CALCULATION OF ISOBARIC PHASE ENTHALPY DIFFERENCES FOR BINARY SYSTEMS FROM VAPOR-LIQUID EQUILIBRIUM DATA

By

STEVEN MERRILL HARVEY

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ABSTRACT

Equations relating isobaric vapor-liquid equilibrium data to heats of vaporization are useful in testing the thermodynamic consistency of experimental VLE data and in the design of distillation equipment. Several researchers have proposed such equations based on the Gibbs-Duhem equation. At low pressures, simplified versions of these equations were successfully used to test the consistency of published VLE and enthalpy data. At high pressures, equilibrium phase enthalpy differences were calculated from rigorous equations using a modified form of the Redlich-Kwong equation to calculate fugacity coefficients. As expected, the relative error of using the simplified equations was found to increase with increasing pressure.

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PREVIOUS METHODS AND THEORY

Othmer, Ricciardi, and Thakar (1953) presented the following equation for binary systems based on the Gibbs-Duhem equation at constant pressure assuming Dalton's law of partial pressures and the Clausius-Clapeyron equation:

$$\frac{L_x}{RT^2} = \left[\frac{x}{y} - \frac{(1-x)}{(1-y)}\right] \left(\frac{dy}{dT}\right)_p \tag{1}$$

where L_x is the latent heat of vaporization based on liquid composition (the integral latent heat of vaporization). They proposed equation (1) be applied to the prediction and correlation of x,y data from vacuum up to moderately high pressures. Earlier, Redlich and Kister (1948) had derived a similar relationship assuming that the variation of activity coefficients with temperature was negligible.

Van Ness (1959) derived a general form of the Gibbs-Duhem equation shown here:

$$\frac{v}{RT}dp + \frac{H^*-H}{RT^2}dT = \sum(z_i d\ln f_i) \tag{2}$$

At constant pressure this reduces to the following:

$$\frac{H^*-H}{RT^2}dT = \sum(z_i d\ln f_i)_p \tag{3}$$

Ljunglin and Van Ness (1962) extended this generalized form to a completely rigorous general coexistence equation for binary mixtures at constant pressure:

$$\Omega\, dT = (y_1-x_1)d\ln\frac{v_1}{v_2} + \frac{y_1-x_1}{y_1(1-y_1)} \tag{4}$$

$$\Omega = \frac{-(\Delta H^v + x_1 H_1^v + x_2 H_2^v - H^L)}{RT^2} \tag{4a}$$

The expression in parentheses ($\Delta H^V + x_1 H_1^V + x_2 H_2^V - H^L$) is a close approximation to the integral heat of vaporization. Another close approximation is as follows:

$$L_x = x_1 L_1 + x_2 L_2 - \Delta H^L \tag{5}$$

Othmer used this approximation in the derivation of equation (1). Equation (5) does not contain a term to account for the enthalpy change necessary to heat the vapor phase from the bubble point to the dew point.

Tao (1968) extended equation (4) to multicomponent systems. Equation (6) is his rigorous equation which describes the relationship between the molar enthalpy difference of two equilibrium phases and the x,y,T data for multicomponent systems:

$$\sum (x_i - y_i) d\ln f_i^V = \frac{L_{xy} - \Delta H^*}{RT^2} dT \tag{6}$$

where L_{xy} is the phase enthalpy difference and ΔH^* is equal to the difference between the ideal gas enthalpy with vapor phase composition and the ideal gas enthalpy with liquid phase composition. Tao also derived the limit forms of equation (6) as the mixture composition approaches that of a pure component (equation 7), as the mixture composition approaches that of an azeotrope (equation 8), and as the mixture approaches its critical point (equation 9).

$$1 - \frac{dy}{dx} = - \frac{L_{xy}}{RT^2} \frac{dT}{dx} \tag{7}$$

$$1/(d(dT/d\ln f_i^V)/d(x_i - y_i)) = L_{xy}/RT^2 \tag{8}$$

$$L_{xy} = 0 \tag{9}$$

Equation (6) can be simplified by assuming that $f_i = y_i P$ (a safe assumption at low pressures), resulting in equation (6a)

for binary mixtures:

$$\frac{L_{xy} - \Delta H^*}{RT^2} = \frac{(x_1 - y_1)}{y_1 y_2}\left(\frac{dy_1}{dT}\right) \tag{6a}$$

In a separate paper, Tao (1968) derived a similar equation relating the integral latent heat of vaporization to vapor- liquid equilibrium data:

$$L_x = x_i RT^2_{yd}\frac{d\ln f^v_x}{dT_{yd}} - x_i RT^2_{xd}\frac{d\ln f^v_x}{dT_{xd}} + (H^*_{xd} - H^*_{xb}) \tag{10}$$

At low pressures, equation (10) can be simplified by assuming that $f^v_y = y_i P$ and $f^v_x = x_i P$, resulting in equation (11):

$$L_x = RT^2_{yd}\frac{x_i dy_i}{y_i dT_{yd}} + (H^*_{xd} - H^*_{xb}) \tag{11}$$

For a binary system, equation (11) rearranges to:

$$L_x = RT^2\left[\frac{x_1}{y_1} - \frac{1-x_1}{1-y_1}\right]\left(\frac{dy_1}{dT}\right)_P + (H^*_{xd} - H^*_{xb}) \tag{11a}$$

Comparing equation (11a) with equation (1) we find they are eqivalent except for the term $(H^*_{xd} - H^*_{xb})$, which represents the enthalpy difference between a vapor mixture of composition x_1 at dewpoint temperature T_{xd} and a vapor mixture of composition x_1 at bubble point temperature T_{xb}. If we compare equation (11a) with equation (6), we find the integral heat of vaporization is related to the equilibrium phase enthalpy difference at low pressures by the expression:

$$L_x = L_{xy} + (H^*_{xd} + H^*_{xb}) \tag{12}$$

where T_{xb} is equivalent to T_{yd}. This is not surprising since the two values are related by definition by the following

expression:

$$L_x = L_{xy} + (H^v_{xd} - H^v_{yd}) \tag{13}$$

Therefore, equation (12) is a good approximation at relatively low pressures when the ideal gas enthalpy difference should approximate the actual enthalpy difference.

Lee and Edmister (1969) calculated phase enthalpy differences using a combination of equation of state calculations and ideal gas enthalpy values to calculate vapor enthalpies and a combination of equation (14) and ideal gas enthalpies to calculate liquid enthalpies:

$$\frac{H^*-H^L}{RT^2} = \sum x_i \left(\frac{\partial \ln\phi_i}{\partial T}\right)_{P,y} + \sum x_i \left(\frac{\partial \ln\phi_i}{\partial y_i}\right)\left(\frac{dy_i}{dT}\right)_P + \sum \frac{1}{K_i}\left(\frac{dy_i}{dT}\right)_P \tag{14}$$

Equation (14) was obtained by combining equation (3) with equation (15):

$$\left(\frac{d\ln f_i}{dT}\right) = \left(\frac{\partial \ln\phi_i}{\partial T}\right)_{P,y} + \left(\frac{\partial \ln\phi_i}{\partial y_i}\right)\left(\frac{dy_i}{dT}\right)_P + \left(\frac{\partial \ln\phi_i}{\partial y_j}\right)\left(\frac{dy_j}{dT}\right)_P + \ldots$$

$$\ldots + \left(\frac{\partial \ln\phi_i}{\partial y_n}\right)\left(\frac{dy_n}{dT}\right)_P + \left(\frac{d\ln y_i}{dT}\right)_P \tag{15}$$

The temperature-composition derivatives $(dy/dT)_P$ were evaluated by fitting a polynomial to a set of six or seven data points to find the empirical constants by least squares, then differentiating the resulting expression to find the derivatives of the middle range points. The two derivatives of $\ln(\phi_i)$ were determined analyticaly from the Benedict-Webb-Rubin and Redlich-Kwong equations of state.

Lee and Edmister concluded that this method of calculating

saturated liquid enthalpy values for mixtures is particularly sensitive to the method used to smooth and differentiate the temperature-composition data, and to a lesser extent, the input data itself and the choice of equation of state. They could not recommend the method until a better procedure for determining the derivative $(dy_i/dT)_P$ is found.

This paper uses Tao's simplified equation (6a) to calculate equilibrium phase enthalpy differences at low pressures. Equation (11a) is used to calculate integral heats of vaporization. Instead of the least squares curve fitting technique used by Lee and Edmister to determine $(dy_i/dT)_P$, this paper uses the Wilson equation to smooth experimental T,y data, and a spline fitting technique to determine the derivative. For higher pressure systems, Tao's equation (6) is rearranged to allow the use of fugacity coefficients calculated from a form of the Redlich-Kwong equation as modified by Prausnitz and Cheuh (1972).

EXTENSION OF TAO'S METHOD FOR BINARY MIXTURES TO HIGHER PRESSURES

Equation (6) can be rearranged to the following form:

$$\sum(x_i-y_i)\left(\frac{d\ln f_i^v}{dT}\right) = \frac{(L_{xy}-\Delta H^*)}{RT^2} \tag{6b}$$

By definition:

$$f_i = \phi_i y_i P \tag{16}$$

At contant pressure:

$$(d\ln f_i/dT)_P = \frac{1}{y_i}\left(\frac{dy_i}{dT}\right)_P + \frac{1}{\phi_i}\left(\frac{d\phi_i}{dT}\right)_P \tag{17}$$

Substituting into equation (6b) for a binary mixture:

$$(x_1-y_1)\left[\frac{1}{y_1}\left(\frac{dy_1}{dT}\right)_P + \frac{1}{\phi_1}\left(\frac{d\phi_1}{dT}\right)_P\right] + (x_2-y_2)\left[\frac{1}{y_2}\left(\frac{dy_2}{dT}\right)_P + \frac{1}{\phi_2}\left(\frac{d\phi_2}{dT}\right)_P\right] = \frac{(L_{xy}-\Delta H^*)}{RT^2} \tag{18}$$

Since $y_2 = 1-y_1$ and $x_2 = 1-x_1$, this rearranges to:

$$\frac{(x_1-y_1)}{y_1y_2}\left(\frac{dy_1}{dT}\right)_P + (x_1-y_1)\left[\left(\frac{d\ln\phi_1}{dT}\right)_P - \left(\frac{d\ln\phi_2}{dT}\right)_P\right] = \frac{(L_{xy}-\Delta H^*)}{RT^2} \tag{19}$$

where for a binary system at constant pressure

$$\left(\frac{d\ln\phi_i}{dT}\right)_P = \left(\frac{d\ln\phi_i}{dy_1}\right)\left(\frac{dy_1}{dT}\right)_P \tag{20}$$

Comparing equation (19) with equation (6a) we find they are identical with the exception of the second term on the left-hand side of equation (19). This term represents the differ-

ence between the actual equilibrium phase enthalpy difference and the value calculated assuming $f_i = y_i P$. In this paper, this term will be referred to as the fugacity contribution to L_{xy}

The derivative $(d\ln\phi_i/dy_1)_P$ can be found by numerically differentiating an equation of state such as the Redlich-Kwong equation. The derivative $(dy_1/dT)_P$ can be found by graphical differentiation or by curve fitting temperature composition data and differentiating the resulting equation.

METHODS OF DETERMINING $(dy/dT)_P$ AND $(d\ln\phi/dy)_P$

In this paper, two methods of obtaining $(dy/dT)_P$ from temperature-composition data were investigated:

1. Representation of T,y data with a single third or fourth order polynomial using the method of King (1962), then differentiation of the resulting equation.
2. Smoothing the T,y data with the Wilson equation, representation of smoothed data with a third degree natural spline function and differentiation of the function using the method of Grenville (1967).

The derivatives $(d\ln\phi_i/dy)$ were determined by numerically differentiating the Redlich-Kwong equation of state as modified by Prausnitz and Chueh (1972). A two phase binary system has two degrees of freedom. In the case of constant pressure, fixing the vapor composition y_1 fixes the liquid composition x_1 and the temperature T. At a specified vapor composition, the molar volume of the gas mixture was determined by solving the Redlich-Kwong equation:

$$P = \frac{RT}{v - b} - \frac{a}{T^{0.5}v(v+b)} \tag{21}$$

where a and b are functions of y_1 and component critical properties and T is a function of y_1. The fugacity coefficients for each component were determined as proposed by Prausnitz and Chueh. The derivatives were obtained by evaluating $\Delta\phi_i/\Delta y_i$ over small increments of y_1.

LOW PRESSURE EXAMPLE: THE ETHANOL-WATER SYSTEM AT 1 ATM THE CALCULATION OF THE EQUILIBRIUM PHASE ENTHALPY DIFFERENCE

The ethanol-water system was chosen for study because it had been studied by Tao (1968) and published enthalpy data were available for comparison. The ethanol-water data of Thomson and Reider (1949) was fit to the Wilson equation to allow interpolation of intermediate values. The smoothed data are presented in table 1. The smoothed data was then fit to third and fourth order polynomials resulting in equations of the form:

$$y_1 = a + bT + cT^2 + dT^3 \tag{22}$$

and

$$y_1 = a + bT + cT^2 + dT^3 + eT^4 \tag{23}$$

Differentiation of equations (22) and (23) led to the following:

$$(dy_1/dT)_P = b + 2cT + 3dT^2 \tag{24}$$

$$(dy_1/dT)_P = b + 2cT + 3dt^2 + 4eT^3 \tag{25}$$

The smoothed data were also fit to a third order natural spline function and differentiated as proposed by Grenville (1967). Using Grenville's method, every set of four smoothed data points was fit to a third order polynomial with the requirement that the values and derivatives at the connecting points, as evaluated by adjacent polynomials, be equivalent. The results are tabulated for each method in table 2, and shown graphically in figure 1.

The derivatives from table 2 were then used to calculate the phase enthalpy difference using equation (6a). Values of L_{xy} are presented in table 3 and compared to the published values of Tao (1968) and Faust (1960).

Figure 1 illustrates that (dy_1/dT) is very sensitive to the method chosen to represent and differentiate T,y data. Assuming that the data of Faust is correct, it is evident from table 3 that the best results were obtained using Grenville's method. A comparison of the Faust data and L_{xy} obtained from equation (6a) is shown graphically in figure 2. The largest relative error occurred at $y_1 = 0.0$ (pure water) where $L_{xy} = L_{H_2O}$ was calculated from equation (7) using two spline functions, one for T,y and the other for T,x representation. Since the heat of vaporization of pure water is well known, the use of equation (7) with this approach is not very accurate. Future research may find it possible to use equation (7) to improve the accuracy of the Wilson equation and other VLE equations in the dilute phase regions.

LOW PRESSURE EXAMPLE: THE TOLUENE-1,2-DICHLOROETHANE SYSTEM AT 686 TORR
THE CALCULATION OF INTEGRAL LATENT HEATS OF VAPORIZATION

The toluene-1,2-dichloroethane system was studied in order to compare values of L_x calculated from equation (11a) with published data. Equation (11a) was selected instead of equation (10) because the pressure was low and f_i could be assumed equal to $y_i P$. The procedure used to determine $(dy/dT)_P$ was the same as that used in the ethanol-water example. Vapor-liquid equilibrium data of Sundaram and Viswanath (1976) was smoothed with the Wilson equation. The smoothed T,y data were then fit to both a fourth order polynomial and a spline function to generate the derivatives and equation (11a) was used to calculate L_x. For purposes of comparison, equation (6a) was used to calculate L_{xy}. Calculated values of L_x and L_{xy} are listed in table 4. The polynomial fit was smoother than the spline fit in this particular case. Figure 3 compares the calculated valus of L_x to the published values. Assuming that the published values of L_x to correct, the maximum error using equation (11a) with the polynomial fit was about 3% which indicates that the VLE data and published latent heat data are reasonably consistent.

It is interesting to note that the maximum calculated difference between the equilibrium phase enthalpy difference and the integral latent heat of vaporization was 229 cal./gm.-mole at $x_1 = 0.7$, or 2.9% of L_x. Thus, the maximum difference between the two parameters was less than the maximum error of the method of calculation. Similarly, the contribution of the term $(H_d^* - H_b^*)_x$ was less than 2.1%. This represents the relative error of using equation (1) in place of equation (11a).

HIGH PRESSURE EXAMPLE: THE ETHANE-BUTANE SYSTEM AT 200 PSIG

The ethane-butane system was selected because it was one of the systems studied by Lee and Edmister (1969) when they concluded that a better method of determining (dy_1/dT) must be found before they could recommend using the isobaric Gibbs-Duhem equation to predict saturated liquid enthalpies from experimental vapor-liquid equilibrium data. Also, published enthalpy values, calculated by other methods, were available in the literature for comparison.

Because of the system pressure (200 psig), it could not be assumed that $f_i = y_i P$. Therefore, equation (19) was used instead of equation (6a). Smoothed T,y,x data were obtained by fitting the experimental data of Chu (1952) to the Wilson equation using Flowtran (1974). The smoothed data were then fit to both a fourth order polynomial and a spline function as previously described for the ethanol-water system. Results using the spline function are shown and compared in table 5 to the calculated values of Steil, Hobson, and Weber (1956). Results using the fourth order polynomial are shown in table 6, and all of the values are compared graphically in figure 4. From figure 4 it is obvious that the spline fit method yielded smoother results than the polynomial method. However, values calculated by both methods were higher than the published values. This indicates that the VLE data used is inconsistent with the published enthalpy values.

Also indicated in table 5 and table 6 are the fugacity contributions of equation (19). In this particular case, the relative fugacity contribution was less than 5% of the phase enthalpy difference throughout the concentration range despite the fact that the fugacity coefficient of butane ranged as low as 0.62. The fugacity contribution represents the difference between the actual phase enthalpy difference and that calculated using the simplified equation (6a).

THE EFFECT OF PRESSURE ON THE FUGACITY CONTRIBUTION TO THE EQUILIBRIUM PHASE ENTHALPY DIFFERENCE

Three systems were studied at various pressures in order to determine how much of a contribution the term

$$\text{fug. cont.} = (x_1 - y_1)\left[(d\ln\phi_1/dT)_P - (d\ln\phi_2/dT)_P\right] RT^2$$

makes to equation (19). The systems studied were:

1. Ethane-butane from 6.8-34.0 atm. (100-500 psia)
2. Carbon dioxide-propane from 33.9-54.3 atm. (500-800 psia)
3. Carbon dioxide-hydrogen sulfide from 20-80 atm. (294-1176 psia)

The T,y,x data used for all systems were obtained from Chu (1952). The x,y data were used directly, but the T,y data were fit to a fourth order polynomial using the method of King (1962) with y_1 as the independent variable. Therefore, T was calculated using equation (23), $(dT/dy_1)_P$ was calculated using equation (25), and $(dy_1/dT)_P = 1/(dT/dy_1)_P$. All calculations were done by digital computer using critical properties from Smith and Van Ness (1959), interaction parameters and constants from Prausnitz and Cheuh (1972), and regression parameters for ideal gas specific heats from Hougen and Watson (1959).

The results of the computerized calculations are summarized in table 7. Note that for each system, the relative fugacity contribution increases with increasing pressure. This confirms that the use of equation (6a) at high pressures could result in errors as high as 12% of calculated L_{xy}, possibly greater.

DISCUSSION OF RESULTS AND CONCLUSIONS

As previously experienced by Lee and Edmister (1969), the calculation of enthalpy differences based on the isobaric Gibbs-Duhem equation is very sensitive to the methods used to smooth and differentiate experimental T,y data. A polynomial expression can be used to directly represent experimental data either by least squares or by the method used in this paper. However, lower order polynomials cannot accurately represent systems of widely varying curvature and higher order polynomials require more data points than are normally available from the literature. A spline function cannot be used directly with experimental data since the resulting function will pass through each data point causing significant errors in the derivative due to normal experimental scatter. The method can be improved by first smoothing the data with using any applicable VLE equation (such as the Wilson equation used in this paper), then fitting the smoothed data to a high order polynomial or a spline function. The accuracy of the derivatives will depend on the accuracy of the VLE equation itself.

The best results for the low pressure, binary systems studied in this paper were achieved by smoothing the data with the Wilson equation, then representing the smoothed data with a spline function. Compared with published data, the average error of calculated values of L_{xy} for the ethanol-water system was 1.4 % using the spline function, 4.7 % using a fourth order polynomial, and 24.9 % using a third order polynomial. The average error of L_x for the toluene-1,2-dichloroethane system was 1.3 % using the spline function and 1.4 % using a fourth order polynomial.

The use of equation (19) to calculate the equilibrium phase enthalpy difference at high pressures has not been confirmed due to a lack of high pressure enthalpy data. L_{xy} values for

the ethane-butane system calculated from equation (19) were found to be, on the average, 20 % higher than the published values of Smith and Weber (1964). Hopefully, accurate methods of measuring latent heats at high pressures will be used in the future to obtain data on this system. Until then one can state only that according to equation (19), the published VLE data is not consistent with the published enthalpy data.

In this paper, several methods of calculating phase enthalpy differences were compared. In addition, several approaches to handling temperature-composition as input to the equations used were tested. Based on the results and comparisons the following were concluded :

1. At low pressures, equations (6a) and (11a) can be used to test the consistency of experimental VLE data for binary systems with latent heats of vaporization. However, it is recommended that the VLE data first be smoothed with a suitable VLE equation, then differentiated using a spline fitting technique.

2. At higher pressures equation (19) should be used in conjunction with an equation of state, such as the Redlich-Kwong equation, rather than the simplified equations. This method requires confirmation due to the lack of published experimental high pressure enthalpy data.

NOMENCLATURE

x_i = mole fraction of i in liquid

y_i = mole fraction of i in vapor

f_i = the fugacity of i in the mixture

L_x = the intergral heat of vaporization at P and x of the system

L_{xy} = the phase enthalpy difference for co-existing equilibrium vapor and liquid at P and T of the system.

L_i = latent heat of pure component i

R = gas constant

ΔH^* = (ideal gas enthalpy with vapor phase composition - ideal gas enthalpy with liquid phase composition)

ΔH^V = vapor phase heat of mixing

ΔH^L = liquid phase heat of mixing

H_i = molal enthalpy of component i

γ_i = activity coefficient of component i in mixture

Ω = defined by equation (4a)

Superscripts

V = of vapor phase

L = of liquid phase

Subscripts

1 = of component 1

2 = of component 2

d = at dew point temperature of mixture

b = at bubble point temperature of mixture

x = at composition x_i

y = at composition y_i

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Table 1

Ethanol-Water Data of Thomson and Reider(18) Smoothed By the Wilson Equation

X	Y	T (K)	X	Y	T (K)
.0000	.0000	373.125	.8400	.8559	350.897
.1000	.4269	359.957	.8500	.8635	350.873
.2000	.5196	356.705	.8600	.8713	350.851
.3000	.5727	355.019	.8700	.8792	350.831
.4000	.6171	353.825	.8800	.8873	350.815
.5000	.6613	352.871	.8900	.8956	350.800
.6000	.7091	352.086	.9000	.9040	350.789
.7000	.7633	351.463	.9100	.9127	350.779
.7500	.7937	351.216	.9200	.9215	350.773
.7600	.8001	351.172	.9300	.9305	350.770
.7700	.8066	351.131	.9400	.9398	350.769
.7800	.8133	351.091	.9500	.9492	350.771
.7900	.8200	351.053	.9600	.9589	350.777
.8000	.8269	351.018	.9700	.9688	350.786
.8100	.8340	350.984	.9800	.9789	350.798
.8200	.8411	350.953	.9900	.9893	350.813
.8300	.8485	350.924	1.0000	1.0000	350.832

Table 2

Ethanol-Water System At 1 Atm.

Comparison of Methods used to represent T-Y data and calculate $(dy1/dT)_P$

X	dy/dT^a	dy/dT^b	dy/dT^c	dy/dT^d
0.000	-.0592	-.0572	-.0343	-.0375
.100	-.0377	-.0287	-.0287	-.0274
.200	-.0303	-.0323	-.0296	-.0280
.300	-.0275	-.0359	-.0340	-.0345
.400	-.0233	-.0405	-.0412	-.0440
.500	-.0297	-.0474	-.0526	-.0538
.600	-.0363	-.0595	-.0714	-.0758
.700	-.0546	-.0878	-.1082	-.1240
.800	-.1688	-.2285	-.2035	-.2128
.900	+.1040	+.2020	-.6816	—
1.000	—	—		+.1720

a. third order polynomial ($0.0 \leq y1 \leq 0.9$)
b. fourth order polynomial ($0.0 \leq y1 \leq 0.9$)
c. third order natural spline function ($0.0 \leq y1 \leq 0.94$)
d. Published by Tao (3)...method of calculation not indicated.

Table 3

Ethanol-Water System

Calculation of L_{xy} From Equation (6a)

and Comparison to Published Data

(P= 1 Atm)

X	L_{xy} [a]	L_{xy} [b]	L_{xy} [c]	L_{xy}(Tao) [e]	L_{xy}(Faust) [f]
.000			9151 [d]	9649	9712
.100	13258	10162	10162	9545	9930
.200	10078	10726	9852	9483	10844
.300	7900	10244	9714	9720	9900
.400	5501	9432	9593	10285	9770
.500	5421	8575	9501	8950	9660
.600	4815	7938	9388	9162	9580
.700	4745	7600	9354	9456	9550
.800	7788	10534	9384	9860	9560
.900	-1163	-2273	7684		
1.000			9432 [4]	9289	9398

a. Third order polynomial used to represent T-Y data
b. Fourth order polynomial used to represent T-Y data
c. Third order natural spline function used to represent T-Y data
d. Calculated using equation (7)
e. Calculated by Tao (3)
f. Published data of Faust (21)

Table 4

Toluene-1,2-Dichloroethane System

at 686 Torr

mole fraction toluene		equil. temp.	$(dy_1/dT)_P$ [a]	term [b]	$(H_d^*-H_b^*)_x$ [c]	ΔH^* [c]	L_x [d]	L_{xy} [e]	L_x [h]
X^f	Y^f	^oK	$^oK^{-1}$	.....calories/g-mole.....					
0.0	0.0000	354.2	.02648	6995[g]	0	0	6995	6995	
0.1	.0482	356.0	.02720	7736	33	-18	7769	7718	7787
0.2	.1022	358.0	.02861	7826	64	-36	7826	7726	7864
0.3	.1633	360.0	.03052	7865	89	-53	7954	7812	7939
0.4	.2333	362.3	.03249	7894	108	-70	8002	7824	8002
0.5	.3143	364.7	.03497	7962	130	-84	8092	7878	8069
0.6	.4087	367.3	.03796	8053	121	-93	8174	7960	8114
0.7	.5198	370.1	.04078	8011	135	-94	8146	7917	8182
0.8	.6516	373.2	.04432	8016	91	-83	8107	7933	8181
0.9	.8094	376.5	.04913	8129	56	-55	8185	8074	8162
1.0	1.0000	380.2	.05339	7666[g]	0	0	7666	7666	

a. Calculated from spline fit to smoothed T-Y data

b. term = $(\frac{x1}{y1} - \frac{1-x1}{1-y1})RT^2(dy1/dT)_P = L_x$ according to equation (1)

c. Calculated using heat capacity data from Hougen, Watson, and Ragatz based on a datum of 273.2 deg. K.

d. Calculated from equation (11a) . L_x = the integral heat of evaporation.

e. Calculated from equation (6a). L_{xy} = the phase enthalpy difference.

f. Data of Sundaram and Viswanath , smoothed with the Wilson equation.

g. Calculated from equation (7)

h. Calculated using T and $(dy1/dT)_P$ from 4th order T-Y polynomial.

Table 5

Ethane-Butane System at 200 Psia

mole fraction ethane x	y	equilibrium temperature °K	term[a]	fug. cont.[b]	ΔH^*	L_{xy}[c]	published data
			.....calories/gram-mole.....				
0	0	367.8					3817
.10	.3849	344.9	4107	-34	-232	3841	3159
.20	.6478	323.3	4128	13	-255	3886	3007
.30	.7830	308.4	4064	100	-180	3984	3039
.40	.8814	291.3	3658	143	- 77	3724	3144
.50	.9313	278.7	3473	132	- 9	3596	3138
.60	.9579	269.8	3479	109	22	3610	3070
.70	.9735	263.3	3531	85	31	3647	2989
.80	.9835	258.5	3439	58	27	3524	2884
.90	.9905	255.4	2797	30	16	2843	2764
1.00	1.0000	252.2					2668

a. term = $\left(\frac{x_1}{y_1} - \frac{1-x_1}{1-y_1}\right)RT^2\left(\frac{dy_1}{dT}\right)_P$ from equation (19)

b. the fugacity contribution = $(x_1-y_1)\left(\left(\frac{d\ln\phi_1}{dT}\right)_P - \left(\frac{d\ln\phi_2}{dT}\right)_P\right)RT^2$

c. L_{xy} = term[a] + fugacity contribution + ΔH^*

Table 6

Ethane-Butane System at 200 Psia.

x_1	y_1	T^a (^oK)	V (l/gmol)	dy_1/dT^b ($x10^2$)	ϕ_1	ϕ_2	$\frac{d\ln\phi_1}{dT}$ ($^oK^{-1}$	$\frac{d\ln\phi_2}{dT}$ $x10^2$..)	Fug. Cont. (cal/gmol	ΔH^* .....)	L_{xy}
.1	.385	344.4	1.698	-1.46	.959	.780	.184	.133	-34.2	-231.8	3878
.2	.648	324.4	1.657	-1.03	.929	.761	.123	.145	12.5	-255.0	3990
.3	.783	307.6	1.580	-.628	.910	.738	.119	.210	83.0	-180.3	3257
.4	.881	288.3	1.468	-.420	.889	.703	.136	.296	127.1	- 76.8	3248
.5	.931	275.2	1.383	-.344	.872	.673	.159	.369	136.3	- 8.9	3616
.6	.958	267.0	1.327	-.310	.860	.652	.177	.424	125.1	22.4	4041
.7	.974	261.8	1.290	-.291	.852	.637	.191	.465	101.9	31.3	4342
.8	.984	258.3	1.265	-.280	.846	.627	.202	.495	71.4	27.3	4303
.9	.991	255.8	1.246	-.273	.841	.619	.210	.518	36.3	15.7	3466

a. Calculated from equation (23)

b. Calculated from equation (25)

Table 7

The Effect of Pressure On the Relative Fugacity Contribution[a]

Ethane-Butane System

System Pressure (Atm.)	Maximum Fugacity Contribution (percent of L_{xy})
6.8	2.5
13.6	3.8
20.4	5.0
27.2	6.0
34.0	8.5

Carbon Dioxide-Propane System

33.9	7.8
40.8	8.7
47.6	11.3
54.3	12.6

Carbon Dioxide-Hydrogen Sulfide System

20.0	2.8
30.0	3.9
40.0	5.1
50.0	6.3
60.0	7.4
70.0	8.3
80.0	7.6[b]

a. The relative fugacity contribution is defined on page 13.

b. Approximately one half of the concentration range was supercritical at 80 Atm.

FIGURE CAPTIONS

Figure 1. Ethanol-Water System at 1 Atmosphere: $(dy_1/dT)_P$ Vs. y_1

Figure 2. Ethanol-Water System at 1 Atmosphere: L_{xy} Vs. y_1

Figure 3. Toluene-1,2-Dichloroethane System at 686 Torr: L_x Vs. x_1

Figure 4. Ethane-n-Butane System at 200 Psia: L_{xy} vs. x_1

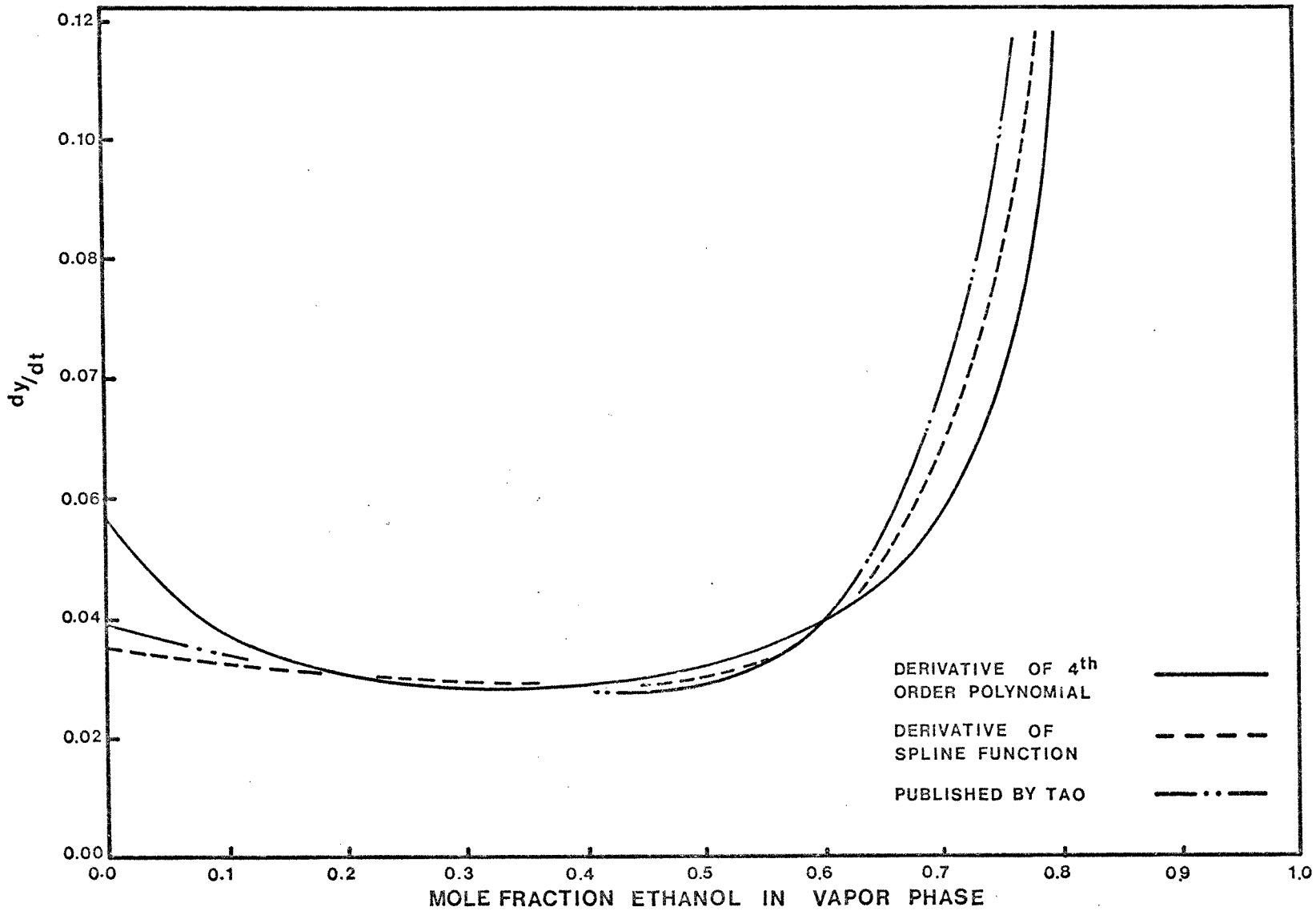
0.12
0.10
0.08
0.07
0.06
0.04
0.02
0.00
dy/dt
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
MOLE FRACTION ETHANOL IN VAPOR PHASE
DERIVATIVE OF 4th ORDER POLYNOMIAL
DERIVATIVE OF SPLINE FUNCTION
PUBLISHED BY TAO

FIGURE 1

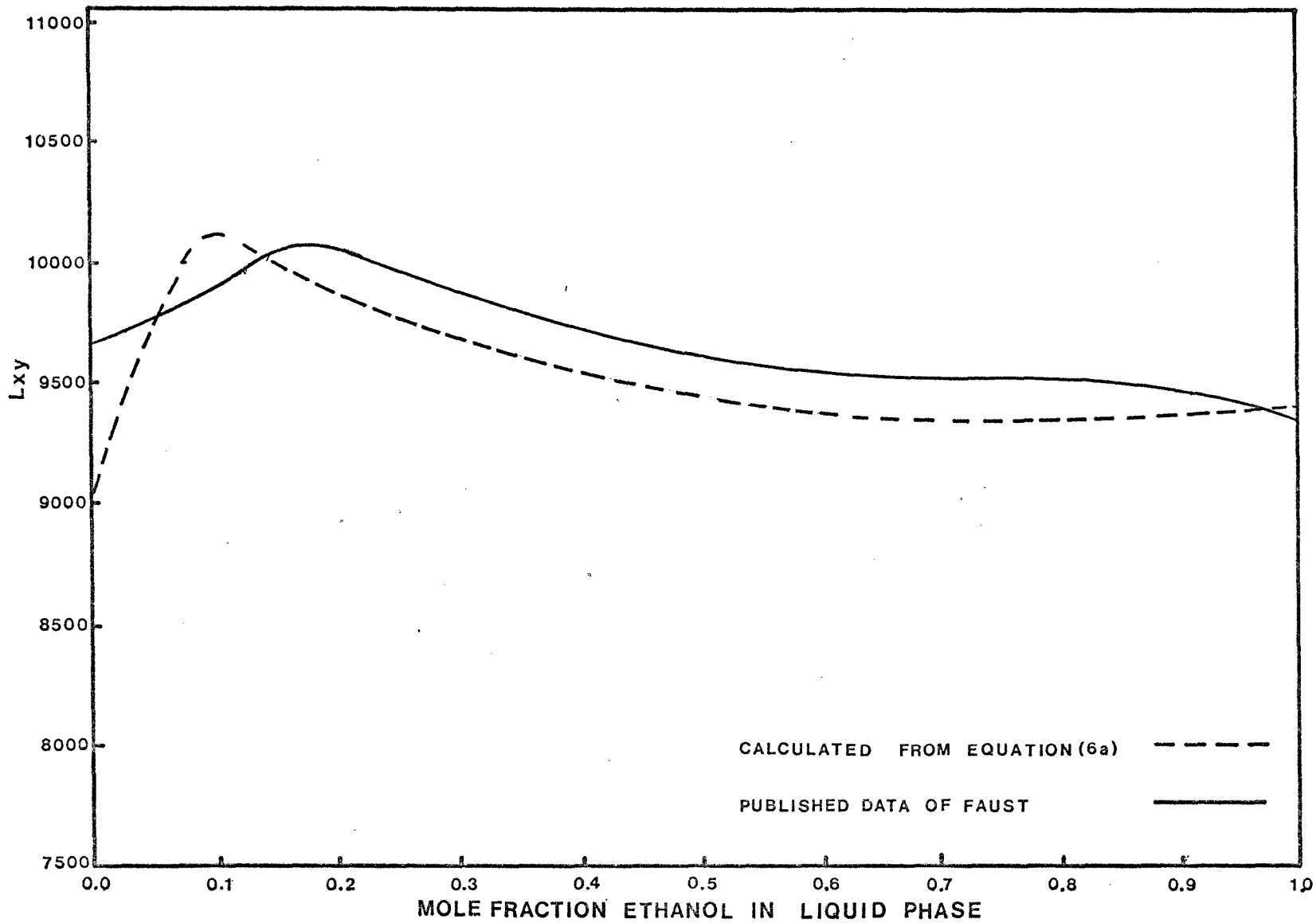
11000
10500
10000
9500
9000
8500
8000
7500
Lxy
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
MOLE FRACTION ETHANOL IN LIQUID PHASE
CALCULATED FROM EQUATION (6a)
PUBLISHED DATA OF FAUST

FIGURE 2

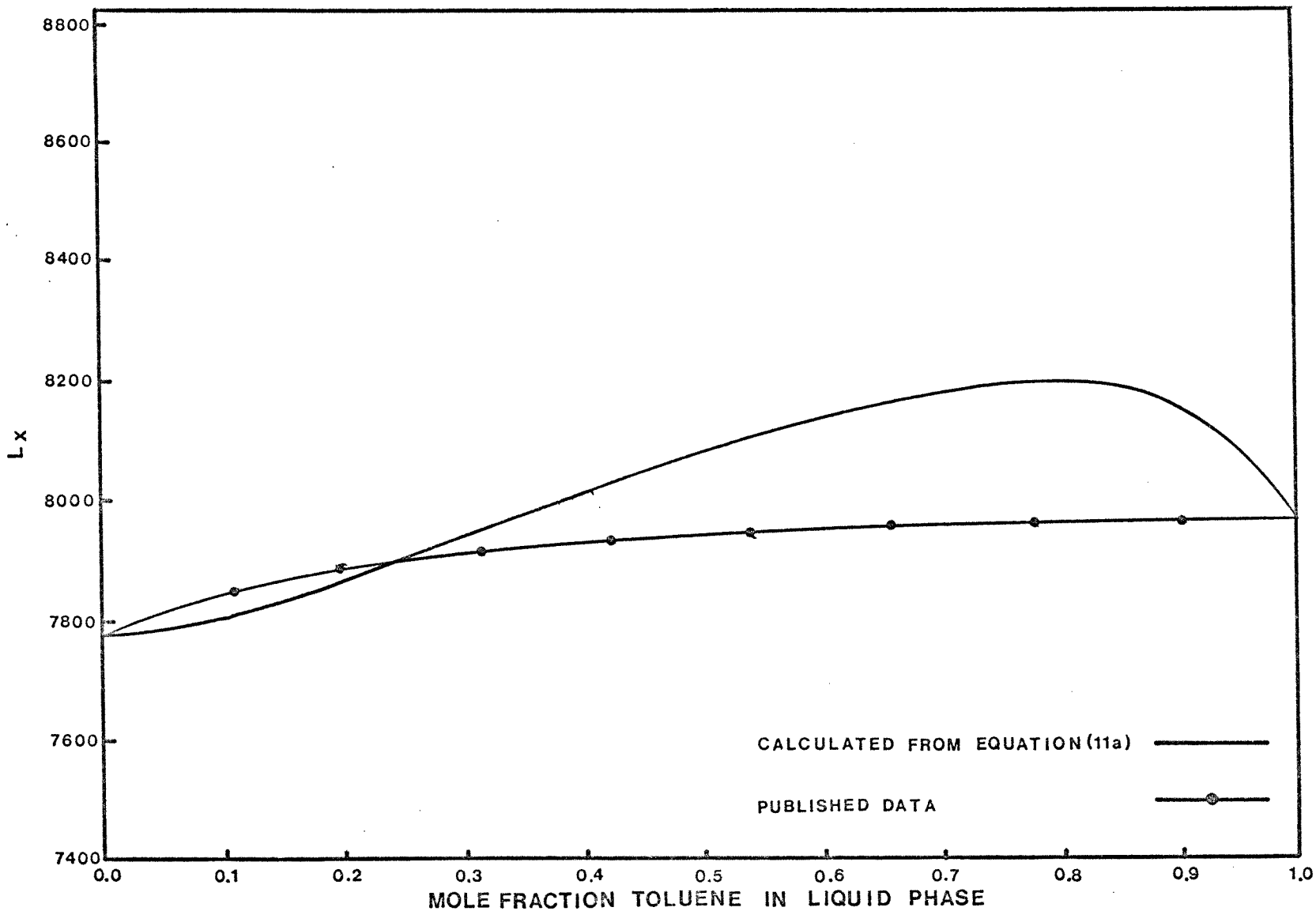
8800
8600
8400
8200
8000
7800
7600
7400
Lx
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
MOLE FRACTION TOLUENE IN LIQUID PHASE
CALCULATED FROM EQUATION (11a)
PUBLISHED DATA

FIGURE 3

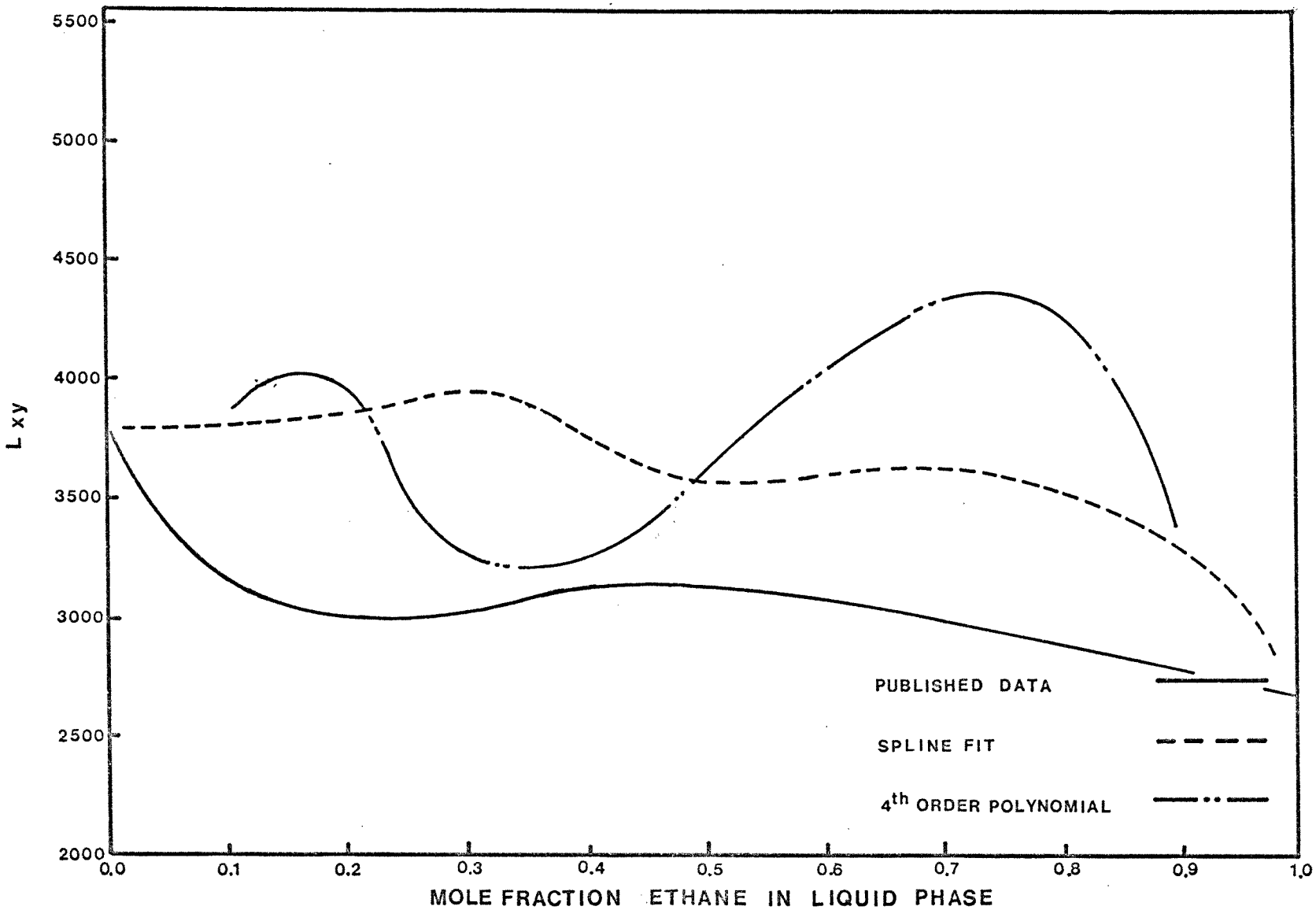
5500
5000
4500
4000
3500
3000
2500
2000
L xy
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
MOLE FRACTION ETHANE IN LIQUID PHASE
PUBLISHED DATA
SPLINE FIT
4th ORDER POLYNOMIAL

FIGURE 4

COMPUTER PROGRAM "ETHANE"

(Used to tabulate the ethane-butane section of table 7)

```
1C        ETHANE --- REVISED FEBRUARY 8, 1978
2C
3C        THIS PROGRAM CALCULATES ISOBARIC INTEGRAL LATENT HEATS OF
4C        VAPORIZATION FOR BINARY MIXTURES FROM HIGH PRESSURE VAPOR-
5C        LIQUID EQUILIBRIUM DATA
6C
7         DIMENSION FG1(99),FG2(99),DDF1(99),DDF2(99),DH(99),CF(99),DHF(999)
8         DIMENSION DAA(99),DBB(99)
9         DIMENSION YV(99),YW(99),YD(99)
10        DIMENSION X(99),Y(99),H(99),T(99),A(99),B(99),YY(99)
11&          ,V(99),DY(99),DV(99),DF(99),FGC1(99),FGC2(99)
20C
21C        ETHANE BUTANE BINARY SYSTEM : ASSIGNED BINARY DATA
22C
23C        TC=COMPONENT CRITICAL TEMP IN DEG K ; PC=CRITICAL PRES IN ATM
24C        VC=CRITICAL VOLUME IN LITERS/GM-MOLE; OMEGA,OMEGB,W,C12=CONSTANTS
25C        USED FOR THE MODIFIED REDLICH-KWONG EQUATION
26C        HA,HB,HC,HD=IDEAL GAS SPECIFIC HEAT REGRESSION COEFFICIENTS
27C        WM=COMPONENT MOLECULAR WEIGHT ; HV=LATENT HEAT OF VAPORIZATION
28C        AT BOILING POINT BP FOR PURE COMPONENT ; CP=AVG SPEC HEAT OF LIQ
29C
30         TC1=305.0
35         TC2=425.0
40         PC1=48.2
45         PC2=37.5
50         VC1=.1479
55         VC2=.2548
60         OMEGA1=0.434
65         OMEGA2=0.445
70         OMEGB1=0.088
75         OMEGB2=0.0906
80         W1=.105
85         W2=.200
90         C12=0.01
100         HA1=1.648
101        HB1=4.124E-2
102        HC1=-1.53E-5
103        HD1=1.74E-9
104        HA2=0.945
105        HB2=8.873E-2
106        HC2=-4.38E-5
107        HD2=8.36E-9
108        WM1=30.07
109        BP1=184.5
110        CP1=.55
111        HV1=3506
112        WM2=58.12
113        BP2=298
114        CP2=.55
115        HV2=5503
116C
116C        THIS SECTION READS IN T-Y REGRESSION DATA, SYSTEM PRESSURE
117C        IN ATM, AND X-Y DATA PAIRS
118C
165 301   CONTINUE
170         PRINT 6
180 6       FORMAT(/"TYPE T-Y REGRESSION DATA: Y0,T0,Y1,T1,Y2,T2,Y3,T3,Y4,T4"/)
200         READ,FY0,FT0,FY1,FT1,FY2,FT2,FY3,FT3,FY4,FT4
202         PRINT 200
204 200     FORMAT(/"TYPE TOTAL PRESSURE IN ATM"/)
```

```
206        READ,P
210 7      CONTINUE
220        PRINT 8
230 8      FORMAT(/"TYPE NO OF Y1,X1 DATA PAIRS OF INPUT"/)
240        READ,L
250        PRINT 9
260 9      FORMAT(/"TYPE Y1,X1 PAIRS, ONE PAIR PER LINE"/)
270        J=1
280        DO 10 I=1,L,1
290        READ,Y(J),X(J)
294       YV(J)=Y(J)*.995
296       YW(J)=Y(J)*1.005
298       YD(J)=YV(J)-YW(J)
300 10     J=J+1
301C
302C       THIS SECTION OF THE PROGRAM CALCULATES SPECIFIC VOLUME
303C       OF THE VAPOR MIXTURE BY SOLVING THE MODIFIED REDLICH
304C       EQUATION FOR THE LARGEST REAL ROOT
305C
310        TC12=(SQRT(TC1*TC2))*(1.-C12)
320        ZC12=.291-.08*((W1+W2)/2.)
330        VC12=(.5*(VC1**(1./3.)+VC2**(1./3.)))**3
340        VCX=VC1/VC2
350        IF(VCX.GE.3.)VC12=(VC1+VC2)/2.
360        A1=(OMEGA1*.006732*(TC1**2.5))/PC1
370        A2=(OMEGA2*.006732*(TC2**2.5))/PC2
380        B1=OMEGB1*.08205*TC1/PC1
390        B2=OMEGB2*.08205*TC2/PC2
400        PC12=ZC12*.08205*TC12/VC12
410        A12=(OMEGA1+OMEGA2)*.006732*(TC12**2.5)/(2.*PC12)
420        RE=(FT4-4.*FT3+6.*FT2-4.*FT1+FT0)/24.
430        RD=(FT3-3.*FT2+3.*FT1-FT0)/6.-6.*RE
440        RC=(6.*FT2-9.*FT1+4.*FT0-FT3)/6.-2.*RD-RE
450        RB=FT1-FT0-RC-RD-RE
460        RA=FT0
470        DELTA=(FY4-FY0)/4.
480        J=1
490        DO 11 M=1,L,1
492       KK=1
493 203   CONTINUE
500        T(J)=RA+RB*(Y(J)-FY0)/DELTA+RC*((Y(J)-FY0)**2)/(DELTA**2)
510        T(J)=T(J)+RD*((Y(J)-FY0)**3)/(DELTA**3)
520        T(J)=T(J)+RE*((Y(J)-FY0)**4)/(DELTA**4)
530        DT=RB/DELTA+(2.*RC/(DELTA**2))*(Y(J)-FY0)
540        DT=DT+(3.*RD/(DELTA**3))*((Y(J)-FY0)**2)
550        DT=DT+(4.*RE/(DELTA**4))*((Y(J)-FY0)**3)
560        DY(J)=1./DT
570        YY(J)=1.-Y(J)
580        A(J)=A1*Y(J)**2+2.*Y(J)*YY(J)*A12+A2*YY(J)**2
590        B(J)=Y(J)*B1+YY(J)*B2
600        CA=-.08205*T(J)/P
610        CB=(A(J)*T(J)**(-.5)-.08205*T(J)*B(J)-P*B(J)**2)/P
620        CC=(-1.)*A(J)*B(J)*(T(J)**(-.5))/P
630        V(J)=CUBIC(CA,CB,CC)
650
657        TZZ=T(J)**(-3./2.)
740        TZ=T(J)**(3./2.)
744        FGC1(J)=FUG(V(J),B(J),B1,TZ,Y(J),A(J),A1,YY(J),A12,P,T(J))
745        FG1(J)=EXP(FGC1(J))
746        FGC2(J)=FUG(V(J),B(J),B2,TZ,YY(J),A(J),A2,Y(J),A12,P,T(J))
749        FG2(J)=EXP(FGC2(J))
750       IF(KK.EQ.2) GO TO 204
751       IF(KK.EQ.3) GO TO 205
755C
756C
761C      THIS SECTION NUMERICALLY DIFFRENTIATES LN(PHI) AS A FUNCTION
762C      OF TEMPERATURE USING THE CHAIN RULE
763C
764C                DLN(PHI)/DT= DLN(PHI)/DY * DY/DT
765C
```

```
770        YPERM=Y(J)
780        YYPERM=YY(J)
790        TPERM=T(J)
800        DYPERM=DY(J)
810        APERM=A(J)
820        BPERM=B(J)
830        VPERM=V(J)
840        FGC1P=FGC1(J)
850        FG1P=FG1(J)
860        FGC2P=FGC2(J)
870        FG2P=FG2(J)
880        Y(J)=YV(J)
890        KK=2
900        GO TO 203
910 204    FGC1A=FGC1(J)
920        FGC2A=FGC2(J)
930        Y(J)=YW(J)
940        KK=3
950        GO TO 203
960 205    FGC1B=FGC1(J)
970        FGC2B=FGC2(J)
980        DDF1(J)=(FGC1A-FGC1B)*DYPERM/YD(J)
990        DDF2(J)=(FGC2A-FGC2B)*DYPERM/YD(J)
1000        Y(J)=YPERM
1010        YY(J)=YYPERM
1020        T(J)=TPERM
1030        DY(J)=DYPERM
1040        A(J)=APERM
1050        B(J)=BPERM
1060        V(J)=VPERM
1070        FGC1(J)=FGC1P
1080        FG1(J)=FG1P
1090        FGC2(J)=FCC2P
2000        FG2(J)=FG2P
2180         DH(J)=((X(J)/Y(J))-((1.-X(J))/(1.-Y(J))))*DY(J)
2190         CF(J)=(X(J)-Y(J))*DDF1(J)+(Y(J)-X(J))*DDF2(J)
2200         DH(J)=DH(J)*1.987*(T(J)**2)
2210         CF(J)=CF(J)*1.987*(T(J)**2)
2220         DHF(J)=DH(J)+CF(J)
2230 11      J=J+1
4000C
4010C
4020C        THIS SECTION OUTPUTS REQUIRED INFORMATION IN TABULAR FORM
4030C
5000         J=1
5001        PRINT 733,P
5002 733    FORMAT(/////5X,"ETHANE-BUTANE BINARY SYSTEM...  P= ",
5003&        F6.1," ATM")
5004 15      FORMAT(//2X,"TC1",8X,"ZC12",6X,"VC12",8X,"PC12",/F7.2,
5005&         4X,F7.3,4X,F7.4,4X,F7.2)
5008 16      FORMAT(//4X,"A1",12X,"A2",11X,"A12",12X,"B1",12X,"B2",
5009&       E10.4,4X,E10.4,4X,E10.4,4X,E10.4,4X,E10.4)
5010         PRINT 13
5012 13     FORMAT(//" Y1",6X,"X1",7X,"TK",7X,"VM",9X,"DYDT",9X,"PHI(1)",
5013&       4X,"PHI(2)")
5014         DO 12 M=1,L,1
5020        PRINT 14,Y(J),X(J),T(J),V(J),DY(J),FG1(J),FG2(J)
5030  14    FORMAT(F6.3,2X,F6.3,2X,F6.1,3X,F7.3,3X,E10.3,3X,E10.3,3X,
5031&       E10.3)
5040 12      J=J+1
5045         J=1
5048         J=1
5050 18     FORMAT(//" Y1",9X,"AM",10X,"BM")
5060         DO 17 N=1,L,1
5080 19      FORMAT(F6.3,3X,E10.3,3X,E10.3,3X,E10.3,3X,E10.3)
5090 17     J=J+1
5100         J=1
5103 202     FORMAT(//2X,"Y1",6X,"PHI(1)",4X,"PHI(2)",4X,
5104&         "LNPHI(1)",5X,"LNPHI(2)")
5110         DO 188 IJ=1,L,1
```

```
5130 189   FORMAT(F6.3,3X,F7.3,3X,F7.3,3X,E10.3,3X,E10.3)
5140 188   J=J+1
5150       J=1
5160       PRINT 208
5165 208   FORMAT(//40X,"IDEAL",8X,"REAL",
5170&      /2X,"Y1",6X,"DLNPHI(1)",4X,"DLNPHI(2)",7X,
5171&     "(HV-H*)",5X,"(HV-H*)",4X,"FUG CONT")
5180       DO 210 JI=1,L,1
5190      PRINT 212,Y(J),DDF1(J),DDF2(J),DH(J),DHF(J),CF(J)
5200 212  FORMAT(F6.3,3X,E10.3,3X,E10.3,3X,F10.1,3X,F10.1,3X,F10.1)
5210 210   J=J+1
5230C
5231C     THIS SECTION CALCULATES DELTA H*=(Y1-X1)*(H2-H1)
5232C     WHERE H1,H2 ARE IDEAL GAS ENTHALPIES OF PURE COMPONENTS
5233C
6080      J=1
6090      PRINT 602
6100 602  FORMAT(//" Y1",6X,"X1",8X,"DELTA H*",5X,"LAT HV")
6110      DO 620 JM=1,L,1
6120      HS=ENT(HA1,HB1,HC1,HD1,Y(J),T(J),
6130&      HA2,HB2,HC2,HD2,X(J))
6140      HLHV=HS+DHF(J)
6150      PRINT 630,Y(J),X(J),HS,HLHV
6160 630  FORMAT(F6.3,2X,F6.3,2X,F10.1,2X,F10.1)
6170 620   J=J+1
7000      PRINT 302
7010 302  FORMAT(///5X,"TYPE 0 TO STOP, 1 TO RERUN WITH NEW COND"/)
7020      READ,I8
7030      IF(I8.EQ.1) GO TO 301
7040      CONTINUE
9500       STOP
9510       END
9511C
9520      REAL FUNCTION CUBIC(G,C,D)
9521C    THIS FUNCTION CALCULATES THE LARGEST REAL ROOT OF A CUBIC
9522C     EQUATION OF THE FORM X**3+ G*X**2+ C*X+ D =0
9523C
9530      IF(G.GE.0.) GO TO 138
9540      EP=(1./3.)*(3.*C-(ABS(G)**2))
9550      GO TO 142
9555 138  CONTINUE
9560      EP=(1./3.)*(3.*C-G**2)
9570 142  IF(G.GE.0.) GO TO 148
9580      EQ=(1./27.)*(27.*D-9.*G*C-2.*(ABS(G)**3))
9590      GO TO 152
9600 148  CONTINUE
9610      EQ=(1./27.)*(27.*D-9.*G*C+2.*G**3)
9620 152  CONTINUE
9630      R=(EP/3.)**3+(EQ/2.)**2
9640      IF(R.LE.0.) GO TO 113
9650      AA1=(-EQ/2.+SQRT(R))
9660      IF(AA1.GE.0.) AA=AA1**(1./3.)
9670      IF(AA1.LT.0.) AA=-1.*(ABS(AA1)**(1./3.))
9680      BB1=(-EQ/2.-SQRT(R))
9690      IF(BB1.GE.0.) BB=BB1**(1./3.)
9700      IF(BB1.LT.0.) BB=-1.*(ABS(BB1)**(1./3.))
9710      Y1=AA+BB
9720      X1=Y1-G/3.
9730      GO TO 30
9740 113  BETA=SQRT(((EQ**2)/4.)/((EP**3)/(-27.)))
9750      THETA=ARCOS(BETA)
9760      X0=SQRT(-4.*EP/3.)*COS(THETA/3.)
9770      IF(EQ.GT.0.) X0=X0*(-1.)
9780      X1=SQRT(-4.*EP/3.)*COS(THETA/3.+2.09439)
9790      IF(EQ.GT.0.) X1=X1*(-1.)
9800      X2=SQRT(-4.*EP/3.)*COS(THETA/3.+4.18879)
9810      IF(EQ.GT.0.) X2=X2*(-1.)
9815      IF(X0.GT.X1) X1=X0
9816      IF(X2.GT.X1) X1=X2
9819      X1=X1-G/3.
```

```
9820 30   CONTINUE
9830      CUBIC=X1
9840      RETURN
9850      END
9859C
9860      REAL FUNCTION FUG(FV,FB,FB1,FTZ,FY1,FA,FA1,FY2,FA12,FP,FT)
9861C
9862C     THIS FUNCTION CALCULATES THE NATURAL LOG OF COMPONENT
9863C     FUGACITY COEFFICIENTS USING MODIFICATIONS OF THE REDLICH
9864C     AND KWONG EQUATION OF STATE AS PROPOSED BY PRAUSNITZ
9865C     AND CHUEH, "COMPUTER CALCULATIONS FOR HIGH PRESSURE VAPOR-
9866C     LIQUID EQUILIBRIA, PRENTICE-HALL, 1968.
9867C
9870      FUG1=ALOG(FV/(FV-FB))+FB1/(FV-FB)
9880      FUG2=(24.3754/(FTZ*FB))*(FY1*FA1+FY2*FA12)*(ALOG((FV+FB)/FV))
9890      FUG3=(FA*FB1/(.08205*FTZ*(FB**2)))*(ALOG((FV+FB)/FV)-(FB/(FV+FB)))
9900      FUG4=ALOG((FP*FV)/(.08205*FT))
9910      FUG=FUG1-FUG2+FUG3-FUG4
9920      RETURN
9930      END
9931C
9940      REAL FUNCTION ENT(A1,B1,C1,D1,Y1,TK,
9941&      A2,B2,C2,D2,X1)
9942C
9950C     THIS FUNCTION CALCULATES IDEAL GAS ENTHA;LPIES FOR GAS
9951C     MIXTURES IN CAL/GM MOLE REFERENCED TO THE LIQ STATE AT
9952C     0 DEG C (273.16 DEG K)
9953C
9955      EH1=A1*(TK-273.16)+
9960&     (B1/2.)*(TK**2-273.16**2)+(C1/3.)*(TK**3-273.16**3)+
9970&     (D1/4.)*(TK**4-273.16**4)
9975      EH2=A2*(TK-273.16)+
9976&     (B2/2.)*(TK**2-273.16**2)+(C2/3.)*(TK**3-273.16**3)+
9977&     (D2/4.)*(TK**4-273.16**4)
9980      ENT=(EH1-EH2)*(Y1-X1)
9985      RETURN
9986      END
```

*B

Directions For Using Program Ethane

1. From experimental or curvefit VLE data, determine T-Y regression data for selected range of y_1. Five pairs of y_1-T values are required at $y_1 = y_a$, $(y_e - y_a).25$, $(y_e - y_a).50$, $(y_e - y_a).75$, y_e, where y_a = lower limit of desired range and y_e = the upper limit. Temperatures must be input in degrees K.

2. Input system pressure in Atmospheres.

3. Input the desired number of experimental or curvefit data pairs.

4. Input data pairs, one pair per line $(y_1, x_1)_P$.

5. Repeat for different system pressures.

6. To run different systems, program text must be edited to include proper component values (lines 34-115).

```
TYPE T-Y REGRESSION DATA: Y0,T0,Y1,T1,Y2,T2,Y3,T3,Y4,T4
=0.0 337.5 .25 324.2 .50 307.3 .75 288.6
=1.0 228.1

TYPE TOTAL PRESSURE IN ATM
=6.804

TYPE NO OF Y1,X1 DATA PAIRS OF INPUT
=11

TYPE Y1,X1 PAIRS, ONE PAIR PER LINE
=.100 .014
=.200 .031
=.300 .050
=.400 .073
=.500 .097
=.600 .124
=.700 .164
=.800 .230
=.900 .342
=.950 .478
=.990 .742
```

ETHANE-BUTANE BINARY SYSTEM... P= 6.8 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.100	0.014	334.5	3.519	-0.189E-01	0.991E 00	0.875E 00
0.200	0.031	327.9	3.475	-0.136E-01	0.983E 00	0.870E 00
0.300	0.050	320.4	3.415	-0.135E-01	0.976E 00	0.863E 00
0.400	0.073	313.4	3.363	-0.153E-01	0.969E 00	0.857E 00
0.500	0.097	307.3	3.323	-0.171E-01	0.963E 00	0.852E 00
0.600	0.124	301.3	3.285	-0.157E-01	0.956E 00	0.849E 00
0.700	0.164	293.8	3.223	-0.109E-01	0.950E 00	0.843E 00
0.800	0.230	281.9	3.098	-0.651E-02	0.941E 00	0.831E 00
0.900	0.342	261.6	2.855	-0.385E-02	0.926E 00	0.804E 00
0.950	0.478	246.9	2.666	-0.301E-02	0.912E 00	0.777E 00
0.990	0.742	232.2	2.470	-0.249E-02	0.896E 00	0.745E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.100	0.138E-02	0.103E-02	4015.9	4009.3	-6.6
0.200	0.998E-03	0.105E-02	3075.1	3076.8	1.7
0.300	0.990E-03	0.103E-02	3281.0	3282.8	1.8
0.400	0.107E-02	0.929E-03	4061.4	4052.4	-9.1
0.500	0.111E-02	0.773E-03	5173.4	5147.7	-25.7
0.600	0.999E-03	0.743E-03	5620.6	5598.5	-22.1
0.700	0.819E-03	0.974E-03	4769.0	4783.3	14.3
0.800	0.761E-03	0.137E-02	3662.5	3717.0	54.5
0.900	0.905E-03	0.200E-02	3247.6	3330.7	83.1
0.950	0.110E-02	0.257E-02	3617.5	3701.4	83.9
0.990	0.138E-02	0.332E-02	6679.3	6730.8	51.5

Y1	X1	DELTA H*	LAT HV
0.100	0.014	-59.4	3949.9
0.200	0.031	-103.4	2973.4
0.300	0.050	-130.6	3152.2
0.400	0.073	-144.1	3908.3
0.500	0.097	-149.1	4998.6
0.600	0.124	-144.1	5454.4
0.700	0.164	-117.5	4665.8
0.800	0.230	-51.7	3665.3
0.900	0.342	65.0	3395.7
0.950	0.478	122.0	3823.5
0.990	0.742	97.3	6828.1

ETHANE-BUTANE BINARY SYSTEM... P= 13.6 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.100	0.023	364.3	1.721	-0.188E-01	0.997E 00	0.804E 00
0.200	0.047	358.1	1.721	-0.145E-01	0.983E 00	0.797E 00
0.300	0.074	350.8	1.711	-0.134E-01	0.970E 00	0.788E 00
0.400	0.104	343.3	1.697	-0.132E-01	0.958E 00	0.779E 00
0.500	0.138	335.6	1.681	-0.126E-01	0.946E 00	0.771E 00
0.600	0.180	327.2	1.658	-0.110E-01	0.934E 00	0.762E 00
0.700	0.235	316.8	1.619	-0.843E-02	0.921E 00	0.750E 00
0.800	0.315	302.7	1.549	-0.596E-02	0.906E 00	0.729E 00
0.900	0.456	282.3	1.427	-0.408E-02	0.881E 00	0.690E 00
0.950	0.591	268.8	1.338	-0.337E-02	0.863E 00	0.657E 00
0.990	0.892	256.0	1.248	-0.290E-02	0.842E 00	0.619E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.100	0.275E-02	0.160E-02	4250.3	4226.9	-23.4
0.200	0.196E-02	0.155E-02	3521.2	3505.1	-16.1
0.300	0.176E-02	0.149E-02	3530.3	3515.5	-14.8
0.400	0.168E-02	0.141E-02	3816.4	3797.6	-18.8
0.500	0.157E-02	0.135E-02	4098.4	4081.0	-17.4
0.600	0.139E-02	0.144E-02	4080.3	4084.1	3.8
0.700	0.125E-02	0.174E-02	3722.4	3767.6	45.2
0.800	0.124E-02	0.227E-02	3288.3	3379.9	91.6
0.900	0.146E-02	0.323E-02	3184.8	3308.9	124.1
0.950	0.173E-02	0.406E-02	3657.4	3777.3	120.0
0.990	0.209E-02	0.510E-02	3740.8	3779.2	38.4

Y1	X1	DELTA H*	LAT HV
0.100	0.023	-82.4	4144.6
0.200	0.047	-151.2	3353.8
0.300	0.074	-202.3	3313.1
0.400	0.104	-236.9	3560.7
0.500	0.138	-255.2	3825.8
0.600	0.180	-253.2	3830.9
0.700	0.235	-223.3	3544.3
0.800	0.315	-154.4	3225.5
0.900	0.456	-42.5	3266.4
0.950	0.591	15.9	3793.2
0.990	0.892	16.8	3796.0

ETHANE-BUTANE BINARY SYSTEM... P= 20.4 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.100	0.028	378.5	1.033	-0.239E-01	0.102E 01	0.736E 00
0.200	0.060	373.8	1.066	-0.190E-01	0.993E 00	0.730E 00
0.300	0.095	368.0	1.086	-0.160E-01	0.971E 00	0.723E 00
0.400	0.129	361.2	1.096	-0.136E-01	0.952E 00	0.715E 00
0.500	0.175	353.2	1.094	-0.113E-01	0.935E 00	0.705E 00
0.600	0.227	343.4	1.081	-0.915E-02	0.917E 00	0.692E 00
0.700	0.295	331.0	1.050	-0.717E-02	0.899E 00	0.673E 00
0.800	0.385	315.1	0.998	-0.553E-02	0.876E 00	0.643E 00
0.900	0.543	294.4	0.915	-0.423E-02	0.843E 00	0.594E 00
0.950	0.687	281.7	0.858	-0.370E-02	0.820E 00	0.558E 00
0.990	0.903	270.3	0.802	-0.333E-02	0.797E 00	0.520E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.100	0.710E-02	0.200E-02	5443.5	5339.0	-104.5
0.200	0.454E-02	0.174E-02	4605.4	4496.8	-108.6
0.300	0.332E-02	0.164E-02	4209.4	4116.4	-93.0
0.400	0.258E-02	0.164E-02	3990.5	3924.6	-65.9
0.500	0.208E-02	0.177E-02	3654.9	3630.5	-24.4
0.600	0.176E-02	0.205E-02	3330.5	3356.0	25.4
0.700	0.162E-02	0.250E-02	3012.4	3090.2	77.8
0.800	0.168E-02	0.322E-02	2829.1	2955.6	126.5
0.900	0.201E-02	0.449E-02	2889.7	3042.5	152.8
0.950	0.235E-02	0.558E-02	3232.6	3366.7	134.1
0.990	0.277E-02	0.690E-02	4248.9	4301.1	52.2

Y1	X1	DELTA H*	LAT HV
0.100	0.028	-90.7	5248.3
0.200	0.060	-167.3	4329.4
0.300	0.095	-229.3	3887.1
0.400	0.129	-279.0	3645.5
0.500	0.175	-300.9	3329.6
0.600	0.227	-299.0	3057.0
0.700	0.295	-263.0	2827.3
0.800	0.385	-191.0	2764.6
0.900	0.543	-80.6	2961.9
0.950	0.687	-23.5	3343.2
0.990	0.903	2.5	4303.6

ETHANE-BUTANE BINARY SYSTEM... P= 27.2 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.100	0.047	398.6	0.732	-0.135E-01	0.105E 01	0.697E 00
0.200	0.086	390.7	0.753	-0.122E-01	0.101E 01	0.683E 00
0.300	0.124	382.4	0.766	-0.118E-01	0.980E 00	0.669E 00
0.400	0.166	373.8	0.775	-0.114E-01	0.953E 00	0.656E 00
0.500	0.214	364.7	0.779	-0.106E-01	0.928E 00	0.643E 00
0.600	0.270	354.7	0.775	-0.925E-02	0.905E 00	0.629E 00
0.700	0.340	342.7	0.761	-0.750E-02	0.881E 00	0.610E 00
0.800	0.440	327.5	0.729	-0.576E-02	0.854E 00	0.579E 00
0.900	0.605	307.3	0.670	-0.429E-02	0.817E 00	0.528E 00
0.950	0.737	294.7	0.625	-0.369E-02	0.791E 00	0.489E 00
0.990	0.925	283.2	0.578	-0.327E-02	0.763E 00	0.446E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.100	0.541E-02	0.275E-02	2506.0	2461.6	-44.4
0.200	0.406E-02	0.252E-02	2646.1	2592.8	-53.3
0.300	0.349E-02	0.234E-02	2866.7	2807.8	-58.9
0.400	0.309E-02	0.219E-02	3081.1	3022.4	-58.7
0.500	0.271E-02	0.217E-02	3207.3	3166.5	-40.7
0.600	0.234E-02	0.238E-02	3178.4	3181.7	3.3
0.700	0.209E-02	0.290E-02	3001.3	3068.9	67.6
0.800	0.207E-02	0.381E-02	2761.0	2894.3	133.2
0.900	0.240E-02	0.546E-02	2638.6	2808.0	169.5
0.950	0.280E-02	0.695E-02	2853.7	3006.3	152.6
0.990	0.334E-02	0.893E-02	3417.2	3475.1	57.9

Y1	X1	DELTA H*	LAT HV
0.100	0.047	-81.5	2380.1
0.200	0.086	-162.7	2430.2
0.300	0.124	-230.9	2576.9
0.400	0.166	-279.7	2742.7
0.500	0.214	-307.4	2859.1
0.600	0.270	-311.7	2870.0
0.700	0.340	-285.4	2783.4
0.800	0.440	-218.3	2675.9
0.900	0.605	-109.3	2698.8
0.950	0.737	-48.9	2957.4
0.990	0.925	-6.8	3468.3

ETHANE-BUTANE BINARY SYSTEM... P= 34.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.100	0.059	409.3	0.475	-0.129E-01	0.114E 01	0.645E 00
0.200	0.106	401.1	0.525	-0.117E-01	0.105E 01	0.629E 00
0.300	0.153	392.3	0.551	-0.111E-01	0.100E 01	0.614E 00
0.400	0.201	383.1	0.568	-0.106E-01	0.951E 00	0.599E 00
0.500	0.256	373.4	0.578	-0.987E-02	0.926E 00	0.585E 00
0.600	0.319	362.7	0.580	-0.874E-02	0.896E 00	0.568E 00
0.700	0.400	350.2	0.572	-0.731E-02	0.866E 00	0.546E 00
0.800	0.505	334.9	0.549	-0.582E-02	0.833E 00	0.513E 00
0.900	0.662	315.4	0.504	-0.450E-02	0.790E 00	0.460E 00
0.950	0.793	303.4	0.468	-0.393E-02	0.761E 00	0.420E 00
0.990	0.945	292.7	0.430	-0.352E-02	0.732E 00	0.377E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.100	0.139E-01	0.304E-02	1959.0	1810.2	-148.8
0.200	0.682E-02	0.286E-02	2195.7	2076.8	-118.9
0.300	0.501E-02	0.268E-02	2376.7	2271.6	-105.1
0.400	0.410E-02	0.255E-02	2566.1	2476.4	-89.7
0.500	0.344E-02	0.258E-02	2670.1	2612.3	-57.8
0.600	0.292E-02	0.287E-02	2675.8	2672.2	-3.6
0.700	0.260E-02	0.351E-02	2545.6	2612.5	66.9
0.800	0.255E-02	0.464E-02	2393.2	2530.8	137.5
0.900	0.291E-02	0.675E-02	2349.6	2530.2	180.6
0.950	0.337E-02	0.875E-02	2374.7	2529.3	154.5
0.990	0.402E-02	0.117E-01	2722.8	2781.[illegible]	58.6

Y1	X1	DELTA H*	LAT HV
0.100	0.059	-69.3	1740.9
0.200	0.106	-147.9	1928.9
0.300	0.153	-213.1	2058.5
0.400	0.201	-263.1	2213.2
0.500	0.256	-290.5	2321.9
0.600	0.319	-294.6	2377.5
0.700	0.400	-266.3	2346.2
0.800	0.505	-205.5	2325.3
0.900	0.662	-110.1	2420.1
0.950	0.793	-51.2	2478.0
0.990	0.945	-9.3	2772.0

Program Revised for the Carbon Dioxide- Propane System *

```
20C
21C       CARBON DIOXIDE- PROPANE BINARY SYSTEM : ASSIGNED BINARY DATA
22C
23C       TC= CRITICAL TEMP IN DEG K
24C       PC= CRITICAL PRES IN ATM
25C       VC= CRITICAL VOL  IN LITERS
26C       OMEGA,OMEGB,C12= BINARY INTERACTION PARAMETERS (PRAUSNITZ& CHUEH)
27C       W= ACCENTRIC FACTOR, WM= MOL. WT., BP= BOILING PT IN DEG K
28C       CP= SPECIFIC HT OF LIQ IN CAL/GM DEG C
29C       HA,HB,HC,HD= VAPOR SP. HT. REG. COEFFICIENTS
30C       HV= LATENT HEAT OF VAPORIZATION AT BP IN CAL/GM MOLE
31C
34        TC1=304.2
30        TC1=304.2
35        TC2=370.0
40        PC1=72.9
45        PC2=42.0
50        VC1=.094
55        VC2=.1995
60        OMEGA1=0.447
65        OMEGA2=0.438
70        OMEGB1=0.0911
75        OMEGB2=0.0889
80        W1=.225
85        W2=.152
90        C12=0.11
100        HA1=5.316
101       HB1=1.4285E-2
102       HC1=-.8362E-5
103       HD1=1.784E-9
104       HA2=-0.966
105       HB2=7.279E-2
106       HC2=-3.755E-5
107       HD2=7.58E-9
108       WM1=44.01
109       BP1=194.7
110       CP1=.55
111       HV1=6030
112       WM2=44.09
113       BP2=298.16
114       CP2=.55
115       HV2=3605
116       TR11=BP1/TC1
117       TR21=BP2/TC2
165 301   CONTINUE
```

*In addition to physical property changes, this program revision includes an extrapolation of the published pure component latent heats using Watson's correlation.

CO2- PROPANE BINARY SYSTEM... P= 33.9 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.300	0.100	340.1	0.552	-0.154E-01	0.995E 00	0.667E 00
0.514	0.200	323.5	0.561	-0.105E-01	0.918E 00	0.651E 00
0.640	0.300	310.0	0.542	-0.849E-02	0.878E 00	0.635E 00
0.731	0.400	298.9	0.520	-0.804E-02	0.848E 00	0.620E 00
0.795	0.500	291.0	0.502	-0.827E-02	0.827E 00	0.610E 00
0.850	0.600	284.6	0.488	-0.905E-02	0.810E 00	0.604E 00
0.900	0.700	279.5	0.477	-0.106E-01	0.796E 00	0.602E 00
0.935	0.800	276.4	0.471	-0.128E-01	0.788E 00	0.604E 00
0.960	0.900	274.7	0.468	-0.156E-01	0.783E 00	0.607E 00
0.980	0.950	273.5	0.468	-0.194E-01	0.780E 00	0.611E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.300	0.672E-02	0.139E-02	3377.7	3133.0	-244.7
0.514	0.363E-02	0.168E-02	2732.5	2605.0	-127.5
0.640	0.309E-02	0.206E-02	2392.6	2325.9	-66.7
0.731	0.310E-02	0.212E-02	2401.1	2343.4	-57.7
0.795	0.323E-02	0.186E-02	2520.3	2452.7	-67.6
0.850	0.337E-02	0.121E-02	2856.1	2769.2	-86.8
0.900	0.348E-02	-0.126E-03	3664.6	3552.6	-112.0
0.935	0.351E-02	-0.197E-02	4316.8	4204.6	-112.2
0.960	0.346E-02	-0.428E-02	3645.6	3576.0	-69.6
0.980	0.336E-02	-0.740E-02	4413.2	4365.3	-47.9

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	PROPANE
0.300	0.100	-176.7	2956.3	0.	2584.7
0.514	0.200	-224.8	2380.1	0.	3054.7
0.640	0.300	-199.7	2126.2	0.	3366.5
0.731	0.400	-161.4	2182.0	1908.5	3590.9
0.795	0.500	-123.8	2328.9	2698.5	3737.5
0.850	0.600	-91.7	2677.5	3135.8	3849.7
0.900	0.700	-65.1	3487.5	3426.3	3936.2
0.935	0.800	-40.7	4163.8	3579.8	3985.7
0.960	0.900	-17.3	3558.7	3665.6	4014.4
0.980	0.950	-8.4	4356.9	3719.6	4032.9

CO2- PROPANE BINARY SYSTEM... P= 40.8 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.255	0.100	351.3	0.423	-0.127E-01	0.104E 01	0.630E 00
0.455	0.200	334.9	0.442	-0.111E-01	0.936E 00	0.611E 00
0.603	0.300	320.3	0.434	-0.933E-02	0.878E 00	0.594E 00
0.703	0.400	309.2	0.420	-0.880E-02	0.842E 00	0.580E 00
0.770	0.500	301.6	0.408	-0.886E-02	0.818E 00	0.572E 00
0.825	0.600	295.5	0.398	-0.927E-02	0.799E 00	0.567E 00
0.877	0.700	290.1	0.388	-0.101E-01	0.782E 00	0.564E 00
0.930	0.800	285.2	0.380	-0.118E-01	0.767E 00	0.566E 00
0.960	0.900	282.8	0.377	-0.136E-01	0.760E 00	0.569E 00
0.980	0.950	281.4	0.375	-0.153E-01	0.756E 00	0.572E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.255	0.766E-02	0.228E-02	2544.3	2339.8	-204.6
0.455	0.495E-02	0.182E-02	2543.5	2365.4	-178.1
0.603	0.393E-02	0.203E-02	2407.2	2290.0	-117.3
0.703	0.376E-02	0.202E-02	2424.6	2324.4	-100.2
0.770	0.380E-02	0.177E-02	2440.4	2341.2	-99.2
0.825	0.388E-02	0.125E-02	2505.4	2402.7	-102.6
0.877	0.395E-02	0.279E-03	2776.3	2667.7	-108.6
0.930	0.395E-02	-0.163E-02	3822.2	3704.9	-117.2
0.960	0.387E-02	-0.349E-02	3367.9	3297.7	-70.2
0.980	0.376E-02	-0.530E-02	3678.4	3635.6	-42.8

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	PROPANE
0.255	0.100	-155.5	2184.3	0.	2162.1
0.455	0.200	-211.6	2153.7	0.	2745.7
0.603	0.300	-207.3	2082.6	0.	3134.5
0.703	0.400	-175.6	2148.8	0.	3384.0
0.770	0.500	-137.9	2203.3	1464.7	3539.3
0.825	0.600	-103.0	2299.8	2306.8	3655.8
0.877	0.700	-72.9	2594.8	2769.4	3754.2
0.930	0.800	-48.3	3656.6	3099.9	3839.7
0.960	0.900	-21.1	3276.6	3241.9	3880.2
0.980	0.950	-10.2	3625.4	3320.6	3903.7

CO2- PROPANE BINARY SYSTEM... P= 47.6 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.380	0.200	347.1	0.348	-0.114E-01	0.980E 00	0.576E 00
0.540	0.300	331.9	0.353	-0.977E-02	0.898E 00	0.557E 00
0.660	0.400	319.1	0.344	-0.904E-02	0.845E 00	0.541E 00
0.728	0.500	311.5	0.335	-0.899E-02	0.817E 00	0.532E 00
0.795	0.600	304.1	0.325	-0.930E-02	0.791E 00	0.525E 00
0.852	0.700	298.2	0.316	-0.999E-02	0.769E 00	0.521E 00
0.902	0.800	293.4	0.309	-0.111E-01	0.753E 00	0.521E 00
0.950	0.900	289.4	0.304	-0.132E-01	0.739E 00	0.526E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.380	0.697E-02	0.208E-02	2085.1	1874.1	-211.0
0.540	0.499E-02	0.223E-02	2065.7	1920.6	-145.1
0.660	0.450E-02	0.228E-02	2119.6	2003.1	-116.5
0.728	0.446E-02	0.210E-02	1996.0	1892.5	-103.5
0.795	0.452E-02	0.159E-02	2045.3	1940.1	-105.2
0.852	0.460E-02	0.634E-03	2127.7	2021.1	-106.6
0.902	0.464E-02	-0.926E-03	2199.9	2102.9	-97.1
0.950	0.455E-02	-0.364E-02	2307.8	2239.7	-68.2

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	PROPANE
0.380	0.200	-172.4	1701.8	0.	2335.8
0.540	0.300	-191.8	1728.8	0.	2833.1
0.660	0.400	-174.8	1828.3	0.	3163.6
0.728	0.500	-137.0	1755.4	0.	3334.5
0.795	0.600	-104.1	1835.9	355.3	3488.0
0.852	0.700	-73.2	1948.0	2000.2	3604.3
0.902	0.800	-44.9	2058.0	2497.4	3693.3
0.950	0.900	-20.3	2219.3	2815.4	3765.3

CO2- PROPANE BINARY SYSTEM... P= 54.3 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.488	0.300	339.9	0.278	-0.102E-01	0.928E 00	0.514E 00
0.600	0.400	328.5	0.277	-0.955E-02	0.865E 00	0.500E 00
0.680	0.500	320.1	0.272	-0.947E-02	0.825E 00	0.490E 00
0.752	0.600	312.5	0.265	-0.973E-02	0.791E 00	0.482E 00
0.820	0.700	305.8	0.258	-0.104E-01	0.763E 00	0.478E 00
0.883	0.800	300.0	0.251	-0.116E-01	0.739E 00	0.479E 00
0.940	0.900	295.4	0.246	-0.136E-01	0.720E 00	0.485E 00
0.968	0.950	293.5	0.244	-0.152E-01	0.713E 00	0.491E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.488	0.677E-02	0.239E-02	1760.7	1571.5	-189.2
0.600	0.575E-02	0.248E-02	1706.5	1565.9	-140.6
0.680	0.551E-02	0.227E-02	1594.5	1475.8	-118.6
0.752	0.547E-02	0.173E-02	1539.7	1429.1	-110.6
0.820	0.552E-02	0.635E-03	1570.1	1461.3	-108.8
0.883	0.552E-02	-0.132E-02	1666.0	1564.5	-101.5
0.940	0.538E-02	-0.458E-02	1671.4	1602.4	-69.0
0.968	0.518E-02	-0.711E-02	1506.9	1469.0	-37.9

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	PROPANE
0.488	0.300	-165.8	1405.8	0.	2590.1
0.600	0.400	-153.0	1412.9	0.	2926.5
0.680	0.500	-122.8	1353.1	0.	3139.7
0.752	0.600	-92.8	1336.3	0.	3311.7
0.820	0.700	-65.8	1395.4	0.	3455.2
0.883	0.800	-41.3	1523.3	1748.9	3569.9
0.940	0.900	-18.3	1584.1	2312.0	3656.8
0.968	0.950	-7.9	1461.1	2495.5	3692.9

Program Revised for the Carbon Dioxide- Hydrogen Sulfide System

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20C
21C       CARBON DIOXIDE- HYDROGEN SULFIDE BINARY SYSTEM : ASSIGNED BINARY DATA.
22C
23C       TC= CRITICAL TEMP IN DEG K
24C       PC= CRITICAL PRES IN ATM
25C       VC= CRITICAL VOL  IN LITERS
26C       OMEGA,OMEGB,C12= BINARY INTERACTION PARAMETERS (PRAUSNITZ& CHUEH)
27C       W= ACCENTRIC FACTOR, WM= MOL. WT., BP= BOILING PT IN DEG K
28C       CP= SPECIFIC HT OF LIQ IN CAL/GM DEG C
29C       HA,HB,HC,HD= VAPOR SP. HT. REG. COEFFICIENTS
30C       HV= LATENT HEAT OF VAPORIZATION AT BP IN CAL/GM MOLE
31C
34        TC1=304.2
35        TC2=374.0
40        PC1=72.9
45        PC2=88.9
50        VC1=.094
55        VC2=.09083
60        OMEGA1=0.447
65        OMEGA2=0.434
70        OMEGB1=0.0911
75        OMEGB2=0.0882
80        W1=.225
85        W2=.1
90        C12=0.08
100        HA1=5.316
101       HB1=1.4285E-2
102       HC1=-.8362E-5
103       HD1=1.784E-9
104       HA2=7.070
105       HB2=.3128E-2
106       HC2=.1364E-5
107       HD2=-.7867E-9
108       WM1=44.01
109       BP1=194.7
110       CP1=.55
111       HV1=6030
112       WM2=34.08
113       BP2=212.9
114       CP2=.55
115       HV2=4463
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CO2- HYDROGEN SULFIDE BINARY SYSTEM... P= 20.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.131	0.020	293.3	1.007	-0.216E-01	0.934E 00	0.848E 00
0.240	0.052	288.3	0.992	-0.213E-01	0.920E 00	0.843E 00
0.341	0.092	283.4	0.977	-0.200E-01	0.907E 00	0.839E 00
0.441	0.142	278.2	0.957	-0.187E-01	0.894E 00	0.835E 00
0.531	0.211	273.3	0.937	-0.179E-01	0.883E 00	0.832E 00
0.665	0.331	265.8	0.904	-0.184E-01	0.866E 00	0.828E 00
0.715	0.431	263.2	0.891	-0.194E-01	0.860E 00	0.828E 00
0.785	0.618	259.8	0.874	-0.221E-01	0.852E 00	0.828E 00
0.810	0.669	258.7	0.868	-0.237E-01	0.850E 00	0.829E 00
0.840	0.748	257.5	0.862	-0.265E-01	0.847E 00	0.830E 00
0.889	0.836	255.8	0.853	-0.346E-01	0.844E 00	0.833E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.131	0.309E-02	0.134E-02	3606.4	3573.2	-33.2
0.240	0.298E-02	0.113E-02	3631.2	3574.0	-57.2
0.341	0.279E-02	0.981E-03	3538.5	3466.5	-72.0
0.441	0.265E-02	0.852E-03	3482.5	3400.0	-82.6
0.531	0.258E-02	0.714E-03	3418.9	3330.3	-88.6
0.665	0.258E-02	0.337E-03	3871.6	3766.3	-105.3
0.715	0.261E-02	0.775E-04	3712.0	3613.2	-98.8
0.785	0.265E-02	-0.526E-03	2931.3	2860.3	-71.0
0.810	0.266E-02	-0.858E-03	2891.6	2825.6	-65.9
0.840	0.268E-02	-0.140E-02	2390.6	2341.3	-49.3
0.889	0.269E-02	-0.290E-02	2418.8	2380.2	-38.5

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	H2S	MIX
0.131	0.020	-12.4	3560.8	2509.	3432.	3311.
0.240	0.052	-21.7	3552.4	2899.	3512.	3365.
0.341	0.092	-29.6	3437.0	3208.	3586.	3457.
0.441	0.142	-36.5	3363.4	3411.	3663.	3587.
0.531	0.211	-40.1	3290.2	3729.	3733.	3731.
0.665	0.331	-43.3	3723.0	4049.	3836.	3977.
0.715	0.431	-37.3	3575.9	4153.	3872.	4073.
0.785	0.618	-22.2	2838.1	4281.	3917.	4203.
0.810	0.669	-18.9	2806.8	4321.	3931.	4247.
0.840	0.748	-12.4	2328.9	4363.	3946.	4297.
0.889	0.836	-7.2	2373.1	4421.	3967.	4371.

CO2- HYDROGEN SULFIDE BINARY SYSTEM... P= 30.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.056	0.010	312.5	0.660	-0.250E-01	0.934E 00	0.809E 00
0.169	0.042	307.7	0.657	-0.222E-01	0.913E 00	0.802E 00
0.261	0.077	303.4	0.650	-0.199E-01	0.897E 00	0.797E 00
0.353	0.122	298.5	0.640	-0.180E-01	0.881E 00	0.792E 00
0.445	0.179	293.2	0.627	-0.169E-01	0.865E 00	0.786E 00
0.531	0.251	288.0	0.613	-0.165E-01	0.850E 00	0.782E 00
0.611	0.349	283.2	0.598	-0.170E-01	0.837E 00	0.779E 00
0.698	0.484	278.3	0.581	-0.188E-01	0.823E 00	0.777E 00
0.808	0.684	273.2	0.563	-0.260E-01	0.808E 00	0.779E 00
0.837	0.732	272.2	0.559	-0.303E-01	0.805E 00	0.781E 00
0.866	0.793	271.3	0.556	-0.374E-01	0.802E 00	0.784E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.056	0.510E-02	0.190E-02	4221.9	4193.4	-28.6
0.169	0.435E-02	0.159E-02	3780.2	3714.3	-66.0
0.261	0.386E-02	0.142E-02	3467.3	3385.3	-82.0
0.353	0.354E-02	0.130E-02	3230.2	3138.5	-91.7
0.445	0.338E-02	0.117E-02	3107.0	3006.7	-100.3
0.531	0.334E-02	0.995E-03	3063.4	2955.1	-108.3
0.611	0.338E-02	0.710E-03	2983.5	2871.9	-111.6
0.698	0.348E-02	0.118E-03	2939.4	2828.6	-110.8
0.808	0.367E-02	-0.177E-02	3082.0	2981.8	-100.1
0.837	0.373E-02	-0.284E-02	3435.2	3333.5	-101.6
0.866	0.381E-02	-0.455E-02	3440.1	3350.9	-89.2

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	H2S	MIX
0.056	0.010	-4.4	4188.9	0.	3095.	2922.
0.169	0.042	-12.7	3701.5	0.	3184.	2646.
0.261	0.077	-19.1	3366.2	952.	3263.	2660.
0.353	0.122	-24.9	3113.7	1964.	3347.	2858.
0.445	0.179	-29.7	2977.0	2519.	3434.	3027.
0.531	0.251	-32.3	2922.8	2915.	3516.	3197.
0.611	0.349	-31.1	2840.8	3218.	3589.	3362.
0.698	0.484	-26.1	2802.4	3485.	3661.	3539.
0.808	0.684	-15.5	2966.3	3733.	3735.	3733.
0.837	0.732	-13.2	3320.3	3780.	3749.	3775.
0.866	0.793	-9.2	3341.6	3819.	3761.	3811.

CO2- HYDROGEN SULFIDE BINARY SYSTEM... P= 40.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.124	0.035	322.9	0.479	-0.210E-01	0.914E 00	0.768E 00
0.216	0.074	318.2	0.476	-0.185E-01	0.893E 00	0.761E 00
0.300	0.117	313.4	0.470	-0.171E-01	0.874E 00	0.755E 00
0.382	0.168	308.5	0.462	-0.163E-01	0.856E 00	0.749E 00
0.467	0.232	303.3	0.452	-0.160E-01	0.837E 00	0.743E 00
0.546	0.313	298.3	0.441	-0.163E-01	0.821E 00	0.738E 00
0.630	0.420	293.3	0.428	-0.171E-01	0.803E 00	0.735E 00
0.720	0.563	288.3	0.414	-0.193E-01	0.786E 00	0.733E 00
0.835	0.756	283.0	0.398	-0.258E-01	0.768E 00	0.738E 00
0.862	0.797	282.1	0.394	-0.288E-01	0.765E 00	0.740E 00
0.899	0.852	280.9	0.390	-0.349E-01	0.761E 00	0.745E 00
0.942	0.916	279.8	0.386	-0.482E-01	0.757E 00	0.751E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.124	0.549E-02	0.208E-02	3560.1	3497.3	-62.9
0.216	0.474E-02	0.188E-02	3127.2	3045.7	-81.5
0.300	0.436E-02	0.174E-02	2914.2	2820.7	-93.5
0.382	0.417E-02	0.160E-02	2799.7	2695.5	-104.2
0.467	0.411E-02	0.141E-02	2765.3	2649.2	-116.1
0.546	0.414E-02	0.114E-02	2701.8	2578.2	-123.6
0.630	0.423E-02	0.680E-03	2640.7	2513.2	-127.5
0.720	0.436E-02	-0.199E-03	2478.3	2360.0	-118.4
0.835	0.450E-02	-0.270E-02	2359.1	2268.5	-90.6
0.862	0.451E-02	-0.380E-02	2489.0	2403.7	-85.3
0.899	0.448E-02	-0.599E-02	2832.1	2754.9	-77.2
0.942	0.436E-02	-0.107E-01	3569.0	3508.3	-60.7

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	H2S	MIX
0.124	0.035	-7.7	3489.5	0.	2886.	2528.
0.216	0.074	-12.9	3032.8	0.	2984.	2339.
0.300	0.117	-17.4	2803.3	0.	3077.	2154.
0.382	0.168	-21.3	2674.2	0.	3170.	1959.
0.467	0.232	-24.4	2624.8	990.	3264.	2202.
0.546	0.313	-25.1	2553.1	1981.	3349.	2602.
0.630	0.420	-23.4	2489.8	2509.	3432.	2851.
0.720	0.563	-18.1	2341.9	2895.	3511.	3068.
0.835	0.756	-9.4	2259.1	3228.	3592.	3288.
0.862	0.797	-7.8	2395.9	3285.	3606.	3329.
0.899	0.852	-5.7	2749.2	3350.	3624.	3378.
0.942	0.916	-3.1	3505.2	3407.	3639.	3421.

CO2- HYDROGEN SULFIDE BINARY SYSTEM... P= 50.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.045	0.010	337.4	0.365	-0.212E-01	0.937E 00	0.743E 00
0.132	0.048	333.0	0.367	-0.185E-01	0.909E 00	0.735E 00
0.216	0.089	328.2	0.365	-0.169E-01	0.885E 00	0.726E 00
0.295	0.135	323.4	0.360	-0.160E-01	0.863E 00	0.719E 00
0.374	0.190	318.4	0.354	-0.156E-01	0.841E 00	0.712E 00
0.455	0.255	313.2	0.346	-0.155E-01	0.820E 00	0.705E 00
0.534	0.336	308.2	0.337	-0.159E-01	0.800E 00	0.699E 00
0.614	0.438	303.3	0.326	-0.169E-01	0.781E 00	0.695E 00
0.701	0.572	298.4	0.314	-0.189E-01	0.761E 00	0.694E 00
0.811	0.739	293.2	0.300	-0.242E-01	0.740E 00	0.693E 00
0.908	0.874	289.8	0.288	-0.364E-01	0.727E 00	0.709E 00
0.950	0.932	288.8	0.283	-0.491E-01	0.723E 00	0.717E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.045	0.763E-02	0.279E-02	3911.4	3873.0	-38.3
0.132	0.618E-02	0.247E-02	2990.9	2922.3	-68.7
0.216	0.544E-02	0.227E-02	2714.4	2628.2	-86.2
0.295	0.508E-02	0.212E-02	2558.8	2460.4	-98.4
0.374	0.491E-02	0.196E-02	2462.9	2353.4	-109.6
0.455	0.489E-02	0.174E-02	2441.1	2318.4	-122.7
0.534	0.495E-02	0.141E-02	2394.1	2261.8	-132.2
0.614	0.508E-02	0.879E-03	2296.6	2161.5	-135.1
0.701	0.526E-02	-0.106E-03	2060.6	1938.0	-122.5
0.811	0.547E-02	-0.267E-02	1944.0	1843.9	-100.1
0.908	0.546E-02	-0.847E-02	2475.3	2396.2	-79.0
0.950	0.525E-02	-0.144E-01	3085.8	3027.4	-58.5

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	H2S	MIX
0.045	0.010	-2.6	3870.5	0.	2541.	2427.
0.132	0.048	-6.5	2915.8	0.	2653.	2303.
0.216	0.089	-10.4	2617.8	0.	2766.	2169.
0.295	0.135	-13.8	2446.6	0.	2874.	2026.
0.374	0.190	-16.7	2336.6	0.	2979.	1865.
0.455	0.255	-19.1	2299.3	0.	3082.	1680.
0.534	0.336	-19.8	2242.1	0.	3177.	1480.
0.614	0.438	-18.3	2143.2	987.	3264.	1866.
0.701	0.572	-13.9	1924.1	1977.	3348.	2387.
0.811	0.739	-8.0	1835.9	2521.	3434.	2694.
0.908	0.874	-3.9	2392.4	2789.	3488.	2853.
0.950	0.932	-2.1	3025.3	2862.	3503.	2894.

CO2- HYDROGEN SULFIDE BINARY SYSTEM... P= 60.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.035	0.009	347.5	0.284	-0.180E-01	0.953E 00	0.716E 00
0.122	0.050	342.4	0.287	-0.166E-01	0.916E 00	0.705E 00
0.194	0.092	338.0	0.286	-0.159E-01	0.889E 00	0.696E 00
0.271	0.137	333.0	0.284	-0.154E-01	0.863E 00	0.687E 00
0.345	0.190	328.2	0.279	-0.151E-01	0.838E 00	0.679E 00
0.423	0.256	323.0	0.273	-0.152E-01	0.814E 00	0.671E 00
0.496	0.330	318.3	0.266	-0.155E-01	0.792E 00	0.665E 00
0.583	0.425	312.8	0.257	-0.164E-01	0.767E 00	0.659E 00
0.662	0.540	308.2	0.247	-0.179E-01	0.746E 00	0.656E 00
0.759	0.687	303.2	0.234	-0.213E-01	0.723E 00	0.657E 00
0.901	0.873	297.7	0.213	-0.348E-01	0.697E 00	0.673E 00
0.938	0.922	296.8	0.207	-0.439E-01	0.693E 00	0.681E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.035	0.859E-02	0.335E-02	3325.0	3292.3	-32.7
0.122	0.710E-02	0.296E-02	2605.5	2536.1	-69.4
0.194	0.641E-02	0.275E-02	2349.7	2264.8	-84.9
0.271	0.600E-02	0.256E-02	2294.9	2193.5	-101.4
0.345	0.579E-02	0.238E-02	2220.4	2107.3	-113.1
0.423	0.573E-02	0.215E-02	2153.7	2029.9	-123.8
0.496	0.578E-02	0.185E-02	2076.5	1945.4	-131.1
0.583	0.593E-02	0.130E-02	2078.1	1935.8	-142.4
0.662	0.614E-02	0.453E-03	1845.1	1714.2	-131.0
0.759	0.645E-02	-0.147E-02	1528.2	1424.1	-104.1
0.901	0.673E-02	-0.979E-02	1924.5	1843.0	-81.5
0.938	0.662E-02	-0.155E-01	2112.2	2050.3	-61.9

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	H2S	MIX
0.035	0.009	-1.6	3290.6	0.	2249.	2171.
0.122	0.050	-4.9	2531.2	0.	2403.	2110.
0.194	0.092	-7.4	2257.4	0.	2526.	2036.
0.271	0.137	-10.4	2183.1	0.	2652.	1934.
0.345	0.190	-12.7	2094.6	0.	2768.	1813.
0.423	0.256	-14.5	2015.4	0.	2882.	1663.
0.496	0.330	-15.1	1930.3	0.	2982.	1503.
0.583	0.425	-15.2	1920.6	0.	3090.	1288.
0.662	0.540	-12.2	1702.0	0.	3176.	1074.
0.759	0.687	-7.5	1416.6	1023.	3265.	1563.
0.901	0.873	-3.0	1840.0	2060.	3359.	2189.
0.938	0.922	-1.7	2048.6	2171.	3375.	2245.

CO2- HYDROGEN SULFIDE BINARY SYSTEM... P= 70.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.090	0.042	352.7	0.226	-0.153E-01	0.945E 00	0.682E 00
0.160	0.086	348.0	0.228	-0.146E-01	0.910E 00	0.671E 00
0.226	0.131	343.4	0.227	-0.142E-01	0.881E 00	0.661E 00
0.300	0.184	338.2	0.224	-0.141E-01	0.850E 00	0.651E 00
0.369	0.243	333.3	0.220	-0.143E-01	0.823E 00	0.642E 00
0.442	0.312	328.3	0.214	-0.148E-01	0.796E 00	0.633E 00
0.532	0.398	322.3	0.205	-0.158E-01	0.765E 00	0.624E 00
0.601	0.489	318.1	0.198	-0.170E-01	0.743E 00	0.620E 00
0.687	0.615	313.4	0.187	-0.193E-01	0.718E 00	0.618E 00
0.796	0.765	308.3	0.170	-0.245E-01	0.690E 00	0.622E 00
0.969	0.967	303.0	0.096	-0.498E-01	0.659E 00	0.654E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.090	0.878E-02	0.357E-02	2217.1	2155.3	-61.9
0.160	0.753E-02	0.334E-02	1930.9	1856.3	-74.6
0.226	0.693E-02	0.318E-02	1808.6	1725.0	-83.5
0.300	0.663E-02	0.301E-02	1771.5	1676.2	-95.3
0.369	0.655E-02	0.282E-02	1706.7	1603.0	-103.7
0.442	0.662E-02	0.254E-02	1665.3	1551.8	-113.5
0.532	0.685E-02	0.200E-02	1754.8	1620.6	-134.2
0.601	0.710E-02	0.133E-02	1599.3	1469.4	-129.9
0.687	0.748E-02	-0.201E-04	1264.1	1158.8	-105.3
0.796	0.802E-02	-0.334E-02	882.2	815.6	-66.5
0.969	0.107E-01	-0.377E-01	605.1	587.4	-17.7

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	H2S	MIX
0.090	0.042	-2.7	2152.6	0.	2069.	1883.
0.160	0.086	-4.6	1851.7	0.	2232.	1875.
0.226	0.131	-6.3	1718.7	0.	2374.	1838.
0.300	0.184	-8.4	1667.9	0.	2521.	1765.
0.369	0.243	-9.7	1593.3	0.	2646.	1670.
0.442	0.312	-10.6	1541.2	0.	2766.	1543.
0.532	0.398	-11.7	1608.9	0.	2897.	1356.
0.601	0.489	-10.2	1459.2	0.	2984.	1191.
0.687	0.615	-6.9	1151.9	0.	3079.	964.
0.796	0.765	-3.1	812.5	0.	3174.	647.
0.969	0.967	-0.2	587.2	1092.	3269.	1160.

CO2- HYDROGEN SULFIDE BINARY SYSTEM... P= 80.0 ATM

Y1	X1	TK	VM	DYDT	PHI(1)	PHI(2)
0.050	0.025	363.7	0.177	-0.154E-01	0.101E 01	0.667E 00
0.127	0.070	357.9	0.182	-0.123E-01	0.948E 00	0.651E 00
0.176	0.116	353.8	0.180	-0.118E-01	0.920E 00	0.640E 00
0.240	0.167	348.4	0.177	-0.120E-01	0.886E 00	0.626E 00
0.308	0.225	342.9	0.172	-0.128E-01	0.852E 00	0.612E 00
0.373	0.292	338.0	0.168	-0.137E-01	0.822E 00	0.601E 00
0.438	0.366	333.4	0.162	-0.140E-01	0.793E 00	0.592E 00
0.508	0.456	328.2	0.153	-0.128E-01	0.764E 00	0.580E 00

Y1	DLNPHI(1)	DLNPHI(2)	IDEAL (HV-H*)	REAL (HV-H*)	FUG CONT
0.050	0.154E-01	0.417E-02	2130.2	2056.3	-73.9
0.127	0.789E-02	0.413E-02	1604.3	1549.7	-54.5
0.176	0.699E-02	0.417E-02	1213.3	1171.2	-42.2
0.240	0.690E-02	0.412E-02	1158.3	1109.3	-49.0
0.308	0.732E-02	0.389E-02	1165.2	1098.6	-66.6
0.373	0.769E-02	0.356E-02	1075.8	999.9	-75.9
0.438	0.759E-02	0.350E-02	901.6	836.6	-65.0
0.508	0.670E-02	0.458E-02	571.0	547.3	-23.7

Y1	X1	DELTA H*	LAT HV	WATKINS EST FOR PURE COMP CO2	H2S	MIX
0.050	0.025	-1.1	2055.1	0.	1571.	1492.
0.127	0.070	-2.9	1546.8	0.	1858.	1622.
0.176	0.116	-3.3	1167.8	0.	2026.	1669.
0.240	0.167	-4.5	1104.8	0.	2217.	1685.
0.308	0.225	-5.6	1093.0	0.	2388.	1652.
0.373	0.292	-5.9	994.0	0.	2525.	1583.
0.438	0.366	-5.5	831.0	0.	2645.	1486.
0.508	0.456	-4.3	543.0	0.	2768.	1362.