

K-VALUES OF POLAR MIXTURES PREDICTED

BY THE SOAVE-REDLICH-KWONG

EQUATION OF STATE

By

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PREFACE

This study is concerned with the prediction of K-values for components in non-ideal mixtures using the Soave-Redlich-Kwong equation of state. Only two semi-empirical correction factors are used in the calculation procedure to correct for system non-idealities.

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NOMENCLATURE

P	- pressure
T	- absolute temperature
R	- ideal gas constant
V	- molar volume
Z	- compressibility factor
a	- component dependent factor in Redlich-Kwong equation
b	- component dependent factor in Redlich-Kwong equation
\bar{f}	- molar fugacity
x	- mole fraction in liquid
y	- mole fraction in vapor
k_{ij}	- binary interaction parameter
Ω_b	- adjusted constant in Soave-Redlich-Kwong equation of state
m	- constant in the Soave-Redlich-Kwong equation of state

Subscripts

R	- reduced value
i,j	- indicate specific components
liq	- indicates liquid phase

vap

- indicates vapor phase

c

- critical value

CHAPTER I

INTRODUCTION

Accurate prediction of the thermodynamic properties of multicomponent mixtures is of critical importance in the design of chemical process equipment. Specifically, the K-values and enthalpies of mixtures must be predicted accurately over wide ranges of temperature, pressure, and composition. These properties are required for the design of various unit operations - distillation columns, absorbers, flash separators, heat exchangers, etc.

The prediction of the thermodynamic properties of hydrocarbon mixtures has been studied extensively. Hydrocarbon mixtures usually exhibit more or less regular behavior; the components are not polar, do not associate in either the vapor or liquid phase, etc. This regular behavior somewhat simplifies the requirements of the thermodynamics prediction procedure. Many excellent methods of predicting K-values and enthalpies for these mixtures are available. These techniques usually follow one of two approaches:

- (1) Use some equation of state to predict the thermodynamic properties of the vapor phase. An alternate equation of state or combination of equations of state would be used to predict the liquid phase properties. This approach is occasionally called the split equation of state approach.

(2) Use a single equation of state to predict the properties of both the vapor and liquid phases. This approach is frequently described as the single equation of state approach.

Each approach has its unique advantages and problems; neither approach has an overall advantage over the other.

Organic compounds, such as acetic acid, methanol, and ethyl acetate, exhibit various forms of highly non-ideal behavior - association, polarity, etc. Mixtures of these kinds of compounds typically exhibit azeotropic behavior or frequently heterogeneous azeotropic behavior, i.e., the liquid may exist in two separate phases around an azeotrope point. Many procedures for describing the thermodynamic behavior of these systems have been proposed. Nearly all of these procedures rely on the split equation of state approach. They require a large number of semi-empirically derived constants to be applied to multicomponent mixtures. The single equation of state approach to predicting the behavior of these highly non-ideal systems has not met with much success until recently (6).

The objective of this study was to determine if the recently proposed Soave-Redlich-Kwong equation of state could be used or modified to reliably predict the thermodynamic behavior of highly non-ideal systems. In this study, the equation of state was applied to both the vapor and liquid phases; i.e., the single equation of state approach. A further objective was to minimize the required number of semi-empirical constants to predict reliable thermodynamic properties of highly non-ideal systems. Systems which exhibit this behavior were selected for the evaluation of the Soave method.

CHAPTER II

LITERATURE REVIEW

The vapor-liquid equilibrium constant or K-value of a component in a two phase mixture is defined as follows:

$$K_i = y_i/x_i \quad (1)$$

where y_i is the component mole fraction in the vapor phase and x_i is the component mole fraction in the liquid phase. When using the split equation of state approach to predicting K-values in equilibrium mixtures, Equation (1) can be modified as follows:

$$K_i = \frac{\gamma_i v_i}{\phi_i P} \quad (2)$$

where ϕ_i is the vapor phase component fugacity coefficient, γ_i is the liquid phase activity coefficient, P is the pressure, and v_i is the component standard state fugacity. For the single equation of state approach, Equation (1) is modified as follows:

$$K_i = \frac{\phi_i^L}{\phi_i^V} \quad (3)$$

where ϕ_i^L and ϕ_i^V are the component partial fugacity coefficients predicted using the same equation for the liquid and vapor phases. Both approaches to calculating K-values require prediction of the vapor phase

component fugacity coefficient while the split equation of state approach also requires prediction of the liquid phase component activity coefficient. Methods of predicting each of these coefficients are discussed below.

Vapor Phase Fugacity Coefficients

The problem of calculating fugacities for components in a gaseous mixture is equivalent to the problem of establishing a reliable equation of state for such a mixture. Once such an equation of state exists, the fugacities can be found by straight-forward computation. For many years, the vapor phase was assumed to be ideal and the ideal gas law was considered a reliable equation of state. This assumption is valid only at pressures less than about 3 atmospheres. Recently, however, it has become necessary to design process equipment for mixtures of extreme non-ideality. Consequently, equations of state that more accurately represent the vapor phase have been developed. One equation of state now used frequently is the virial equation of state. The virial equation gives the compressibility factor as a power series in the reciprocal molar volume $1/V$:

$$Z = 1 + \frac{B_{\text{mix}}}{V} + \frac{C_{\text{mix}}}{V^2} + \frac{D_{\text{mix}}}{V^3} + \dots \quad (4)$$

The principal problem involved in using this equation is calculating the virial coefficients B_{mix} , C_{mix} , D_{mix} , etc., for a given system. The equations for calculating these coefficients and the many interaction potential functions necessary for the calculation have been outlined by Prausnitz (1). The component fugacity coefficient is

calculated using the virial equation truncated after the third term as follows:

$$\ln\phi_i = \frac{2}{v} \sum_{j=1}^m y_j B_{ij} + \frac{3}{2} \cdot \frac{1}{v^2} \sum_{j=1}^m \sum_{k=1}^m y_j y_k C_{ijk} - \ln Z_{\text{mix}} \quad (5)$$

It should be noted that many system dependent constants are necessary to use Equation (5). This is true of most other equations of state with similar accuracy. Further this approach is limited to systems which do not form dimers (or trimers) in the vapor phase. When these effects are found, more elegant methods must be used.

Liquid Phase Activity Coefficients

Liquid phase activity coefficients are calculated using a technique based on defining an ideal liquid solution and by describing deviations from ideal behavior in terms of excess functions. Activity coefficients can be calculated using various relationships to describe these excess functions.

An expression for the excess Gibbs energy of solution has been developed by Wohl (2). Equations for the activity coefficients in a binary mixture developed from a truncated form of Wohl's expression are as follows:

$$\ln\gamma_1 = A' / \left[1 + \frac{A'}{B'} \frac{x_1}{x_2} \right]^2 \quad (6)$$

$$\ln\gamma_2 = B' / \left[1 + \frac{B'}{A'} \frac{x_2}{x_1} \right]^2 \quad (7)$$

These are commonly known as the van Laar equations (1). They contain two system dependent constants, A' and B'. The van Laar equations have become popular because of their flexibility and because of their mathematical simplicity relative to many other equations which have been proposed.

Another expression for the excess Gibbs energy of solution is that derived by Wilson (3,4):

$$\frac{gE}{RT} = - \sum_{i=1}^m x_i \ln \left[\sum_{j=1}^m x_j \Lambda_{ij} \right] \quad (8)$$

The activity coefficient for any component is given by:

$$\ln \gamma_k = - \ln \left[\sum_{j=1}^m x_j \Lambda_{kj} \right] + 1 - \frac{\sum_{i=1}^m x_i \Lambda_{ij}}{\sum_{j=1}^m x_j \Lambda_{ij}} \quad (9)$$

This equation requires only parameters which can be obtained from binary data; for each possible binary pair in the multicomponent solution, two parameters are needed. Orye (4) has tested this equation for a variety of miscible ternary mixtures, using only binary data, and found that for most cases good results are obtained. The most serious disadvantage of Wilson's equation lies in its inability to predict limited or partial miscibility.

A third expression for the excess Gibbs energy of solution has been developed by Renon (5):

$$\frac{gE}{RT} = \sum_{i=1}^m x_i \frac{\sum_{j=1}^m \tau_{ji} G_{ji} x_j}{\sum_{l=1}^m G_{li} x_l} \quad (10)$$

$$G_{ji} = \exp(-\alpha_{ji} \tau_{ji})$$

The activity coefficient for a component k is given by:

$$\ln \gamma_k = \frac{\sum_{j=1}^m \tau_{ji} G_{ji} x_j}{\sum_{l=1}^m G_{li} x_l} + \frac{\sum_{j=1}^m \frac{x_j G_{ij}}{m}}{\sum_{l=1}^m G_{lj} x_l} \left(\tau_{ij} - \frac{\sum_{r=1}^m x_r \tau_{rj} G_{rj}}{m} \right) \quad (10)$$

Renon's NRTL (Non-Random, Two-Liquid) equation, unlike Wilson's, is applicable to partially miscible as well as completely miscible systems. The NRTL equation contains three parameters but reduction of experimental data for a large number of binary systems indicates that one of them varies very little from system to system and can be held constant when experimental data are scarce. For strongly non-ideal mixtures, and especially for partially immiscible systems, the NRTL equation provides a good representation of experimental data. Palmer and Smith have developed an equation identical to the Renon equation but they use different parameters to describe the arbitrary constants (6).

Other important work on K-value prediction has been done by Peter and Wenzel (7), and Bonner, Bazua, and Prausnitz (8).

The above review is by no means a complete review of the work that has been done in the area of K-value prediction. It represents only some of the important recent developments.

CHAPTER III

DEVELOPMENT OF PROCEDURE

The original Redlich-Kwong equation of state is:

$$P = \frac{RT}{V - b_{\text{mix}}} - \frac{a_{\text{mix}}/T^{0.5}}{V(V + b_{\text{mix}})} \quad (1)$$

This equation is commonly considered the best of two-parameter equations of state for describing the thermodynamic properties of the vapor phase. However, the Redlich-Kwong equation was not developed with application to the liquid phase as a condition of development. Consequently poor results are obtained when the Redlich-Kwong is used in the single equation of state approach. In an effort to improve this situation, Soave (9) modified the equation by replacing the term $a_{\text{mix}}/T^{0.5}$ with a more general temperature dependent term $a_{\text{mix}}(T)$:

$$P = \frac{RT}{V - b_{\text{mix}}} - \frac{a_{\text{mix}}(T)}{V(V + b_{\text{mix}})} \quad (2)$$

Letting:

$$V = Z \frac{RT}{P}$$

$$\frac{a_{\text{mix}} P}{R^2 T^2} = A \quad (3)$$

$$\frac{b_{\text{mix}} P}{RT} = B \quad (4)$$

Equation (2) can also be written:

$$Z^3 - Z^2 + Z(A-B-B^2) - AB = 0 \quad (5)$$

For any given component, Soave defined:

$$a_i(T) = a_{ci} \alpha_i(T) \quad (6)$$

$$b_i = 0.08664 \frac{RT_{ci}}{P_{ci}} \quad (7)$$

where:

$$a_{ci} = 0.42747 \frac{R^2 T_{ci}^2}{P_{ci}} \quad (8)$$

Soave related the value of α_i in Equation (6) to a value, m_i , which is a constant for each component. The value of $\alpha_i^{0.5}$ as a function of temperature is calculated from:

$$\alpha_i^{0.5} = 1 + m_i (1 - T_{Ri}^{0.5}) \quad (9)$$

For application to non-polar mixtures the following mixing rules were recommended:

$$a_{\text{mix}} = \left(\sum_{i=1}^N x_i a_i^{0.5} \right)^2 \quad (10)$$

$$b_{\text{mix}} = \sum_{i=1}^N x_i b_i \quad (11)$$

Since polar systems were being studied, the introduction of a semi-empirical correction factor into the mixing rule calculations was necessary to account for the large change in intermolecular forces between the various components. Therefore an a_{ij} for each component pair was calculated as recommended by Soave from:

$$a_{ij} = (1 - k_{ij})(a_i a_j)^{1/2} \quad (12)$$

where k_{ij} is the correction factor. The mixing rule for a_{mix} was changed to:

$$a_{\text{mix}} = \sum_{i=1}^N \sum_{j=1}^N x_i x_j a_{ij} \quad (13)$$

After reviewing the results of a few preliminary calculations, the introduction of a second correction factor was deemed necessary. Therefore, following the lead of Prausnitz (1), Equation (7) was changed to:

$$b_i = \Omega b \frac{RT_{ci}}{P_{ci}} \quad (14)$$

where Ωb is the semi-empirical correction factor and replaces the constant value 0.08664. The mixing rule for b_{mix} was not changed.

The fugacity coefficient of a component in a mixture is given by:

$$\ln \frac{f_i}{P x_i} = \int_{\infty}^V \left[\frac{1}{V} - \frac{1}{RT} \left(\frac{dp}{dn_i} \right)_{T,P,n_j} \right] dv - \ln Z \quad (15)$$

Applying Equations (2), (3), (4), (11), and (13) to Equation (15) gives the final express for predicting the partial fugacity of a component:

$$\ln \frac{\bar{f}_i}{P x_i} = \frac{b_i}{b_{\text{mix}}}(Z - 1) - \ln(Z - B) - \frac{A}{B} \left(\frac{\sum_{k=1}^N x_k a_{ik}}{a_{\text{mix}}} - \frac{b_i}{b_{\text{mix}}} \right) \left[\ln \left(1 + \frac{B}{Z} \right) \right] \quad (16)$$

The compressibility factor Z for each phase is found by solving Equation (5) once for the liquid phase and once for the vapor phase. When three real roots are found the smallest is used for the liquid phase and the largest for the vapor phase.

Values of m_i in Equation (9) are dependent only on the component identity. The appropriate values of m_i were calculated by a trial and error procedure which forced the pure component fugacity coefficients for the vapor and liquid phases to be equal at the normal boiling point of the pure component.

CHAPTER IV

CORRELATION PROCEDURE AND RESULTS

As stated in the last chapter, two semi-empirical correction factors, Ω_b and k_{ij} , were introduced into the equations for predicting the thermodynamic behavior of non-ideal systems. The work of Prausnitz, et al., in which similar adjustments were made, provided the basis for these arbitrary modifications. The term Ω_b was assumed to be constant for a given component. Further, the binary interaction parameter k_{ij} was assumed constant for a given binary system. Both constants were assumed to be independent of temperature. These assumptions were the basis of the correlation of experimental data in this study.

Correlation Procedure

Parameter estimation for systems containing water is especially difficult. Therefore it was decided that the values of Ω_b for each component in the systems to be studied would be determined by finding the values of Ω_b that best predicted the K-values for binary systems of each component and water. A computer program using the calculation procedure described in the last chapter was written for this purpose. This program allowed for the calculation of K-values using all combinations of Ω_b s for the two components and k_{ij} s within arbitrary ranges. In this way the combination of Ω_b s and k_{ij} that gives the minimum error could be determined. Before determining the Ω_b values for the

other components, however, it was necessary to find a suitable value of Ω_b for water. To accomplish this, three binary systems containing water were selected. Points on the three-dimensional surface described by the two Ω_b s and the percent error were calculated for each system for a range of k_{ij} s. These points represented several three-dimensional surfaces, one for each values of k_{ij} . The plane described by the Ω_b for water and percent error axes was plotted at two points along the Ω_b axis of the other component for each binary system. These graphs are shown in Figures 1, 2, and 3. As can be seen from these figures the values of Ω_b for water at the minimum percent error can be kept within a range of 0.07155 to 0.11926 by using reasonable values of k_{ij} . This range applies from system to system and within each system as the Ω_b of the other component is varied. Therefore the value of Ω_b for water was set equal to 0.09541. The Ω_b values for the other components were then found by computing points in the plane described by the Ω_b value of the component and the percent error, with the Ω_b for water held constant. The Ω_b values associated with the points with minimum percent error were used. The values for the components studied are shown in Table I. The k_{ij} values associated with these points were used as the k_{ij} s for the binary pairs. It should be noted here that the values of Ω_b in Table I are all relative to the value of Ω_b for water. This is not the case for Ω_b as used by Prausnitz. The k_{ij} values for binary pairs not containing water were found by using the Ω_b values calculated above, calculating points in a plane described by the k_{ij} values and the percent error, and finding the point with minimum percent error. The k_{ij} values for the binary pairs studied along with the minimum percent error for each pair are shown in Table II. The total of the average percent errors

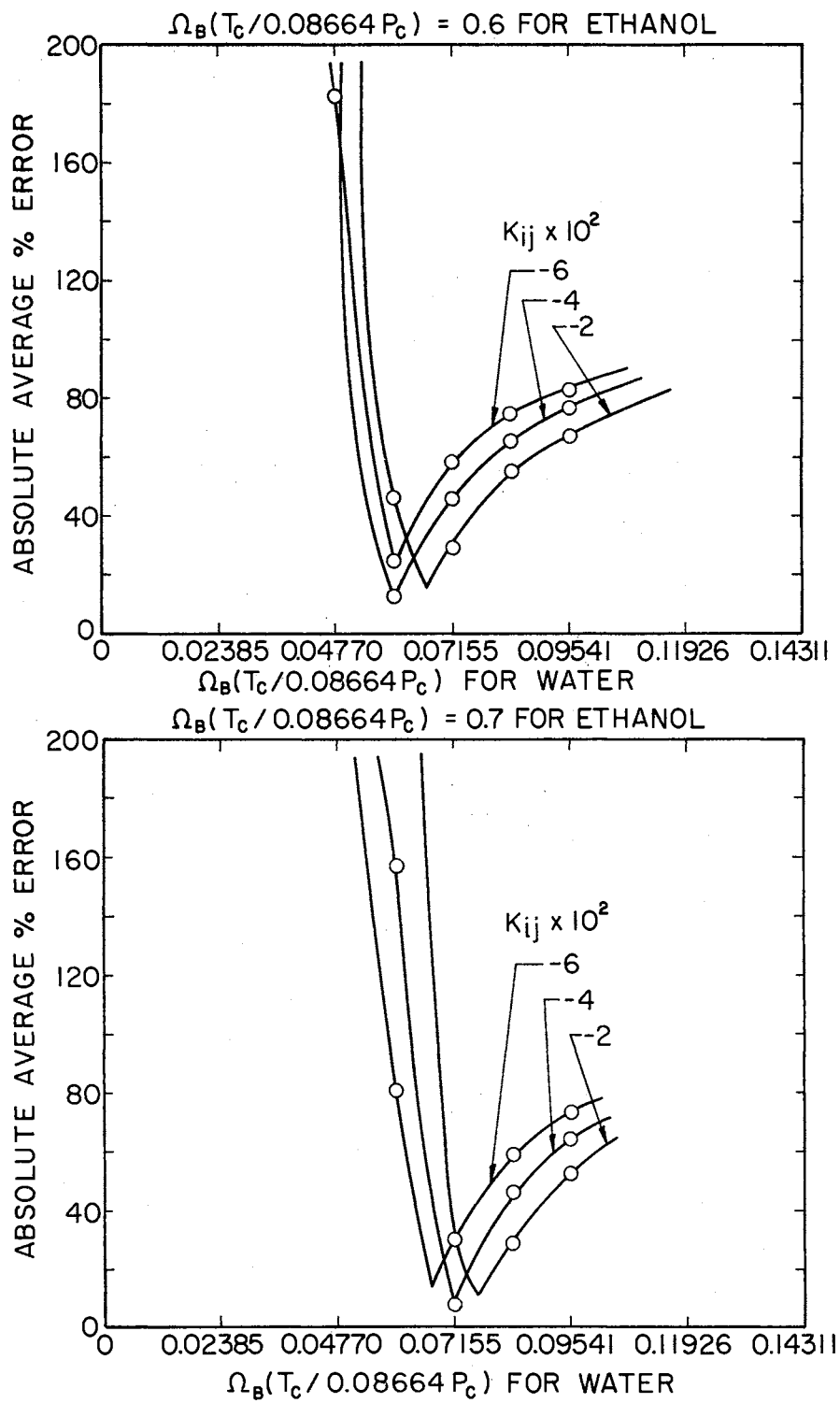


Figure 1. Two Planes from Three-Dimensional Surface for Ethanol-Water System

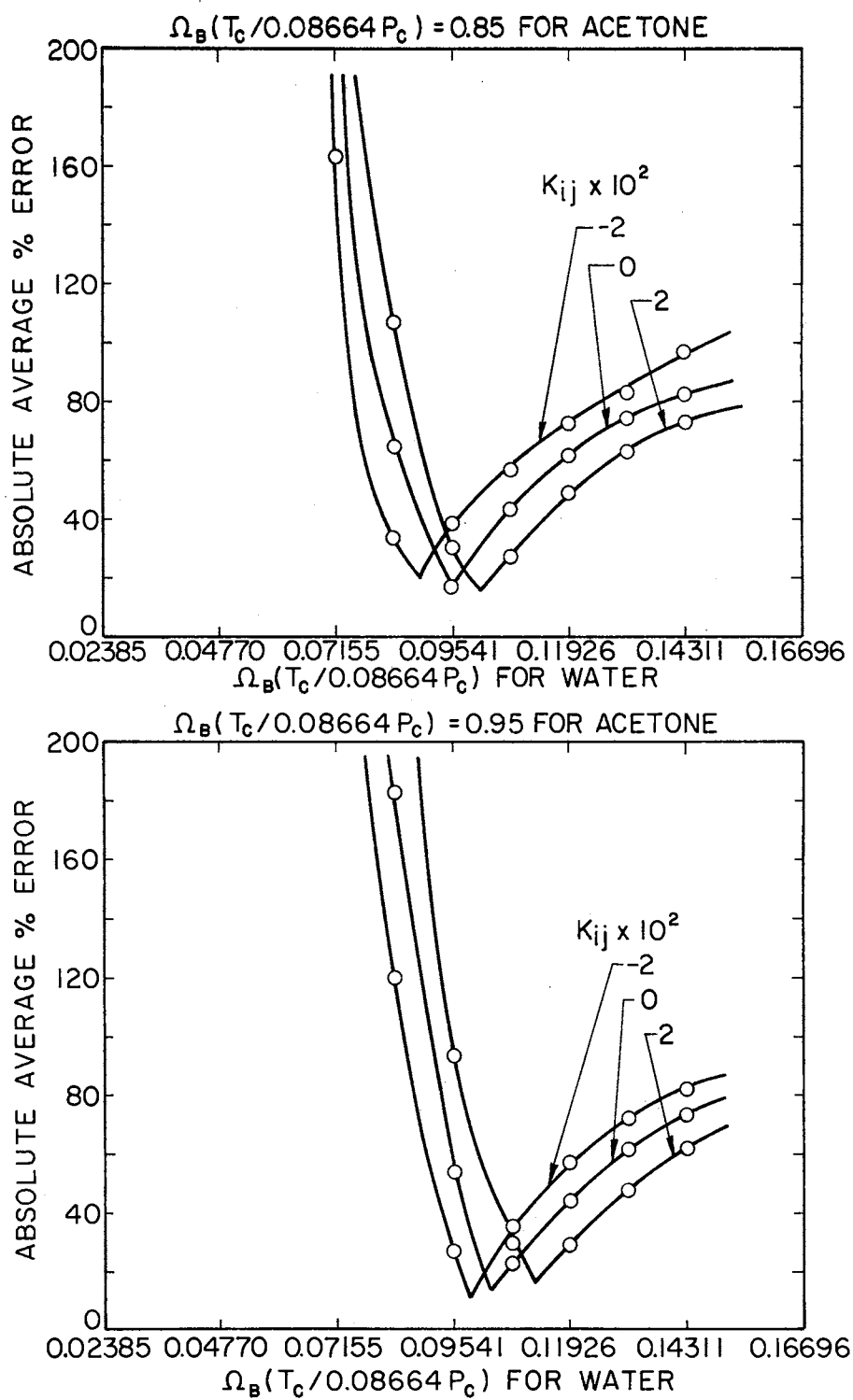


Figure 2. Two Planes from Three-Dimensional Surface for Acetone-Water System

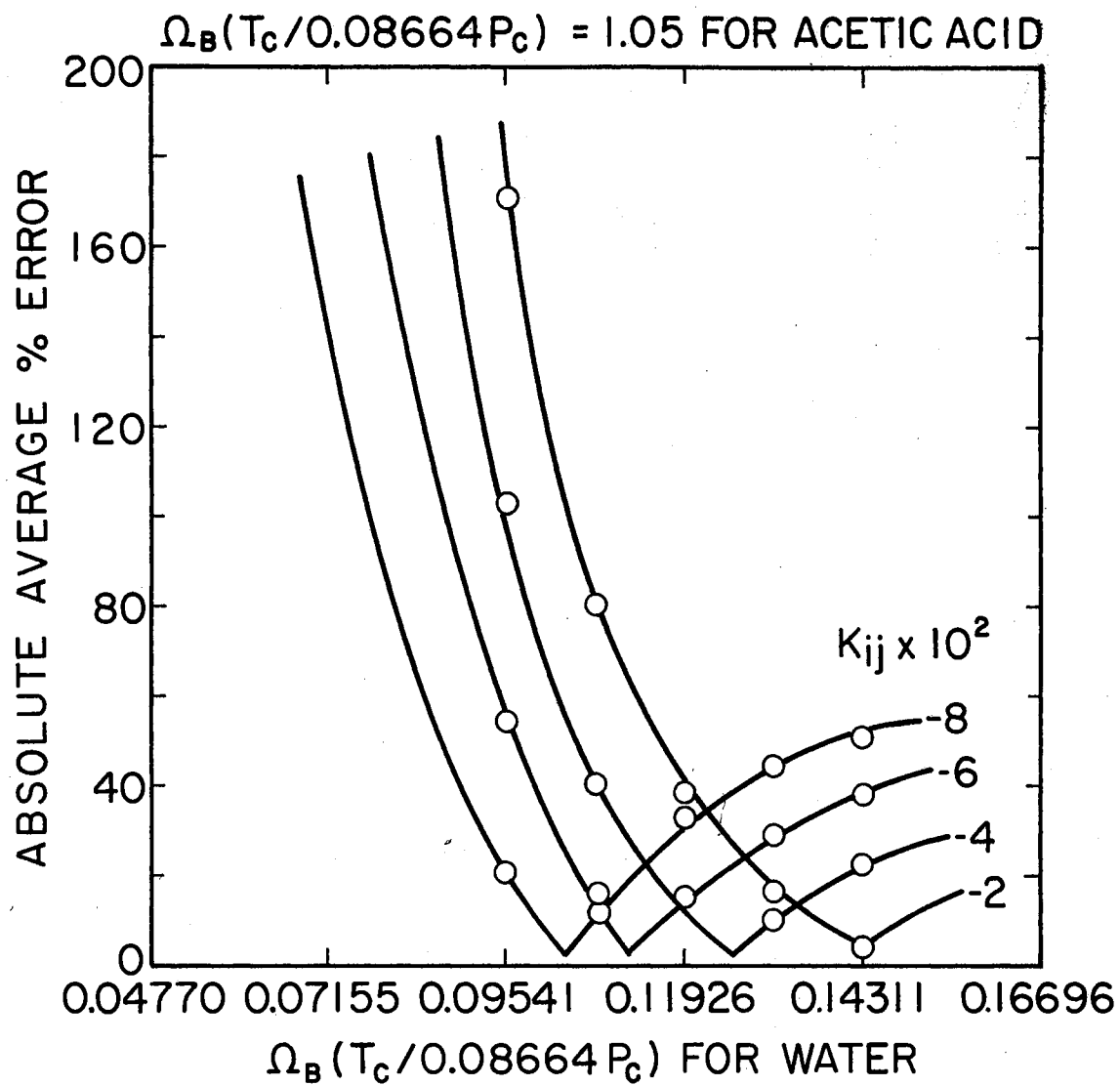


Figure 3. Plane from Three-Dimensional Surface for Acetic Acid-Water System

TABLE I
VALUES OF Ω_b FOR COMPONENTS STUDIED

Compound	Ω_b
Acetone (14.7 psia.)	0.05507
Acetone (500 psia.)	0.08747
Methyl Ethyl Ketone	0.08615
Methanol	0.07718
Ethanol	0.06901
N-Propyl Alcohol	0.06724
N-Butyl Alcohol	0.07388
Isopropyl Alcohol	0.05889
Formic Acid	0.04626
Acetic Acid	0.06122
Propionic Acid	0.07166
Water	0.09541

TABLE II
VALUES OF k_{ij} FOR THE BINARY PAIRS STUDIED

Binary Pair	$k_{ij} \times 10^2$	Total Abs. Avg. % Error
N-Propyl Alcohol-Water	-1.0	10.81
Acetone-Methyl Ethyl Ketone	-2.6	28.43 (14.7 psia.)
Acetone-Methyl Ethyl Ketone	0.0	6.71 (500 psia.)
Isopropyl Alcohol-Water	0.0	7.50
Water-Propionic Acid	-4.5	19.53
Methanol-Water	-2.0	11.98
Acetone-Water	-8.0	20.88
Methyl Ethyl Ketone-Water	-4.5	21.74
Ethanol-Water	0.0	9.58
Formic Acid-Acetic Acid	-4.0	8.49
Water-Acetic Acid	-7.0	5.80
Water-Formic Acid	-6.0	5.98
Methanol-Ethanol	0.0	5.32
Acetone-Methanol	4.0	3.11
Acetone-Ethanol	5.0	7.74

for each component was used as a convenient number to minimize. The interrelationship between Ω_b , k_{ij} , and percent error is shown for the Isopropyl Alcohol-Water system in Figure 4 and for the Acetone-Water system in Figure 5. Figure 4 shows the typical relationship for the systems studied for which a minimum error of 10% or less was found, while Figure 5 shows the typical relationship for systems with a higher percent error.

A computer program was written incorporating the K-value prediction method being studied in to a flash calculation using a standard Newton-Raphson convergence procedure. This was thought to be the best way of testing the method because this is the type of calculation in which it would normally be used. Using the values of Ω_b and k_{ij} found as described above, each of the binary systems was subjected to the flash calculation. The results are shown in Tables III-XVII. Four ternary systems were also subjected to the calculation and these results are shown in Tables XVIII-XXI. A summary of the results for the binary and ternary systems is given in Table XXII.

Discussion of Results

The results given in Tables III-XXI show that the K-value prediction method using the Redlich-Kwong equation of state as modified by Soave gives very good results for the fifteen binary and four ternary systems studied. The absolute average percent errors for the components are all under 33% with most under 10%.

Absolute average percent errors under 10% were obtained for systems without an azeotrope and with all components present in quantities greater than about 10 mole percent. Two examples are the Formic

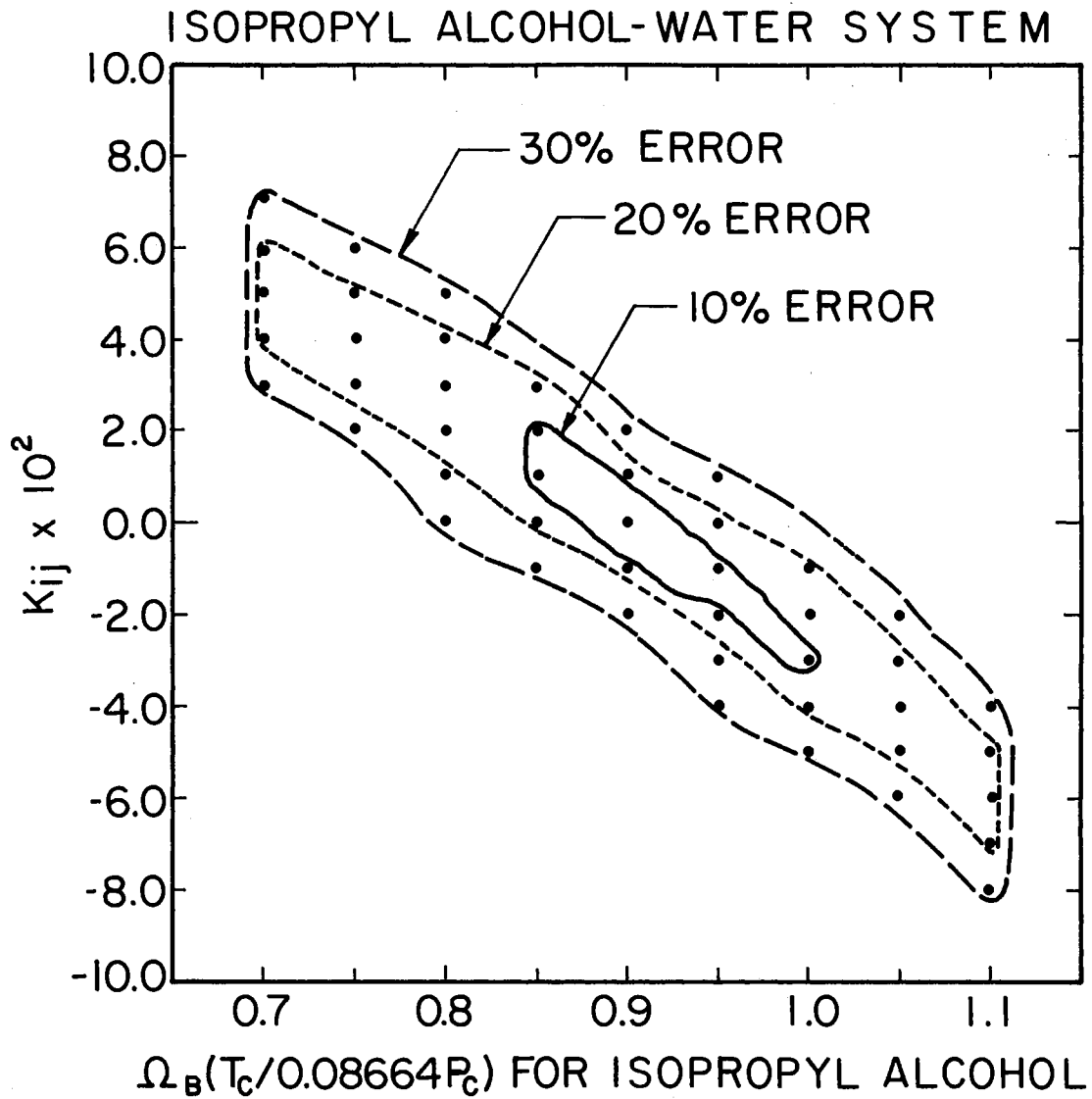


Figure 4. Low Percent Error Relationship Between k_{ij} , Ω_b , and Percent Error

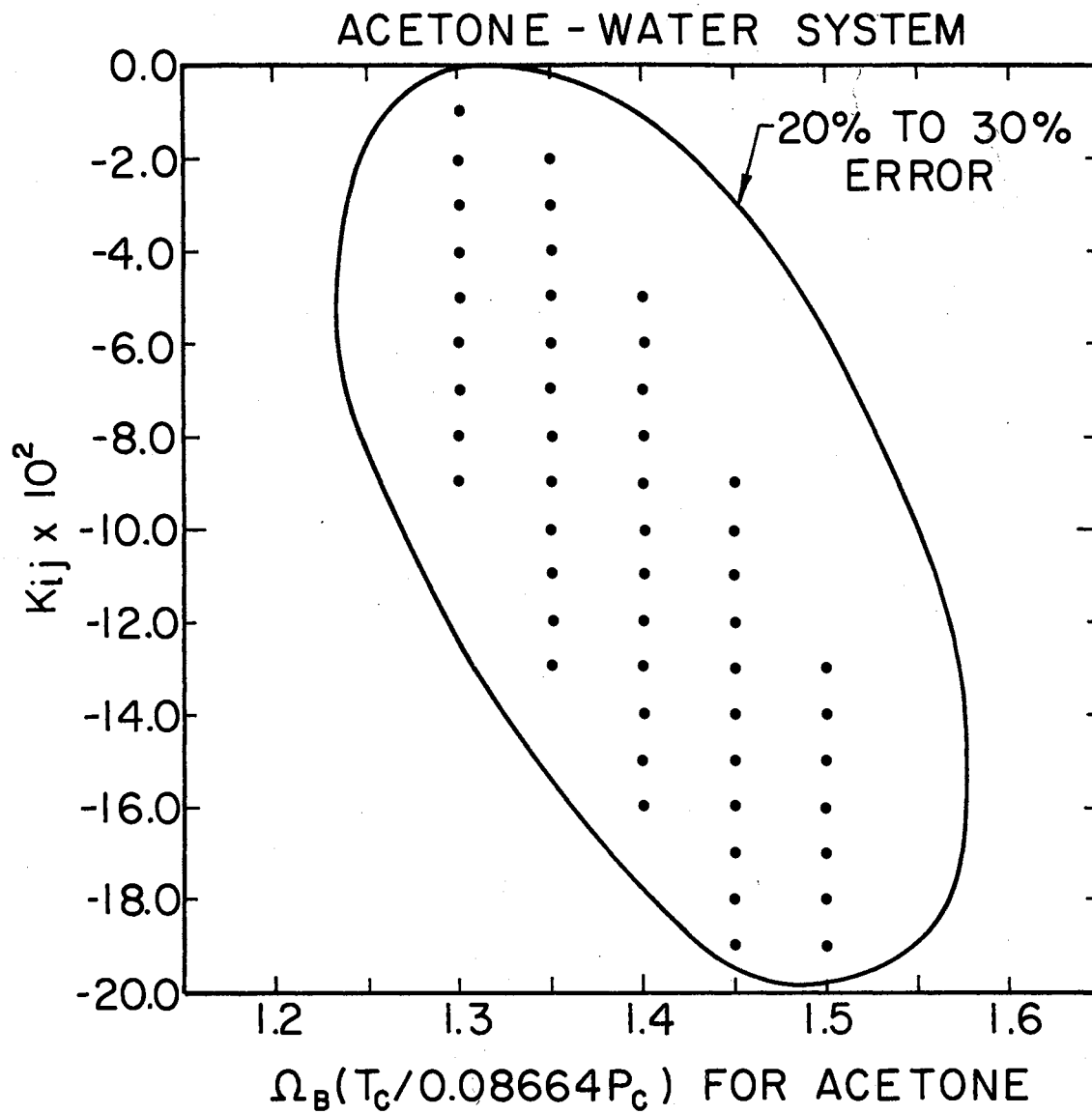


Figure 5. High Percent Error Relationship Between k_{ij} , Ω_b , and Percent Error

TABLE III

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM ACETONE-METHYL ETHYL KETONE

TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	COMP NUM		COMP NUM		COMP NUM		COMP NUM		COMP NUM	
	1	2	1	2	1	2	1	2	1	2
56.90	0.9500	0.0500	0.9720	0.0280	1.0232	0.5600	1.0116	0.4929	-1.13	-11.99
57.90	0.8910	0.1090	0.9420	0.0580	1.0572	0.5321	1.0321	0.5162	-2.38	-2.98
58.90	0.8170	0.1830	0.9030	0.0970	1.1053	0.5301	1.0516	0.5396	-4.86	1.81
60.00	0.7380	0.2620	0.8570	0.1430	1.1612	0.5458	1.0721	0.5652	-7.67	3.56
60.30	0.7270	0.2730	0.8400	0.1600	1.1554	0.5861	1.0776	0.5721	-6.73	-2.39
61.00	0.6860	0.3140	0.8170	0.1830	1.1910	0.5828	1.0899	0.5884	-8.48	0.96
61.10	0.6760	0.3240	0.8170	0.1830	1.2086	0.5648	1.0917	0.5908	-9.67	4.59 *
62.10	0.6200	0.3800	0.7750	0.2250	1.2500	0.5921	1.1086	0.6138	-11.31	3.67
64.10	0.5440	0.4560	0.7150	0.2850	1.3143	0.6250	1.1401	0.6600	-13.26	5.61
65.10	0.5100	0.4900	0.6570	0.3430	1.2882	0.7000	1.1541	0.6833	-10.41	-2.38
67.00	0.4500	0.5500	0.6400	0.3600	1.4222	0.6545	1.1787	0.7272	-17.12	11.11
69.00	0.3730	0.6270	0.5710	0.4290	1.5308	0.6842	1.2001	0.7734	-21.60	13.04
71.40	0.2450	0.7550	0.4370	0.5630	1.7837	0.7457	1.2187	0.8287	-31.67	11.13
74.20	0.1530	0.8470	0.2900	0.7100	1.8954	0.8383	1.2266	0.8923	-35.29	6.45
76.60	0.0810	0.9190	0.1530	0.8470	1.8889	0.9217	1.2138	0.9451	-35.74	2.55
78.50	0.0260	0.9740	0.0500	0.9500	1.9231	0.9754	1.1156	0.9861	-41.99	1.10 *
ABSOLUTE AVERAGE PERCENT ERROR									16.21	5.33

* FLASH CALCULATION DID NOT CONVERGE

TABLE IV
 COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
 THE BINARY SYSTEM N-PROPYL ALCOHOL-WATER

COMPONENT 1 = N-PROPYL ALCOHOL COMPONENT 2 = WATER PRESSURE = 14.5 PSIA										
TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
92.35	0.0390	0.9610	0.2810	0.7190	7.2051	0.7482	8.0745	0.7562	12.07	1.08 *
88.85	0.0720	0.9280	0.3600	0.6400	5.0000	0.6897	4.4762	0.6772	-10.48	-1.81 *
89.05	0.0750	0.9250	0.3750	0.6250	5.0000	0.6757	4.7727	0.6789	-4.55	0.48
87.95	0.1790	0.8210	0.3880	0.6120	2.1676	0.7454	0.9649	1.0266	-55.49	37.72 *
88.00	0.2000	0.8000	0.3790	0.6210	1.8950	0.7763	1.0210	0.9839	-46.12	26.75 *
87.50	0.4250	0.5750	0.4260	0.5740	1.0024	0.9983	0.8651	1.1135	-13.69	11.54 *
87.80	0.4820	0.5180	0.4380	0.5620	0.9087	1.0849	1.0661	0.9436	17.32	-13.03 *
89.20	0.7120	0.2880	0.5600	0.4400	0.7865	1.5278	0.8387	1.3499	6.63	-11.64
91.70	0.8500	0.1500	0.6850	0.3150	0.8059	2.1000	0.8682	1.6709	7.74	-20.43
95.00	0.9400	0.0600	0.8550	0.1450	0.9096	2.4167	0.9493	2.0201	4.37	-16.41
ABSOLUTE AVERAGE PERCENT ERROR									17.84	14.09

* FLASH CALCULATION DID NOT CONVERGE

TABLE V

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM ISOPROPYL ALCOHOL-WATER

COMPONENT 1 = ISOPROPYL ALCOHOL COMPONENT 2 = WATER PRESSURE = 14.7 PSIA										
TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
81.48	0.9535	0.0465	0.9325	0.0675	0.9780	1.4516	0.9817	1.3184	0.38	-9.18
80.70	0.8725	0.1275	0.8340	0.1660	0.9559	1.3020	0.9699	1.1860	1.47	-8.91
80.37	0.8090	0.1910	0.7745	0.2255	0.9574	1.1806	0.9748	1.0978	1.82	-7.01
80.23	0.7650	0.2350	0.7370	0.2630	0.9634	1.1191	0.9939	1.0163	3.17	-9.19 *
80.11	0.6955	0.3045	0.6915	0.3085	0.9942	1.0131	1.0343	0.9216	4.03	-9.04 *
80.16	0.6605	0.3395	0.6715	0.3285	1.0167	0.9676	1.0419	0.9135	2.48	-5.60 *
80.15	0.6460	0.3540	0.6645	0.3355	1.0286	0.9477	0.9904	1.0166	-3.72	7.26 *
80.31	0.5590	0.4410	0.6255	0.3745	1.1190	0.8492	1.0436	0.9225	-6.73	8.63
80.38	0.5145	0.4855	0.6075	0.3925	1.1808	0.8084	1.0650	0.8967	-9.80	10.92
80.67	0.4460	0.5540	0.5920	0.4080	1.3274	0.7365	1.1566	0.8209	-12.87	11.47
80.90	0.3835	0.6165	0.5700	0.4300	1.4863	0.6975	1.2380	0.7771	-16.71	11.42
81.28	0.2980	0.7020	0.5510	0.4490	1.8490	0.6396	1.4228	0.7117	-23.05	11.28
81.29	0.2975	0.7025	0.5540	0.4460	1.8622	0.6349	1.4304	0.7096	-23.19	11.77
81.23	0.2835	0.7165	0.5530	0.4470	1.9506	0.6239	1.3963	0.7191	-28.42	15.27
81.62	0.2450	0.7550	0.5390	0.4610	2.2000	0.6106	1.7530	0.6444	-20.32	5.54
81.75	0.1935	0.8065	0.5320	0.4680	2.7494	0.5803	2.1769	0.5950	-20.82	2.54 *

TABLE V (Continued)

TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
81.58	0.1895	0.8105	0.5375	0.4625	2.8364	0.5706	1.7304	0.6472	-38.99	13.43
81.99	0.1665	0.8335	0.5215	0.4785	3.1321	0.5741	3.4063	0.5361	8.75	-6.61 *
82.32	0.1215	0.8785	0.5120	0.4880	4.2140	0.5555	4.4496	0.5215	5.59	-6.13 *
82.70	0.1000	0.9000	0.5015	0.4985	5.0150	0.5539	4.9349	0.5231	-1.60	-5.57 *
84.57	0.0570	0.9430	0.4565	0.5435	8.0088	0.5764	6.8610	0.5515	-14.33	-4.31 *
88.05	0.0365	0.9635	0.3655	0.6345	10.0137	0.6585	9.0218	0.6280	-9.91	-4.63
93.40	0.0160	0.9840	0.2115	0.7885	13.2188	0.8013	11.9316	0.7749	-9.74	-3.30 *
95.17	0.0115	0.9885	0.1630	0.8370	14.1739	0.8467	12.7323	0.8298	-10.17	-2.00
ABSOLUTE AVERAGE PERCENT ERROR									11.59	7.96

* FLASH CALCULATION DID NOT CONVERGE

TABLE VI

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM WATER-PROPIONIC ACID

COMPONENT 1 = WATER COMPONENT 2 = PROPIONIC ACID PRESSURE = 14.7 PSIA										
TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
99.20	0.9636	0.0364	0.9596	0.0404	0.9958	1.1099	0.9783	1.1015	-1.76	-0.76 *
99.10	0.9522	0.0478	0.9519	0.0481	0.9997	1.0063	0.9717	1.0913	-2.80	8.44 *
99.30	0.9321	0.0679	0.9403	0.0597	1.0088	0.8792	0.9801	1.1348	-2.85	29.07 *
99.35	0.9187	0.0813	0.9345	0.0655	1.0172	0.8057	1.0037	0.7791	-1.33	-3.29 *
99.45	0.9018	0.0982	0.9302	0.0698	1.0315	0.7108	0.9837	1.1578	-4.63	62.88 *
99.50	0.8847	0.1153	0.9248	0.0752	1.0453	0.6522	1.0022	0.8451	-4.12	29.57 *
100.50	0.7190	0.2810	0.8670	0.1330	1.2058	0.4733	1.1452	0.4622	-5.03	-2.34
101.50	0.6200	0.3800	0.8450	0.1550	1.3629	0.4079	1.2730	0.3897	-6.59	-4.46
102.10	0.5700	0.4300	0.8430	0.1570	1.4789	0.3651	1.3352	0.3759	-9.72	2.94
103.70	0.4906	0.5094	0.8206	0.1794	1.6726	0.3522	1.4845	0.3656	-11.25	3.30
106.10	0.3646	0.6354	0.7645	0.2355	2.0968	0.3706	1.6862	0.3756	-19.58	1.34
107.80	0.3212	0.6788	0.7415	0.2585	2.3085	0.3808	1.8227	0.3898	-21.04	2.35
110.00	0.2738	0.7262	0.7141	0.2859	2.6081	0.3937	1.9974	0.4126	-23.42	4.81
112.90	0.2229	0.7771	0.6775	0.3225	3.0395	0.4150	2.2308	0.4480	-26.61	7.94
116.40	0.1571	0.8429	0.6080	0.3920	3.8701	0.4651	2.5214	0.4967	-34.85	6.81
118.50	0.1392	0.8608	0.5846	0.4114	4.1997	0.4779	2.7033	0.5288	-35.63	10.65 *

TABLE VI (Continued)

TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
122.20	0.1008	0.8992	0.4850	0.5150	4.8115	0.5727	3.0393	0.5903	-36.83	3.07
127.90	0.0444	0.9556	0.3606	0.6394	8.1216	0.6691	3.5958	0.6975	-55.73	4.24
ABSOLUTE AVERAGE PERCENT ERROR									16.88	10.49

* FLASH CALCULATION DID NOT CONVERGE

TABLE VII
 COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
 THE BINARY SYSTEM METHANOL-WATER

TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
96.40	0.0200	0.9800	0.1340	0.8660	6.7000	0.8837	7.8978	0.8702	17.88	-1.52 *
93.50	0.0400	0.9600	0.2300	0.7700	5.7500	0.8021	6.8639	0.7770	19.37	-3.13 *
91.20	0.0600	0.9400	0.3040	0.6960	5.0667	0.7404	6.2368	0.7112	23.09	-3.95
89.30	0.0800	0.9200	0.3650	0.6350	4.5625	0.6902	5.5467	0.6596	21.57	-4.44 *
87.70	0.1000	0.9000	0.4180	0.5820	4.1800	0.5467	5.0434	0.6198	20.66	-4.15 *
84.40	0.1500	0.8500	0.5170	0.4830	3.4467	0.5682	4.1329	0.5471	19.91	-3.71
81.70	0.2000	0.8000	0.5790	0.4210	2.8950	0.5262	3.3534	0.4977	15.83	-5.42 *
78.00	0.3000	0.7000	0.6650	0.3350	2.2167	0.4786	2.4651	0.4477	11.21	-6.45
75.30	0.4000	0.6000	0.7290	0.2710	1.8225	0.4517	1.9318	0.4277	6.00	-5.31 *
73.10	0.5000	0.5000	0.7790	0.2210	1.5580	0.4420	1.6113	0.4201	3.42	-4.95
71.20	0.6000	0.4000	0.8250	0.1750	1.3750	0.4375	1.4033	0.4190	2.06	-4.23
69.30	0.7000	0.3000	0.8700	0.1300	1.2429	0.4333	1.2486	0.4201	0.46	-3.05
67.60	0.8000	0.2000	0.9150	0.0850	1.1437	0.4250	1.1417	0.4225	-0.18	-0.60
66.00	0.9000	0.1000	0.9580	0.0420	1.0644	0.4200	1.0614	0.4253	-0.29	1.26
65.00	0.9500	0.0500	0.9790	0.0210	1.0305	0.4200	1.0188	0.4273	-1.14	1.75
ABSOLUTE AVERAGE PERCENT ERROR									10.87	3.60

* FLASH CALCULATION DID NOT CONVERGE

TABLE VIII

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM ACETONE-WATER

COMPONENT 1 = ACETONE COMPONENT 2 = WATER PRESSURE = 500.0 PSIA										
TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
211.10	0.9390	0.0610	0.9210	0.0790	0.9808	1.2951	0.9928	1.0953	1.22	-15.43
209.20	0.8840	0.1160	0.8530	0.1470	0.9649	1.2672	0.9807	1.0686	1.64	-15.68
208.50	0.7890	0.2110	0.7500	0.2500	0.9506	1.1848	0.9793	1.0487	3.03	-11.49
206.00	0.6690	0.3310	0.6630	0.3370	0.9910	1.0181	0.9984	0.9605	0.75	-5.66 *
207.50	0.5470	0.4530	0.5850	0.4150	1.0695	0.9161	0.9846	1.0115	-7.93	10.42 *
208.60	0.4120	0.5880	0.5270	0.4730	1.2791	0.8044	1.0963	0.9368	-14.29	16.45
210.60	0.2910	0.7090	0.4650	0.5350	1.5979	0.7546	1.4521	0.8573	-9.13	13.61
212.70	0.1850	0.8150	0.4080	0.5920	2.2054	0.7264	2.5777	0.7891	16.88	8.63
218.90	0.0920	0.9080	0.3180	0.6820	3.4565	0.7511	5.6494	0.8221	63.44	9.46
230.00	0.0230	0.9770	0.1400	0.8600	6.0870	0.8802	8.5659	0.9753	40.79	10.80
ABSOLUTE AVERAGE PERCENT ERROR									15.91	11.76

* FLASH CALCULATION DID NOT CONVERGE

TABLE IX

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM METHYL ETHYL KETONE-WATER

TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	COMP NUM		COMP NUM		COMP NUM		COMP NUM		COMP NUM	
	1	2	1	2	1	2	1	2	1	2
242.20	0.9450	0.0550	0.9010	0.0990	0.9534	1.8000	0.9596	1.3747	0.64	-23.63
240.00	0.9170	0.0830	0.8680	0.1320	0.9466	1.5904	0.9449	1.3748	-0.18	-13.56
239.40	0.9090	0.0910	0.8630	0.1370	0.9494	1.5055	0.9408	1.3742	-0.91	-8.72
231.10	0.8320	0.1680	0.7380	0.2620	0.8870	1.5595	0.8790	1.3405	-0.90	-14.04
226.70	0.7720	0.2280	0.6740	0.3260	0.8731	1.4298	0.8452	1.3022	-3.20	-8.92
223.30	0.7030	0.2970	0.5740	0.4260	0.8165	1.4343	0.8212	1.2602	0.57	-12.14
219.40	0.6190	0.3810	0.5020	0.4980	0.8110	1.3071	0.8042	1.1904	-0.84	-8.93
217.20	0.5360	0.4640	0.4610	0.5390	0.8601	1.1616	0.8175	1.1268	-4.96	-3.00
216.10	0.4100	0.5900	0.4090	0.5910	0.9976	1.0017	0.8677	1.0669	-13.02	6.51
216.50	0.3650	0.6350	0.3900	0.6100	1.0685	0.9606	0.8388	1.0945	-21.50	13.93
216.80	0.2700	0.7300	0.3660	0.6340	1.3556	0.8685	0.8273	1.1096	-38.97	27.77
218.00	0.1810	0.8190	0.3520	0.6480	1.9448	0.7912	0.8078	1.1540	-58.46	45.85
221.10	0.0860	0.9140	0.2840	0.7160	3.3023	0.7834	9.7809	0.8458	196.18	7.96
227.20	0.0210	0.9790	0.1720	0.8280	8.1905	0.8458	11.7760	0.9329	43.78	10.31
233.90	0.0110	0.9890	0.1000	0.9000	9.0909	0.9100	12.3759	1.0362	36.14	13.87 *
ABSOLUTE AVERAGE PERCENT ERROR									28.02	14.61

* FLASH CALCULATION DID NOT CONVERGE

TABLE X

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM ACETONE-METHYL ETHYL KETONE

TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2
214.50	0.9550	0.0450	0.9710	0.0290	1.0168	0.6444	1.0144	0.8037	-0.24	24.71
215.60	0.9130	0.0870	0.9330	0.0670	1.0219	0.7701	1.0212	0.8103	-0.07	5.21
218.00	0.8550	0.1450	0.8810	0.1190	1.0304	0.8207	1.0359	0.8247	0.53	0.49
220.10	0.7950	0.2050	0.8300	0.1700	1.0440	0.8293	1.0486	0.8373	0.43	0.97
222.60	0.7130	0.2870	0.7610	0.2390	1.0673	0.8328	1.0634	0.8523	-0.37	2.34
223.20	0.7010	0.2990	0.7570	0.2430	1.0799	0.8127	1.0669	0.8559	-1.21	5.31
225.00	0.5700	0.4300	0.6220	0.3780	1.0912	0.8791	1.0772	0.8666	-1.28	-1.42
227.40	0.6500	0.3500	0.6910	0.3090	1.0631	0.8829	1.0907	0.8808	2.60	-0.23
233.50	0.3970	0.6030	0.4500	0.5500	1.1335	0.9121	1.1231	0.9163	-0.92	0.46
235.60	0.3350	0.6650	0.3830	0.6170	1.1433	0.9278	1.1334	0.9282	-0.86	0.04
238.90	0.2520	0.7480	0.2950	0.7050	1.1706	0.9425	1.1488	0.9465	-1.87	0.42
241.40	0.1900	0.8100	0.2230	0.7770	1.1737	0.9593	1.1596	0.9600	-1.20	0.08
243.00	0.1510	0.8490	0.1850	0.8150	1.2252	0.9600	1.1661	0.9684	-4.82	0.88
247.80	0.0620	0.9380	0.0860	0.9140	1.3871	0.9744	1.1836	0.9926	-14.67	1.86
240.40	0.0500	0.9500	0.0780	0.9220	1.5600	0.9705	1.1855	0.9954	-24.00	2.57
ABSOLUTE AVERAGE PERCENT ERROR									3.67	3.13

TABLE XI
COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM ETHANOL-WATER

TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
98.40	0.0050	0.9950	0.0650	0.9350	13.0000	0.9397	10.4453	0.9415	-19.65	0.19
97.10	0.0100	0.9900	0.1100	0.8900	11.0000	0.8990	9.8055	0.8954	-10.86	-0.40
94.90	0.0200	0.9800	0.1750	0.8250	8.7500	0.8418	8.7063	0.8219	-0.50	-2.36
93.50	0.0300	0.9700	0.2310	0.7690	7.7000	0.7928	8.1341	0.7792	5.64	-1.72
91.80	0.0400	0.9600	0.2730	0.7270	6.8250	0.7573	7.2983	0.7294	6.93	-3.68
89.50	0.0600	0.9400	0.3400	0.6600	5.6667	0.7021	6.1180	0.6682	7.97	-4.83
88.50	0.0700	0.9300	0.3670	0.6330	5.2429	0.6806	5.6192	0.6441	7.18	-5.38
84.80	0.1400	0.8600	0.4820	0.5180	3.4429	0.6023	3.5872	0.5753	4.19	-4.50
81.20	0.3500	0.6500	0.5950	0.4050	1.7000	0.6231	1.5477	0.6367	-8.96	2.18
78.50	0.7500	0.2500	0.7870	0.2130	1.0493	0.8520	1.0276	0.8829	-2.07	3.63
78.40	0.8000	0.2000	0.8280	0.1720	1.0350	0.8600	1.0170	0.9087	-1.74	5.66
78.30	0.8500	0.1500	0.8550	0.1450	1.0059	0.9667	1.0066	0.9465	0.07	-2.09
78.20	0.9000	0.1000	0.8980	0.1020	0.9978	1.0200	0.9993	0.9831	0.15	-3.61 *
78.30	0.9500	0.0500	0.9420	0.0580	0.9916	1.1600	1.0004	1.0429	0.89	-10.09 *
ABSOLUTE AVERAGE PERCENT ERROR									5.49	3.59

* FLASH CALCULATION DID NOT CONVERGE

TABLE XII

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM FORMIC ACID-ACETIC ACID

TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2
101.20	0.9255	0.0745	0.9423	0.0577	1.0182	0.7745	1.0156	0.8048	-0.25	3.91
101.90	0.8693	0.1307	0.8940	0.1060	1.0284	0.8110	1.0331	0.7817	0.46	-3.62
102.90	0.7922	0.2078	0.8324	0.1676	1.0507	0.8065	1.0607	0.7668	0.94	-4.93
104.00	0.7088	0.2912	0.7625	0.2375	1.0758	0.8156	1.0920	0.7637	1.51	-6.36
105.30	0.6136	0.3864	0.6721	0.3279	1.0953	0.8486	1.1302	0.7703	3.18	-9.23
106.60	0.5214	0.4786	0.5992	0.4008	1.1492	0.8374	1.1688	0.7836	1.71	-6.43
107.90	0.4475	0.5525	0.5224	0.4776	1.1674	0.8644	1.2076	0.8013	3.45	-7.31
109.40	0.3739	0.6261	0.4423	0.5577	1.1829	0.8908	1.2521	0.8248	5.84	-7.41
110.80	0.2793	0.7207	0.3521	0.6479	1.2607	0.8990	1.2938	0.8496	2.63	-5.50
112.30	0.2179	0.7821	0.2804	0.7196	1.2868	0.9201	1.3385	0.8781	4.02	-4.56
113.30	0.1752	0.8248	0.2297	0.7703	1.3111	0.9339	1.3685	0.8983	4.38	-3.81
114.20	0.1266	0.8734	0.1800	0.8200	1.4218	0.9389	1.3955	0.9170	-1.85	-2.33
ABSOLUTE AVERAGE PERCENT ERROR									2.52	5.45

TABLE XIII

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM WATER-ACETIC ACID

TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
109.70	0.2080	0.7920	0.3310	0.6690	1.5913	0.8447	1.3988	0.8159	-12.10	-3.41
107.20	0.3270	0.6730	0.4410	0.5590	1.3486	0.8306	1.2990	0.7636	-3.68	-8.07
105.40	0.4680	0.5320	0.6020	0.3980	1.2863	0.7481	1.2268	0.7283	-4.63	-2.65
104.00	0.5920	0.4080	0.7130	0.2870	1.2044	0.7034	1.1695	0.7036	-2.90	0.03
102.70	0.6880	0.3120	0.7870	0.2130	1.1439	0.6827	1.1149	0.6854	-2.54	0.40
101.70	0.7790	0.2210	0.8520	0.1480	1.0937	0.6697	1.0716	0.6783	-2.02	1.29
101.50	0.8450	0.1550	0.8950	0.1050	1.0592	0.6774	1.0626	0.6779	0.32	0.07
100.90	0.8840	0.1160	0.9180	0.0820	1.0385	0.7069	1.0368	0.6836	-0.16	-3.29 *
100.70	0.9190	0.0810	0.9430	0.0570	1.0261	0.7037	1.0289	0.6877	0.27	-2.27
100.30	0.9700	0.0300	0.9780	0.0220	1.0082	0.7333	1.0143	0.7013	0.50	-4.37
100.20	0.9870	0.0130	0.9910	0.0090	1.0041	0.6923	1.0083	0.7218	0.42	4.26
ABSOLUTE AVERAGE PERCENT ERROR									2.69	2.74

* FLASH CALCULATION DID NOT CONVERGE

TABLE XIV

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM WATER-FORMIC ACID

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR THE BINARY SYSTEM WATER-FORMIC ACID										
COMPONENT 1 = WATER COMPONENT 2 = FORMIC ACID PRESSURE = 14.7 PSIA										
TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	1	2	1	2	1	2	1	2	1	2
100.40	0.9697	0.0303	0.9860	0.0140	1.0168	0.4620	1.0195	0.4044	0.27	-12.47 *
101.00	0.9359	0.0641	0.9697	0.0303	1.0361	0.4727	1.0377	0.4409	0.15	-6.73
101.50	0.8990	0.1010	0.9502	0.0498	1.0570	0.4931	1.0525	0.4691	-0.42	-4.87
102.00	0.8696	0.1304	0.9325	0.0675	1.0723	0.5176	1.0677	0.5004	-0.43	-3.32
102.50	0.8359	0.1641	0.9119	0.0881	1.0909	0.5369	1.0768	0.5251	-1.29	-2.20 *
103.30	0.7889	0.2111	0.8769	0.1231	1.1115	0.5831	1.0980	0.5734	-1.22	-1.67 *
103.70	0.7699	0.2301	0.8616	0.1384	1.1191	0.6015	1.1030	0.5960	-1.44	-0.91
104.40	0.7315	0.2685	0.8278	0.1722	1.1316	0.6413	1.1168	0.6425	-1.31	0.19 *
105.10	0.6878	0.3122	0.7813	0.2187	1.1359	0.7005	1.1225	0.6886	-1.19	-1.70
106.10	0.6163	0.3837	0.6555	0.3045	1.1285	0.7936	1.1255	0.7565	-0.27	-4.68 *
106.60	0.5758	0.4242	0.6359	0.3641	1.1044	0.8583	1.1247	0.7889	1.84	-8.08 *
107.10	0.5215	0.4785	0.5605	0.4395	1.0748	0.9185	1.1169	0.8337	3.92	-9.23 *
107.40	0.4533	0.5467	0.4639	0.5361	1.0234	0.9806	1.1045	0.8591	7.92	-12.39 *
107.30	0.3793	0.6207	0.3593	0.6407	0.9473	1.0322	0.8101	1.0680	-14.48	3.47
106.80	0.3241	0.6759	0.2816	0.7184	0.8689	1.0629	0.7683	1.0725	-11.57	0.91 *
ABSOLUTE AVERAGE PERCENT ERROR									3.18	4.85

* FLASH CALCULATION DID NOT CONVERGE

TABLE XV

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM METHANOL-ETHANOL

TEMP DEG C	LIQ MOL FRAC COMP NUM		VAP MOL FRAC COMP NUM		EXP K VALUES COMP NUM		CAL K VALUES COMP NUM		K VALUE % ERROR COMP NUM	
	1	2	1	2	1	2	1	2	1	2
65.80	0.8880	0.1120	0.9320	0.0680	1.0495	0.6071	1.0491	0.6522	-0.04	7.42
67.60	0.7250	0.2750	0.8200	0.1800	1.1310	0.6545	1.1219	0.6943	-0.81	6.08
69.20	0.6000	0.4000	0.7250	0.2750	1.2083	0.6875	1.1895	0.7342	-1.56	6.79
70.90	0.4700	0.5300	0.6000	0.4000	1.2766	0.7547	1.2652	0.7786	-0.89	3.17
72.30	0.3750	0.6250	0.5050	0.4950	1.3467	0.7920	1.3302	0.8170	-1.22	3.16
74.00	0.2480	0.7520	0.3620	0.6380	1.4597	0.8484	1.4128	0.8658	-3.21	2.05
75.80	0.1420	0.8580	0.2220	0.7780	1.5634	0.9068	1.5055	0.9201	-3.71	1.47
77.00	0.0730	0.9270	0.1200	0.8800	1.6438	0.9493	1.5684	0.9577	-4.59	0.88
76.60	0.1340	0.8660	0.1830	0.8170	1.3657	0.9434	1.5470	0.9450	13.28	0.17
75.00	0.2420	0.7580	0.3260	0.6740	1.3471	0.8892	1.4641	0.8957	8.69	0.73
73.60	0.3200	0.6800	0.4280	0.5720	1.3375	0.8412	1.3932	0.8541	4.16	1.54
72.30	0.4010	0.5990	0.5290	0.4710	1.3192	0.7863	1.3300	0.8171	0.82	3.91
71.70	0.4350	0.5650	0.5660	0.4340	1.3011	0.7681	1.3023	0.8004	0.09	4.20
70.00	0.5420	0.4580	0.6760	0.3240	1.2472	0.7074	1.2247	0.7548	-1.80	6.70
68.60	0.6520	0.3480	0.7590	0.2410	1.1641	0.6925	1.1636	0.7190	-0.04	3.83
67.70	0.7280	0.2720	0.8130	0.1870	1.1168	0.6875	1.1259	0.6968	0.82	1.35

TABLE XV (Continued)

TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2
66.90	0.7900	0.2100	0.8580	0.1420	1.0861	0.6762	1.0930	0.6777	0.63	0.22
66.60	0.8140	0.1860	0.8750	0.1250	1.0749	0.6720	1.0812	0.6705	0.58	-0.24
65.80	0.8730	0.1270	0.9190	0.0810	1.0527	0.6378	1.0491	0.6522	-0.34	2.25
65.60	0.9100	0.0900	0.9370	0.0630	1.0297	0.7000	1.0414	0.6476	1.14	-7.49
ABSOLUTE AVERAGE PERCENT ERROR									2.42	3.18

TABLE XVI

COMPARISON OF THE EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM ACETONE-METHANOL

TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2
63.50	0.0360	0.9640	0.0820	0.9180	2.2778	0.9523	2.2390	0.9632	-1.70	1.14
62.20	0.0810	0.9190	0.1610	0.8390	1.9877	0.9129	2.0531	0.9200	3.29	0.77
60.70	0.1410	0.8590	0.2510	0.7490	1.7801	0.8719	1.8356	0.8768	3.12	0.56
59.40	0.2060	0.7940	0.3360	0.6640	1.6311	0.8363	1.6529	0.8470	1.34	1.28
58.10	0.2930	0.7070	0.4230	0.5770	1.4437	0.8161	1.4737	0.8274	2.08	1.38
56.90	0.3940	0.6060	0.5000	0.5000	1.2690	0.8251	1.3099	0.8247	3.22	-0.04
56.20	0.5130	0.4870	0.5800	0.4200	1.1306	0.8624	1.2163	0.8351	7.58	-3.17
55.90	0.5840	0.4160	0.6390	0.3610	1.0942	0.8678	1.1759	0.8444	7.47	-2.70
55.80	0.6830	0.3170	0.7050	0.2950	1.0322	0.9306	1.1622	0.8485	12.59	-8.82 *
55.80	0.7420	0.2580	0.7450	0.2550	1.0040	0.9884	0.9891	1.2585	-1.49	27.33
55.80	0.8230	0.1770	0.8060	0.1940	0.9793	1.0960	0.9891	1.2585	1.00	14.82
55.80	0.8610	0.1390	0.8430	0.1570	0.9791	1.1295	0.9891	1.2585	1.02	11.42
ABSOLUTE AVERAGE PERCENT ERROR									3.82	6.12

* FLASH CALCULATION DID NOT CONVERGE

TABLE XVII

COMPARISON OF THE EXPERIMENTAL AND CALCULATED K-VALUES FOR
THE BINARY SYSTEM ACETONE-ETHANOL

TEMP DEG C	LIQ MOL FRAC		VAP MOL FRAC		EXP K VALUES		CAL K VALUES		K VALUE % ERROR	
	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2	COMP NUM 1	COMP NUM 2
	COMPONENT 1 = ACETONE COMPONENT 2 = ETHANOL PRESSURE = 14.7 PSIA									
76.40	0.0330	0.9670	0.1110	0.8890	3.3636	0.9193	2.9491	0.9393	-12.33	2.17
74.00	0.0780	0.9220	0.2160	0.7840	2.7692	0.8503	2.6764	0.8692	-3.35	2.22
70.80	0.1490	0.8510	0.3450	0.6550	2.3154	0.7697	2.3111	0.7873	-0.19	2.29
69.10	0.1950	0.8050	0.4100	0.5900	2.1026	0.7329	2.1315	0.7496	1.38	2.28
65.60	0.3160	0.6840	0.5340	0.4660	1.6899	0.6813	1.7564	0.6895	3.94	1.21
63.40	0.4140	0.5860	0.6140	0.3860	1.4831	0.6587	1.5338	0.6686	3.42	1.50
61.30	0.5320	0.4680	0.6970	0.3030	1.3102	0.6474	1.3375	0.6684	2.08	3.24
59.00	0.6910	0.3090	0.7960	0.2040	1.1520	0.6602	1.1505	0.7091	-0.12	7.41
57.30	0.8520	0.1480	0.8960	0.1040	1.0516	0.7027	1.0436	0.7973	-0.76	13.46
	ABSOLUTE AVERAGE PERCENT ERROR								3.06	3.97

TABLE XVIII

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR THE
TERNARY SYSTEM ACETONE-METHANOL-ETHANOL

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
76.50	0.0190	0.0460	0.9350	0.0600	0.0700	0.8700	3.1579	1.5217	0.9305	3.0161	1.5406	0.9421	-4.49	1.24	1.25
75.90	0.0190	0.1000	0.8810	0.0630	0.1460	0.7910	3.3158	1.4600	0.8978	2.9863	1.5088	0.9233	-9.94	3.34	2.84
74.80	0.0220	0.1600	0.8180	0.0740	0.2220	0.7040	3.3636	1.3875	0.8606	2.9121	1.4525	0.8899	-13.42	4.68	3.40
74.00	0.0180	0.2200	0.7620	0.0520	0.3130	0.6350	2.8889	1.4227	0.8333	2.8760	1.4121	0.8661	-0.45	-0.75	3.93
73.00	0.0170	0.2810	0.7020	0.0570	0.3700	0.5730	3.3529	1.3167	0.8162	2.8161	1.3638	0.8372	-16.01	3.57	2.57 *
72.30	0.0170	0.3300	0.6530	0.0480	0.4340	0.5180	2.8235	1.3152	0.7933	2.7763	1.3297	0.8174	-1.67	1.11	3.04
71.30	0.0220	0.3800	0.5980	0.0530	0.5890	0.4580	2.4091	1.5500	0.7659	2.7164	1.2830	0.7898	12.75	-17.23	3.13 *
70.70	0.0200	0.4290	0.5510	0.0480	0.5520	0.4000	2.4000	1.2867	0.7260	2.6816	1.2558	0.7737	11.73	-2.40	6.58
69.80	0.0210	0.4850	0.4940	0.0530	0.5910	0.3560	2.5238	1.2186	0.7206	2.6229	1.2156	0.7501	3.92	-0.24	4.08
69.30	0.0190	0.5350	0.4460	0.0450	0.6450	0.3100	2.3684	1.2056	0.6951	2.6027	1.1937	0.7371	9.89	-0.99	5.05
69.00	0.0130	0.5830	0.4040	0.0350	0.6800	0.2850	2.6923	1.1664	0.7054	2.5963	1.1805	0.7294	-3.57	1.21	3.40
68.00	0.0170	0.6490	0.3340	0.0450	0.7300	0.2250	2.6471	1.1248	0.6737	2.5272	1.1380	0.7047	-4.53	1.17	4.60
67.30	0.0170	0.7030	0.2800	0.0450	0.7700	0.1850	2.6471	1.0953	0.6607	2.4901	1.1092	0.6876	-5.93	1.27	4.07
67.20	0.0200	0.6900	0.2900	0.0570	0.7580	0.1850	2.8500	1.0985	0.6379	2.4741	1.1054	0.6853	-13.19	0.62	7.42
66.00	0.0180	0.7960	0.1860	0.0450	0.8370	0.1180	2.5000	1.0515	0.6344	2.4167	1.0573	0.6570	-3.33	0.55	3.57
65.60	0.0110	0.8500	0.1390	0.0340	0.8820	0.0840	3.0909	1.0376	0.6043	2.4060	1.0414	0.6479	-22.16	0.36	7.21

TABLE XVIII (Continued)

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
65.00	0.0170	0.8960	0.0870	0.0410	0.9110	0.0480	2.4118	1.0167	0.5517	2.3676	1.0184	0.6345	-1.83	0.17	15.00 *
64.40	0.0200	0.9370	0.0430	0.0400	0.9310	0.0290	2.0000	0.9936	0.6744	2.3254	0.9958	0.6215	16.27	0.22	-7.85
74.80	0.0490	0.0450	0.9060	0.1550	0.0690	0.7760	3.1633	1.5333	0.8565	2.8153	1.4514	0.8910	-11.00	-5.34	4.02
73.40	0.0620	0.1050	0.8330	0.1700	0.1500	0.6800	2.7419	1.4286	0.8163	2.7107	1.3822	0.8503	-1.14	-3.24	4.16
72.40	0.0600	0.1680	0.7720	0.1570	0.2330	0.6100	2.6167	1.3869	0.7902	2.6563	1.3344	0.8219	1.52	-3.79	4.02
71.4C	0.0600	0.2400	0.7000	0.1520	0.3130	0.5350	2.5333	1.3042	0.7643	2.5986	1.2874	0.7943	2.58	-1.29	3.93
70.50	0.0620	0.3030	0.6350	0.1550	0.3750	0.4700	2.5000	1.2376	0.7402	2.5444	1.2466	0.7703	1.78	0.73	4.07
69.70	0.0580	0.3790	0.5630	0.1390	0.4590	0.4020	2.3966	1.2111	0.7140	2.5182	1.2113	0.7490	5.08	0.02	4.90
70.00	0.0430	0.3930	0.5640	0.1100	0.4800	0.4100	2.5581	1.2214	0.7270	2.5674	1.2244	0.7562	0.36	0.25	4.02
68.30	0.0640	0.4700	0.4660	0.1520	0.5360	0.3120	2.3750	1.1404	0.6695	2.4266	1.1516	0.7139	2.17	0.98	6.63
67.70	0.0600	0.5310	0.4090	0.1430	0.5850	0.2720	2.3833	1.1017	0.6650	2.4045	1.1267	0.6990	0.89	2.27	5.10
66.90	0.0610	0.5810	0.3580	0.1410	0.6360	0.2230	2.3115	1.0947	0.6229	2.3573	1.0942	0.6799	1.98	-0.04	3.14
66.20	0.0590	0.6420	0.2990	0.1350	0.6820	0.1830	2.2881	1.0623	0.6120	2.3234	1.0664	0.6634	1.54	0.38	8.39 *
65.40	0.0620	0.6910	0.2470	0.1330	0.7160	0.1510	2.1452	1.0362	0.6113	2.2633	1.0351	0.6456	5.51	-0.11	5.61
65.00	0.0580	0.7360	0.2060	0.1300	0.7490	0.1210	2.2414	1.0177	0.5874	2.2508	1.0198	0.6364	0.42	0.21	8.35
64.30	0.0590	0.7930	0.1460	0.1330	0.7850	0.0840	2.2542	0.9899	0.5753	2.2088	0.9936	0.6212	-2.01	0.38	7.98
63.80	0.0600	0.8400	0.1000	0.1310	0.8150	0.0540	2.1833	0.9702	0.5400	2.1852	0.9753	0.6104	0.08	0.52	13.04
63.20	0.0580	0.8900	0.0520	0.1260	0.8400	0.0340	2.1724	0.9438	0.6538	2.1415	0.9538	0.5982	-1.42	1.06	-8.51

TABLE XVIII (Continued)

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
71.40	0.1180	0.0510	0.8310	0.2800	0.0830	0.6370	2.3729	1.6274	0.7665	2.4388	1.2907	0.7991	2.78	-20.69	4.25
70.30	0.1230	0.1200	0.7570	0.2860	0.1620	0.5520	2.3252	1.3500	0.7292	2.3678	1.2409	0.7701	1.83	-8.08	5.62
69.90	0.1130	0.1880	0.6990	0.2570	0.2360	0.5070	2.2743	1.2553	0.7253	2.3820	1.2226	0.7583	4.73	-2.61	4.55
69.10	0.1140	0.2530	0.6330	0.2510	0.3020	0.4470	2.2018	1.1937	0.7062	2.3458	1.1881	0.7376	6.54	-0.47	4.45
67.90	0.1220	0.3170	0.5610	0.2690	0.3560	0.3750	2.2049	1.1230	0.6684	2.2603	1.1387	0.7087	2.51	1.39	6.02
66.60	0.1270	0.4040	0.4690	0.2600	0.4400	0.3000	2.0472	1.0891	0.6397	2.1832	1.0863	0.6780	6.64	-0.26	6.00
66.40	0.1220	0.4350	0.4430	0.2530	0.4670	0.2800	2.0738	1.0736	0.6321	2.1853	1.0781	0.6728	5.38	0.42	5.45
65.50	0.1250	0.4970	0.3780	0.2500	0.5150	0.2350	2.0000	1.0362	0.6217	2.1310	1.0436	0.6525	6.55	0.71	4.96
65.10	0.1130	0.5620	0.3250	0.2350	0.5720	0.1930	2.0796	1.0178	0.5938	2.1329	1.0274	0.6426	2.56	0.94	8.21
64.30	0.1180	0.6150	0.2670	0.2400	0.6140	0.1460	2.0339	0.9984	0.5468	2.0848	0.9979	0.6253	2.50	-0.05	14.35
63.70	0.1160	0.6670	0.2170	0.2340	0.6520	0.1140	2.0172	0.9775	0.5253	2.0494	0.9759	0.6128	1.59	-0.17	16.64
63.10	0.1070	0.7350	0.1580	0.2210	0.6990	0.0800	2.0654	0.9510	0.5063	2.0297	0.9541	0.5996	-1.73	0.32	18.43
62.60	0.1060	0.7870	0.1070	0.2190	0.7340	0.0470	2.0660	0.9327	0.4393	2.0121	0.9363	0.5890	-2.61	0.39	34.09
61.80	0.1150	0.8380	0.0470	0.2200	0.7610	0.0190	1.9130	0.9081	0.4043	1.9505	0.9097	0.5740	1.96	0.17	41.99
68.80	0.1850	0.0630	0.7520	0.3890	0.0860	0.5250	2.1027	1.3651	0.6981	2.1573	1.1839	0.7391	2.60	-13.27	5.86
67.70	0.1920	0.1280	0.6800	0.3860	0.1630	0.4510	2.0104	1.2734	0.6632	2.0895	1.1388	0.7128	3.93	-10.57	7.47
ABSOLUTE AVERAGE PERCENT ERROR												5.02	2.44	7.62	

* FLASH CALCULATION DID NOT CONVERGE

TABLE XIX

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR THE
TERNARY SYSTEM METHANOL--ETHANOL--WATER

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
	COMPONENT 1 = METHANOL COMPONENT 2 = ETHANOL COMPONENT 3 = WATER PRESSURE = 14.7 PSIA														
68.10	0.7500	0.1410	0.1090	0.8500	0.0960	0.0540	1.1333	0.6809	0.4954	1.1409	0.7436	0.4826	0.66	9.22	-2.58
68.10	0.7560	0.1420	0.1020	0.8520	0.0960	0.0520	1.1270	0.6761	0.5098	1.1408	0.7427	0.4836	1.23	9.86	-5.13
74.20	0.3020	0.5900	0.1080	0.4180	0.4900	0.0920	1.3841	0.8305	0.8519	1.3910	0.8920	0.7260	0.49	7.41	-14.77 *
71.70	0.5300	0.2300	0.2400	0.6950	0.1800	0.1250	1.3113	0.7826	0.5208	1.3098	0.9067	0.5162	-0.11	15.85	-0.90
75.00	0.2600	0.5200	0.2200	0.3600	0.4700	0.1700	1.3846	0.9038	0.7727	1.4252	0.9542	0.6724	2.93	5.57	-12.99
81.20	0.0490	0.2480	0.7030	0.1300	0.5120	0.3580	2.6531	2.0645	0.5092	2.2170	1.9582	0.5638	-16.44	-5.15	10.72 *
74.50	0.3600	0.2930	0.3470	0.5250	0.2900	0.1850	1.4583	0.9898	0.5331	1.4599	1.0551	0.5498	0.11	6.60	3.12
76.30	0.2030	0.4750	0.3220	0.3280	0.4700	0.2020	1.6158	0.9895	0.6273	1.5030	1.0527	0.6456	-6.98	6.39	2.92
77.20	0.2160	0.3100	0.4740	0.3900	0.3650	0.2450	1.8056	1.1774	0.5169	1.6740	1.2948	0.5576	-7.29	9.97	7.88
71.90	0.4900	0.3600	0.1500	0.6350	0.2900	0.0750	1.2959	0.8056	0.5000	1.2924	0.8500	0.5935	-0.27	5.52	18.71
79.00	0.1020	0.3680	0.5300	0.1970	0.5100	0.2930	1.9314	1.3859	0.5528	1.7573	1.3637	0.6052	-9.01	-1.60	9.47
75.80	0.2840	0.2960	0.4200	0.4400	0.3550	0.2050	1.5493	1.1993	0.4881	1.5400	1.1392	0.5629	-0.60	-5.01	15.33
80.50	0.0350	0.3500	0.6150	0.0810	0.5540	0.3650	2.3143	1.5829	0.5935	1.9019	1.5306	0.6139	-17.82	-3.30	3.43
83.00	0.0430	0.0620	0.8950	0.1850	0.3100	0.5050	4.3023	5.0000	0.5642	3.1553	3.2355	0.5381	-26.66	-35.29	-4.63
87.50	0.0610	0.0330	0.9060	0.2800	0.2200	0.5000	4.5902	6.6667	0.5519	4.7796	5.4517	0.6173	4.13	-18.22	11.85 *
83.00	0.1380	0.0410	0.8210	0.4250	0.1500	0.4250	3.0797	3.6585	0.5177	3.4984	3.7292	0.5257	13.59	1.93	1.55 *

TABLE XIX (Continued)

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
79.00	0.2400	0.0600	0.7000	0.5500	0.1600	0.2900	2.2917	2.6667	0.4143	2.4320	2.3076	0.4755	6.12	-13.47	14.79
81.00	0.0550	0.2550	0.6900	0.1600	0.4850	0.3550	2.9091	1.9020	0.5145	2.2159	1.9566	0.5585	-23.83	2.87	8.54
82.70	0.0530	0.1450	0.8020	0.1450	0.4300	0.4250	2.7358	2.9655	0.5299	2.8884	2.8624	0.5435	5.58	-3.48	2.56
82.70	0.0930	0.0980	0.8090	0.3100	0.3000	0.3900	3.3333	3.0612	0.4821	3.1984	3.3011	0.5289	-4.05	7.84	9.72 *
ABSOLUTE AVERAGE PERCENT ERROR												7.39	8.73	8.08	

* FLASH CALCULATION DID NOT CONVERGE

TABLE XX

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR THE
TERNARY SYSTEM ACETONE-METHYL ETHYL KETONE-WATER

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
213.60	0.7830	0.1380	0.0790	0.7870	0.0990	0.1140	1.0051	0.7174	1.4430	1.0097	0.7821	1.1233	0.45	9.03	-22.16
218.50	0.6920	0.2460	0.0620	0.7260	0.1850	0.0890	1.0491	0.7520	1.4355	1.0414	0.8174	1.1702	-0.73	8.69	-18.48
212.30	0.6210	0.1730	0.2060	0.6220	0.1280	0.2500	1.0016	0.7399	1.2136	1.0029	0.7619	1.1069	0.13	2.98	-8.79
212.80	0.6000	0.1950	0.2050	0.6050	0.1440	0.2510	1.0083	0.7385	1.2244	1.0063	0.7649	1.1136	-0.20	3.57	-9.05
215.60	0.4840	0.2780	0.2380	0.4990	0.2030	0.2980	1.0310	0.7302	1.2521	1.0260	0.7810	1.1504	-0.49	6.95	-8.12
209.20	0.4830	0.1080	0.4090	0.5210	0.0870	0.3920	1.0787	0.8056	0.9584	1.0026	0.7601	1.0258	-7.05	-5.64	7.03
214.10	0.4600	0.2780	0.3220	0.4260	0.2080	0.3660	1.0650	0.7482	1.1366	1.0191	0.7710	1.1236	-4.31	3.05	-1.14
209.60	0.3980	0.0710	0.5310	0.4770	0.0620	0.4610	1.1985	0.8732	0.8682	1.0199	0.7785	1.0137	-14.90	-10.85	16.76
225.40	0.3850	0.5100	0.1050	0.4050	0.4040	0.1910	1.0519	0.7922	1.8190	1.0895	0.8529	1.2506	3.57	7.67	-31.25
214.10	0.3740	0.2730	0.3530	0.3930	0.2070	0.4000	1.0508	0.7582	1.1331	1.0205	0.7718	1.1208	-2.89	1.79	-1.09
211.40	0.3660	0.1840	0.4500	0.4040	0.1470	0.4490	1.1038	0.7989	0.9978	1.0172	0.7722	1.0572	-7.85	-3.35	5.96
211.20	0.2790	0.0960	0.6250	0.3970	0.0980	0.5050	1.4229	1.0208	0.8080	1.0449	0.8042	1.0218	-26.56	-21.23	26.46
215.90	0.2580	0.3660	0.3760	0.2870	0.2850	0.4280	1.1124	0.7787	1.1383	1.0336	0.7821	1.1452	-7.09	0.44	0.61
214.00	0.2570	0.2220	0.5210	0.3130	0.1830	0.5040	1.2179	0.8243	0.9674	1.0290	0.7804	1.1027	-15.51	-5.33	13.99
219.40	0.2420	0.5070	0.2510	0.2660	0.4210	0.3130	1.0992	0.8304	1.2470	1.0538	0.8010	1.2022	-4.13	-3.54	-3.60
212.80	0.2360	0.1090	0.6550	0.3400	0.1160	0.5440	1.4407	1.0642	0.8305	1.0381	0.7934	1.0625	-27.94	-25.45	27.92

TABLE XX (Continued)

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
216.40	0.2070	0.3970	0.3960	0.2290	0.3150	0.4560	1.1063	0.7935	1.1515	1.0383	0.7860	1.1498	-6.15	-0.94	-0.15
214.40	0.1630	0.0690	0.7680	0.2980	0.1090	0.5930	1.8282	1.5797	0.7721	3.6325	4.3484	0.7818	98.69	175.27	1.25
214.70	0.1420	0.8310	0.0270	0.1700	0.7850	0.0450	1.1972	0.9446	1.6667	1.0155	0.8060	1.1242	-15.18	-14.68	-32.55
216.40	0.1350	0.3410	0.5240	0.1670	0.2990	0.5340	1.2370	0.8768	1.0191	1.0436	0.7920	1.1398	-15.64	-9.67	11.84
215.60	0.1260	0.1920	0.6820	0.1750	0.2320	0.5930	1.3889	1.2083	0.8695	1.0463	0.7973	1.1155	-24.67	-34.01	29.30
216.50	0.1250	0.1310	0.7440	0.2200	0.1800	0.6000	1.7600	1.3740	0.8065	1.0431	0.7911	1.1434	-40.74	-42.43	41.78
216.00	0.1080	0.2400	0.6520	0.1490	0.2710	0.5800	1.3796	1.1292	0.8896	1.0477	0.7981	1.1230	-24.06	-29.32	26.24
216.10	0.0880	0.0930	0.8190	0.1870	0.1880	0.6250	2.1250	2.0215	0.7631	4.8076	6.2412	0.7887	126.24	208.74	3.36
221.10	0.0530	0.1890	0.7580	0.0870	0.2850	0.3720	1.6415	1.5079	0.4908	1.0000	1.0000	1.0000	-39.08	-33.68	103.76
221.00	0.0510	0.0600	0.8890	0.1580	0.1700	0.6720	3.0980	2.8333	0.7559	6.5928	9.1870	0.8462	112.81	224.25	11.94
247.30	0.0470	0.9410	0.0120	0.0690	0.9160	0.0150	1.4681	0.9734	1.2500	1.1840	0.9900	1.3468	-19.35	1.70	7.74
225.70	0.0400	0.3730	0.5870	0.0540	0.3570	0.5890	1.3500	0.9571	1.0034	1.0984	0.8390	1.2887	-18.63	-12.34	28.43
ABSOLUTE AVERAGE PERCENT ERROR												23.75	32.38	17.85	

TABLE XXI

COMPARISON OF EXPERIMENTAL AND CALCULATED K-VALUES FOR THE TERNARY
SYSTEM ACETIC ACID-FORMIC ACID-WATER

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
107.60	0.6120	0.0730	0.3150	0.5100	0.0730	0.4170	0.8333	1.0000	1.3238	0.7910	1.0023	1.2732	-5.08	0.23	-3.83
105.80	0.3990	0.1350	0.4670	0.3340	0.1130	0.5530	0.8371	0.8370	1.1842	0.7916	0.8727	1.1774	-5.44	4.26	-0.57
105.20	0.2390	0.1950	0.5660	0.2000	0.1520	0.6480	0.8368	0.7795	1.1449	0.8527	0.8014	1.1234	1.89	2.81	-1.88
105.80	0.1830	0.2700	0.5470	0.1670	0.2160	0.6160	0.9126	0.8000	1.1261	0.9416	0.8313	1.1011	3.19	3.91	-2.22 *
106.60	0.0920	0.3930	0.5150	0.0920	0.3420	0.5660	1.0000	0.8702	1.0990	1.1522	0.8620	1.0744	15.22	-0.95	-2.24
107.00	0.1140	0.4350	0.4510	0.1150	0.4030	0.4820	1.0088	0.9264	1.0687	1.1281	0.9186	1.0452	11.83	-0.85	-2.21
107.10	0.0670	0.4640	0.4690	0.0720	0.4320	0.4960	1.0746	0.9310	1.0576	1.2109	0.9031	1.0523	12.68	-3.00	-0.50 *
107.20	0.0620	0.4980	0.4400	0.0680	0.4750	0.4570	1.0968	0.9538	1.0386	1.2083	0.9230	1.0402	10.17	-3.24	0.15 *
107.20	0.1450	0.5130	0.3420	0.1520	0.5250	0.3230	1.0483	1.0234	0.9444	1.1210	0.9914	0.9707	6.94	-3.12	2.78 *
106.50	0.1030	0.6250	0.2720	0.1070	0.6650	0.2280	1.0383	1.0640	0.8382	1.0835	1.0457	0.8358	4.30	-1.72	-0.29
105.90	0.0900	0.6770	0.2330	0.0900	0.7240	0.1870	1.0000	1.0694	0.8026	1.0696	1.0539	0.7711	6.96	-1.45	-3.93
104.80	0.0580	0.7510	0.1910	0.0640	0.7840	0.1520	1.1034	1.0439	0.7958	1.0485	1.0547	0.6767	-4.98	1.03	-14.96
103.60	0.0390	0.8000	0.1610	0.0400	0.8420	0.1180	1.0256	1.0525	0.7329	1.0038	1.0451	0.5945	-2.13	-0.70	-18.88 *
106.60	0.0150	0.4100	0.5750	0.0150	0.3500	0.6350	1.0000	0.8537	1.1043	1.3599	0.8116	1.1093	35.99	-4.92	0.45
105.60	0.0120	0.3340	0.6540	0.0140	0.2490	0.7360	1.1667	0.7455	1.1254	1.2741	0.7317	1.1184	9.21	-1.85	-0.62 *
104.00	0.0260	0.2270	0.7470	0.0230	0.1450	0.8320	0.8846	0.6388	1.1138	1.0912	0.6315	1.1020	23.35	-1.13	-1.06

TABLE XXI (Continued)

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
102.00	0.0130	0.1130	0.8750	0.0120	0.0580	0.9300	0.9231	0.5133	1.0629	0.9174	0.5051	1.0623	-0.61	-1.59	-0.05 *
102.00	0.0500	0.0940	0.8570	0.0390	0.0500	0.9110	0.7800	0.5319	1.0630	0.8550	0.5211	1.0623	9.61	-2.03	-0.07 *
102.40	0.0770	0.1140	0.8090	0.0410	0.0580	0.9010	0.5325	0.5088	1.1137	0.8602	0.5514	1.0696	61.56	8.37	-3.96
103.40	0.1840	0.1170	0.6980	0.1410	0.0760	0.7830	0.7663	0.6496	1.1218	0.7979	0.6610	1.0988	4.13	1.76	-2.05
104.60	0.3200	0.0900	0.5900	0.2520	0.0630	0.6850	0.7875	0.7000	1.1610	0.7603	0.7820	1.1532	-3.46	11.72	-0.67
106.60	0.3760	0.1770	0.4460	0.3200	0.1590	0.5210	0.8511	0.8983	1.1629	0.8193	0.9319	1.1773	-3.73	3.75	1.23
107.40	0.4190	0.1990	0.3820	0.3650	0.1800	0.4540	0.8711	0.9045	1.1885	0.8264	0.9958	1.1944	-5.13	10.09	0.49
108.30	0.5290	0.1440	0.3270	0.4650	0.1380	0.3980	0.8790	0.9583	1.2171	0.8185	1.0543	1.2589	-6.88	10.01	3.43
109.20	0.5440	0.2210	0.2350	0.4800	0.2550	0.2640	0.8824	1.1538	1.1234	0.8439	1.1347	1.2304	-4.36	-1.66	9.53
109.00	0.5290	0.2940	0.1780	0.4620	0.3360	0.2030	0.8733	1.1429	1.1404	0.8485	1.1506	1.1659	-2.84	0.68	2.23
110.30	0.6310	0.2230	0.1470	0.5620	0.2620	0.1770	0.8906	1.1749	1.2041	0.8548	1.2082	1.2646	-4.03	2.83	5.03
107.10	0.3930	0.4770	0.1300	0.3420	0.5250	0.1330	0.8702	1.1006	1.0231	0.8491	1.1181	0.9493	-2.42	1.59	-7.21
107.20	0.1930	0.4830	0.3240	0.1880	0.5010	0.3110	0.9741	1.0373	0.9599	1.1035	0.9895	0.9763	13.28	-4.61	1.71 *
106.70	0.1770	0.5540	0.2690	0.1740	0.5860	0.2370	0.9831	1.0632	0.8810	0.9929	1.0466	0.8898	1.00	-1.56	0.99
105.80	0.1270	0.6530	0.2200	0.1220	0.6850	0.1930	0.9606	1.0490	0.8773	1.0096	1.0558	0.7805	5.10	0.65	-11.03
107.00	0.1600	0.5350	0.3040	0.1660	0.5700	0.2640	1.0375	1.0654	0.8684	1.0350	1.0238	0.9357	-0.24	-3.91	7.75 *
106.10	0.1040	0.6470	0.2500	0.1100	0.6700	0.2210	1.0577	1.0355	0.8840	1.0462	1.0525	0.7966	-1.08	1.54	-9.89
105.60	0.0930	0.6680	0.2390	0.0860	0.7110	0.2030	0.9247	1.0644	0.8494	1.0483	1.0563	0.7476	13.36	-0.76	-11.98 *

TABLE XXI (Continued)

TEMP DEG C	LIQUID MOLE FRACTION COMP NUM			VAPOR MOLE FRACTION COMP NUM			EXP K VALUES COMP NUM			CAL K VALUES COMP NUM			% ERROR IN K VALUES COMP NUM		
	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
104.70	0.0680	0.7220	0.2100	0.0640	0.7610	0.1750	0.9412	1.0540	0.8333	1.0330	1.0541	0.6744	9.75	0.01	-19.07 *
106.90	0.0510	0.6270	0.3220	0.0520	0.6630	0.2840	1.0196	1.0574	0.8820	1.1947	1.0448	0.8411	17.17	-1.20	-4.64 *
107.20	0.0640	0.4540	0.4820	0.0650	0.4310	0.5040	1.0156	0.9493	1.0456	1.2592	0.9089	1.0506	23.99	-4.26	0.47 *
107.00	0.1550	0.3930	0.4520	0.1540	0.3790	0.4670	0.9935	0.9644	1.0332	1.0927	0.9398	1.0316	9.98	-2.55	-0.15 *
107.20	0.2580	0.3370	0.4040	0.2470	0.3330	0.4210	0.9574	0.9881	1.0421	0.8994	0.9911	1.0908	-6.06	0.30	4.67
107.90	0.4070	0.2590	0.3340	0.3760	0.2580	0.3670	0.9238	0.9961	1.0988	0.8463	1.0441	1.1702	-8.39	4.82	6.50
ABSOLUTE AVERAGE PERCENT ERROR												9.44	2.94	4.28	

* FLASH CALCULATION DID NOT CONVERGE

TABLE XXII
 SUMMARY OF RESULTS FOR THE BINARY AND TERNARY
 SYSTEMS STUDIED

System	Abs. Avg. % Error Comp. No.		
	1	2	3
Acetone-Methyl Ethyl Ketone	16.21	5.33	(14.7 psia.)
N-Propyl Alcohol-Water	17.84	14.09	
Isopropyl Alcohol-Water	11.59	7.96	
Water-Propionic Acid	16.88	10.49	
Methanol-Water	10.87	3.60	
Acetone-Water	15.91	11.76	
Methyl Ethyl Ketone-Water	28.02	14.61	
Acetone-Methyl Ethyl Ketone	3.67	3.13	(500 psia.)
Ethanol-Water	5.49	3.59	
Formic Acid-Acetic Acid	2.52	5.45	
Water-Acetic Acid	2.69	2.74	
Water-Formic Acid	3.18	4.85	
Methanol-Ethanol	2.42	3.18	
Acetone-Methanol	3.82	6.12	
Acetone-Ethanol	3.06	3.97	
Acetone-Methanol-Ethanol	5.02	2.44	7.62
Methanol-Ethanol-Water	7.39	8.73	8.08
Acetone-Methyl Ethyl Ketone-Water	23.75	32.38	17.85
Acetic Acid-Formic Acid-Water	9.44	2.94	4.28

Acid-Acetic Acid system given in Table XII and the Methanol-Ethanol system given in Table XV. An x-y plot is given in Figure 6 for the Formic Acid-Acetic Acid system as an example of the type of system behavior for which the method studied works best. The method gives absolute average percent errors greater than 10% around azeotrope points and points where one or more component mole percents are less than 10%. Poor behavior around an azeotrope point is illustrated by the Methyl Ethyl Ketone-Water system given in Table IX. For the first nine points of the system the method worked well. On the other side of the azeotrope at the tenth point, however, the experimental K-values show component one to be the most volatile but the calculated K-values show component two to be the most volatile. This failure to correctly predict the relative volatilities continues until the thirteenth point when the prediction method over corrects the relative volatilities and predicts a K-value much higher than the experimental K-value for component one. Poor behavior at small component mole fractions can also be seen in this system but is better illustrated by the Ethanol-Water system in Table XI. For the first two points of this system the mole fractions of ethanol in the liquid are 0.005 and 0.01. The corresponding errors in the K-values for ethanol are -19.65 and -10.86 percent. For the rest of the points the mole fraction of ethanol in the liquid is over twice as large and the K-value error is much less than 10%. An x-y plot for the Methyl Ethyl Ketone-Water system is given in Figure 7 as an illustration of the type of system behavior which gives the least accurate results for the systems studied. For all systems studied the errors in K-values above 10% seem to be caused by bad behavior around azeotrope points or points with component mole

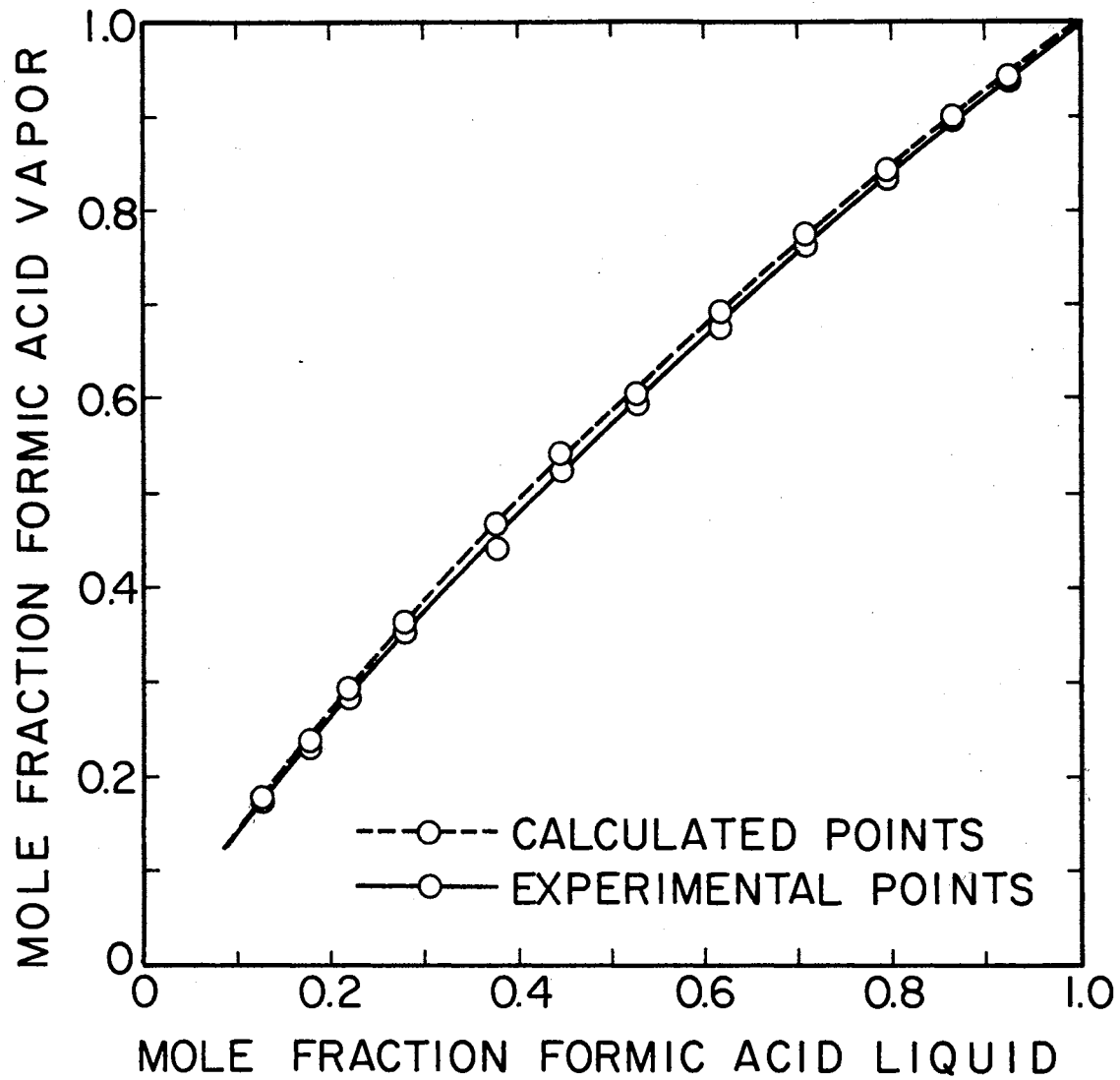


Figure 6. Comparison of Calculated and Experimental Values for Formic Acid-Acetic Acid System

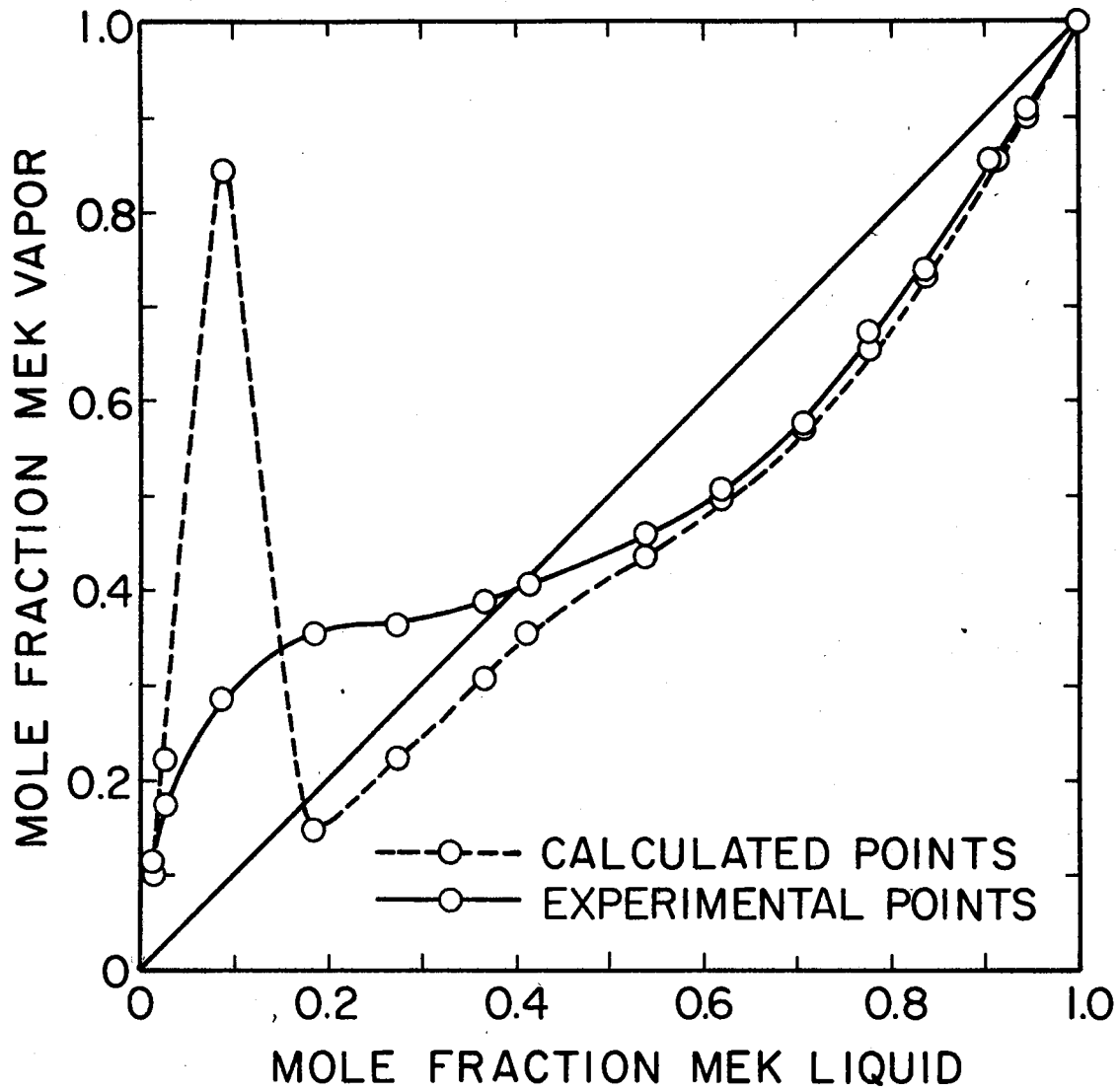


Figure 7. Comparison of Calculated and Experimental Values for Methyl Ethyl Ketone-Water System

percents less than 10% or occasionally bad experimental data. The poor behavior around azeotrope points could be caused by the equation of state giving incorrect liquid densities in that region. However, this may or may not be the only problem.

CHAPTER V

CONCLUSION AND RECOMMENDATIONS

The results of this study clearly show that for many highly non-ideal binary systems K-value prediction using the Soave modification of the Redlich-Kwong equation of state gives K-value percent errors of less than 10%. These results are particularly good in light of the fact that only two semi-empirical correction factors, an Ω_b for each component and a k_{ij} for each component pair, are used in the calculation procedure. It has been shown, using values of Ω_b and k_{ij} predicted from binary data, that K-values of ternary systems can be predicted with almost the same accuracy as binary systems. This indicates that values of Ω_b and k_{ij} predicted from binary data should work well for systems with any number of components.

In light of the findings of this study it is recommended that this K-value prediction method be further developed. The first subject of future work should be the improvement of the method's accuracy around azeotrope points and at component mole percents less than 10%. This should cause the relationship of Ω_b , k_{ij} , and percent error for all systems to be similar to that in Figure 4 and very distinct values of Ω_b and k_{ij} for the minimum percent error could then be determined. After finding values of Ω_b for many compounds and k_{ij} for many binary pairs, some type of correlation should be developed for calculating these values. A study should also be made of how Ω_b and k_{ij} vary with

pressure. As can be seen from the values of Ω_b for Acetone in Table I, at 14.7 and 500.0 psia., there is some indication that Ω_b , at least, varies considerably with pressure. Finally, a comparison should be made between the analytical and iterative procedures for solving the cubic form of the equation of state. There is some indication that the iterative procedure gives more accurate results because of significant computer round off error in the analytical procedure.

BIBLIOGRAPHY

1. Prausnitz, J. M., Molecular Thermodynamics of Fluid-Phase Equilibria, Englewood Cliffs, N. J.: Prentice-Hall, 1969.
2. Wohl, K., Trans. A.I.Ch.E., 42, (1946)215.
3. Wilson, G. M., J. Am. Chem. Soc., 86, (1964)127.
4. Orye, R. V., and J. M. Prausnitz, Ind. Eng. Chem., 57, No. 5, (1965)19.
5. Renon, H., and J. M. Prausnitz, A.I.Ch.E. Journal, 14, (1968)135.
6. Palmer, P. A., and Smith, Ind. Eng. Chem. Process Des. and Devel., 11, (1972)114.
7. Peter, S., and H. Wenzel, Chemie. Ing. Techn., 43, (1971)623.
8. Bonner, D. C., E. R. Bazua, and J. M. Prausnitz, Ind. Eng. Chem. Fundam., 12, No. 2, (1973)254.
9. Soave, G., Chem. Eng. Sci., 27, (1972)1197.

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