

COMPUTER EVALUATION OF BINARY
VAPOR-LIQUID EQUILIBRIUM DATA

by

JOHN WARREN MACAN

A THESIS

submitted to

OREGON STATE COLLEGE

in partial fulfillment of
the requirements for the
degree of

MASTER OF SCIENCE

June 1960

APPROVED:

Redacted for Privacy

Associate Professor of Chemical Engineering

In Charge of Major

Redacted for Privacy

Head of Department of Chemical Engineering

Redacted for Privacy

Chairman of School Graduate Committee

Redacted for Privacy

Dean of Graduate School

Date thesis is presented October 7, 1959

Typed by Miriam Schubert

ACKNOWLEDGEMENT

The author wishes to express his appreciation to Dr. C. E. Wicks, Mr. Donald Amos and Mr. A. A. Faruqui for their assistance in making this work possible. The author also wishes to thank the Mathematics Department for suggesting various power series and for the use of the computer.

TABLE OF CONTENTS

	Page
INTRODUCTION	1
THEORY	3
DISCUSSION OF COMPUTER OPERATIONS	12
DISCUSSION OF RESULTS	16
CONCLUSIONS	22
RECOMMENDATIONS	23
NOMENCLATURE	24
BIBLIOGRAPHY	25
APPENDIX	27

FIGURES

	Page
1. Diagram of Computer Operations	13
2. Comparison of Results System: Ethyl Acetate - Ethanol	19
3. Comparison of Results System: Carbon Tetrachloride - Ethyl Acetate	20

TABLES OF EXPERIMENTAL AND CALCULATED DATA

Table No.		Page
1.	Acetone - Acetic Acid	27
2.	Acetone - Methanol	28
3.	Acetone - Water	29
4.	Benzene - Cyclohexane	31
5.	Benzene - Ethylene Dichloride	32
6.	Carbon Disulfide - Acetone	33
7.	Carbon Tetrachloride - Ethyl Acetate	34
8.	Carbon Tetrachloride - n-Propanol	35
9.	Cyclohexane - Cyclohexene	36
10.	Cyclohexane - 2,2,3 Trimethylbutane	37
11.	Ethanol - Trichloroethylene	38
12.	Ethanol - Water	39
13.	Ethyl Acetate - Benzene	40
14.	Ethyl Acetate - Ethanol	41
15.	Ethyl Acetate - Ethylene Dichloride	42
16.	n-Heptane - Methyl Cyclohexane	43
17.	n-Heptane - Toluene	44
18.	Methanol - Benzene	45
19.	Methanol - Trichloroethylene	46
20.	Methanol - Water	47
21.	Isooctane - Toluene	48

TABLES OF EXPERIMENTAL AND CALCULATED DATA, Continued

Table No.		page
22. n-Propanol - Water		49
23. Toluene - n-Octane		50
24. Toluene - Phenol		52
25. Water - Acetic Acid		53
26. Water - n-Butanol		55

COMPUTER EVALUATION OF BINARY VAPOR-LIQUID EQUILIBRIUM DATA

INTRODUCTION

Binary vapor-liquid equilibrium data are used in the design and performance evaluation of costly equipment involved in various separation processes. Therefore, it is important to have accurate data on which to rely.

There is a vast amount of vapor-liquid equilibrium data in the literature reported at either constant temperature or constant pressure. Unfortunately, the accuracy of much of this data is questionable. For many systems, conflicting results have been reported thus presenting a confusing problem to the user of such data.

Consequently, O. Redlich and A. T. Kister (7), (8) have proposed two methods based on thermodynamic relations for testing such data. The first method, which is known as the area test, can be used to evaluate the thermodynamic consistency of experimental data. The slope test, as the second method is called, can be used to pinpoint the errors in the inconsistent data.

Redlich and Kister (7), (8) also developed a power series for smoothing experimental data which could be

used to classify the systems according to which terms were necessary to define the data. However, Stockett (12) found that all of the terms are necessary to define the data; and therefore, it would be difficult to classify binary systems using this power series. Therefore, it is proposed that a new series of orthogonal polynomials be used for this purpose.

The Alwac III-E digital computer was used to evaluate previously published data for thermodynamic consistency by means of the area test using the proposed orthogonal polynomial series. For each set of data, the computer also determined the coefficients of the new power series so that each system could be classified according to the terms necessary to define the data.

THEORY

For binary mixtures, the basic equation used to predict vapor-liquid equilibria is a combination of the laws of Raoult and Dalton expressed as

$$(1) \quad y\pi = xP^{\circ}.$$

This equation is applicable only for systems of ideal solutions and ideal vapors. Since such systems seldom are encountered in practice, it is therefore necessary to correct for these deviations from ideality.

To correct for the vapor phase deviations, Lewis and Randall (4, p. 221, 328) suggested that the pressure terms in equation (1) be replaced by fugacities. However, when operating near atmospheric pressure, the fugacity and pressure terms are nearly equal for most substances and the use of either is acceptable.

The deviations of the liquid phase are more important than those of the vapor phase and, in general, are greater in magnitude. Even at low pressures most liquids deviate from ideality. These liquid phase deviations are corrected for by a factor, γ , called the activity coefficient. For low pressures where the fugacity is equal to the pressure, equation (1) now becomes

$$(2) \quad y\pi = \gamma xP^{\circ}.$$

The activity coefficient is obtained easily by rearranging equation (2) to the form

$$(3) \quad \gamma = \frac{\pi}{x P^0} .$$

In a binary mixture, the activity coefficients for each component are not equal; but are related by the Duhem equation in the form

$$(4) \quad x_1 \left[\frac{\partial \log \gamma_1}{\partial x_1} \right]_{\pi, t} + (1-x_1) \left[\frac{\partial \log \gamma_2}{\partial x_1} \right]_{\pi, t} = 0$$

It would involve a considerable amount of calculations to solve the Duhem equation precisely. Consequently, Margules (9, p. 54-56), van Laar (9, p. 56-60), Scatchard (9, p. 59), and others have devised approximation methods for predicting the required activity coefficients from experimental data. The use of these approximation formulas introduces some uncertainty as to whether the deviations of the original values, as determined by equation (3), from the smoothed values are due to experimental errors or to the insufficient validity of the approximation formulas.

If experimental data are to be used to calculate activity coefficients, some procedure must be used to smooth the data. Also the data should be checked for thermodynamic consistency to insure the best possible results. Redlich and Kister (7), (8) have proposed a method for binary systems which will smooth experimental

data and also indicate its thermodynamic consistency.

A form of Scatchard's "excess free energy" equation (11) is used as a starting point.

$$(5) \quad Q = x_1 \log \gamma_1 + (1-x_1) \log \gamma_2$$

Applying the boundary conditions that $\gamma_1 = 1$ for $x_1 = 1$, and $\gamma_2 = 1$ for $x_2 = 1$, the excess free energy function, Q , becomes zero for any pure component. Differentiation of equation (5) with respect to x_1 yields the more useful relation

$$(6) \quad \frac{dQ}{dx_1} = \log \gamma_1 - \log \gamma_2 + x_1 \left[\frac{\partial \log \gamma_1}{\partial x_1} \right] + (1-x_1) \left[\frac{\partial \log \gamma_2}{\partial x_1} \right].$$

At constant temperature and pressure, equations (4) and (6) can be combined to yield

$$(7) \quad \frac{dQ}{dx_1} = \log \frac{\gamma_1}{\gamma_2}.$$

Applying the boundary conditions that $Q = 0$ at $x_1 = 0$ and $x_1 = 1$, it is evident that on integrating, equation (7) becomes

$$(8) \quad Q = \int_0^1 \log \frac{\gamma_1}{\gamma_2} dx_1 = 0.$$

Equation (8) can be used to evaluate the thermodynamic consistency of experimental data. The activity coefficients of the two components can be determined by means of equation (3); and if the logarithm of their ratio is plotted against the mole fraction of the more volatile component in the liquid phase, the net area under the

resulting curve must equal zero or the experimental data is not thermodynamically consistent. This area test is strictly applicable only at constant temperature and pressure. However, for practical purposes it can be extended to data obtained over a moderately small boiling range with little discrepancy.

Unfortunately, the area test does not give a clue as to the source of any error in the experimental data. That is, it does not tell whether the source of error is due to the liquid or to the vapor composition. Therefore, Redlich and Kister (7), (8) have proposed a "slope test" in order to pinpoint these errors. In this test, equation (2) is logarithmically differentiated and substituted into the Duhem equation, equation (4), to obtain

$$(9) \quad \frac{dt}{dy_1} = \frac{0.4343 (x_1 - y_1)}{y_1 (1-y_1)} \left[\frac{1}{x_1 \frac{d \log P_1^{\circ}}{dt} + (1-x_1) \frac{d \log P_2^{\circ}}{dt}} \right].$$

This equation may be used to calculate the slope of the dewpoint curve (y_1 vs t) at various experimental points. Unless the experimental data are thermodynamically consistent, the calculated slopes will not lie tangent to the curve drawn through the data. This calculation is very sensitive to differences in composition. If the vapor composition is high or the liquid composition low, the calculated slope will be greater than the experimental slope; and if the reverse is true, the calculated slope

will be smaller. Equation (9), having been obtained through the use of the Duhem equation, is strictly applicable only at constant temperature and pressure. However, it is sufficiently accurate to allow for small changes in either temperature or pressure.

In order to smooth experimental data, Redlich and Kister (7), (8) suggested that the function Q be represented by a power series in x_1 . Since $Q = 0$ for $x_1 = 0$ and $x_1 = 1$, it was necessary to include the factor $x_1(1-x_1)$ in every term of the series. It was also desirable to develop the series with respect to a variable which is symmetric with respect to the two components.

The simplest variable of this kind is $(2x_1-1)$. Application of these conditions gave for Q the series

$$(10) \quad Q = x_1(1-x_1) [B + C(2x_1-1) + D(2x_1-1)^2 + E(2x_1-1)^3].$$

Differentiating equation (10) with respect to x_1 yields

$$(11) \quad \frac{dQ}{dx_1} = B(1-2x_1) + C[-1 + 6x_1(1-x_1)] + \\ D(2x_1-1)[-1 + 8x_1(1-x_1)] + E(2x_1-1)^2[-1+10x_1(1-x_1)].$$

Combining equations (7) and (11) yields

$$(12) \quad \log \frac{x_1}{\delta_2} = B(1-2x_1) + C[-1 + 6x_1(1-x_1)] + \\ D(2x_1-1)[-1 + 8x_1(1-x_1)] + E(2x_1-1)^2[-1+10x_1(1-x_1)].$$

Not only is this series flexible and convenient to use, but it also furnishes a natural method for classifying systems. A system may be classified according to

which terms are necessary to define the function $\log(\gamma_1/\gamma_2)$. Redlich and Kister (7, p. 346) suggest five different types of systems ranging from a perfect solution where all the coefficients are equal to zero to a highly imperfect solution which would require four terms.

Using the Alwac III-E digital computer, Stockett (12) calculated the coefficients to equation (12) from experimental data obtained on several systems that ranged from nearly ideal to extremely imperfect. The author concluded that "satisfying the method of classifying binary systems, as proposed by Redlich and Kister, would be difficult unless one beforehand has some idea as to which classification a system in question belongs."

Consequently, it has been suggested that the function $\log(\gamma_1/\gamma_2)$ might be represented better by a series of orthogonal polynomials, such as the Legendre polynomials for the interval zero to one. Thus, $\log(\gamma_1/\gamma_2)$ would be represented by the series

$$(13) \quad \log \frac{\gamma_1}{\gamma_2} = aP_0(x_1) + bP_1(x_1) + cP_2(x_1) + dP_3(x_1) + eP_4(x_1)$$

where (6, p. 260)

$$(14) \quad P_0(x_1) = 1,$$

$$(15) \quad P_1(x_1) = 1 - 2x_1,$$

$$(16) \quad P_2(x_1) = 1 - 6x_1 + 6x_1^2,$$

$$(17) \quad P_3(x_1) = 1 - 12x_1 + 30x_1^2 - 20x_1^3,$$

and

$$(18) \quad P_4(x_1) = 1 - 20x_1 + 90x_1^2 - 140x_1^3 + 70x_1^4.$$

These orthogonal polynomials have two very important properties, namely (6, p. 260-261)

$$(19) \quad \int_0^1 P_m(x_1) P_n(x_1) dx_1 = 0$$

when $m \neq n$, and

$$(20) \quad \int_0^1 P_m^2(x_1) dx_1 = \frac{1}{2m+1}$$

when $m = n$.

Multiplying both sides of equation (13) by $P_0(x_1)$ dx_1 and integrating between the limits $x_1 = 0$ and $x_1 = 1$, yields

$$(21) \quad \begin{aligned} \int_0^1 P_0(x_1) \log \frac{x_1}{\delta_2} dx_1 &= a \int_0^1 P_0^2(x_1) dx_1 \\ &+ b \int_0^1 P_0(x_1) P_1(x_1) dx_1 + c \int_0^1 P_0(x_1) P_2(x_1) dx_1 \\ &+ d \int_0^1 P_0(x_1) P_3(x_1) dx_1 + e \int_0^1 P_0(x_1) P_4(x_1) dx_1. \end{aligned}$$

From the conditions given by equations (14), (19), and (20), equation (21) reduces to

$$(22) \quad \int_0^1 \log \frac{x_1}{\delta_2} dx_1 = a.$$

In comparing equations (8) and (22), it will be noted that in order for the experimental data to be thermodynamically consistent equation (22), and consequently the coefficient "a", must be equal to zero. Thus, the first coefficient of this series indicates the results of the area test.

The remaining coefficients, b, c, d, and e, of equation (13) can be determined by multiplying both sides of that equation by $P_1(x_1) dx_1$, $P_2(x_1) dx_1$, $P_3(x_1) dx_1$, or $P_4(x_1) dx_1$ respectively and integrating between the limits $x_1 = 0$ and $x_1 = 1$. Expressed mathematically,

$$(23) \quad b = \int_0^1 P_1(x_1) \log \frac{\gamma_1}{\gamma_2} dx_1 ,$$

$$(24) \quad c = \int_0^1 P_2(x_1) \log \frac{\gamma_1}{\gamma_2} dx_1 ,$$

$$(25) \quad d = \int_0^1 P_3(x_1) \log \frac{\gamma_1}{\gamma_2} dx_1 ,$$

$$(26) \quad e = \int_0^1 P_4(x_1) \log \frac{\gamma_1}{\gamma_2} dx_1 .$$

It will be noted that all the coefficients in the Legendre polynomial series can be evaluated by plotting the function $P_n(x_1) \log (\gamma_1/\gamma_2)$ against x_1 and determining the net area under the curves. This method for evaluating the coefficients has the advantage that terms can be dropped from the series without affecting the

value of the remaining coefficients. That is, for a given set of data, the value of each coefficient is independent of the number of terms in the series.

Like the series proposed by Redlich and Kister, this series can be used to classify various systems. The greater the deviation of a system from ideality, the greater the number of terms necessary to define the function $\log (\gamma_1/\gamma_2)$.

DISCUSSION OF COMPUTER OPERATION

To test binary vapor-liquid equilibrium data obtained from the literature for thermodynamic consistency, the mathematical relationships involved were programmed on the Alwac III-E digital computer.

The overall routine consists of twenty-one channels of instruction and twenty-two channels for information storage. Up to twenty experimental points can be handled by the routine. Figure 1 is a schematic diagram of the calculations made by the computer for each set of data.

In order to apply the area test as expressed by equation (8), it was necessary to obtain vapor pressure data for each component under consideration. This was accomplished by using the Antoine equation,

$$(27) \log P^{\circ} = A - \frac{B}{C + t}$$

which expresses the logarithm of the vapor pressure as a function of three constants and the temperature. In most cases, the constants in this equation were readily available (3), (10, p. 336-367).

Most vapor-liquid equilibrium data found in the literature are presented in tabular form with the compositions of the more volatile component in both liquid and vapor phases given at various temperatures; the total

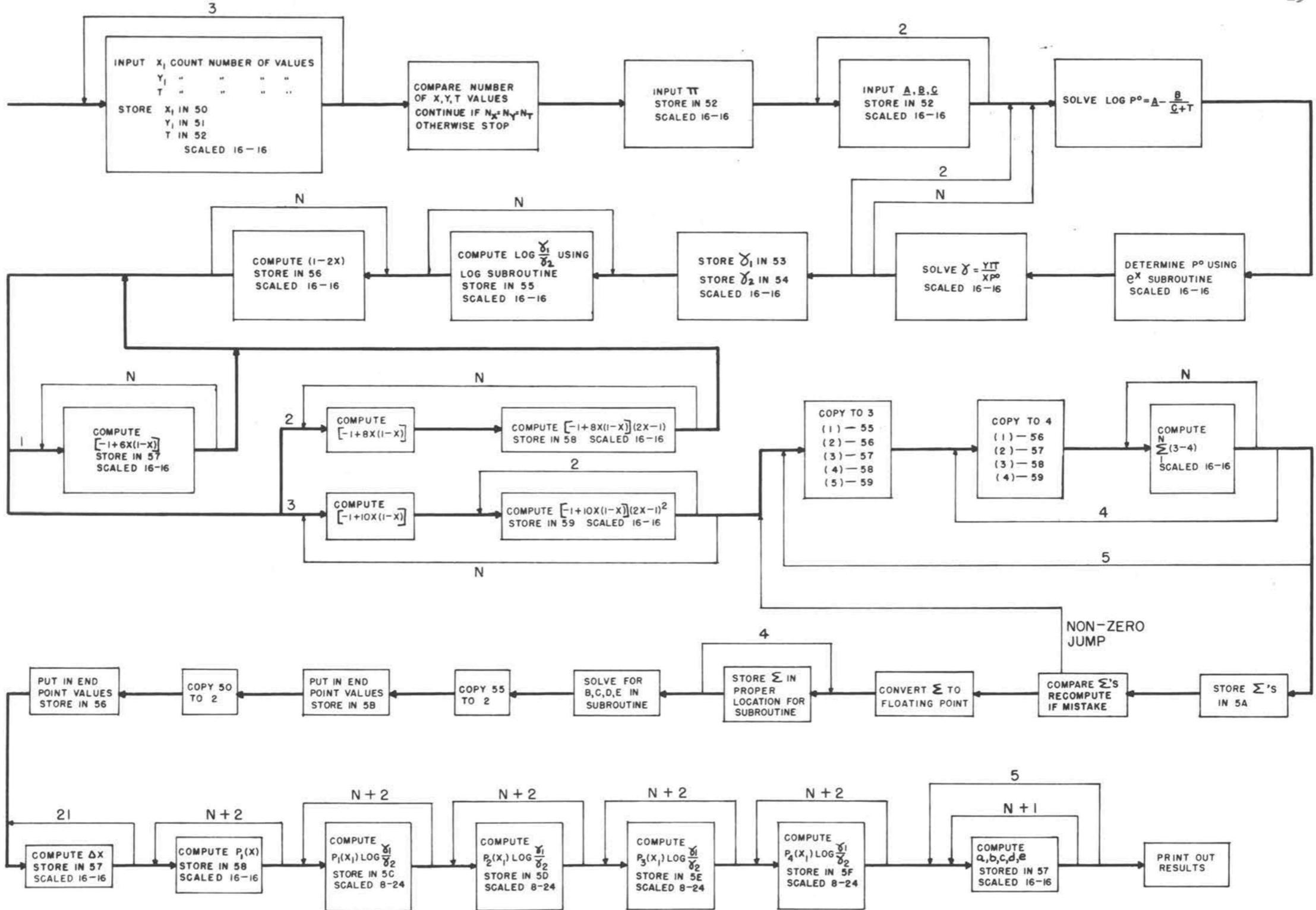


DIAGRAM OF COMPUTER OPERATIONS

FIGURE I

pressure of the system remaining constant. Each set of x , y , t data followed by the total pressure and the constants for the Antoine equation were punched on tape. As each punched tape of data was fed to the computer, a scheme checked to see that the same number of x , y , and t data points were accepted by the machine. If the computer did not accept the same number of x , y , and t values, it was instructed to stop. It then would be necessary to correct the error and resubmit the data.

Once the necessary data were inserted and stored, the computer proceeded to calculate vapor pressures, activity coefficients, and the logarithm of the ratio of the activity coefficients for each experimental point.

For each experimental point, the computer next calculated the polynomials represented by the right half of equation (12). Utilizing this data and the logarithms of the ratio of the activity coefficients, the computer proceeded to determine the coefficients of equation (12) by the method of least squares.

These coefficients then were used to determine the values of the logarithm of the ratio of the activity coefficients at the end points; e.g.

at $x_1 = 0$

$$(28) \quad \log \frac{y_1}{y_2} = B - C + D - E$$

and at $x_1 = 1$

$$(29) \quad \log \frac{\gamma_1}{\gamma_2} = -B - C - D - E$$

The next step in the routine involved the calculation of the product of the logarithm of the ratio of the activity coefficients and the proper Legendre polynomial for each data point. This was done by making use of the recurrence relationship

$$(30) \quad \left(\log \frac{\gamma_1}{\gamma_2} \right) P_{n+1}(x_1) = \left(\frac{2n+1}{n+1} \right) \left(\log \frac{\gamma_1}{\gamma_2} \right) (1-2x_1) P_n(x_1) \\ - \left(\frac{n}{n+1} \right) \left(\log \frac{\gamma_1}{\gamma_2} \right) P_{n-1}(x_1).$$

The trapezoidal rule in the form of

$$(31) \quad \int_0^1 P_n(x_1) \log \frac{\gamma_1}{\gamma_2} dx_1 = \frac{1}{2} \sum_{k=0}^{k=N+1} \left[\left(P_n(x_1) \log \frac{\gamma_1}{\gamma_2} \right)_k + \left(P_n(x_1) \log \frac{\gamma_1}{\gamma_2} \right)_{k+1} \right] (x_{k+1} - x_k)$$

was used in evaluating the coefficients of equation (13). Upon substituting these coefficients (a, b, c, d, and e) into equation (13), the resulting expression best represents the smoothed data. The first coefficient, a, represents the results of the area test and indicates the thermodynamic consistency of the experimental data.

DISCUSSION OF RESULTS

The experimental and calculated results are presented in tables 1 through 26 for the systems acetone - acetic acid (2, p. 10), acetone - methanol (2, p. 19), acetone - water (2, p. 22-23), benzene - cyclohexane (2, p. 29), benzene - ethylene dichloride (2, p. 33), carbon disulfide - acetone (2, p. 49), carbon tetrachloride - ethyl acetate (2, p. 58), carbon tetrachloride - n-propanol (2, p. 59), cyclohexane - cyclohexene (2, p. 67), cyclohexane - 2, 2, 3 trimethylbutane (2, p. 69), ethanol - trichloroethylene (2, p. 86), ethanol - water (2, p. 91-92), ethyl acetate - benzene (5, p. 62-64), ethyl acetate - ethanol (2, p. 95), ethyl acetate - ethylene dichloride (5, p. 60-61), n-heptane - methyl cyclohexane (2, p. 108), n-heptane - toluene (2, p. 109), methanol - benzene (2, p. 138), methanol - trichloroethylene (2, p. 142), methanol - water (2, p. 143), isoctane - toluene (2, p. 178), n-propanol - water (2, p. 193), toluene - n-octane (2, p. 200-202), toluene - phenol (2, p. 203), water - acetic acid (2, p. 208-210), and water - n-butanol (2, p. 213). Two sets of data, each at a different pressure, were examined for the systems acetone - water and toluene - n-octane. Two sets of data at the same pressure were examined for the system water -

acetic acid.

As previously stated, the area test as proposed by Redlich and Kister is applicable for data obtained over a moderately small boiling range. The greatest temperature difference encountered was approximately sixty degrees centigrade. However, nearly all of the data had a temperature range of less than thirty degrees centigrade. Redlich and Kister have applied the area test to data where the boiling range was about fourty-six degrees centigrade. Along with this, it was stated (8, p. 51) that this interval was "somewhat too large for the strict validity of equation (8), but any likely deviation from (8) would increase the discrepancy." The results of the area test for the systems acetone - acetic acid and toluene - phenol can be considered only approximations due to the large temperature range.

By means of the area test, the computer checked the experimental data for thermodynamic consistency. It also calculated the coefficients of equations (12) and (13).

To evaluate the coefficients of equation (13), it was necessary to extrapolate the function $\log (\gamma_1 / \gamma_2)$ to the end points $x_1 = 0$ and $x_1 = 1$. The ccoefficients of equation (12) in the form expressed by equations (28) and (29) were used for this purpose. It is felt that this was the best method of extrapolating as all the experimental

points were used and not just the values near the end points.

For each set of data, experimental and calculated values of the function $\log(\gamma_1/\gamma_2)$ were obtained. The experimental values were determined by means of equation (3); and equation (13) was used to determine the calculated values.

It was found that the experimental results and those determined by means of equation (13) agreed quite well even though the data were not thermodynamically consistent. However, this was not true for the series proposed by Redlich and Kister. If the data were consistent or nearly so, the results determined by means of the Redlich Kister series, equation (12), and the Legendre polynomial series, equation (13), agreed very well with the experimental results (see figure 2). For inconsistent data, the results determined means of equation (12) did not agree with the experimental results (see figure 3). When the two series are compared term by term, the reason for this discrepancy becomes apparent. The first term in the Legendre polynomial series is a constant which is equal to zero only if the experimental data is thermodynamically consistent. The Redlich Kister series does not contain such a term.

It was found that the data for most of the systems

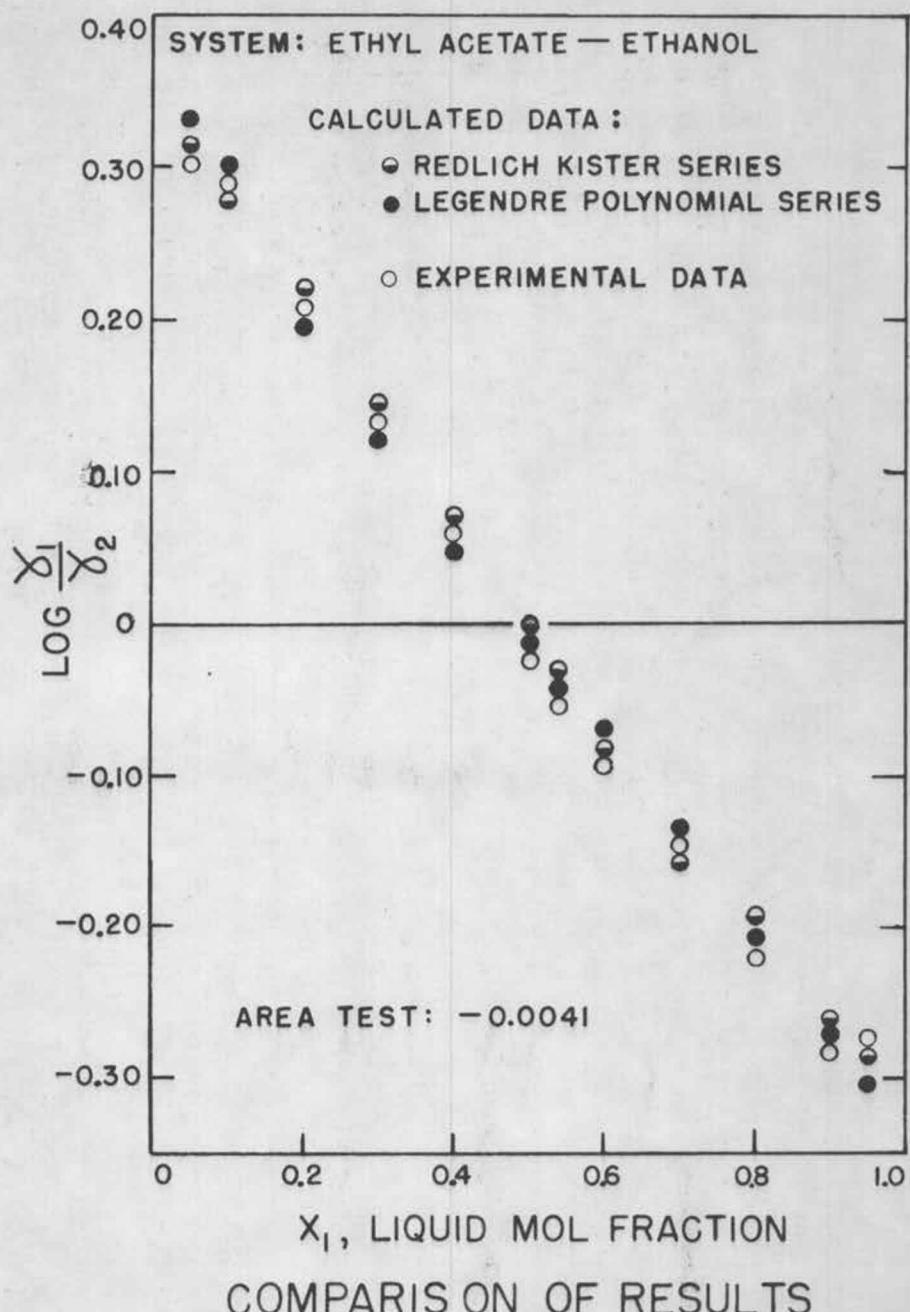
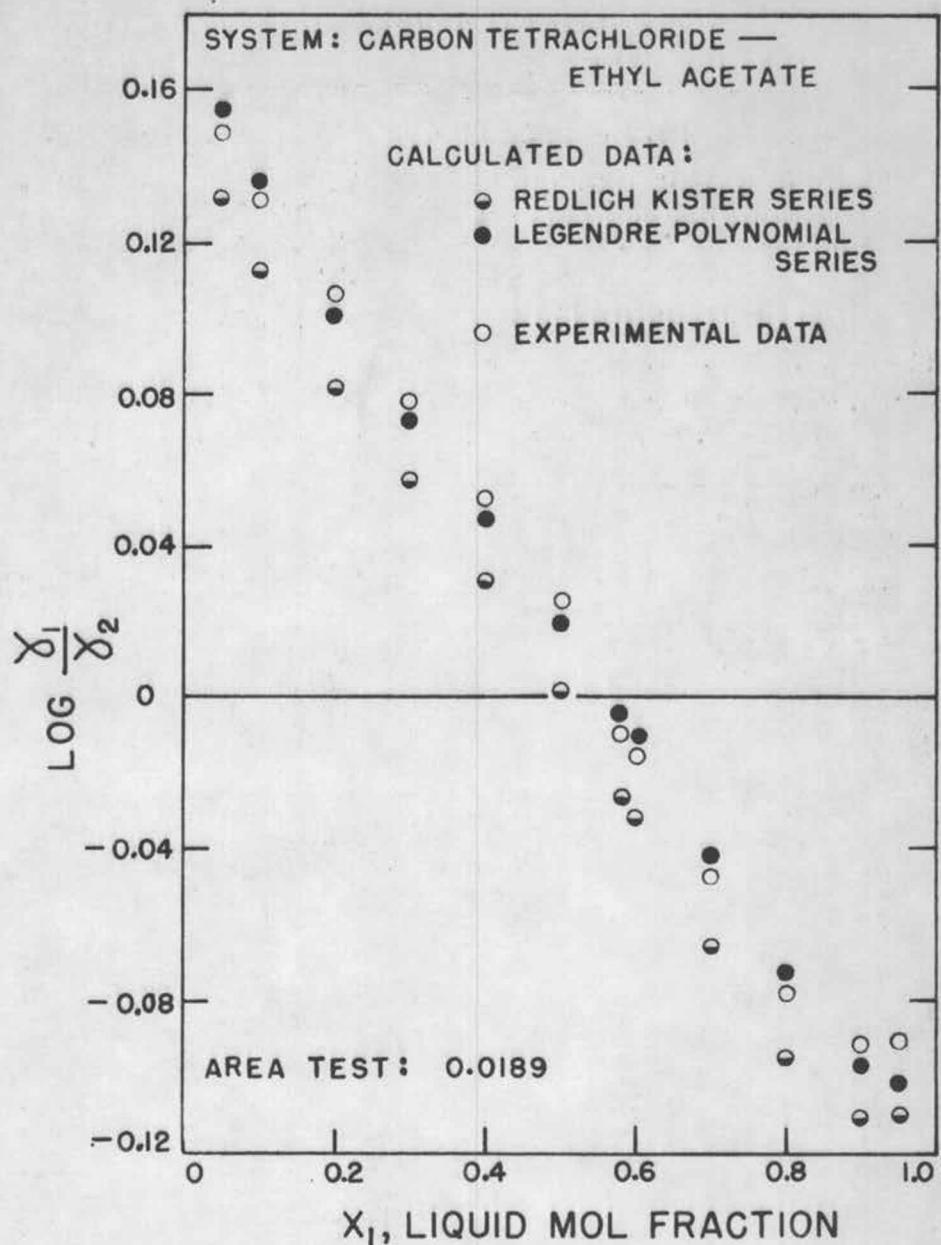


FIGURE 2



COMPARISON OF RESULTS

FIGURE 3

studied were not thermodynamically consistent. Data for the systems benzene - cyclohexane, ethyl acetate - benzene, ethyl acetate - ethanol, ethyl acetate - ethylene dichloride, n-heptane - toluene, methanol - benzene, methanol - trichloroethylene, and isoctane - toluene were found to be fairly consistent. The only thermodynamically consistent data were for the systems benzene - ethylene dichloride and ethanol - trichloroethylene. For all practical purposes, the system benzene - ethylene dichloride can be considered an ideal system because the activity coefficients were all very close to one. For an ideal system, the function $\log (\gamma_1/\gamma_2)$ equals zero for all values of x_1 .

For nearly all the systems studied, it was found that the experimental data were represented best by using all the terms in equation (13). The systems whose data were found to be consistent or nearly so, possibly could be classified as Redlich and Kister proposed since some of the coefficients were relatively small.

CONCLUSIONS

1. The majority of the vapor-liquid equilibrium data studied did not satisfy the Redlich and Kister area test for thermodynamic consistency.
2. The Legendre polynomial series will define the function $\log(\gamma_1/\gamma_2)$ very satisfactorily even though the experimental data may be thermodynamically inconsistent. The Redlich-Kister series will give as good results only if the experimental data is consistent.
3. The Legendre polynomial series has the added advantage over the Redlich-Kister series in that the first coefficient indicates the thermodynamic consistency of the experimental data.
4. Experimental data that satisfies the Redlich and Kister area test possibly could be classified according to the number of terms in the proposed series that are necessary to define the data. In order to classify the systems it will first be necessary to determine the importance of each term in the series by means of statistical analysis. The data appeared to be represented best when all of the terms in the proposed series were used.

RECOMMENDATIONS

1. It strongly is recommended that work be continued to evaluate binary vapor-liquid equilibrium data for thermodynamic consistency.
2. The author advises that the proposed Legendre polynomial series be used to define the function $\log(\gamma_1/\gamma_2)$.
3. Statistical analysis should be used to determine the importance of each coefficient in the Legendre polynomial series.

NOMENCLATURE

<u>Symbol</u>	<u>Description</u>	<u>Units</u>
A, B, C	constants of the Antcine equation	none
B, C, D, E	coefficients of the Redlich Kister power series	none
a, b, c, d, e	coefficients of the Legendre polynomial series	none
k, m, n	integers 0, 1, 2, 3, 4, . . .	none
N	number of experimental data points	none
P°	vapor pressure of a pure component	mm Hg
P _m (x ₁), P _n (x ₁)	Legendre polynomials of order m and n	none
Q	excess free energy function	none
t	temperature	°C
x	mole fraction in the liquid phase	none
y	mole fraction in the vapor phase	none
γ	activity coefficient	none
π	total pressure	mm Hg
1	subscript denoting more volatile component	none
2	subscript denoting less volatile component	none

BIBLIOGRAPHY

1. Chemical Rubber Company, Cleveland. Handbook of chemistry and physics. 35th ed. Cleveland, Chemical Rubber, 1953. 3163 p.
2. Chu, Ju Chin, et al. Distillation equilibrium data. New York, Reinhold, 1950. 304 p.
3. Dreisbach, Robert R. Physical properties of chemical substances. Midland, Michigan, Dow Chemical, 1952. 2 vols. (various paging)
4. Lewis, Gilbert Newton, and Merle Randall. Thermodynamics. New York, McGraw-Hill, 1923. 653 p.
5. Miller, Richard Linn. An improved vapor-liquid equilibrium still. Master's thesis. Corvallis, Oregon State College, 1958. 66 numb. leaves.
6. Milne, William Edmund. Numerical calculus. Princeton, Princeton University Press, 1949. 393 p.
7. Redlich, Otto, and A. T. Kister. Thermodynamics of nonelectrolyte solutions. Industrial and Engineering Chemistry 40:341-348. 1948.
8. Redlich, Otto, A. T. Kister, and C. E. Turnquist. Thermodynamics of solutions. In: American Institute of Chemical Engineers. Chemical Engineering Progress Symposium series. no.2 New York, 1952. p. 49-61.
9. Robinson, Clark Shove, and Edwin Richard Gilliland. Elements of fractional distillation. 4th ed. New York, McGraw-Hill, 1950. 492 p.
10. Rossini, Frederick D. Selected values of physical and thermodynamic properties of hydrocarbons and related compounds. American Petroleum Institute Research Project 44. Pittsburgh, Carnegie Press, 1953. 1050 p.
11. Scatchard, George. Equilibria in nonelectrolyte solutions in relation to the vapor pressures and densities of the components. Chemical Reviews 8:321-333. 1931.

12. Stockett, Alan Lee. Testing vapor-liquid equilibrium data with thermodynamic relations. Master's thesis. Corvallis, Oregon State College, 1958. 46 numb. leaves.

APPENDIX

TABLE 1

EXPERIMENTAL AND CALCULATED DATA

System: Acetone - Acetic Acid

Antoine Constants:

$$\begin{array}{ll} A_1 = 7.0247 & A_2 = 7.29963 \\ B_1 = 1161.0 & B_2 = 1479.02 \\ C_1 = 224.0 & C_2 = 216.81 \end{array}$$

Boiling Points:

Acetone - 56.5°C (l, p. 703)

Acetic Acid - 118.1°C (l, p. 695)

Total Pressure: 760 mm Hg

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt.</u> <u>log γ₁</u>	<u>Calc.</u> <u>log γ₁</u>
.0420	.1079	112.10	.5251	1.1141	-.3266	-.3187
.0820	.2250	108.80	.6068	1.1218	-.2669	-.3334
.1030	.2570	107.40	.5709	1.1515	-.3047	-.3323
.1200	.2890	106.30	.5660	1.1641	-.3132	-.3276
.1270	.3100	106.10	.5765	1.1463	-.2985	-.3248
.1580	.3560	104.60	.5521	1.1652	-.3244	-.3070
.1940	.4330	101.40	.5925	1.1922	-.3037	-.2772
.2260	.5640	94.30	.7957	1.2188	-.1852	-.2447
.2360	.5800	92.50	.8220	1.2676	-.1881	-.2337
.2710	.6300	90.40	.8227	1.2618	-.1858	-.1932
.2940	.6600	87.00	.8718	1.3554	-.1917	-.1654
.3070	.7090	86.30	.9144	1.2129	-.1227	-.1496
.4330	.8440	78.60	.9610	1.0651	-.0447	-.0056
.5380	.9200	74.20	.9604	.7980	.0805	.0824
.5500	.9180	70.80	1.0396	.9643	.0326	.0902
.6680	.9660	65.60	1.0599	.6739	.1967	.1503
.7610	.9810	63.60	1.0075	.5701	.2473	.1962
.9350	.9970	60.70	.9161	.3766	.3861	.4211

a = .0235

b = -.4242

c = .0267

d = -.0191

e = .1185

B = -.4045

C = .0058

D = .0402

E = -.0276

TABLE 2

EXPERIMENTAL AND CALCULATED DATA

System: Acetone - Methanol

Antoine Constants:

$$\begin{array}{ll} A_1 = 7.0247 & A_2 = 8.07246 \\ B_1 = 1161.0 & B_2 = 1574.99 \\ C_1 = 224.0 & C_2 = 238.86 \end{array}$$

Boiling Points:

Acetone - 56.5°C (1, p. 703)

Methanol - 64.65°C (1, p. 1023)

Total Pressure: 760 mm Hg

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt.</u>	<u>Calc.</u>
					<u>$\log \frac{\gamma_1}{\gamma_2}$</u>	<u>$\log \frac{\gamma_1}{\gamma_2}$</u>
.0480	.1400	62.90	2.3316	.9628	.3841	.4317
.1760	.3170	60.10	1.5785	.9887	.2032	.1992
.2800	.4200	58.30	1.3958	1.0341	.1302	.1009
.4000	.5160	57.20	1.2458	1.0836	.0606	.0423
.6000	.6560	56.10	1.0960	1.2092	-.0427	-.0229
.6760	.7100	55.10	1.0895	1.3123	-.0808	-.0574
.8000	.8000	55.60	1.0197	1.4358	-.1486	-.1379
.9500	.9400	55.60	1.0090	1.7228	-.2324	-.2754
.9820	.9760	56.10	.9963	1.8744	-.2745	-.3089

$$\begin{array}{ll} a = .0275 & B = .3006 \\ b = .3282 & C = -.0424 \\ c = .0578 & D = .0651 \\ d = .1181 & E = -.0409 \\ e = .0328 & \end{array}$$

TABLE 3

EXPERIMENTAL AND CALCULATED DATA

System: Acetone - Water

Antoine Constants:

$$\begin{array}{ll} A_1 = 7.0247 & A_2 = 7.96681 \\ B_1 = 1161.0 & B_2 = 1668.21 \\ C_1 = 224.0 & C_2 = 228.0 \end{array}$$

Boiling Points:

Acetone - 56.5°C (1, p. 703)Water - 100°C (1, p. 623)

Total Pressure: 200 mm Hg

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt. $\log \frac{\gamma_1}{\gamma_2}$</u>	<u>Calc. $\log \frac{\gamma_1}{\gamma_2}$</u>
.0340	.6010	48.10	6.1740	.9823	.7983	.9130
.0550	.7150	41.50	5.7970	1.0084	.7596	.8141
.1540	.7920	33.20	3.1733	1.2930	.3899	.4558
.1770	.8390	30.70	3.2390	1.1859	.4364	.3934
.3110	.8620	27.60	2.1554	1.4539	.1710	.1301
.4680	.8760	25.90	1.5647	1.8708	-.0776	-.0742
.6120	.8850	24.80	1.2674	2.5411	-.3021	-.2636
.7800	.9090	23.80	1.0666	3.7669	-.5480	-.5342
.9030	.9470	22.80	1.0028	5.2871	-.7220	-.7439
.9680	.9820	22.30	.9915	5.6149	-.7530	-.8400

a = -.0874

b = .8419

c = .1136

d = .1447

e = .0812

B = .7755

C = .0219

D = .0771

E = -.1512

TABLE 3 (Continued)

System: Acetone-Water
 Total Pressure: 500 mm Hg

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	Expt. $\log \frac{\gamma_1}{\gamma_2}$	Calc. $\log \frac{\gamma_1}{\gamma_2}$
.0609	.7329	62.30	6.4503	.8562	.8770	.8785
.0750	.7260	59.60	5.6746	1.0098	.7497	.8243
.1100	.7710	56.80	4.5137	1.0002	.6544	.7019
.1490	.7870	55.00	3.6169	1.0601	.5330	.5842
.1570	.8140	52.70	3.8448	1.0444	.5660	.5622
.2460	.8350	51.30	2.6438	1.1094	.3771	.3577
.3920	.8570	49.40	1.8217	1.3102	.1431	.1233
.4860	.8650	48.60	1.5263	1.5227	.0010	-.0020
.6400	.8740	47.90	1.2010	2.1022	-.2431	-.2158
.7650	.8930	46.50	1.0802	2.9357	-.4342	-.4127
.8820	.9330	45.70	1.0080	3.8141	-.5779	-.6059
.9480	.9650	45.10	.9917	4.6630	-.6723	-.7079

a = .0128	B = .8048
b = .8440	C = -.0604
c = .1125	D = .0800
d = .1211	E = -.1296
e = .0614	

TABLE 4

EXPERIMENTAL AND CALCULATED DATA

System: Benzene - Cyclohexane

Antoine Constants:

$$\begin{array}{ll} A_1 = 6.90565 & A_2 = 6.84498 \\ B_1 = 1211.033 & B_2 = 1203.526 \\ C_1 = 220.79 & C_2 = 222.863 \end{array}$$

Boiling Points:

Benzene - 80.1°C (l, p. 755)

Cyclohexane - 80.74°C (l, p. 869)

Total Pressure: 759 mm Hg

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt.</u> <u>log γ₁</u>	<u>Calc.</u> <u>log γ₁</u>
.0450	.0590	80.20	1.3055	1.0001	.1157	.1215
.0660	.0840	80.00	1.2750	1.0014	.1049	.1136
.1050	.1290	79.50	1.2499	1.0089	.0930	.1006
.1180	.1450	79.30	1.2579	1.0111	.0949	.0966
.2540	.2900	78.20	1.2093	1.0265	.0712	.0631
.3830	.4070	77.50	1.1505	1.0591	.0359	.0322
.4490	.4610	77.40	1.1151	1.0812	.0134	.0136
.5020	.5020	77.40	1.0861	1.1053	-.0076	-.0031
.5540	.5450	77.40	1.0684	1.1276	-.0234	-.0208
.5970	.5800	77.50	1.0518	1.1484	-.0381	-.0364
.6450	.6210	77.60	1.0391	1.1728	-.0526	-.0542
.7200	.6820	77.70	1.0191	1.2438	-.0865	-.0817
.7530	.7170	78.00	1.0149	1.2434	-.0882	-.0930
.7980	.7580	78.20	1.0061	1.2921	-.1087	-.1069
.8350	.7980	78.30	1.0092	1.3164	-.1154	-.1165
.8790	.8470	78.70	1.0049	1.3431	-.1260	-.1249
.8929	.8650	78.90	1.0040	1.3313	-.1226	-.1267
.9280	.9070	79.20	1.0036	1.3512	-.1292	-.1291
.9370	.9180	79.30	1.0029	1.3575	-.1315	-.1292
.9600	.9480	79.50	1.0046	1.3480	-.1277	-.1282

a = -.0088

b = .1447

c = .0006

d = -.0129

e = .0178

B = .1534

C = .0161

D = -.0332

E = -.0176

TABLE 5

EXPERIMENTAL AND CALCULATED DATA

System: Benzene - Ethylene Dichloride
 Antoine Constants:

$$\begin{array}{ll} A_1 = 6.90565 & A_2 = 7.18431 \\ B_1 = 1211.033 & B_2 = 1358.46 \\ C_1 = 220.79 & C_2 = 232.2 \end{array}$$

Boiling Points:

Benzene - 80.1°C (l, p. 755)

Ethylene Dichloride - 83.5°C (l, p. 917)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y₁</u>	<u>t</u>	<u>y₁</u>	<u>y₂</u>	<u>Expt. log y₁/y₂</u>	<u>Calc. log y₁/y₂</u>
.0500	.0550	83.32	.9969	.9992	-.0010	.0002
.1000	.1100	83.14	1.0025	.9990	.0015	-.0001
.2000	.2170	82.79	.9994	.9997	-.0001	.0000
.3000	.3220	82.45	.9989	1.0000	-.0005	.0004
.4000	.4260	82.10	1.0017	.9987	.0013	.0006
.5000	.5260	81.77	.9995	1.0000	-.0002	.0005
.6000	.6250	81.43	1.0000	.9997	.0001	.0001
.7000	.7220	81.09	1.0005	.9989	.0007	-.0004
.8000	.8160	80.76	.9995	1.0022	-.0012	-.0007
.9000	.9090	80.42	1.0001	1.0021	-.0009	.0000
.9500	.9550	80.27	1.0000	.9958	.0018	.0010

$$\begin{array}{ll} a = .0002 \\ b = .0000 \\ c = .0003 \\ d = -.0009 \\ e = .0012 \end{array}$$

$$\begin{array}{ll} B = .0003 \\ C = .0005 \\ D = -.0013 \\ E = -.0018 \end{array}$$

TABLE 6

EXPERIMENTAL AND CALCULATED DATA

System: Carbon Disulfide - Acetone

Antoine Constants:

$$\begin{array}{ll} A_1 = 6.85145 & A_2 = 7.0247 \\ B_1 = 1122.5 & B_2 = 1161.0 \\ C_1 = 236.46 & C_2 = 224.0 \end{array}$$

Boiling Points:

Carbon Disulfide - 46.3°C (1, p. 837)Acetone - 56.5°C (1, p. 703)

Total Pressure: 760 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt.</u> $\log \frac{\gamma_1}{\gamma_2}$	<u>Calc.</u> $\log \frac{\gamma_1}{\gamma_2}$
.0190	.0832	54.00	3.4306	1.0069	.5324	.5628
.0476	.1850	51.40	3.2984	1.0096	.5142	.5308
.1340	.3510	46.60	2.5890	1.0502	.3918	.4294
.1858	.4430	44.00	2.5647	1.0552	.3857	.3681
.2912	.5275	41.40	2.1241	1.1337	.2727	.2486
.3798	.5740	40.30	1.8389	1.2182	.1788	.1562
.4477	.5980	39.80	1.6530	1.3158	.0991	.0898
.5360	.6270	39.30	1.4724	1.4815	-.0027	.0045
.6530	.6610	39.10	1.2828	1.8145	-.1150	-.1218
.7894	.7050	39.30	1.1241	2.5815	-.3611	-.3303
.8023	.7230	39.60	1.1228	2.5526	-.3567	-.3558
.8799	.7600	40.50	1.0439	3.5171	-.5275	-.5390
.9683	.8860	43.50	1.0006	5.6524	-.7520	-.8272

a = -.0115

b = .6547

c = -.1335

d = .1152

e = -.0417

B = .6248

C = .1086

D = .0677

E = .0316

TABLE 7

EXPERIMENTAL AND CALCULATED DATA

System: Carbon Tetrachloride - Ethyl Acetate
 Antoine Constants:

$$\begin{array}{ll} A_1 = 6.93390 & A_2 = 7.09808 \\ B_1 = 1242.43 & B_2 = 1238.71 \\ C_1 = 230.0 & C_2 = 217.0 \end{array}$$

Boiling Points:

Carbon Tetrachloride - 76.8°C (1, p. 839)

Ethyl Acetate - 77.15°C (1, p. 695)

Total Pressure: 685 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt. log γ₁/γ₂</u>	<u>Calc. log γ₁/γ₂</u>
.0500	.0699	73.60	1.3800	.9794	.1489	.1552
.1000	.1330	73.10	1.3325	.9802	.1333	.1343
.2000	.2450	72.50	1.2506	.9800	.1059	.1012
.3000	.3420	72.10	1.1785	.9895	.0759	.0741
.4000	.4330	71.80	1.1297	1.0051	.0508	.0479
.5000	.5180	71.60	1.0880	1.0323	.0228	.0199
.5820	.5820	71.56	1.0514	1.0723	-.0085	-.0051
.6000	.5970	71.60	1.0449	1.0789	-.0139	-.0107
.7000	.6810	71.80	1.0152	1.1309	-.0468	-.0428
.8000	.7730	72.10	.9989	1.1949	-.0778	-.0728
.9000	.8810	72.60	.9196	1.2316	-.0921	-.0955
.9550	.9400	72.90	.9976	1.2292	-.0906	-.1019

$$\begin{array}{ll} a = .0189 & B = .1437 \\ b = .1438 & C = .0015 \\ c = .0073 & D = -.0143 \\ d = -.0020 & E = -.0277 \\ e = .0123 & \end{array}$$

TABLE 8

EXPERIMENTAL AND CALCULATED DATA

System: Carbon Tetrachloride - n-Propanol
 Antoine Constants:

$$\begin{array}{ll} A_1 = 6.93390 & A_2 = 7.99733 \\ B_1 = 1242.43 & B_2 = 1569.70 \\ C_1 = 230.0 & C_2 = 209.5 \end{array}$$

Boiling Points:

Carbon Tetrachloride - 76.8°C (1, p. 839)
 n-Propanol - 97.19°C (1, p. 1115)

Total Pressure: 760 mm Hg.

Expt. Calc.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>log γ₁/γ₂</u>	<u>log γ₁/γ₂</u>
.0580	.2530	90.80	2.8810	1.0229	.4497	.4965
.1410	.4500	84.50	2.5198	1.0690	.3772	.3831
.3000	.6330	78.50	1.9884	1.1308	.2451	.2094
.4410	.7070	75.80	1.6398	1.2731	.1099	.0943
.5220	.7390	74.70	1.4977	1.3929	.0315	.0324
.6830	.7820	73.90	1.2416	1.8184	-.1657	-.1298
.8180	.8180	73.40	1.1014	2.7045	-.3902	-.3755
.8510	.8310	73.60	1.0688	3.0400	-.4540	-.4612
.9500	.8950	74.20	1.0122	5.4778	-.7334	-.8027

$$\begin{array}{ll} a = -.0197 & \\ b = .6395 & B = .5986 \\ c = -.1673 & C = .1481 \\ d = .1691 & D = .0965 \\ e = -.0381 & E = .0404 \end{array}$$

TABLE 9

EXPERIMENTAL AND CALCULATED DATA

System: Cyclohexane - Cyclohexene

Antoine Constants:

$$\begin{array}{ll} A_1 = 6.84498 & A_2 = 6.88617 \\ B_1 = 1203.526 & B_2 = 1229.973 \\ C_1 = 222.863 & C_2 = 224.104 \end{array}$$

Boiling Points:

Cyclohexane - 80.74°C (1, p. 869)Cyclohexene - 83°C (1, p. 873)

Total Pressure: 741 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt.</u>	<u>Calc.</u>
					<u>$\log \frac{\gamma_1}{\gamma_2}$</u>	<u>$\log \frac{\gamma_1}{\gamma_2}$</u>
.0150	.0349	82.10	2.1806	.9808	.3470	.4361
.0990	.1350	82.00	1.2802	.9640	.1232	.1162
.1990	.2000	81.70	.9520	1.0121	-.0266	-.0369
.5400	.5650	80.90	1.0152	.9818	.0145	.0410
.5780	.6000	80.80	1.0102	.9871	.0100	.0432
.6630	.6800	80.60	1.0041	.9949	.0040	.0311
.7050	.7350	80.50	1.0238	.9441	.0352	.0193
.7420	.7600	80.40	1.0088	.9807	.0123	.0087
.8320	.8450	80.30	1.0034	.9756	.0122	-.0012
.9040	.9190	80.20	1.0074	.8949	.0514	.0345
.9400	.9550	80.10	1.0097	.7979	.1022	.0781

$$\begin{array}{l} a = .0436 \\ b = .0401 \\ c = .14855 \\ d = .1161 \\ e = .1700 \end{array}$$

$$\begin{array}{l} B = -.0264 \\ C = -.1065 \\ D = .1758 \\ E = -.1559 \end{array}$$

TABLE 10

EXPERIMENTAL AND CALCULATED DATA

System: Cyclohexane - 2,2,3 Trimethylbutane
Antoine Constants:

$$\begin{array}{ll} A_1 = 6.84498 & A_2 = 6.79230 \\ B_1 = 1203.526 & B_2 = 1200.563 \\ C_1 = 222.863 & C_2 = 226.05 \end{array}$$

Boiling Points:

Cyclohexane - 80.74°C (l, p. 869)

2,2,3 Trimethylbutane - 80.88°C (l, p. 807)

Total Pressure: 744 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt. $\log \frac{\gamma_1}{\gamma_2}$</u>	<u>Calc. $\log \frac{\gamma_1}{\gamma_2}$</u>
.0420	.0660	80.00	1.5725	.9795	.2056	.2021
.1180	.1490	79.90	1.2678	.9722	.1153	.1296
.2250	.2550	79.80	1.1413	.9715	.0699	.0635
.2790	.3060	79.70	1.1078	.9757	.0551	.0424
.3790	.3960	79.60	1.0586	.9888	.0296	.0188
.4350	.4430	79.50	1.0349	1.0052	.0126	.0116
.4840	.4910	79.40	1.0340	1.0088	.0107	.0071
.5170	.5180	79.40	1.0213	1.0205	.0003	.0047
.5220	.5220	79.40	1.0193	1.0227	-.0014	.0044
.6650	.6540	79.40	1.0024	1.0562	-.0227	-.0080
.7570	.7480	79.50	1.0041	1.0574	-.0225	-.0241
.8340	.8230	79.60	.9998	1.0840	-.0351	-.0462
.8710	.8600	79.70	.9973	1.1001	-.0426	-.0603
.9120	.9000	79.80	.9937	1.1486	-.0629	-.0789
.9400	.9270	79.90	.9901	1.2260	-.0928	-.0936
.9630	.9520	80.00	.9895	1.3034	-.1197	-.1069

$$a = .0211$$

$$b = .1299$$

$$c = .0346$$

$$d = .0623$$

$$e = .0056$$

$$B = .1088$$

$$C = -.0366$$

$$D = .0631$$

$$E = .0061$$

TABLE 11

EXPERIMENTAL AND CALCULATED DATA

System: Ethanol - Trichloroethylene
 Antoine Constants:

$$\begin{array}{ll} A_1 = 8.16290 & A_2 = 7.02808 \\ B_1 = 1623.22 & B_2 = 1315.04 \\ C_1 = 228.98 & C_2 = 230.0 \end{array}$$

Boiling Points:

Ethanol - 78.5°C (1, p. 913)

Trichloroethylene - 87°C (1, p. 917)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt. $\log \frac{\gamma_1}{\gamma_2}$</u>	<u>Calc. $\log \frac{\gamma_1}{\gamma_2}$</u>
.0143	.0999	83.40	5.7189	1.0217	.7480	1.0254
.0226	.1480	81.60	5.7609	1.0313	.7471	.9967
.0282	.2400	78.70	8.3864	1.0136	.9177	.9776
.0550	.3570	74.20	7.6602	1.0197	.8758	.8884
.0680	.3720	73.00	6.7799	1.0504	.8099	.8466
.1130	.4200	71.60	4.8791	1.0677	.6599	.7097
.2810	.4810	71.20	2.2847	1.1945	.2816	.2894
.5200	.5250	70.80	1.3701	1.6596	-.0832	-.1256
.5420	.5280	70.80	1.3220	1.7283	-.1164	-.1562
.6280	.5500	70.90	1.1836	2.0219	-.2326	-.2677
.7160	.5640	71.00	1.0601	2.5575	-.3825	-.3711
.7720	.6080	71.30	1.0468	2.8356	-.4328	-.4333
.8080	.6260	71.40	1.0256	3.2018	-.4944	-.4723
.8500	.6570	72.20	.9899	3.6602	-.5679	-.5173
.8860	.7520	73.00	1.0518	3.3912	-.5084	-.5557
.9090	.7730	73.40	1.0367	3.8375	-.5684	-.5803
.9269	.8220	74.20	1.0464	3.6509	-.5427	-.5995
.9440	.8480	75.00	1.0262	3.9625	-.5868	-.6178
.9640	.8890	75.60	1.0282	4.4148	-.6328	-.6395
.9770	.9210	76.20	1.0260	4.8240	-.6722	-.6536

$$a = -.0004$$

$$b = .8183$$

$$c = .1956$$

$$d = .0592$$

$$e = .0036$$

$$B = .7960$$

$$C = -.1633$$

$$D = -.0272$$

$$E = .0711$$

TABLE 12

EXPERIMENTAL AND CALCULATED DATA

System: Ethanol - Water

Antoine Constants:

$$\begin{array}{ll} A_1 = 8.16290 & A_2 = 7.96681 \\ B_1 = 1623.22 & B_2 = 1668.21 \\ C_1 = 228.98 & C_2 = 228.0 \end{array}$$

Boiling Points:

Ethanol - 78.5°C (1, p. 913)Water - 100°C (1, p. 623)

Total Pressure: 380 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt. log γ₁</u>	<u>Calc. log γ₁</u>
					<u>log γ₂</u>	<u>log γ₂</u>
.0160	.1469	78.10	4.6314	1.0019	.6649	.7130
.0315	.2505	76.00	4.3635	.9753	.6507	.6743
.0600	.3765	72.40	3.9853	.9727	.6125	.6054
.0855	.4300	69.30	3.6335	1.0444	.5415	.5462
.1465	.5005	67.70	2.6407	1.0516	.3999	.4140
.2060	.5415	67.50	2.0492	1.0468	.2917	.2979
.2360	.5600	67.10	1.8816	1.0626	.2482	.2441
.3495	.5945	65.30	1.4571	1.2457	.0680	.0689
.4675	.6410	64.70	1.2054	1.3839	-.0600	-.0702
.4875	.6425	64.30	1.1789	1.4579	-.0923	-.0900
.5800	.6890	64.40	1.0580	1.5407	-.1632	-.1693
.6525	.7250	64.20	.9982	1.6614	-.2212	-.2206
.7000	.7495	63.80	.9788	1.7849	-.2609	-.2508
.7175	.7680	63.20	1.0045	1.8037	-.2542	-.2615
.7890	.8111	63.80	.9398	1.9137	-.3089	-.3042
.8420	.8488	62.70	.9670	2.1500	-.3470	-.3368
.8749	.8767	62.50	.9698	2.2338	-.3624	-.3584
.8967	.8973	63.60	.9228	2.1445	-.3662	-.3735
.9483	.9440	63.50	.9220	2.3471	-.4058	-.4130
.9727	.9692	63.00	.9433	2.5013	-.4235	-.4338

a = -.0123

b = .5503

c = .1707

d = .0562

e = -.0111

B = .5365

C = -.1620

D = .0435

E = .0173

TABLE 13

EXPERIMENTAL AND CALCULATED DATA

System: Ethyl Acetate - Benzene

Antoine Constants:

$$\begin{array}{ll} A_1 = 7.09808 & A_2 = 6.90565 \\ B_1 = 1238.71 & B_2 = 1211.033 \\ C_1 = 217 & C_2 = 220.79 \end{array}$$

Boiling Points:

Ethyl Acetate - 77.15°C (1, p. 695)Benzene - 80.1°C (1, p. 755)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y₁</u>	<u>t</u>	<u>y₁</u>	<u>y₂</u>	Expt. $\log \frac{y_1}{y_2}$	Calc. $\log \frac{y_1}{y_2}$
.0640	.0760	79.74	1.0760	.9982	.0326	.0381
.0860	.1010	79.62	1.0681	.9982	.0294	.0323
.1370	.1580	79.32	1.0592	.9994	.0253	.0217
.1415	.1615	79.30	1.0489	1.0011	.0203	.0209
.1825	.2060	79.07	1.0451	1.0026	.0180	.0150
.1970	.2210	79.02	1.0403	1.0030	.0159	.0133
.2565	.2830	78.77	1.0316	1.0048	.0114	.0079
.3040	.3310	78.60	1.0237	1.0069	.0072	.0050
.3575	.3825	78.32	1.0152	1.0155	-.0001	.0024
.4230	.4492	78.14	1.0135	1.0144	-.0004	-.0005
.4665	.4925	77.98	1.0129	1.0159	-.0013	-.0027
.5230	.5450	77.87	1.0034	1.0222	-.0080	-.0061
.5740	.5935	77.74	.9999	1.0267	-.0115	-.0097
.6340	.6500	77.60	.9960	1.0335	-.0160	-.0146
.7020	.7140	77.44	.9933	1.0424	-.0209	-.0209
.7575	.7665	77.34	.9914	1.0492	-.0246	-.0259
.8135	.8190	77.28	.9884	1.0595	-.0301	-.0303
.8740	.8775	77.23	.9873	1.0629	-.0320	-.0335
.9115	.9135	77.20	.9865	1.0696	-.0351	-.0341
.9732	.9740	77.17	.9861	1.0629	-.0326	-.0316

a = -.0042

b = .0388

c = .0091

d = .0059

e = .0109

B = .0367

C = -.0006

D = .0052

E = -.0154

TABLE 14

EXPERIMENTAL AND CALCULATED DATA

System: Ethyl Acetate - Ethanol

Antoine Constants:

$$\begin{array}{ll} A_1 = 7.09808 & A_2 = 8.16290 \\ B_1 = 1238.71 & B_2 = 1623.22 \\ C_1 = 217.0 & C_2 = 228.98 \end{array}$$

Boiling Points:

Ethyl Acetate - 77.15°C (1, p. 695)Ethanol - 78.5°C (1, p. 913)

Total Pressure: 760 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt.</u>	<u>Calc.</u>
					<u>log γ₁</u>	<u>log γ₂</u>
.0500	.1020	76.60	2.0483	1.0125	.3060	.3331
.1000	.1870	75.50	1.9473	1.0113	.2845	.2850
.2000	.3050	73.90	1.6757	1.0377	.2081	.1990
.3000	.3890	72.80	1.4788	1.0906	.1322	.1229
.4000	.4570	72.10	1.3344	1.1638	.0594	.0529
.5000	.5160	71.80	1.2178	1.2603	-.0149	-.0139
.5400	.5400	71.80	1.1800	1.3020	-.0427	-.0402
.6000	.5760	71.90	1.1289	1.3744	-.0854	-.0794
.7000	.6440	72.20	1.0709	1.5197	-.1520	-.1446
.8000	.7260	73.00	1.0280	1.6978	-.2179	-.2097
.9000	.8370	74.70	.9948	1.8846	-.2775	-.2739
.9500	.9140	76.00	.9854	1.8870	-.2822	-.3051

a = -.0041

b = .3480

c = .0237

d = .0123

e = .0055

B = .3480

C = -.0187

D = -.0246

E = -.0055

TABLE 15

EXPERIMENTAL AND CALCULATED DATA

System: Ethyl Acetate - Ethylene Dichloride
Antcine Constants:

$$\begin{array}{ll} A_1 = 7.09808 & A_2 = 7.18431 \\ B_1 = 1238.71 & B_2 = 1358.46 \\ C_1 = 217 & C_2 = 232.2 \end{array}$$

Boiling Points:

Ethyl Acetate - 77.15°C (l, p. 695)

Ethylene Dichloride - 83.5°C (l, p. 917)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt.</u>	<u>Calc.</u>
					<u>$\log \frac{\gamma_1}{\gamma_2}$</u>	<u>$\log \frac{\gamma_1}{\gamma_2}$</u>
.0517	.0521	83.44	.8110	1.0003	-.0911	-.0891
.0959	.0979	83.43	.8219	.9988	-.0847	-.0882
.1311	.1336	83.39	.8215	.9994	-.0851	-.0845
.1777	.1849	83.37	.8393	.9942	-.0735	-.0769
.2148	.2269	83.27	.8548	.9906	-.0640	-.0692
.2715	.2900	83.03	.8709	.9880	-.0548	-.0560
.3185	.3440	82.87	.8851	.9807	-.0446	-.0447
.3935	.4265	82.56	.8970	.9729	-.0353	-.0273
.4645	.5080	82.13	.9176	.9582	-.0188	-.0128
.5105	.5610	81.84	.9306	.9440	-.0062	-.0046
.5320	.5850	81.76	.9336	.9357	-.0010	-.0011
.5670	.6205	81.46	.9380	.9337	.0020	.0044
.6230	.6805	81.04	.9489	.9150	.0158	.0130
.6998	.7580	80.35	.9621	.8898	.0340	.0260
.7485	.8038	79.90	.9679	.8736	.0445	.0368
.8002	.8503	79.38	.9740	.8532	.0575	.0519
.8362	.8825	78.96	.9807	.8279	.0735	.0656
.9240	.9485	78.05	.9827	.8055	.0863	.1152
.9628	.9789	77.55	.9894	.6854	.1594	.1467

$$a = -.0016$$

$$b = -.1148$$

$$c = .0277$$

$$d = -.0189$$

$$e = .0241$$

$$B = -.1113$$

$$C = -.0135$$

$$D = -.0181$$

$$E = -.0311$$

TABLE 16

EXPERIMENTAL AND CALCULATED DATA

System: n-Heptane - Methyl Cyclohexane
 Antoine Constants:

$$\begin{array}{ll} A_1 = 6.90240 & A_2 = 6.82689 \\ B_1 = 1268.115 & B_2 = 1272.864 \\ C_1 = 216.9 & C_2 = 221.63 \end{array}$$

Boiling Points:

n-Heptane - 94.43°C (1, p. 951)

Methyl Cyclohexane - 100.3°C (1, p. 869)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt.</u> <u>$\log \frac{\gamma_1}{\gamma_2}$</u>	<u>Calc.</u> <u>$\log \frac{\gamma_1}{\gamma_2}$</u>
.0309	.0350	100.70	1.0586	1.0024	.0237	.0225
.0580	.0620	100.60	1.0032	1.0052	-.0008	.0133
.0950	.1030	100.50	1.0205	1.0034	.0074	.0048
.1330	.1430	100.40	1.0150	1.0035	.0050	.0000
.1800	.1920	100.30	1.0099	1.0031	.0029	-.0018
.2715	.2890	100.00	1.0166	1.0021	.0063	.0017
.3630	.3810	99.90	1.0053	1.0006	.0020	.0074
.4010	.4200	99.80	1.0061	.9998	.0027	.0089
.4560	.4750	99.60	1.0065	1.0022	.0019	.0096
.5010	.5210	99.30	1.0136	1.0054	.0035	.0087
.5990	.6180	99.00	1.0145	1.0063	.0035	.0032
.6470	.6660	98.90	1.0151	1.0023	.0055	-.0002
.7090	.7280	98.80	1.0156	.9930	.0098	-.0029
.7960	.8100	98.60	1.0124	.9952	.0074	.0014
.8430	.8535	98.60	1.0073	.9970	.0044	.0111
.8790	.8900	98.50	1.0103	.9741	.0158	.0237
.9060	.9130	98.50	1.0055	.9918	.0059	.0367
.9310	.9400	98.50	1.0075	.9317	.0339	.0519
.9540	.9625	98.50	1.0067	.8736	.0616	.0690
.9800	.9860	98.40	1.0069	.7525	.1265	.0922

$$\begin{array}{ll} a = .0121 \\ b = -.0163 \\ c = .0308 \\ d = -.0220 \\ e = .0322 \end{array}$$

$$\begin{array}{ll} B = -.0096 \\ C = -.0064 \\ D = -.0321 \\ E = -.0689 \end{array}$$

TABLE 17

EXPERIMENTAL AND CALCULATED DATA

System: n-Heptane - Toluene

Antoine Constants:

$$\begin{array}{ll} A_1 = 6.90240 & A_2 = 6.95464 \\ B_1 = 1268.115 & B_2 = 1344.8 \\ C_1 = 216.9 & C_2 = 219.482 \end{array}$$

Boiling Points:

n-Heptane - 94.43°C (1, p. 951)Toluene - 110.63°C (1, p. 1173)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt. $\log \frac{\gamma_1}{\gamma_2}$</u>	<u>Calc. $\log \frac{\gamma_1}{\gamma_2}$</u>
.0250	.0480	110.75	1.3555	.9729	.1441	.1287
.0620	.1070	108.60	1.2921	1.0088	.1075	.1191
.1290	.2050	106.80	1.2507	1.0188	.0890	.0974
.1850	.2750	105.65	1.2080	1.0269	.0706	.0771
.2350	.3330	104.80	1.1795	1.0319	.0580	.0588
.2500	.3490	104.50	1.1719	1.0364	.0533	.0534
.2860	.3960	103.83	1.1846	1.0303	.0606	.0409
.3540	.4540	102.95	1.1250	1.0567	.0272	.0195
.4120	.5040	102.25	1.0948	1.0768	.0072	.0041
.4480	.5410	101.78	1.0954	1.0766	.0075	-.0041
.4550	.5400	101.72	1.0784	1.0947	-.0065	-.0056
.4970	.5770	101.35	1.0663	1.1029	-.0147	-.0135
.5680	.6370	100.70	1.0495	1.1238	-.0297	-.0243
.5800	.6470	100.60	1.0470	1.1275	-.0322	-.0259
.6920	.7420	99.73	1.0322	1.1537	-.0484	-.0405
.8430	.8640	98.90	1.0107	1.2237	-.0830	-.0766
.9400	.9480	98.50	1.0063	1.2394	-.0905	-.1288
.9750	.9760	98.40	1.0018	1.3775	-.1383	-.1568
.9940	.9930	98.33	1.0018	1.6789	-.2243	-.1745

a = -.0044

b = .1287

c = .0029

d = .0285

e = -.0218

B = .1187

C = -.0244

D = .0412

E = .0530

TABLE 18

EXPERIMENTAL AND CALCULATED DATA

System: Methanol - Benzene

Antoine Constants:

$$\begin{array}{ll} A_1 = 8.07246 & A_2 = 6.90565 \\ B_1 = 1574.99 & B_2 = 1211.033 \\ C_1 = 238.86 & C_2 = 220.79 \end{array}$$

Boiling Points:

Methanol - 64.65°C (l, p. 1023)Benzene - 80.1°C (l, p. 755)

Total Pressure: 760 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	Expt. <u>log γ₁/γ₂</u>	Calc. <u>log γ₁/γ₂</u>
.0280	.3100	69.40	9.1587	.9990	.9622	1.0810
.0500	.3950	66.80	7.2226	.9776	.8685	.9906
.0570	.4200	65.70	7.0311	.9799	.8558	.9631
.0900	.4850	61.40	6.0992	1.0459	.7658	.8409
.1180	.5650	59.00	5.9732	.9920	.7797	.7464
.1200	.5660	59.20	5.7744	.9986	.7621	.7400
.2700	.5750	58.00	2.7678	1.2137	.3580	.3487
.4400	.5850	57.80	1.7423	1.5560	.0491	.0460
.5860	.6100	57.70	1.3697	1.9851	-.1611	-.1741
.6950	.6250	57.60	1.1882	2.6003	-.3401	-.3457
.8170	.6550	58.10	1.0377	3.9162	-.5768	-.5620
.8830	.7000	58.90	.9930	5.1760	-.7171	-.6927
.9020	.7300	59.60	.9852	5.4245	-.7408	-.7321
.9340	.8010	60.40	1.0106	5.7720	-.7568	-.8005
.9450	.8220	61.20	.9924	6.0234	-.7832	-.8245
.9680	.9000	62.40	1.0109	5.5776	-.7418	-.8755
.9879	.9420	63.40	.9963	8.2941	-.9204	-.9206

a = -.0029

b = .9458

c = .1048

d = .1308

e = .0265

B = .9127

C = -.0688

D = .0427

E = .0013

TABLE 19

EXPERIMENTAL AND CALCULATED DATA

System: Methanol - Trichloroethylene
 Antoine Constants:

$$\begin{array}{ll} A_1 = 8.07246 & A_2 = 7.02808 \\ B_1 = 1574.99 & B_2 = 1315.04 \\ C_1 = 238.86 & C_2 = 230.0 \end{array}$$

Boiling Points:

Methanol - 64.65°C (1, p. 1023)

Trichloroethylene - 87°C (1, p. 917)

Total Pressure: 760 mm Hg.

x_1	y_1	t	γ_1	γ_2	Expt. $\log \frac{\gamma_1}{\gamma_2}$	Calc. $\log \frac{\gamma_1}{\gamma_2}$
.0009	.0450	83.50	23.5199	1.0662	1.3436	1.1839
.0280	.1880	78.20	4.0071	1.1002	.5614	1.0707
.0320	.2540	75.30	5.2650	1.1142	.6744	1.0547
.0400	.3600	70.10	7.2505	1.1446	.8017	1.0233
.0450	.4430	67.30	8.8284	1.1012	.9040	1.0040
.0510	.4720	66.10	8.6962	1.0947	.9000	.9812
.0940	.6000	60.90	7.3717	1.0429	.8493	.8290
.2370	.6440	60.40	3.2020	1.1221	.4554	.4369
.3000	.6420	60.10	2.5526	1.2433	.3124	.3045
.3480	.6400	60.10	2.1936	1.3423	.2133	.2146
.5760	.6600	59.60	1.3948	1.9848	-.1532	-.1514
.6460	.6700	59.40	1.2729	2.3242	-.2615	-.2615
.7240	.6890	59.40	1.1679	2.8094	-.3812	-.3903
.8200	.7290	59.50	1.0866	3.7402	-.5368	-.5610
.8880	.7780	60.10	1.0450	4.8186	-.6638	-.6907
.9240	.8200	60.70	1.0332	5.6345	-.7367	-.7621
.9440	.8460	61.00	1.0307	6.4732	-.7980	-.8025
.9640	.9020	61.80	1.0421	6.2285	-.7765	-.8434
.9800	.9330	62.50	1.0310	7.4739	-.8603	-.8764
.9920	.9630	63.30	1.0183	10.0396	-.9939	-.9013

$$\begin{array}{ll} a = .0068 & \\ b = .9410 & B = .8548 \\ c = .1018 & C = -.0164 \\ d = .1120 & D = .1002 \\ e = .0264 & E = -.0134 \end{array}$$

TABLE 20

EXPERIMENTAL AND CALCULATED DATA

System: Methanol - Water

Antoine Constants:

$$\begin{array}{ll} A_1 = 8.07246 & A_2 = 7.96681 \\ B_1 = 1574.99 & B_2 = 1668.21 \\ C_1 = 238.86 & C_2 = 228.0 \end{array}$$

Boiling Points:

Methanol - 64.65°C (1, p. 1023)Water - 100°C (1, p. 623)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt. $\log \frac{\gamma_1}{\gamma_2}$</u>	<u>Calc. $\log \frac{\gamma_1}{\gamma_2}$</u>
.0200	.1339	96.40	2.1476	1.0064	.3292	.3258
.0400	.2300	93.50	2.0271	1.0164	.2998	.3081
.0600	.3040	91.20	1.9271	1.0226	.2752	.2902
.0800	.3650	89.30	1.8493	1.0244	.2565	.2720
.1000	.4180	87.70	1.7884	1.0205	.2436	.2539
.1500	.5170	84.40	1.6519	1.0197	.2095	.2085
.2000	.5790	81.70	1.5249	1.0513	.1615	.1638
.3000	.6650	78.00	1.3324	1.1107	.0790	.0798
.4000	.7290	75.30	1.2088	1.1722	.0134	.0065
.5000	.7790	73.10	1.1210	1.2583	-.0502	-.0542
.6000	.8250	71.20	1.0623	1.3507	-.1043	-.1023
.7000	.8700	69.30	1.0321	1.4522	-.1483	-.1407
.8000	.9150	67.60	1.0138	1.5342	-.1799	-.1741
.9000	.9580	66.00	1.0040	1.6273	-.2097	-.2101
.9500	.9790	65.00	1.0108	1.7009	-.2260	-.2320

a = -.0137

b = .2888

c = .0703

d = .0120

e = -.0141

B = .2816

C = -.0589

D = -.0019

E = -.0035

TABLE 21

EXPERIMENTAL AND CALCULATED DATA

System: Isooctane - Toluene

Antoine Constants:

$$\begin{array}{ll} A_1 = 6.81984 & A_2 = 6.95464 \\ B_1 = 1262.49 & B_2 = 1344.8 \\ C_1 = 221.271 & C_2 = 219.482 \end{array}$$

Boiling Points:

Isooctane - 99.3°C (1, p. 1069)Toluene - 110.63°C (1, p. 1173)

Total Pressure: 760 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt.</u> <u>log γ₁/γ₂</u>	<u>Calc.</u> <u>log γ₁/γ₂</u>
.0201	.0345	110.30	1.2656	.9945	.1047	.1116
.0699	.1125	109.10	1.2277	.9966	.0905	.0955
.0736	.1238	109.00	1.2865	.9907	.1134	.0943
.1400	.2030	107.30	1.1607	1.0196	.0563	.0747
.2180	.3020	107.20	1.1118	.9848	.0527	.0539
.2864	.3806	107.30	1.0637	.9549	.0468	.0377
.4097	.5050	103.90	1.0823	1.0191	.0261	.0122
.4712	.5490	103.30	1.0400	1.0552	-.0063	.0008
.5204	.5960	103.10	1.0280	1.0484	-.0086	-.0080
.5793	.6392	102.80	.9987	1.0769	-.0328	-.0184
.6180	.6746	101.70	1.0186	1.1055	-.0355	-.0254
.7220	.7673	101.10	1.0085	1.1061	-.0401	-.0456
.8020	.8290	100.20	1.0059	1.1727	-.0666	-.0638
.8870	.9010	100.00	.9941	1.1968	-.0806	-.0873
.9181	.9260	99.60	.9983	1.2496	-.0975	-.0973
.9661	.9685	99.40	.9978	1.2923	-.1123	-.1145

a = -.0033

b = .1097

c = .0005

d = .0137

e = -.0021

B = .1074

C = -.0052

D = .0095

E = .0085

TABLE 22

EXPERIMENTAL AND CALCULATED DATA

System: n-Propanol - Water

Antoine Constants:

$$\begin{array}{ll} A_1 = 7.99733 & A_2 = 7.96681 \\ B_1 = 1569.70 & B_2 = 1668.21 \\ C_1 = 209.5 & C_2 = 228.0 \end{array}$$

Boiling Points:

n-Propanol - 97.19°C (1, p. 1115)Water - 100°C (1, p. 623)

Total Pressure: 760 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	Expt. <u>log γ₁/γ₂</u>	Calc. <u>log γ₁/γ₂</u>
.0100	.1100	95.00	12.0259	1.0777	1.0476	1.2147
.0200	.2160	92.00	13.2776	1.0721	1.0929	1.1511
.0400	.3200	90.50	10.4469	1.0045	1.0170	1.0317
.0600	.3510	89.30	8.0167	1.0248	.8934	.9218
.1000	.3720	88.50	5.2654	1.0679	.6929	.7280
.2000	.3920	88.10	2.8201	1.1811	.3780	.3696
.3000	.4040	87.90	1.9535	1.3334	.1659	.1417
.4000	.4240	87.80	1.5440	1.5092	.0091	-.0068
.4320	.4320	87.80	1.4566	1.5721	-.0332	-.0443
.5000	.4520	87.90	1.3114	1.7164	-.1169	-.1144
.6000	.4920	88.30	1.1702	1.9585	-.2236	-.2068
.7000	.5510	89.00	1.0918	2.2470	-.3135	-.2969
.8000	.6410	90.50	1.0461	2.5455	-.3862	-.3849
.8500	.7040	91.50	1.0389	2.6949	-.4140	-.4248
.9000	.7780	92.80	1.0298	2.8872	-.4477	-.4585
.9600	.9000	95.00	1.0243	2.9976	-.4663	-.4857

a = .0109

b = .7254

c = .3076

d = .1611

e = .0757

B = .6869

C = -.2626

D = .1367

E = -.0795

TABLE 23

EXPERIMENTAL AND CALCULATED DATA

System: Toluene - n-Octane

Antoine Constants:

$$\begin{array}{ll} A_1 = 6.95464 & A_2 = 6.92377 \\ B_1 = 1344.8 & B_2 = 1355.126 \\ C_1 = 219.482 & C_2 = 209.517 \end{array}$$

Boiling Points:

Toluene - 110.63°C (l, p. 1173)n-Octane - 125.80°C (l, p. 1053)

Total Pressure: 400 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt.</u> <u>$\log \frac{\gamma_1}{\gamma_2}$</u>	<u>Calc.</u> <u>$\log \frac{\gamma_1}{\gamma_2}$</u>
.0179	.0670	101.60	2.5580	1.0273	.3962	.3422
.0520	.1500	100.00	2.0739	1.0212	.3077	.3262
.0950	.2330	98.50	1.8459	1.0138	.2603	.3031
.1650	.3650	97.00	1.7437	.9559	.2610	.2619
.2200	.4400	95.40	1.6567	.9520	.2406	.2287
.2880	.5100	94.50	1.5088	.9406	.2052	.1893
.3050	.5400	94.40	1.5133	.9077	.2220	.1799
.4030	.5950	93.70	1.2901	.9526	.1317	.1320
.4750	.6330	93.50	1.1718	.9884	.0739	.1038
.5050	.6700	92.50	1.2042	.9753	.0916	.0938
.5450	.6950	92.00	1.1761	.9975	.0715	.0817
.5800	.7050	91.50	1.1390	1.0634	.0298	.0721
.6660	.8020	91.20	1.1394	.9068	.0992	.0504
.7550	.8400	90.70	1.0697	1.0164	.0222	.0249
.8200	.8620	90.30	1.0238	1.2099	-.0725	-.0012
.8400	.8950	89.60	1.0615	1.0611	.0002	-.0113
.8900	.9220	89.20	1.0455	1.1628	-.0461	-.0425
.9300	.9560	88.90	1.0477	1.0416	.0025	-.0748
.9630	.9700	88.80	1.0299	1.3481	-.1169	-.1075

a = .1125

b = .2153

c = .0137

d = .0354

e = -.0274

B = .2059

C = -.0573

D = .0341

E = .0033

TABLE 23, Continued

System: Toluene - n-Octane
 Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	Expt. <u>$\log \frac{\gamma_1}{\gamma_2}$</u>	Calc. <u>$\log \frac{\gamma_1}{\gamma_2}$</u>
.0090	.0340	124.00	2.6208	1.0211	.4093	.3429
.0300	.0780	123.00	1.8527	1.0241	.2574	.3065
.0600	.1500	122.20	1.8194	.9966	.2614	.2618
.1100	.2200	120.70	1.5149	1.0080	.1769	.2037
.1950	.3300	119.00	1.3417	1.0053	.1254	.1422
.2500	.4250	117.40	1.4077	.9701	.1617	.1205
.3250	.4800	116.20	1.2639	1.0097	.0975	.1051
.4000	.5800	115.00	1.2826	.9505	.1301	.0983
.5000	.6550	113.80	1.1980	.9710	.0912	.0904
.5900	.7000	113.00	1.1095	1.0546	.0220	.0758
.6750	.7900	112.30	1.1162	.9511	.0695	.0508
.7650	.8400	111.60	1.0681	1.0236	.0185	.0114
.8400	.8850	111.00	1.0424	1.1004	-.0235	-.0299
.9170	.9330	110.50	1.0210	1.2550	-.0896	-.0768
.9570	.9670	110.20	1.0227	1.2041	-.0709	-.1012

$$\begin{aligned} a &= .0798 \\ b &= .1675 \\ c &= .0038 \\ d &= .0753 \\ e &= .0333 \end{aligned}$$

$$\begin{aligned} B &= .1573 \\ C &= -.0058 \\ D &= .0911 \\ E &= -.0979 \end{aligned}$$

TABLE 24

EXPERIMENTAL AND CALCULATED DATA

System: Toluene - Phenol

Antoine Constants:

$$\begin{array}{ll} A_1 = 6.95464 & A_2 = 7.13617 \\ B_1 = 1344.8 & B_2 = 1518.1 \\ C_1 = 219.482 & C_2 = 175.0 \end{array}$$

Boiling Points:

Toluene - 110.63°C (1, p. 1173)Phenol - 182°C (1, p. 1077)

Total Pressure: 760 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt.</u> <u>log γ₁</u>	<u>Calc.</u> <u>log γ₂</u>
.0435	.3409	172.70	1.7757	.8892	.3003	.3014
.0872	.5120	159.40	1.7550	1.0291	.2318	.2713
.1186	.6210	153.80	1.7693	.9890	.2526	.2491
.1248	.6250	149.40	1.8683	1.1383	.2151	.2447
.2190	.7850	142.20	1.5805	.9340	.2284	.1761
.2750	.8070	133.80	1.5860	1.2189	.1143	.1342
.4080	.8725	128.30	1.3275	1.2109	.0399	.0328
.4800	.8901	126.70	1.1996	1.2631	-.0224	-.0229
.5898	.9159	122.20	1.1302	1.4604	-.1113	-.1087
.6348	.9280	120.20	1.1222	1.5208	-.1320	-.1442
.6512	.9260	120.00	1.0975	1.6497	-.1770	-.1572
.7400	.9463	119.70	.9949	1.6254	-.2132	-.2280
.7730	.9536	119.40	.9676	1.6283	-.2260	-.2546
.8012	.9545	115.60	1.0365	2.1294	-.3127	-.2775
.8840	.9750	112.70	1.0402	2.2631	-.3376	-.3460
.9108	.9796	112.20	1.0287	2.4534	-.3775	-.3686
.9394	.9861	113.30	.9735	2.3493	-.3826	-.3930
.9770	.9948	111.10	1.0046	2.5437	-.4035	-.4256
.9910	.9980	111.10	.9936	2.4960	-.4001	-.4379
.9973	.9993	110.50	1.0056	2.9978	-.4744	-.4435

a = -.0436

b = .3886

c = -.0119

d = -.0005

e = -.0022

B = .3978

C = .0496

D = -.0244

E = .0005

TABLE 25

EXPERIMENTAL AND CALCULATED DATA

System: Water - Acetic Acid

Antoine Constants:

$$\begin{array}{ll} A_1 = 7.96681 & A_2 = 7.29963 \\ B_1 = 1668.21 & B_2 = 1479.02 \\ C_1 = 228.0 & C_2 = 216.81 \end{array}$$

Boiling Points:

Water - 100°C (l, p. 623)Acetic Acid - 118.1°C (l, p. 695)

Total Pressure: 760 mm Hg.

<u>x₁</u>	<u>y₁</u>	<u>t</u>	<u>γ₁</u>	<u>γ₂</u>	<u>Expt. log γ₁/γ₂</u>	<u>Calc. log γ₁/γ₂</u>
.0045	.0114	117.50	1.4048	1.0051	.1454	.1597
.0890	.1560	109.10	1.2777	1.2193	.0203	.0511
.1730	.2810	105.60	1.3344	1.2817	.0175	.0066
.3285	.4760	103.00	1.3031	1.2536	.0168	.0045
.4740	.6240	101.60	1.2437	1.2033	.0143	.0134
.5575	.6850	101.20	1.1774	1.2146	-.0135	.0033
.6360	.7450	100.90	1.1344	1.2074	-.0271	-.0183
.7430	.8170	100.60	1.0763	1.2397	-.0614	-.0588
.8400	.8860	100.40	1.0398	1.2489	-.0796	-.0886
.9540	.9680	100.10	1.0110	1.2316	-.0857	-.0763

a = -.0112

b = .0814

c = .0052

d = .0245

e = .0681

B = .0783

C = .0454

D = .0131

E = -.0991

TABLE 25, Continued

System: Water - Acetic Acid
 Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	Expt. $\log \frac{\gamma_1}{\gamma_2}$	Calc. $\log \frac{\gamma_1}{\gamma_2}$
.0500	.0920	115.40	1.0881	1.0318	.0231	.0305
.1000	.1670	113.80	1.0408	1.0500	-.0038	.0075
.2000	.3020	110.10	1.0643	1.1122	-.0191	-.0195
.3000	.4250	107.50	1.0904	1.1383	-.0187	-.0285
.4000	.5300	105.80	1.0810	1.1472	-.0258	-.0276
.5000	.6260	104.40	1.0722	1.1471	-.0293	-.0238
.6000	.7160	103.20	1.0657	1.1330	-.0266	-.0231
.7000	.7950	102.10	1.0542	1.1312	-.0306	-.0304
.8000	.8640	101.30	1.0312	1.1563	-.0497	-.0499
.9000	.9300	100.60	1.0114	1.2188	-.0810	-.0844
.9500	.9630	100.30	1.0029	1.3015	-.1132	-.1079

$$\begin{array}{ll}
 a = -.0318 & \\
 b = .0528 & B = .0410 \\
 c = -.0115 & C = .0287 \\
 d = .0458 & D = .0494 \\
 e = .0060 & E = -.0101
 \end{array}$$

TABLE 26

EXPERIMENTAL AND CALCULATED DATA

System: Water - n-Butanol
 Antoine Constants:

$$\begin{array}{ll} A_1 = 7.96681 & A_2 = 7.51697 \\ B_1 = 1668.21 & B_2 = 1392.66 \\ C_1 = 228.0 & C_2 = 182.66 \end{array}$$

Boiling Points:

Water - 100°C (l, p. 623)
 n-Butanol - 117.71°C (l, p. 813)

Total Pressure: 760 mm Hg.

<u>x</u>	<u>y</u>	<u>t</u>	<u>γ_1</u>	<u>γ_2</u>	<u>Expt.</u>	<u>Calc.</u>
					<u>$\log \frac{\gamma_1}{\gamma_2}$</u>	<u>$\log \frac{\gamma_1}{\gamma_2}$</u>
.0389	.2670	111.50	4.6113	.9562	.6833	.6203
.0470	.2990	110.60	4.4093	.9536	.6650	.6829
.0550	.3230	109.60	4.2099	.9641	.6401	.7358
.0700	.3520	108.80	3.7027	.9664	.5834	.8125
.2570	.6290	97.90	2.6393	1.0619	.3954	.3575
.2920	.6550	96.70	2.5266	1.0884	.3657	.1845
.3050	.6620	96.30	2.4808	1.1043	.3515	.1254
.4960	.7360	93.50	1.8802	1.3365	.1482	-.0917
.5060	.7400	93.40	1.8601	1.3485	.1397	-.0656
.5520	.7500	92.90	1.7606	1.4603	.0812	.0906
.5730	.7500	92.80	1.7024	1.5385	.0439	.1762
.9750	.7520	92.70	1.0069	26.1850	-1.4152	-4.4909
.9800	.7560	93.00	.9959	31.7832	-1.5041	-4.7565
.9850	.7750	93.40	1.0007	38.4358	-1.5845	-5.0322
.9880	.8080	93.70	1.0286	40.5042	-1.5953	-5.2023
.9920	.8430	95.40	1.0038	46.2777	-1.6639	-5.4340
.9940	.8839	96.80	.9980	43.0521	-1.6349	-5.5520
.9970	.9290	98.30	.9904	49.4198	-1.6982	-5.7316
.9980	.9510	98.40	1.0092	51.0781	-1.7045	-5.7929
.9990	.9810	99.40	1.0033	37.7513	-1.5757	-5.8536

$$\begin{array}{l} a = -.1038 \\ b = 1.3091 \\ c = -.1.2118 \\ d = 1.7344 \\ e = -.1.5567 \end{array}$$

$$\begin{array}{l} B = .8334 \\ C = .2843 \\ D = .3548 \\ E = .2232 \end{array}$$