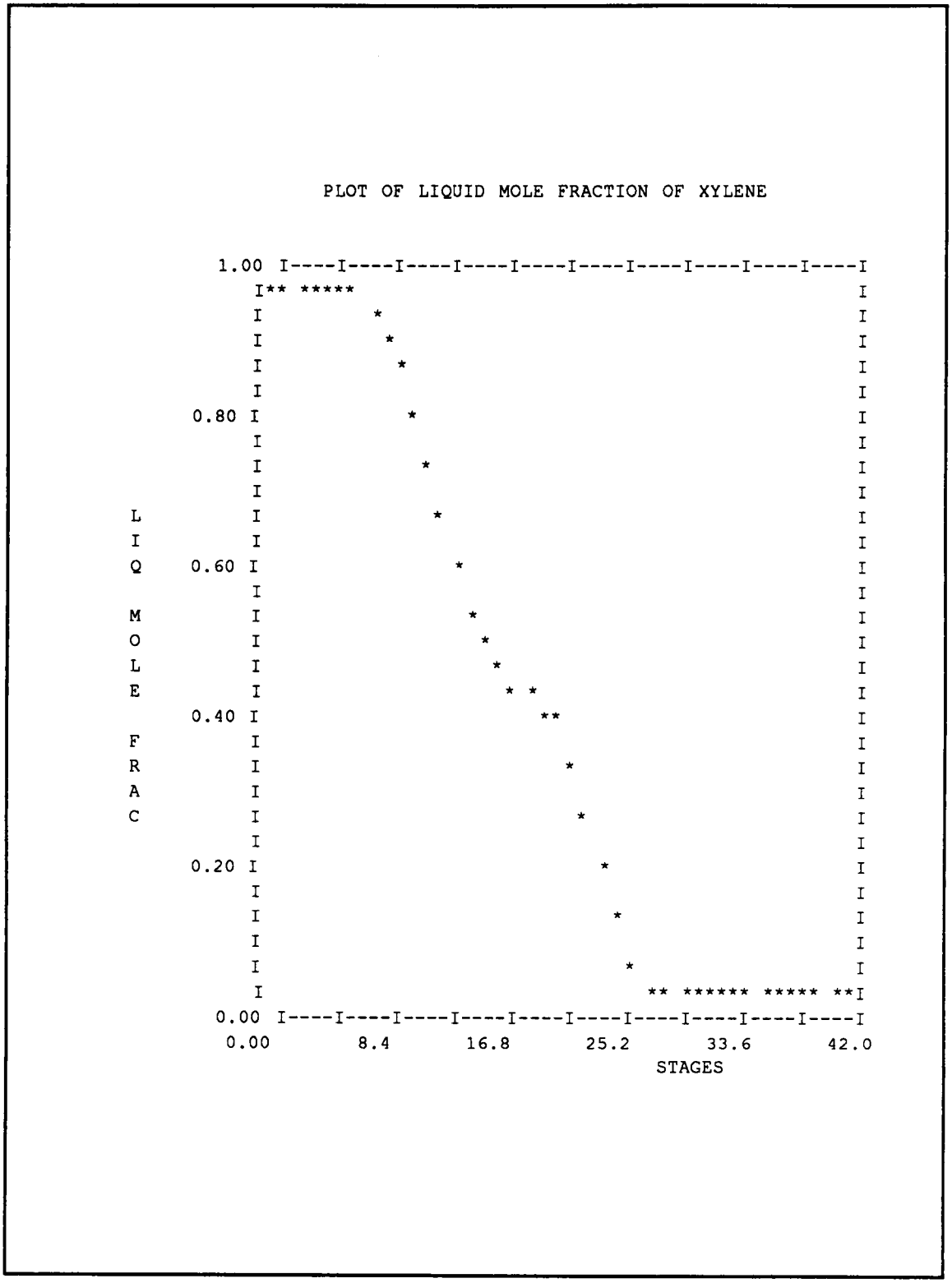
STAGES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0.40
0.20
0.00
LIQ MOLE FRAC
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8.4
16.8
25.2
33.6
42.0
STAGES

APPENDIX E

SVD ANALYSES SUMMARY FOR A SOLE CONTROLLED VARIABLE

SVD ANALYSIS

Page 1 of 4

Index Number	Measured Variable	Manipulated Variables			Original CN	Partial CN	ΔCN (Orig. - Part.)
		Top	Bottom	Side			
1.	T	L	Q	S	259.1187		
2.	X1	L	Q	S	472.3389		
3.	X2	L	Q	S	173.7246	165.0395	8.6851
4.	X3	L	Q	S	23093.89		
5.	Y1	L	Q	S	235.7361		
6.	Y2	L	Q	S	320.4635		
7.	Y3	L	Q	S	68209.30		
8.	T	L	Q	none	44.05356	36.5846	7.46896
9.	X1	L	Q	none	353.8140		
10.	X2	L	Q	none	34.68688	28.8131	5.87378
11.	X3	L	Q	none	143.5962	133.2951	10.3011
12.	Y1	L	Q	none	168.4132	380.0000	-211.5868
13.	Y2	L	Q	none	45.81887	37.1705	8.64837
14.	Y3	L	Q	none	309.2491		
15.	T	L	none	S	9.195785	7.4978	1.697985
16.	X1	L	none	S	84.22099	128.4673	-44.24631
17.	X2	L	none	S	7.079255	5.5054	1.573855
18.	X3	L	none	S	10625.37		
19.	Y1	L	none	S	74.58906	96.6194	-22.03034
20.	Y2	L	none	S	9.526671	7.4978	2.028871
21.	Y3	L	none	S	29357.15		
22.	T	none	Q	S	10.12945	6.5435	3.58595
23.	X1	none	Q	S	98.39391	149.5335	-51.13959
24.	X2	none	Q	S	7.809926	6.1160	1.693926
25.	X3	none	Q	S	138.9215	128.8253	10.0962
26.	Y1	none	Q	S	88.16980	112.7273	-24.55750
27.	Y2	none	Q	S	10.49367	8.2970	2.19667
28.	Y3	none	Q	S	298.1074		
29.	T	D	Q	S	119.5906	117.7150	1.8756
30.	X1	D	Q	S	76.58048	131.5969	-55.01642
31.	X2	D	Q	S	80.08843	75.7170	4.37143
32.	X3	D	Q	S	47601.29		

SVD ANALYSIS

Index Number	Measured Variable	Manipulated Variables			Original CN	Partial CN	ΔCN (Orig. - Part.)
		Top	Bottom	Side			
33.	Y1	D	Q	S	47.33159	344.9692	-297.63761
34.	Y2	D	Q	S	147.5988	160.6579	-13.0591
35.	Y3	D	Q	S	139949.5		
36.	T	D	Q	none	5.471786	4.5161	0.955686
37.	X1	D	Q	none	52.29942	11.0148	-58.71538
38.	X2	D	Q	none	4.245379		
39.	X3	D	Q	none	18.94985	17.7490	1.20085
40.	Y1	D	Q	none	24.27958	53.8235	-29.54392
41.	Y2	D	Q	none	5.714140	4.5802	1.133940
42.	Y3	D	Q	none	40.90382	43.7504	-2.84658
43.	T	D	none	S	21.42264	17.1204	4.30224
44.	X1	D	none	S	33.76470	51.0948	-17.33010
45.	X2	D	none	S	16.43137	12.7361	3.69527
46.	X3	D	none	S	26764.68		
47.	Y1	D	none	S	29.31978	38.8673	-9.54752
48.	Y2	D	none	S	22.20443	17.4111	4.79333
49.	Y3	D	none	S	73848.60		
50.	T	L	B	S	146.5506	147.2064	-0.6558
51.	X1	L	B	S	633.7013		
52.	X2	L	B	S	100.4147	244.6395	-144.2248
53.	X3	L	B	S	16826.78		
54.	Y1	L	B	S	445.7145		
55.	Y2	L	B	S	181.2378	244.6395	-63.4017
56.	Y3	L	B	S	49674.33		
57.	T	L	B	none	35.08376	29.7201	5.36366
58.	X1	L	B	none	294.6158		
59.	X2	L	B	none	27.70097	23.1056	4.59537
60.	X3	L	B	none	118.2852	110.6406	7.6446
61.	Y1	L	B	none	137.3886	298.7838	-161.3952
62.	Y2	L	B	none	36.48356	29.6268	6.85676
63.	Y3	L	B	none	254.1007		
64.	T	none	B	S	5.213522	4.4402	0.773322

SVD ANALYSIS

Index Number	Measured Variable	Manipulated Variables			Original CN	Partial CN	ΔCN (Orig. - Part.)
		Top	Bottom	Side			
65.	X1	none	B	S	367.2041		
66.	X2	none	B	S	4.200342	3.5619	0.638442
67.	X3	none	B	S	70.06191	65.5121	4.54981
68.	Y1	none	B	S	321.8230		
69.	Y2	none	B	S	5.387666	4.4402	0.947466
70.	Y3	none	B	S	150.2047	160.8276	-10.6229
71.	T	R	Q	S	159.5239	155.88577	3.63813
72.	X1	R	Q	S	88.84530	156.3373	-67.49200
73.	X2	R	Q	S	106.7123	99.6731	7.0392
74.	X3	R	Q	S	63412.66		
75.	Y1	R	Q	S	47.42105	297.1247	-249.70365
76.	Y2	R	Q	S	197.3389	211.6191	-14.2802
77.	Y3	R	Q	S	186686.2		
78.	T	R	Q	none	16.11245	13.2812	2.83125
79.	X1	R	Q	none	67.76505	144.7166	-76.95155
80.	X2	R	Q	none	12.43256	10.0404	2.39216
81.	X3	R	Q	none	55.53206	51.7072	3.82486
82.	Y1	R	Q	none	32.01587	69.8425	-37.82663
83.	Y2	R	Q	none	16.84640	13.3928	3.45360
84.	Y3	R	Q	none	120.06262	127.4825	-7.41988
85.	T	R	none	S	28.19500	22.4756	5.71940
86.	X1	R	none	S	24.73749	37.4228	-12.68531
87.	X2	R	none	S	21.62608	16.6657	4.96038
88.	X3	R	none	S	34636.69		
89.	Y1	R	none	S	21.59514	28.4541	-6.85896
90.	Y2	R	none	S	29.22327	22.7804	6.44287
91.	Y3	R	none	S	95603.18		
92.	T	R	B	S	181.0963	213.6145	-32.5182
93.	X1	R	B	S	407.4987		
94.	X2	R	B	S	122.5569	116.1089	6.4480
95.	X3	R	B	S	103204.2		
96.	Y1	R	B	S	329.0449		

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Index Number	Measured Variable	Manipulated Variables			Original CN	Partial CN	ΔCN (Orig. - Part.)
		Top	Bottom	Side			
97.	Y2	R	B	S	223.9757		
98.	Y3	R	B	S	305815.0		
99.	T	R	B	none	73.03233	59.9289	13.10343
100.	X1	R	B	none	182.3341	380.2083	-197.8742
101.	X2	R	B	none	56.03359	45.3140	10.71959
102.	X3	R	B	none	255.0136		
103.	Y1	R	B	none	86.73897	187.0968	-100.35783
104.	Y2	R	B	none	76.48984	61.0943	15.39554
105.	Y3	R	B	none	552.0690		

VITA

Clemence Marie McCain Noakes was born on January 2, 1958, in Memphis, TN, to Robert Earl and Clemence Wadley McCain. She graduated from Raleigh-Egypt High School in 1976 and attended her freshman year at Southwestern of Memphis Liberal Arts College pursuing a major in chemistry. Clemence transferred to the University of Tennessee at Knoxville and graduated in 1980 with a Bachelor of Science in Science Education with a major in chemistry and a minor in biology. In the autumn of 1980 she married Mark William Noakes. Through the influence and encouragement of her husband, an electrical engineer, Clemence reentered UTK in March, 1982, to obtain a degree in chemical engineering. She received her Bachelor of Science in Chemical Engineering in June, 1984, and began graduate studies in chemical engineering in September, 1984. After completing one year of classes, Clemence changed her status to part-time student and obtained employment with United Engineers of Kingsport/Knoxville, TN. In May, 1987, Clemence acquired a position at the Oak Ridge National Laboratory as an Instrument Engineer in the Engineering Division. She has chaired a committee to formulate instrumentation and controls standards for Martin Marietta Energy Systems, and has worked on a national level with the Instrument Society of America to develop standards for industrial use. She is an active member of the Society of Women Engineers and the Instrument Society of America and hold offices in each.