

6-30-1964

## Gas phase fugacity coefficients

Harvey Joel Klee  
*New Jersey Institute of Technology*

Follow this and additional works at: <https://digitalcommons.njit.edu/theses>



Part of the [Chemical Engineering Commons](#)

---

### Recommended Citation

Klee, Harvey Joel, "Gas phase fugacity coefficients" (1964). *Theses*. 2110.  
<https://digitalcommons.njit.edu/theses/2110>

This Thesis is brought to you for free and open access by the Electronic Theses and Dissertations at Digital Commons @ NJIT. It has been accepted for inclusion in Theses by an authorized administrator of Digital Commons @ NJIT. For more information, please contact [digitalcommons@njit.edu](mailto:digitalcommons@njit.edu).

## **Copyright Warning & Restrictions**

The copyright law of the United States (Title 17, United States Code) governs the making of photocopies or other reproductions of copyrighted material.

Under certain conditions specified in the law, libraries and archives are authorized to furnish a photocopy or other reproduction. One of these specified conditions is that the photocopy or reproduction is not to be “used for any purpose other than private study, scholarship, or research.” If a user makes a request for, or later uses, a photocopy or reproduction for purposes in excess of “fair use” that user may be liable for copyright infringement,

This institution reserves the right to refuse to accept a copying order if, in its judgment, fulfillment of the order would involve violation of copyright law.

**Please Note: The author retains the copyright while the New Jersey Institute of Technology reserves the right to distribute this thesis or dissertation**

Printing note: If you do not wish to print this page, then select “Pages from: first page # to: last page #” on the print dialog screen

The Van Houten library has removed some of the personal information and all signatures from the approval page and biographical sketches of theses and dissertations in order to protect the identity of NJIT graduates and faculty.

GAS PHASE FUGACITY COEFFICIENTS

BY

HARVEY J. KLEE

A THESIS

PRESENTED IN PARTIAL FULFILLMENT OF

THE REQUIREMENTS FOR THE DEGREE

OF

MASTER OF SCIENCE IN CHEMICAL ENGINEERING

AT

THE NEWARK COLLEGE OF ENGINEERING

This thesis is to be used only with due regard to the rights of the author. Bibliographical references may be noted, but passages must not be copied without permission of the College and without credit being given in subsequent written or published work.

Newark, New Jersey

1964

## ABSTRACT

A method is presented for calculation of fugacity coefficients in gas mixtures. This work is based on a recent paper by Leland, Gamson, and Chappellear, wherein they presented a new method for evaluation of ideal K values. The information required for the method presented here includes pure component physical properties, and generalized tables or equations for compressibility factors, fugacity coefficients, and real gas enthalpy departure terms. Pseudo-critical temperatures and pressures for the mixture are calculated using the expressions presented by Leland and Mueller.

Five different binary systems consisting of paraffin hydrocarbon and CO<sub>2</sub> mixtures containing 318 separate points were used to test this method. The results were compared with fugacity coefficients calculated from experimental data. For mixtures containing molecules of small size, this work predicts fairly accurate coefficients. For mixtures containing molecules with an appreciable difference in molecular size, the component with the larger molecule displays substantial deviations from the experimental fugacity coefficient. The one-non-hydrocarbon molecule studied, carbon dioxide, was accurately treated by this method. For binary systems containing two paraffinic components, this method will predict fugacity coefficients higher than experimental data for both components.

By comparison of this method with Pitzer's for the same set of data, it was established that the Pitzer method was more accurate,

but does require experimental data on equimolal mixtures. The method considered here requires further study to determine what modifications can be made so systems with large differences in molecular size can be accurately treated.

APPROVAL OF THESIS  
FOR  
DEPARTMENT OF CHEMICAL ENGINEERING  
NEWARK COLLEGE OF ENGINEERING  
BY  
FACULTY COMMITTEE

APPROVED: \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

NEWARK, NEW JERSEY

JUNE, 1964

### ACKNOWLEDGMENTS

The author wishes to thank Professor Joseph Joffe for his generous advice and guidance which led to the successful conclusion of this work.

This work was done with the computer facilities of Socony Mobil Oil Company, Inc. in New York City. The author wishes also to express his appreciation to the corporate Engineering Department for donating computer operating time for this problem.

The author is grateful to his wife for her encouragement and assistance during the course of this work.



## TABLE OF CONTENTS

	<u>Page</u>
Abstract	i
Approval of Thesis	iii
Acknowledgements	iv
List of Tables	vii
Introduction	
Object	1
Definitions	1
Methods of Calculating Fugacity Coefficients	5
Garnson, Leland and Chappelaar Method	13
Sample Calculation	17
Description of Computer Program	24
Discussion	
General	27
Statistical Definitions	29
Specific Results	30
Comparison with Other Methods	35
Conclusion	37
Recommendations	38
Comparison of Results with Experimental Data	
Table 1	39
Pure Component Critical Properties - Table 2	40

Nomenclature	41
References	43
Appendix	45
Computer Program	46
Nomenclature for Computer Program	57
Machine Calculations, Tables 1 and 2	61

LIST OF TABLES

<u>Table</u>	<u>Title</u>	<u>Page Number</u>
Text		
1	Comparison of Results with Experimental Data and the Pitzer Method	39
2	Pure Component Critical Properties	40
Appendix		
1	Calculated Fugacity Coefficients	61
2	Intermediate Values in Calculations	70

## INTRODUCTION

### Object

Accurate fugacity values are of importance when dealing with chemical reactions and equilibrium systems. A reliable method for predicting fugacities for components in solution, can be of great utility in calculating ideal K values or equilibrium constants. Equilibrium constants find widespread use in chemical engineering calculations.

This work is an attempt to evaluate a new method for calculating fugacity coefficients for components in gaseous mixtures. The only information required is the pure component critical properties and generalized tables of thermodynamic properties. The method is based on the principle of corresponding states. This discussion deals with binary gas mixtures, but can be extended to multicomponent systems.

### Definitions

Fugacity is an arbitrarily defined thermodynamic function related to the free energy. For a pure substance:

$$\left(\frac{dG}{T}\right) = \left(RT d \ln f\right) \quad (1)$$

For a solution, the fugacity of a component is related to the partial molal free energy and chemical potential by:

$$\left(\frac{d\bar{G}}{T}\right) = \left(d\mu_1\right) = \left(RT d \ln f_1\right) \quad (2)$$

Fugacity can be considered as a measure of the escaping tendency from a phase. At equilibrium, the escaping tendency or chemical potential must be equal in all phases or else there will be a net transfer of mass between phases. Fugacity is therefore a measure of equilibrium since it is directly related to the chemical potential in solution. As the pressure approaches zero, the fugacity of a pure component becomes equivalent to the pressure.

An ideal gas is one whose P-V-T relationships are exactly defined by the ideal gas law. For 1 mole of gas, the relationship is:

$$PV = RT \quad (3)$$

An ideal solution is one in which the fugacity of a component in solution equals the product of its mole fraction and the pure component fugacity at the same temperature, pressure and physical state. (11) Thus,

$$f_1 = N_1 f_1^{\circ} \quad (4)$$

This is known as the Lewis and Randall rule. An ideal solution exhibits no heat evolution or volume change on isothermal formation from its components. Dalton's law for ideal gases and Raoult's law for ideal solutions are less general modifications of the Lewis and Randall rule. Thus for an ideal gas mixture in contact with an ideal liquid solution: (31)

$$f_1 = y_1 f_1^{\circ} = y_1 P = p_1 = \kappa_1 P^{\circ} \quad (5)$$

The fugacity in a gas mixture is then equal to its partial pressure.

Various combination of ideality in coexisting phases are possible. For example, an ideal gas phase may be in equilibrium with a non-ideal liquid phase. Ideal gases and ideal solutions are not corequisites, although they may both be approached in the gas phase at very low pressures. Ideal gases will necessarily form ideal solutions, while it is possible for non-ideal gases to form ideal solutions.

The activity of a substance is arbitrarily defined as the ratio of the fugacity of the component in any state to the fugacity in the standard state.

$$(a_i)_T = (f_i/f_i^{\circ})_T \quad (6)$$

The standard state for fugacity is arbitrarily chosen for convenience. Two standard states are in general use for gases. Both states are based on the pure component at the temperature of the system. One is based on one atmosphere pressure and the ideal gaseous state, while the other uses the system pressure. When the standard state is taken as the ideal gas at one atmosphere, the activity becomes equal to the fugacity in atmospheres, since the fugacity of an ideal gas equals its partial pressure.

A function related to the activity is the activity coefficient, as defined:

$$\gamma_i = a_i/N_i = f_i / f_i^{\circ} N_i \quad (7)$$

The activity coefficient is an empirical correction factor for the departure from ideal solution behavior. The activity coefficient finds its greatest use in considering the non-ideal behavior of the liquid phase. The actual value of this factor depends on the standard state selected for fugacity and the concentration unit selected for the composition.

Another function derived from the fugacity is the fugacity coefficient. For a pure substance this is defined as the ratio of the fugacity to the absolute pressure.

$$\phi = (f/p)_T \quad (8)$$

For a component in solution, the fugacity coefficient is equal to the fugacity divided by the product of the pressure and its mole fraction.

$$\phi_1 = (f_1/N_1 P)_T \quad (9)$$

Generalized tables of fugacity coefficients have been developed. (24, 26) The fugacity coefficient is related to the activity coefficient by the following:

$$\phi_1 = \gamma_1 \left( \frac{f_1^0}{P} \right) = \gamma_1 \phi_1^0 \quad (10)$$

Where  $\phi_1^0$  is the fugacity coefficient in the standard state. The fugacity coefficient is also a measure of the deviation from ideal behavior.

Another important law is the Theorem of Corresponding States.

This law leads to the conclusion that all pure gases when measured under the same reduced conditions of temperature and pressure, display the same compressibility factor. (33) This can be expressed mathematically as:

$$Z = f(P_R, T_R) \quad (11)$$

It has been shown recently that two parameters are not adequate to describe a reduced condition and that a third is required. The third parameter can be the critical compressibility,  $Z_c$ , or the acentric factor,  $w$ .

#### Methods of Calculating Fugacity Coefficients

Lewis and Randall. If a gas mixture forms an ideal solution or is at a sufficiently low pressure such that ideal solution behavior may be assumed, the Lewis and Randall rule may be used. This defines the fugacity coefficient in solution as the product of the mole fraction of the component and its pure component fugacity at the same temperature and pressure. (23)

$$f_1 = y f_1^0 \quad (12)$$

At high pressures this rule can give a large error but may be suitable for approximations if the reduced pressure of the component of interest is less than 0.6. (30)

Partial residual molal volume. At constant temperature the fugacity of a component in solution may be given by:

$$(d \ln f_1)_T = \frac{(\bar{V}_1 dP)}{RT} \quad (13)$$



where  $\bar{V}_i$  is the partial molal volume of component  $i$  in solution and  $P$  is the total pressure. Integrating equation (13) from some low pressure  $P^*$ , where ideal solution behavior is exhibited, to some existing pressure  $P$ , and substituting

$$f_i^* = N_i P^*$$

will give,

$$\ln \frac{f_i}{N_i P^*} = \frac{1}{RT} \int_{P^*}^P \bar{V}_i dP \quad (14)$$

Equation (14) will allow calculation of the fugacity of each component in a solution if P-V-T data is available.

The evaluation of the fugacity is facilitated by introduction of the residual molal volume,  $\alpha$ .

$$\alpha = V^* - V = \frac{RT}{P} - V \quad (15)$$

Equation (15) can be differentiated at constant pressure, temperature and composition to give:

$$\left( \frac{\partial \alpha}{\partial n_i} \right)_{P,T,n_j} = \left( \frac{\partial V^*}{\partial n_i} \right)_{P,T,n_j} - \left( \frac{\partial V}{\partial n_i} \right)_{P,T,n_j}$$

or  $\bar{\alpha}_i = \bar{V}_i^* - \bar{V}_i \quad (16)$

where the bar denotes partial molal quantities.

For an ideal gas, the partial molal volume equals the molal

volume of the mixture and

$$\bar{V}_1^* = V^* = RT/P \quad (17)$$

Substituting (17) in (16), the partial molal residual volume then becomes:

$$\bar{\alpha}_1 = \frac{RT}{P} - \bar{V}_1$$

or  $\bar{V}_1 = \frac{RT}{P} - \bar{\alpha}_1 \quad (18)$

Multiplying through by  $dP$  and integrating between  $P^*$  and  $P$ ,

$$\int_{P^*}^P \bar{V}_1 dP = RT \ln \frac{P}{P^*} - \int_{P^*}^P \bar{\alpha}_1 dP \quad (19)$$

Substituting (19) in (14), the final working equation results,

$$\ln \frac{f_1}{N_1 P} = - \frac{1}{RT} \int_{P^*}^P \bar{\alpha}_1 dP \quad (20)$$

$\bar{\alpha}_1$  is evaluated by plotting residual molal volumes against composition for varying pressures. By extrapolating the tangent to the curve at a given composition to zero mole fraction, the intercept is the partial residual molal volume,  $\bar{\alpha}_1$ . Residual molal volumes are obtained from the compressibility factors of the gas mixture by:

$$\alpha = (1 - Z) RT/P \quad (21)$$

The integral in equation (20) is evaluated by plotting  $\bar{\alpha}_i$  against pressure and graphically integrating the result between zero and the system pressure. The integral is at constant temperature and composition. Substituting the result in equation (20), the fugacity coefficient is evaluated directly.

This procedure was used in developing most of the experimental data with which this work is compared. The work of Lacey and Sage was among the earliest examples of this method.<sup>(17)</sup> As evident from the preceding discussion, this method of calculation of the fugacity coefficient is involved, tedious, and time consuming. The method requires experimental P-V-T data on the system which may not be readily available.

Gamson and Watson. Various authors have proposed methods of calculating the fugacity coefficient in gaseous mixtures based on generalized correlations. Gamson and Watson developed an equation based on the Corresponding States Theorem and Kay's rule pseudo-critical properties.<sup>(8)</sup>

The correlation was further refined by Gamson<sup>(6)</sup> to include Joffe's definition of pseudo-critical properties.<sup>(15)</sup>

Joffe. A similar method was proposed by Joffe using Kay's rule and the Corresponding States Theory.<sup>(16)</sup> The equation for the relationship is:

$$\ln \frac{f_i}{y_i f_M} = \left( \frac{T_c' - T_{c1}}{RT} \right) \left( \frac{H^* - H}{T_c'} \right) + \left( \frac{P_{c1} - P_c'}{P_c'} \right) (Z_M - 1) \quad (22)$$

This work was originally developed for use with the then existing two parameter generalized correlations.

Benedict, Webb, Rubin and Friend. Other authors have established correlations based on equations of state. Benedict, Webb, Rubin and Friend developed correlations based on mixtures of twelve light hydrocarbons and their equation of state. The liquid molal average boiling point was selected as a composition parameter. They developed a series of 276 charts of K factors,  $(y/X)$ , or fugacity coefficients to cover a pressure range to 3,600 psia. (2)

The charts were replotted by DePriester with two parameters. The number was significantly reduced and the accuracy improved. (4)

Edmister and Ruby. Edmister and Ruby developed a four parameter relationship based on the original work of Benedict et al. The parameters were reduced temperature, pressure, boiling point, and an intermediate temperature-composition scale. For vapors, two charts of  $B_R$  as a function of  $T_R$  and  $\theta$ , one being for methane only, and one of  $(f_1/yP)$  versus  $P_R$  and  $\theta$ , were developed. The results are applicable for olefin and paraffin systems and are said to agree within 3-4% of the original data. (5)

Redlich, et al. Redlich has also developed a method based on a modified equation of state, given by:

$$P = \frac{RT}{(V-b)} - \frac{0.5a}{V(V+b)} T^{1/2} \quad (23)$$

Charts were developed from this equation to be used in conjunction with generalized thermodynamic charts in estimating fugacity coefficients. (29)

Pitzer Method. Pitzer has defined a parameter which he designates as the "acentric factor".

$$w = -\log P_R - 1.0 \quad (24)$$

where  $P_R$  is the reduced saturation pressure at a reduced temperature of 0.70. (28) The  $w$  function is intended to serve as a third parameter for the two-parameter Corresponding States Theorem proposed by Van Der Waals in 1873. (33) In this sense, it is analogous to the critical compressibility factor,  $Z_c$ , used in the Lydersen, Greenkorn and Hougen, Generalized Thermodynamic Property Tables. (24) These tables were published by Hougen, Watson and Ragatz in their thermodynamics text. The acentric factor measures the deviation of the intermolecular potential function of a substance from that of a simple spherical molecule. The  $Z_c$  and  $w$  functions are related by: (13)

$$Z_c = \frac{1}{1.28w + 3.41} \quad (25)$$

Using this third parameter, Pitzer has developed series of generalized Thermodynamic Property Tables. (26) These tables are limited to normal fluids as defined by Hildebrand. (9) Normal fluids are defined in terms of the hypothetical surface tension and molal volume at 0°K, and the acentric factor:

$$\frac{\sigma_{0VO}^{2/3}}{T_c} = 1.86 + 1.18w \quad (26)$$

where  $\sigma_0$  = hypothetical surface tension at  $0^\circ\text{K}$ ,  
dynes/cm

$V_0$  = hypothetical molal volume at  $0^\circ\text{K}$ ,  
cc./g - mole

Compounds that deviate less than 5% from the definition are "normal fluids". In general substances that are polar, form hydrogen bonds or associate in some way, are non-"normal". Methane and the heavier rare gases are "normal fluids", while acetic acid, ammonia, hydrogen cyanide, methanol and water manifest appreciable deviations from equation (26). The quantum fluids,  $\text{H}_2$  and He, are not covered by these correlations. Pitzer states that a group of gaseous substances with the same acentric factor will conform to the corresponding states principle within the group.

The thermodynamic properties of a substance at any reduced condition are given from the table values by an equation linear in the acentric function:

$$X = X^{(0)} + wX^{(1)} \quad (27)$$

where the  $X^{(0)}$  and  $X^{(1)}$  are the separate table values of any function at a given reduced temperature and pressure. The original function is a power series where all terms higher than the second, are considered not important. (26) In some binary systems the pseudo-critical temperature and pressure, and the acentric factor can be assumed linear with composition, but this assumes no interaction occurs. Therefore Pitzer and Hultgren, developed equations to handle non-linear behavior. Their equations are in terms of the given mixture, the pure components,

and equimolal mixtures as follows:

$$T_{cM} = x_1 T_{c1} + x_2 T_{c2} + 2x_1 x_2 (2T_{cMix} - T_{c1} - T_{c2}) \quad (28)$$

$$P_{cM} = x_1 P_{c1} + x_2 P_{c2} + 2x_1 x_2 (2P_{cMix} - P_{c1} - P_{c2}) \quad (29)$$

$$w_M = x_1 w_1 + x_2 w_2 + 2x_1 x_2 (2w_{Mix} - w_1 - w_2) \quad (30)$$

where the subscripts;

M are for the given mixture

Mix are for equimolal mixtures

1,2 are for components 1 and 2.

For binary systems the following equation for fugacity coefficients were developed by Pitzer for components 1 and 2 respectively. (27)

$$\log \frac{f_1}{x_1 P} = \log \left( \frac{f}{P} \right)_M + x_2 Y \quad (31)$$

$$\log \frac{f_2}{x_2 P} = \log \left( \frac{f}{P} \right)_M - x_1 Y \quad (32)$$

The term Y was defined as:

$$Y = \left[ \frac{H^* - H}{RTc'} \right]_M \frac{[T_{c2} - T_{c1} + 2(1-2x_2)(2T_{cMix} - T_{c1} - T_{c2})]}{2,303 T} \\ + (Z_M - 1) \frac{[P_{c2} - P_{c1} + 2(1-2x_2)(2P_{cMix} - P_{c1} - P_{c2})]}{2,303 P_{cM}} \\ - \log \left( \frac{f}{P} \right)^{(1)} (w_2 - w_1) \quad (33)$$

Equations (27) through (33) were the basis for the work of Mazzei. (25)

### Gamson, Leland, and Chappellear Method

Gamson, Leland and Chappellear recently presented a method for determining a new ideal K value which is not based on the Lewis and Randall ideal solution rule but on composition dependent pseudocritical properties and the corresponding states principle. (7) For each phase it was shown that the following expression holds:

$$\ln\left(\frac{f_1}{x_1}\right) = \ln f + n \left( \frac{\partial \ln f}{\partial \ln n_1} \right)_{T,P,n_2,n_3,\dots} \quad (34)$$

The second term on the right of the equation was designated  $\Psi$  and defined by:

$$\Psi = - \frac{1}{RT} \left[ \frac{H^* - H}{T_c} \right] \left[ \frac{\partial T_c'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial T_c'}{\partial x_i} \right] - \left[ \frac{Z-1}{Pc'} \right] \left[ \frac{\partial Pc'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial Pc'}{\partial x_i} \right] \quad (35)$$

The partial derivative terms are given for component 1 by:

$$\left[ \frac{\partial T_c'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial T_c'}{\partial x_i} \right] = \left( \frac{2}{\alpha} \right) \left[ \frac{\sum_{i=1}^c x_i a_1 a_i}{\sum_{i=1}^c \sum_{j=1}^c x_i x_j a_i a_j} - \frac{\sum_{i=1}^c x_i (b_1 + b_i)^3}{\sum_{i=1}^c \sum_{j=1}^c x_i x_j (b_i + b_j)^3} \right] T_c' \quad (36)$$

$$\left[ \frac{\partial Pc'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial Pc'}{\partial x_i} \right] = \left( \frac{2}{\alpha} \right) \left[ \frac{\sum_{i=1}^c x_i a_1 a_i}{\sum_{i=1}^c \sum_{j=1}^c x_i x_j a_i a_j} \right]$$



$$\begin{aligned}
 & - (1 + \alpha) \left( \frac{2}{\alpha} \right) \frac{\sum_{i=1}^c x_i (b_i + b_i)^3}{\sum_{i=1}^c \sum_{j=1}^c x_i x_j (b_i + b_j)^3} \\
 & + \left( 1 + \frac{Z_{c1}}{\sum_{i=1}^c x_i Z_{ci}} \right) \Bigg]_{Pc'} \quad (37)
 \end{aligned}$$

It should be noted that separate values for equations (37) and (39) can be calculated for each component of a mixture. Therefore, there will be a distinct  $\Psi$  value for every component in each phase.

Using an equation of the form of (34) for the liquid and vapor phases, and equating  $f_{iG}$  to  $f_{iL}$  at equilibrium, the final working equation was developed:

$$\ln (K_1)_{\text{ideal}} = \ln \frac{f_{iL}}{f_{iG}} + (\Psi_{iL} - \Psi_{iG}) \quad (38)$$

Equation (38) can be solved for the ideal K value by determining  $f$ ,  $(H^* - H)/Tc'$ , and  $Z$ , for each phase separately at the pseudoreduced conditions from generalized charts or tables. The pseudocritical temperature and pressure are given by the Leland and Mueller modification of Joffe's definitions as follows: <sup>(22)</sup>

$$Tc' = \left[ \frac{\sum_{i=1}^c \sum_{j=1}^c x_i x_j a_i a_j}{\sum_{i=1}^c \sum_{j=1}^c x_i x_j (b_i + b_j)^3} \right]^{1/\alpha} \quad (39)$$

$$Pc' = \left[ \frac{Tc' \sum_{i=1}^c x_i (Zc)_i}{\sum_{i=1}^c \sum_{j=1}^c x_i x_j (b_i + b_j)^3} \right] \quad (40)$$

where

$$a_i = \left[ \frac{Z_c T_c^{\alpha+1}}{P_c} \right]_i^{\frac{1}{2}} \quad (41)$$

and

$$b_i = \frac{1}{2} \left[ \frac{Z_c T_c}{P_c} \right]_i^{1/3} \quad (42)$$

$$\alpha = 1.0 + \exp \left[ -10 \left( \frac{P}{\sum x_i P_{ci}} - 1 \right)^2 \right] \quad (43)$$

The pseudocritical compressibility was taken as the Kay's rule value:

$$Z_c' = x_1 Z_{c1} + x_2 Z_{c2} + \dots + x_n Z_{cn} \quad (44)$$

The authors also suggest using a reference substance whose thermodynamic properties are known or may be calculated from an equation of state, to determine the  $f$ ,  $(H^*-H) / T_c'$ , and  $Z$  terms. The properties would be evaluated at an equivalent temperature and pressure defined as:

$$T^0 = (T_{R}') T_c^0$$

$$P^0 = (P_{R}') P_c^0$$

where  $T_c^0$  and  $P_c^0$  are the criticals of the reference substance. A reference substance is chosen so it has as much molecular similarity as possible with the mixture. Two methods of choice were proposed. The first was to choose a substance with a critical compressibility,  $Z_c$ , close to that of the molar average of the mixture.  $Z_c$  can be considered to be an empirical shape factor. The alternate procedure was to use the molecular length/width ratio as a shape factor and

chose a substance with a ratio similar to the molal average of the mixture. The authors state that this method will give inaccurate results for extremely dissimilar molecules, and is not directly applicable to polar molecules although the results may be usable approximations.

If equation (34) is rewritten with  $\Psi$  replacing the second term, then for gaseous mixtures:

$$\ln \frac{f_1}{x_1} = \ln f_M + \Psi_G \quad (45)$$

Raising each term to the base e:

$$\left( \frac{f_1}{x_1} \right) / f_M = e^{\Psi_G} \quad (46)$$

Dividing the numerator and denominator of the left side by the pressure and taking the logarithm of the equation, gives:

$$\ln \left( \frac{f}{xP} \right)_1 = \ln \left( \frac{f}{P} \right)_M + \Psi_{1G} \quad (47)$$

Equation (47) is the basis for this work. This relates the fugacity coefficient in solution to the mixture fugacity coefficient and a correction term for non-ideal behavior,  $\Psi$ . The  $\Psi$  term is given by equation (35). The mixture fugacity coefficient is determined from a generalized table along with the mixture compressibility factor and enthalpy departure term.

### SAMPLE CALCULATION

Given: Point number 60

T 310.94 °K

P 400.00 atm.

$x_1$  0.204

$\phi_1$  exp. 1.417

$\phi_2$  exp. 0.252

component 1 CH<sub>4</sub>

component 2 CO<sub>2</sub>

Critical Properties	1	2
T <sub>c</sub>	191.06	304.2
P <sub>c</sub>	45.80	72.9
Z <sub>c</sub>	0.289	0.275

#### Step (1) Calculation of alpha.

$$\alpha = 1.0 + \exp \left[ -10 \left( \frac{P}{P_{c1}x_1 + P_{c2}x_2} - 1 \right)^2 \right] \quad (43)$$

$$= 1.0 + \exp \left[ -10 \left( \frac{400.00}{.204 \times 45.80 + .796 \times 72.9} - 1.0 \right)^2 \right]$$

$$\alpha = 1.000$$

#### Step (2) Calculation of a and b constants.

$$a_i = \left[ \frac{Z_c T_c}{P_c} \right]_i^{\alpha + 1} \quad (41)$$

$$a_1 = \left( \frac{0.289 \times (191.06)^{2.0}}{45.80} \right)^{1/2} = 15.177$$

$$a_2 = \left( \frac{0.275 \times (304.2)^{2.0}}{72.9} \right)^{1/2} = 18.684$$

$$b_i = \frac{1}{2} \left( \frac{Z_c T_c}{P_c} \right)_i^{1/3} \quad (42)$$

$$b_1 = \frac{1}{2} \left( \frac{0.289 \times 191.06}{45.80} \right)^{1/3} = 0.5322$$

$$b_2 = \frac{1}{2} \left( \frac{0.275 \times 304.2}{72.9} \right)^{1/3} = 0.5235$$

Step (3) Calculation of pseudocritical compressibility.

$$Z_c' = x_1 Z_{c1} + x_2 Z_{c2} \quad (44)$$

$$Z_c' = 0.204 \times 0.289 + 0.796 \times 0.275 = 0.278$$

Step (4) Calculation of pseudocritical temperature.

$$T_c' = \left[ \frac{(x_1 a_1 + x_2 a_2)^2}{x_1^2 (2b_1)^3 + 2x_1 x_2 (b_1 + b_2)^3 + x_2^2 (2b_2)^3} \right]^{1/\alpha} \quad (39)$$

$$= \left[ \frac{(.204 \times 15.177 + .796 \times 18.684)^2}{(.204)^2 (2 \times .5322)^3 + 2 \times .204 \times .796 (1.0557)^3 + (.796)^2 (2 \times .5235)^3} \right]^{1.0}$$

$$T_c' = 278.44 \text{ } ^\circ\text{K}$$

Step (5) Calculation of pseudocritical pressure.

$$P_c' = \left[ \frac{(T_c') (Z_c')}{x_1^2 (2b_1)^3 + 2x_1 x_2 (b_1 + b_2)^3 + x_2^2 (2b_2)^3} \right] \quad (40)$$

$$= \frac{278.44 \times 0.278}{(\text{same denominator as } Tc')}$$

$$Pc' = 66.753 \text{ atm.}$$

Step (6) Calculation of temperature-composition partial derivative term for component 1.

$$\left[ \frac{\partial Tc'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial Tc'}{\partial x_i} \right] = \frac{2Tc'}{\alpha} \left[ \frac{x_1 a_1^2 + x_2 a_1 a_2}{(x_1 a_1 + x_2 a_2)^2} \right. \\ \left. - \frac{x_1 (2b_1)^3 + x_2 (b_1 + b_2)^3}{x_1^2 (2b_1)^3 + 2x_1 x_2 (b_1 + b_2)^3 + x_2^2 (2b_2)^3} \right] \quad (36)$$

$$= \frac{2Tc'}{1.0} \left[ \frac{.204x(15.177)^2 + .796x(15.177 \times 18.684)}{(.204 \times 15.177 + .796 \times 18.684)^2} \right. \\ \left. - \frac{.204x(2 \times .5322)^3 + .796(.5322 + .5235)^3}{(\text{same denominator as } Tc')} \right]$$

$$= 2(0.84469 - 1.01983) Tc'$$

$$= -0.35028 Tc'$$

Step (7) Calculation of pressure-composition partial derivative term for component 1.

$$\left[ \frac{\partial Pc'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial Pc'}{\partial x_i} \right] = \left[ \frac{2}{\alpha} \left( \frac{x_1 a_1^2 + x_2 a_1 a_2}{(x_1 a_1 + x_2 a_2)^2} \right) \right. \\ \left. - \frac{(1+\alpha) (x_1 (2b_1)^3 + x_2 (b_1 + b_2)^3)}{x_1^2 (2b_1)^3 + 2x_1 x_2 (b_1 + b_2)^3 + x_2^2 (2b_2)^3} \right] + \left( \frac{1+Zc_1}{Zc'} \right) Pc' \quad (37)$$

$$= \left[ \frac{2}{1.0} \left( \text{first term of equation (36)} - (1+1.0) \times \text{second term of} \right. \right. \\ \left. \left. \text{equation (36)} \right) + \left( 1 + \frac{0.289}{0.278} \right) \right] Pc'$$

$$= \frac{2}{1.0} (0.84469 - (2) 1.01983) + 2.03957$$

$$= - 0.35037 P_c'$$

Step (8) Calculation of reduced temperature and pressure.

$$T_R = \frac{T}{T_c'} = \frac{310.94}{278.44} = 1.1167$$

$$P_R = \frac{P}{P_c'} = \frac{400.00}{66.753} = 5.9922$$

Step (9) Table look up for generalized functions.

$$\text{Basis: } T_R = 1.1167$$

$$P_R = 5.9922$$

$$Z'_c = 0.278$$

$$\frac{H^*-H}{T_c'} = 7.55 \frac{\text{g-cal}}{\text{g-mole-}^\circ\text{K}} \quad Z = .772$$

$$\phi_M = 0.3534$$

Step (10) Evaluation of psi (1).

$$\Psi_1 = - \frac{1}{RT} \left[ \frac{H^*-H}{T_c'} \right] \left[ \frac{\partial T_c'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial T_c'}{\partial x_i} \right] + \frac{(1-Z)}{P_c'} \left[ \frac{\partial P_c'}{\partial x_1} - \sum_{i=1}^c x_i \frac{\partial P_c'}{\partial x_i} \right] \quad (35)$$

$$= \frac{-7.55 \times (-.35028) \times 278.43}{1.987 \times 310.94} + \frac{(1-0.772)}{P_c'} \times (-.35037 P_c')$$

$$\Psi_1 = 1.19179 - 0.07988 = 1.1119$$

(note: R=1.987 cal/g. mole - °K)

Step (11) Calculation of  $\phi_1$ .

$$\log \phi_1 = \log \phi_M + \frac{\Psi_1}{2.303} \quad (47)$$

$$\log \phi_1 = \log 0.3534 + \frac{1.1119}{2.303}$$

$$\phi_1 = 1.0741$$

$$\phi_1 \text{ exp.} = 1.417$$

$$\% \text{ DEV } 1 = \frac{1.417 - 1.0741}{1.417} \times 100 \% = 24.3 \%$$

Step (12) Calculation of temperature-composition partial derivative term for component 2.

$$\left[ \frac{\partial Tc'}{\partial x_2} - \sum_{i=1}^G x_i \frac{\partial Tc'}{\partial x_i} \right] = \left[ \frac{x_2 a_2^2 + x_1 a_1 a_2}{(x_1 a_1 + x_2 a_2)^2} \right. \\ \left. - \frac{x_2 (2b_2)^3 + x_1 (b_1 + b_2)^3}{x_1^2 (2b_1)^3 + 2x_1 x_2 (b_1 + b_2)^3 + x_2^2 (2b_2)^3} \right] \frac{2Tc'}{\alpha} \quad (36)$$

$$= \frac{2Tc'}{1.0} \left[ \frac{.796x(18.684)^2 + .204(15.177x18.684)}{\text{Same as for comp. 1}} \right. \\ \left. - \frac{.796(2x.5235)^3 + .204(.5322 \& .5235)^3}{\text{Same as for comp. 1}} \right]$$

$$= 2(1.03989 - .99482)Tc' = 0.09014 Tc'$$

Step (13) Calculation of pressure-composition partial derivative term for component 2.



$$\left[ \frac{\partial P_c'}{\partial x_2} - \sum_{i=1}^c x_i \frac{\partial P_c'}{\partial x_i} \right] = \left[ \frac{2}{\alpha} \right] \text{ (first term of equation (36) above)}$$

- (1.+ $\alpha$ )\* second term of equation (36) above)

$$+ \left( 1 + \frac{Zc_2}{Zc'} \right) P_c' \quad (37)$$

$$= \left[ \frac{2}{1.0} (1.03989 - (1 + 1.0) \times .99482) + (1 + \frac{.275}{278}) \right] P_c'$$

$$= 0.0897 P_c'$$

Step (14) Evaluation of  $\psi_1$  (2).

$$\psi_2 = -\frac{1}{RT} \left[ \frac{H^* - H}{Tc'} \right] \left[ \frac{\partial Tc'}{\partial x_2} - \sum_{i=1}^c x_i \frac{\partial Tc'}{\partial x_i} \right] + \frac{(1-Z)}{Pc'} \left[ \frac{\partial P_c'}{\partial x_2} - \sum_{i=1}^c x_i \frac{\partial P_c'}{\partial x_i} \right] \quad (35)$$

RT,  $\frac{H^* - H}{Tc'}$ , and Z are the same values as used for comp. 1 previously.

$$\psi_2 = - \frac{7.55 \times .09014 \times 278.43}{1.987 \times 310.94} + \frac{(1 - .772)}{Pc'} \times (.0897 P_c')$$

$$\psi_2 = - 0.28624$$

Step (15) Calculation of  $\theta_2$ .

$$\log \theta_2 = \log \theta_M + \frac{\psi_2}{2.303} \quad (47)$$

$$= \log 0.3534 - \frac{0.28624}{2.303}$$

$$\theta_2 = 0.26544$$

$$\theta_2 \text{ exp.} = 0.252$$

$$\% \text{ DEV } 2 = \frac{0,252 - 0,26544}{0,252} \times 100 \% = - 5,15 \%$$

Note: The critical properties used in this example for CO<sub>2</sub> are slightly different from those used for the computer calculation.

## DESCRIPTION OF PROGRAM

The fugacity coefficient calculation of this problem was programmed for solution on an IBM 7094 computer in "FORTRAN" II machine language. The pertinent sections of the tables given in Hougen et al, <sup>(14)</sup> for real gas enthalpy departure terms, fugacity coefficients, and compressibilities, were punched on IBM cards and submitted to the computer along with the other input information. The table range used for reduced temperatures was 0.80 to 3.00, and for reduced pressure, 0.20 to 10.0.

For each binary system, the critical temperature, pressure, and compressibility were given for each component. Data for the critical properties were obtained from API Project 44 <sup>(1)</sup> for the hydrocarbons and miscellaneous sources for carbon dioxide. Table 2 lists these values.

The input information for each point was also punched on cards, 2 points per card. For each point, the following information was supplied:

1. system temperature
2. system pressure
3. mole fraction of component 1
4. experimental fugacity coefficient for component 1
5. experimental fugacity coefficient for component 2

The total information supplied was therefore composed of sections

of the generalized tables, the pure component critical properties, and the temperature, pressure and composition for each point.

The program calculated 318 points one at a time in numerical order. The points were in six groups in the following sequence:

1. methane - carbon dioxide	34 points.
2. methane - ethane	69 points
3. butane - carbon dioxide	41 points
4. methane - pentane	40 points
5. methane - butane	34 points
6. methane - butane	100 points

Groups three through five were saturated systems, while groups one, two, and six were in the superheated region.

The program consists of four sections. The main program and three subroutines. Subroutine Table gives instructions for the table search and interpolation, while OUTPT 1 and OUTPT 2 describe the format and contents of tables 1 and 2 in the appendix.

The Hougen et al tables are calculated for a critical compressibility of  $Z_c = 0.27$ . For other values of  $Z_c$ , a correction factor is given. The correction  $D_A$  or  $D_B$  is used depending on whether  $Z_c$  for the point is greater or less than 0.27, respectively. For reduced pressures greater than 1.2, the correction given at  $P_R = 1.2$  was used. When the reduced temperature was between the saturation temperature and the first entry in the table, the correction for the first value

was used. Linear interpolation was used between the various table entries. Because the saturation temperature increases with increase in the reduced pressure, the first reduced temperature in each column was not generally the same between  $P_R = 0.2$  and 1.0. In order to interpolate between any two adjacent columns at or near the saturation temperature, it was necessary to linearly extrapolate the first reduced temperature in one of the columns. The extrapolated point was in the hypothetical vapor region. By this device, the first reduced temperature in any two adjacent columns used for interpolation, was the same. At reduced pressures greater than 1.0, the saturated region disappears and no extrapolation is required.

A test is made in the program to insure that the reduced properties of a point fall within the range of the table sections used. All the points selected did.

The actual calculation procedure is exactly analogous to the hand calculation given previously.

The running time for the "debugged" program depends on the number of points processed, and was 2.3 minutes for the 318 points used. An estimate of the time required for a hand calculation of one point is about 4-5 hours.

Component 1 in Tables 1 and 2 of the Appendix is the first species in the system name except for the two  $\text{CO}_2$  systems. In those mixtures  $\text{CO}_2$  is component 2.

## DISCUSSION

### General

The work of Mazzei used all the available data for the six binary systems. (25) The present work selected approximately one third of the data for use in comparing the two methods. The selection of points was by necessity a somewhat arbitrary procedure. An attempt was made to select those points in areas of composition or P-V-T conditions that might be expected to give the greatest deviations from ideal solution behavior. The primary guide used was the percentage deviation from experimental data found by use of the Pitzer method.

Binary systems were used in the evaluation of this method because data was more readily available than for multicomponent mixtures.

All the experimental values which are used in this work were determined by calculation from P-V-T data for the mixtures. Most of the data was obtained by use of the Partial Residual Molar Volume method discussed previously. For the system methane-carbon dioxide, the experimental data was determined by the method of H. C. Van Ness, (34) using the Redlich and Kwong equation of state. The sources of the experimental values are given as follows:

<u>System</u>	<u>Reference</u>
methane-CO <sub>2</sub>	3, 32
methane-ethane	17
n-butane-CO <sub>2</sub>	20

Methane-n-pentane	21
methane-n-butane (saturated)	19
methane-n-butane (superheated)	18

This method, as mentioned previously, is based on the use of generalized thermodynamic tables for  $(H^*-H)/Tc'$ ,  $(f/p)$ , and  $Z$ . In this work, the tables given in Hougen, Watson, and Ragatz, were employed. <sup>(14)</sup> The correction terms for  $Z_c$  values other than 0.27 were not supplied for every area of the tables and certain simplifications were required. Above a  $P_R = 1.2$ , the corrections at 1.2 were used. It should be noted that in the area bounded by reduced temperatures between 0.8 and 1.2, and reduced pressures greater than 1.2, the correction is not reliable. <sup>(12)</sup> The question of whether the correction terms are significant, or can be neglected, depends to a great extent on what area of reduced conditions is under consideration.

The correction terms tend to become insignificant as the reduced temperature is increased and approach zero at a  $T_R$  near 2.0. The corrections also become negligible as the reduced pressure approaches zero.

There would be some improvement in the use of this method, if smooth equations were used for estimating the functions, instead of tables. Also, an elaboration of the region beyond  $P_R = 1.2$  for compounds with a  $Z_c \neq 0.27$  would be desirable. Hirshfelder, Buehler, McGee, and Sutton have developed a generalized, reduced equation of state which incorporates the  $Z_c$  parameter. <sup>(10)</sup>

### Statistical Definitions

The program calculated the percent deviation of both components at each point from the experimental values. The percent deviation is defined as follows for either component:

$$\% \text{ DEV} = \left( \frac{\phi_{\text{exp}} - \phi_{\text{calc.}}}{\phi_{\text{exp.}}} \right) \times 100\% \quad (48)$$

For each system the average deviation for each component was calculated from the absolute values of the % DEV terms as:

$$\text{a.d.} = \frac{\sum |\% \text{ DEV.}|}{\text{No. points}} \quad (49)$$

An additional short computer program was developed to calculate a modified standard deviation defined by:

$$\% \text{ s.d.} = \left( \frac{\sum (\% \text{ DEV})^2}{\text{No. points}} \right)^{\frac{1}{2}} = \frac{1}{\sum \phi_{\text{exp}}} \left( \frac{\sum (\phi_{\text{exp}} - \phi_{\text{calc.}})^2}{\text{No. points}} \right)^{\frac{1}{2}} \quad (50)$$

This differs from the usual statistical definition of standard deviation which is given by:

$$\text{s.d.} = \left( \frac{\sum (\phi_{\text{exp}} - \phi_{\text{calc.}})^2}{\text{No. points}} \right)^{\frac{1}{2}} \quad (51)$$

The advantage of the % s.d. is that it gives an indication of the relative rather than absolute value. The standard deviation is an indication of the spread of the data from the mean. When viewed in conjunction with the bias and the average deviation, an indication of the type of correlation can be obtained. A large s.d. indicates a wide spread of values from the mean. For a normal or bell type



distribution curve the standard deviation has a special meaning. In this case it can be shown that 68% of the points will fall within the area bounded by  $\pm 1.0$  s.d. from the mean, and 95% will be within  $\pm 2.0$  s.d.

The third quantity calculated was the bias. The bias is defined as:

$$\% \text{ bias} = \frac{\sum (\% \text{ DEV})}{\text{No. points}} \quad (52)$$

where the summation is with regard to the sign of the individual % DEV terms. Using the previous definition of the % DEV, a positive value for the bias indicates that the calculated values are generally lower than the experimental values and vice versa. This gives an indication of whether the method of calculation is systematically biased in one direction or another from the experimental values. The bias is equivalent to the algebraic mean in this work.

### Specific Results

The calculated bias, average and standard deviations for all six systems are tabulated in Table 1. In those systems where the components have a large relative difference in molecular size, the larger component shows the widest deviation from the experimental fugacity coefficient. Small molecules which may be considered to approximate a spherical shape, gave fairly good agreement in all the systems. The one non-hydrocarbon molecule used, CO<sub>2</sub>, gave good agreement in the two systems studied. The results for CO<sub>2</sub> were

generally equal to or slightly better than the methane results. The components in all paraffin systems had a negative bias, although methane or butane when in mixtures with CO<sub>2</sub>, displayed a positive bias. Therefore, calculated fugacity coefficients in all paraffin systems are generally higher than the experimental values.

If equation (47) is examined, it can be seen that for very low values of the correction term  $\Psi_{1, \text{exp}}$   $\Psi_1$  approaches 1.0 and:

$$\begin{aligned}
 (f/py)_1 &= (f/p)_M \\
 \text{or } f_1 &= yf_M
 \end{aligned}
 \tag{53}$$

The fugacity in solution becomes equal to its mole fraction times the fugacity of the mixture. This is analogous to the Lewis and Randall rule, with the mixture fugacity replacing the pure component fugacity. For example, for point number 973,  $\psi$  for methane is 0.020,  $\Psi_{\text{exp}}$  is about 1.02, and equation (53) above is a good approximation.

It is possible that better results may be obtained, if a reference substance is used to determine the compressibility, fugacity coefficient, and enthalpy departure term, instead of generalized charts. For mixtures of hydrocarbons and non-hydrocarbons, or adjacent members of a homologous series, it would be difficult to select such a reference compound. Though no attempt has been made in this work to test this variation of the method, it might be used, for example, in the methane-butane or methane-pentane system. A normal paraffin with a length/width ratio close to the molal average

of the mixture would be selected as the reference substance.

System methane - CO<sub>2</sub> (superheated). This mixture appears to give moderately good results for both components. The correlation seems to represent this system well, as the percentage deviation terms seem symmetrically scattered. If it is assumed that this system gives a normal type distribution curve then 95% of the calculated fugacity coefficients will fall within  $\pm 18.42\%$  and  $\pm 12.70\%$  of the experimental values for methane and carbon dioxide respectively. The largest deviations are obtained at high pressure for the component present in relatively low concentration; i.e., mole fraction less than about 0.2.

System methane-ethane (superheated). For both components, the bias is approximately equal to the average deviation. Since the bias is negative, the correlation gives values, for fugacity coefficients which are generally higher than the experimental data. The distribution of deviations about zero % Dev, is nonsymmetrical. For methane appreciable deviations are found even in a range of mole fraction of 0.3 - 0.7, whereas for ethane the larger deviations occurred when the mole fraction was relatively low. The average deviation for methane and ethane respectively were 8.50% and 12.9%. In this mixture, methane behaves more ideally than ethane.

System n-butane - CO<sub>2</sub> (saturated). As in the methane - CO<sub>2</sub> system, CO<sub>2</sub> gives good results, approximating an even distribution, about 0% DEV. 95% of the calculated CO<sub>2</sub> fugacities will fall within

$\pm$  13.38% of the experimental value. For n-butane the results are poorer. The bias is positive and approximately equal to the % a.d. The correlation therefore gives results which are generally lower than the experimental values, and is not symmetrical with respect to the origin, or 0% DEV. The average deviation for n-butane is 20.8%. The larger of the % DEV terms for CO<sub>2</sub> were scattered through a range of mole fractions, temperatures, and pressures, and therefore no conclusions can be drawn. For n-butane, very few points were available at mole fractions above 0.5, and it is difficult to generalize on the effect of concentration. At below about thirty atmospheres, the deviations are greatly reduced. Increasing temperature negates to some extent the effect of the higher pressures.

System methane-n-pentane (saturated). The results for methane are in fair agreement with the experimental values. The bias is negative and again almost equal to the average deviation, so that the distribution of deviations favors the negative side. The calculated fugacity coefficients are generally slightly higher than the experimental values. The a.d. for methane is 4.43% for this system. Based on limited data, it appears that the composition range of 0 to 0.35 mole fraction methane, is where the greatest deviations occur.

For n-pentane, the bias and average deviation were exactly the same, - 22.4%. All the % DEV terms were negative. The results are then strongly biased, the calculated fugacity coefficients being consistently higher than the experimental values. High deviations

are evident through most of the composition range although not too many points were available in the range of n-butane mole fraction of 0.5 - 1.0.

System methane-n-butane (saturated). As in the methane-n-pentane system, the bias and a.d. for methane are very close. The bias is negative and the a.d. for methane is 5.46%. The calculated values are therefore generally a little higher than the experimental data. Most of the high % deviations occur at low mole fractions of methane.

For n-butane, the correlation is poor, the results are worse than for the n-butane - CO<sub>2</sub> saturated system. As with n-pentane previously, the bias and the a.d. are exactly equal, and all the % DEV terms are consistently negative. The calculated values are therefore always higher than the experimental ones. Most of the points were in the range of 0.6 to 0.92 n-butane mole fraction. The substantial % DEV terms were distributed fairly evenly over this range.

System methane-n-butane (superheated). This system had more data points available than any of the others and should give a good check on the method of calculation for this mixture. A range of  $T_R$  of 1.00 - 2.00 and for  $P_R$  0.6 - 4.5 was covered. Unfortunately, the range of composition covered was limited to methane mole fractions of 0.6 to 1.0.

The results for methane are fairly good, producing better agreement with experimental data than for methane in any of the other

binary systems. The correlation is slightly biased from the origin. The a.d. is approximately equal to the bias, and calculated fugacities will tend to run slightly higher than experimental ones.

For n-butane, the results were the poorest of the three systems including it. The a.d. and the bias were exactly equal at -62.3%. All the deviation terms were negative, indicating calculated values always higher than experimental ones. The large deviations calculated appear well distributed over the composition range studied. Because the methane-n-butane saturated system had 1/3 as many points as the superheated system, it may be that the indicated difference in accuracy is not correct.

#### Comparison with other Methods

A point worth noting when comparing two different methods for the same mixture is that the results may have limited significance if they are not based on the same data points. Similarly it is difficult to directly compare the performance of a component in two different mixtures. Most methods show varying agreement with experimental data in different areas of temperature, pressure and composition. A reported value for the accuracy of a mixture is therefore dependent on the P-V-T region in which the system is situated.

Mazzel has compared the Pitzer method with the methods of Redlich et al, and Edmister and Ruby, for the methane-ethane and methane-butane systems. For the superheated region of these two systems, the method of Pitzer was found to be as good as the others.

It appeared to be better than the method of Edmister and Ruby for the saturated methane-n-butane system. (25) The calculated fugacity coefficients for this method are compared with those of Pitzer, for the same points, in Table 1. It can be seen that the results are generally poorer than for the Pitzer method. The only instance where better performance was obtained is for methane in the methane-n-butane saturated mixture. This method gave a 5.46% a.d., while the Pitzer method gave 8.98% for the same points. By inference, this method should give poorer results than the Redlich et al and Edmister and Ruby methods for the systems compared by Mazzei. This work gives slightly better results for the saturated methane-n-butane system than for the superheated, but this may only be a question of point selection. Interestingly, of the two saturated hydrocarbon systems, the n-pentane gives better agreement than the n-butane. Again, this is based on limited data, and the selection of points that are comparative is very difficult, if not impossible, over a range of temperature, pressure and composition.

## CONCLUSIONS

The method under investigation has been shown to give satisfactory results for binary systems of small molecules, i.e., CO<sub>2</sub> - methane, methane-ethane. For systems with a large relative molecular size difference, the larger molecule exhibits an appreciable deviation between the calculated and experimental fugacity coefficient. For these systems, the method predicts usable fugacity coefficients for the smaller molecule. The predicted coefficients for the larger molecule are of very limited utility. An example of this type of behavior is the methane-n-butane system. For binary systems with two paraffinic components, this correlation will give fugacity coefficients that are consistently higher than experimental values for both components. The one non-hydrocarbon studied gave predicted fugacity coefficients in good agreement with those calculated from experimental data.

This method has been shown to be poorer than the Pitzer method in most instances. The only exception was for methane in the saturated methane-n-butane system. The Pitzer method depends on data for equimolar mixtures, while the method tested in this work requires no experimental data on mixtures. For the methane-ethane and methane-n-butane mixtures, the methods of Edmister and Ruby, and Redlich et al, give more accurate results. For these systems, the Pitzer method has been shown to give equivalent results.



## RECOMMENDATIONS

Further work could be done in several areas. It would be of interest to evaluate binary systems containing non-hydrocarbon compounds other than carbon dioxide, and systems of two non-hydrocarbons. If data is available on multi-component mixtures, then this would certainly be amenable to evaluation.

This method should be studied to determine a modification or variation that would enable it to successfully handle mixtures containing molecules with a large size difference. The concept of a reference substance may be useful in this type of mixture, but it would have to be tested.

TABLE 1

COMPARISON OF RESULTS WITH EXPERIMENTAL DATA AND FITZER'S METHOD

<u>SYSTEM</u>	<u>NO. PTS.</u>	<u>THIS WORK</u>						<u>FITZER'S METHOD</u>	
		<u>COMPONENT 1</u>			<u>COMPONENT 2</u>			<u>COMP. 1</u>	<u>COMP. 2</u>
		a.d.%	s.d.%	bias%	a.d.%	s.d.%	bias%	a.d.%	a.d.%
CH <sub>4</sub> -CO <sub>2</sub>	34	5.67	9.21	+2.86	4.50	6.35	-1.20	4.49	3.94
CH <sub>4</sub> -C <sub>2</sub> H <sub>6</sub>	69	8.50	9.17	-8.49	12.9	17.3	-12.7	4.22	6.86
C <sub>4</sub> H <sub>10</sub> -CO <sub>2</sub>	41	20.8	33.2	+19.3	5.01	6.69	-1.37	5.15	2.46
CH <sub>4</sub> -n-C <sub>5</sub> H <sub>12</sub>	40	4.43	8.53	-4.12	22.4	26.1	-22.4	3.24	6.40
CH <sub>4</sub> -n-C <sub>4</sub> H <sub>10</sub> (saturated)	33	5.46	7.94	-5.41	53.6	60.2	-53.6	8.98	31.7
CH <sub>4</sub> -n-C <sub>4</sub> H <sub>10</sub> (superheated)	100	3.68	4.47	-3.45	62.3	67.8	-62.3	2.21	37.3

Notes: a) Component 1 is the first species listed in each system's title.

b) Average Deviation for Pitzer's Method is based on the same points.

TABLE 2PURE COMPONENT CRITICAL PROPERTIES

	Temperature, °K	Pressure, atm.	Compressibility
Methane	191.06	45.80	0.289
Ethane	305.56	48.30	0.285
n-Butane	425.17	37.47	0.274
n-Pentane	469.78	33.31	0.269
Carbon dioxide	304.12	72.93	0.275

NOMENCLATURE

a	Activity.
a,b	Constants in equations of state.
a <sub>1,2</sub>	$\left[ \frac{Z_c T_c^{\alpha+1}}{P_c} \right]_{1,2}^{\frac{1}{2}}$
b <sub>1,2</sub>	$\frac{1}{2} \left[ \frac{Z_c T_c}{P_c} \right]_{1,2}^{1/3}$
e	Base of Naparian logarithms.
K	Ideal equilibrium constant, $\bar{v}_y/x$
f	Fugacity.
(f/p), (f/py)	Fugacity coefficient, pure component, component in solution.
G	Free energy.
(H*-H) / Tc'	Real gas enthalpy departure term.
N	Mole fraction any phase.
n	Number moles.
p <sup>o</sup>	Vapor pressure.
P	Total pressure.
P	Partial pressure.
R	Universal gas constant.
T	Temperature.
V	Volume.
w	Acentric factor.
x	Mole fraction liquid phase.
x <sup>(o)</sup> , x <sup>(1)</sup>	Pitzer table values for H, $\bar{v}$ or Z function.
y	Mole fraction vapor phase.
Z	Compressibility factor.

$\alpha$	Residual molar volume.
$\alpha$	$1.0 + e \left[ -10 \left( \frac{P}{\sum x_i P_{ci}} - 1.0 \right)^2 \right]$ ; empirical factor.
$\theta$	Intermediate temperature-composition scale.
$\gamma$	Activity coefficient.
$\mu$	Chemical potential.
$\Sigma$	Summation.
$\sigma_0$	Hypothetical surface tension at 0° K.
$\phi$	Fugacity coefficient.
$\psi$	Correction term in Leland, et al, equation for ideal K or $\phi$ .

SUPERSCRIPTS

-	Partial molar property.
o	Standard state.
*	Ideal gas state.
'	Pseudo state.
c	Number of components in mixture.

SUBSCRIPTS

c	Critical property.
i, j, n	Components in a mixture.
M	Mixture.
Mix	Equimolar mixture.
n	Number of moles.
R	Reduced property.
calc.	Calculated.
exp.	Experimental.

REFERENCES

1. Amer. Pat. Inst., "Research Project No. 44", Carnegie Inst. of Tech., 1958.
2. Benedict, M., G. B. Webb, L. C. Rubin, and L. Friend, Chem. Eng. Progr., Vol. 47, 1951, pp. 419, 449, 571, 609.
3. Capik, R. J., "Fugacity and Activity Coefficients", Thesis, Newark Coll. of Eng., Newark, New Jersey, 1959.
4. De Priester, C. L., Chem. Eng. Progr. Symposium Series, Vol. 49, No. 7, 1953, p. 1.
5. Edmister, W. C. and C. L. Ruby, Chem. Eng. Progr., Vol. 51, No. 2, 1955, p. 97-F.
6. Gamson, B. W., Ind. Eng. Chem., Vol. 40, 1948, p. 2439.
7. Gamson, B. W., T. W. Leland, Jr., and P. S. Chappellear, A. I. Ch. E. Journal, Vol. 8, No. 4, Sept. 1962, p. 482.
8. Gamson, B. W., and K. M. Watson, Natl. Pat. News, Vol. 36 1944, p. R-623.
9. Hildebrand, J. H., "Solubility", First Edition, New York: The Chemical Catalog Co., 1924, pp. 90-95.
10. Hirschfelder, J. O., R. J. Buehler, H. A. McGee, Jr., and J. R. Sutton, Ind. Eng. Chem., Vol. 50, 1958, p. 375.
11. Hougen, Olaf A., Kenneth M. Watson, and Roland A. Ragatz, Chemical Process Principles - Part II Thermodynamics, Second Edition. New York: John Wiley and Sons, Inc., 1959, p. 548.
12. Ibid, p. 576.
13. Ibid, p. 572.
14. Ibid, pp. 588-604.
15. Joffe, J., Ind. Eng. Chem., Vol. 39, 1947, p. 837.
16. Joffe, J., Ind. Eng. Chem., Vol. 40, 1948, p. 1738.
17. Lacey, W. N. and B. H. Sage, Ind. Eng. Chem., Vol. 31, No. 12, December, 1939, p. 1497.
18. Lacey, W. N., B. H. Sage, and R. A. Budenholzer, Ind. Eng. Chem., Vol. 32, 1940, p. 1262.

19. Lacey, W. N., B. H. Sage, and B. L. Hicks, Ind. Eng. Chem., Vol. 32, 1940, p. 1085.
20. Lacey, W. N., B. H. Sage, H. H. Reamer, and R. H. Olds, Ind. Eng. Chem., Vol. 41, 1949, p. 475.
21. Lacey, W. N., B. H. Sage, H. H. Reamer, R. H. Olds, Ind. Eng. Chem., Vol. 34, 1942, p. 1108.
22. Leland, T. W., Jr., and W. H. Mueller, Ind. Eng. Chem., Vol. 51, 1959, p. 597.
23. Lewis, G. N., and M. Randall, "Thermodynamics and the Free Energy of Chemical Substances." New York: Mc Graw Hill, 1923.
24. Lyderson, A. L., R. A. Greenkorn, and O. A. Hougen, "Generalized Thermodynamic Properties of Pure Fluids," Univ. Wisconsin Eng. Exp. Station Report No. 4, Oct. 1955.
25. Mazzei, Louis D., Jr., "Fugacity Coefficients of Gases," Thesis, Newark College of Engineering, Newark, New Jersey, 1961.
26. Pitzer, K. S. and R. F. Curl, Jr., Ind. Eng. Chem., Vol. 50, No. 2, February, 1958, p. 265.
27. Pitzer, K. S. and G. O. Hultgren, J. Am. Chem. Soc., Vol. 80, 1958, p. 4793.
28. Pitzer, K. S., D. Z. Lippman, R. F. Curl, Jr., C. M. Huggins, and D. E. Petersen, J. Am. Chem. Soc., Vol. 77, 1955, p. 3433.
29. Redlich, O., A. T. Kister and C. E. Turnquist, Chem. Eng. Progr. Symposium Series, Vol. 48, No. 2, 1952, p. 42.
30. Reid, R. C. and T. K. Sherwood, "Properties of Liquids and Gases", First Edition. New York: McGraw Hill, 1958, p. 306.
31. Ibid, pp. 313, 319.
32. Sievering, P. J., "Fugacity and Activity Coefficients", Thesis, Newark College of Engineering, Newark, New Jersey, 1958.
33. Van Der Waals, J., Dissertation, Leiden, 1873.
34. Van Ness, H. C., A. I. Ch. E. Journal, Vol. 1, 1955, p. 100

**APPENDIX**



```

C   DIMENSION F TABLE ENTRIES
DIMENSION FTR(31,20),FDA(31,20),H(31,20),HCB(31,20),FHS(20),FS(20)
1,PSI(2),FC(2)
C   Z TABLE ENTRIES
DIMENSION ZTR(31,20),ZCA(31,20),Z(31,20),ZCB(31,20),ZTS(20),ZS(20)
C   F TABLE ENTRIES
DIMENSION FTR(31,20),FDA(31,20),F(31,20),FCB(31,20),FHS(20),FS(20)
COMMON FTR,FDA,F,FCB,HTS,HS,ZTR,ZCA,Z,ZCB,ZTS,ZS,FTR,FDA,F,FCB,FHS
1,FS
C   DIMENSION TAB(31)
TABLE OF VALUES FOR Z, H, AND F TABLE ASSIGNMENTS
TAB( 1)=-.8C
TAB( 2)=-.9C
TAB( 3)=-.92
TAB( 4)=-.94
TAB( 5)=-.96
TAB( 6)=-.98
TAB( 7)=1.0C
TAB( 8)=1.01
TAB( 9)=1.02
TAB(10)=1.03
TAB(11)=1.04
TAB(12)=1.05
TAB(13)=1.06
TAB(14)=1.07
TAB(15)=1.08
TAB(16)=1.09
TAB(17)=1.1C
TAB(18)=1.12
TAB(19)=1.14
TAB(20)=1.16
TAB(21)=1.18
TAB(22)=1.2C
TAB(23)=1.30
TAB(24)=1.4C
TAB(25)=1.5C
TAB(26)=1.6C
TAB(27)=1.7C
TAB(28)=1.8C
TAB(29)=1.9C
TAB(30)=2.0C
TAB(31)=2.0C
C   READ TABLES INTO CORE
ICT=C
K=C
C   READ F TABLE
4 READ 1,PR,TR,CP,T,DA,TS,T1
1 F2RMAT(F5.C,F5.C,3F6.0,F5.C,F6.C)
C   ASSIGN TO PROPER PLACE IN TABLE FIRST PRINT AND SATURATION VALUE
D2 21 I=1,31
IF(TR-TAB(I))21,24,21
21 CONTINUE
24 K=K+1
FTR(I,K)=TR
FDA(I,K)=DA
F(I,K)=T
FCB(I,K)=CP
FHS(K)=TS
FS(K)=T1
D2 2 I=2,3C,2
READ 3,TR,CP,F,CA,TR1,CP1,I1,CA1
3 F2RMAT(5X,F5.C,F6.C,F6.C,F6.C,F6.C,F5.C,3F6.C)
C   ASSIGN TO PROPER PLACE IN TABLE ALL REMAINING VALUES
D2 25 L=1,31

```

```

IF (TR-TAB(L))25,26,25
25 CONTINUE
G2 T2 2
26 FTR(L,K)=TR
FCA(L,K)=CA
F(L,K)=T
FCB(L,K)=CB
FTR(L+1,K)=TR1
FCA(L+1,K)=CA1
F(L+1,K)=T1
2 FCB(L+1,K)=CB1
IF(K-20)4,5,5
5 K=C
C READ Z TABLE
7 READ 1,PR,TR,CR,T,DA,TS,T1
C ASSIGN TO PROPER PLACE IN TABLE FIRST POINT AND SATURATION VALUE
D2 27 I=1,31
IF (TR-TAB(I))27,28,27
27 CONTINUE
28 K=K+1
ZTR(I,K)=TR
ZCA(I,K)=CA
ZCB(I,K)=CB
Z(I,K)=T
ZTS(K)=TS
ZS(K)=T1
D2 6 I=2,3C,2
READ 3,TR,CR,T,DA,TR1,CB1,T1,CA1
C ASSIGN TO PROPER PLACE IN TABLE ALL REMAINING VALUES
D2 29 L=1,31
IF (TR-TAB(L))29,30,29
29 CONTINUE
G2 T2 6
30 ZTR(L,K)=TR
ZCA(L,K)=CA
Z(L,K)=T
ZCB(L,K)=CB
ZTR(L+1,K)=TR1
ZCA(L+1,K)=CA1
Z(L+1,K)=T1
6 ZCB(L+1,K)=CB1
IF(K-20)7,8,8
8 K=C
C READ F TABLE
10 READ 1,PR,TR,CR,T,DA,TS,T1
C ASSIGN TO PROPER PLACE IN TABLE FIRST POINT AND SATURATION VALUE
D2 31 I=1,31
IF (TR-TAB(I))31,32,31
31 CONTINUE
32 K=K+1
FTR(I,K)=TR
FCA(I,K)=CA
F(I,K)=T
FCB(I,K)=CB
FIS(K)=TS
FS(K)=T1
D2 9 I=2,3C,2
READ 3,TR,CR,T,DA,TR1,CB1,T1,CA1
C ASSIGN TO PROPER PLACE IN TABLE ALL REMAINING VALUES
D2 33 L=1,31
IF (TR-TAB(L))33,34,33
33 CONTINUE
G2 T2 9
34 FTR(L,K)=TR
FCA(L,K)=CA
F(L,K)=T

```

```

FCB(L,K)=CB
FTR(L+1,K)=TR1
FCA(L+1,K)=CA1
FCB(L+1,K)=CB1
9 F(L+1,K)=I1
  IF(K-ZO)IC,11,11
C  EXTRAPOLATE INTO HYPOTHETICAL REGION IF LOWEST VALUE IN TABLE I IS
C  HIGHER THAN LOWEST VALUE IN PRECEDING TABLE I-1
11 ICT=ICT+1
  GO 4C N=3,8
  I=11-N
  GO 41 M=1,7
  K=B-M
  IF(FTR(K,I)-FTR(K,I+1))41,41,42
41 CONTINUE
  GO TO 4C
42 J=I+1
  L=K+1
  IF(J-5)43,44,44
44 BLINE=(F(L,J)-F(L+1,J))/(FTR(L,J)-FTR(L+1,J))
  ALINE=(F(L,J)-PLINE*HTR(L,J))
  BZLINE=(Z(L,J)-Z(L+1,J))/(ZTR(L,J)-ZTR(L+1,J))
  AZLINE=Z(L,J)-BZLINE*ZTR(L,J)
  BFLINE=(F(L,J)-F(L+1,J))/(FTR(L,J)-FTR(L+1,J))
  AFLINE=F(L,J)-BFLINE*FTR(L,J)
  GO TO 45
43 BLINE=(FS(J)+F(L,J))/(FTS(J)-HTR(L,J))
  ALINE=FS(J)-BLINE*HTR(L,J)
  BZLINE=(ZS(J)-Z(L,J))/(ZTS(J)-ZTR(L,J))
  AZLINE=ZS(J)-BZLINE*ZTS(J)
  BFLINE=(FS(J)-F(L,J))/(FTS(J)-FTR(L,J))
  AFLINE=FS(J)-BFLINE*FTR(L,J)
45 F(K,J)=ALINE+BLINE*HTR(K,I)
  Z(K,J)=AZLINE+BZLINE*ZTR(K,I)
  F(K,J)=AFLINE+BFLINE*FTR(K,I)
  HTR(K,J)=HTR(K,I)
  ZTR(K,J)=ZTR(K,I)
  FTR(K,J)=FTR(K,I)
C  USE SAME CA-CB FOR EXTRAPOLATED POINT AS UPPERMOST POINT IN TABLE
  FCA(K,J)=FCA(L,J)
  FCB(K,J)=FCB(L,J)
  ZCA(K,J)=ZCA(L,J)
  ZCB(K,J)=ZCB(L,J)
  FCA(K,J)=FCA(L,J)
  FCB(K,J)=FCB(L,J)
40 CONTINUE
  GO TO(11,46),ICT
C  START CALC. OF MIXTURE FUGACITIES
C  READ CRITICAL PROPERTIES
46 READ 12,TC1,TC2,PC1,PC2,ZC1,ZC2
12 FORMAT(6F7.0)
  CASE=CASE+1.
  I2=1
C  IS LAST CASE, YES- END OF JOB, NO- READ DATA POINT
  IF(1CT1-9999.)13,2C,2C
C  READ DATA POINT
13 READ 15,PIN,T,P,X1,FE1,FE2
15 FORMAT(F6.C,F8.0,F8.C,F7.C,F7.0)
  I=1
C  IS LAST POINT IN SYSTEM, YES- READ NEXT SYSTEM, NO- CALCULATE
  IF(1)46,46,14
14 ALPHA=1.C+EXP(-1C.*(P/(X1*PC1+(1.-X1)*PC2)-1.))**2)
  A1=SCRIF (((ZC1*(TC1)**(ALPHA+1.)))/PC1)
  A2=SCRIF (((ZC2*(TC2)**(ALPHA+1.)))/PC2)
  B1=.5*((ZC1*TC1)/PC1)**.33333333
  B2=.5*((ZC2*TC2)/PC2)**.33333333

```

```

ZC=X1*ZC1+(1.-X1)*ZC2
CAX=(X1*A1+(1.-X1)*A2)**2
CBX=(X1*X1*((2.*B1)**3)+2.*X1*(1.-X1)*((B1+B2)**3)+((1.-X1)**2)*
1(2.*B2)**3)
TC=(CAX/CBX)**(1./ALPHA)
PC=(TC*ZC)/CBX
DTX=(2./ALPHA)*(((X1*A1+A1+(1.-X1)*A1*A2)/CAX)-((X1*((2.*B1)**3)+
11.-X1)*((B1+B2)**3))/CBX))
CPX=(2./ALPHA)*(((X1*A1+A1+(1.-X1)*A1*A2)/CAX)-((1.+ALPHA)*(X1
1 )*((2.*B1)**3)+(1.-X1)*((B1+B2)**3)))/CBX)+(1.+ZC1/ZC)
TR=T/TC
PR=P/PC
C CALL TABLE L22KUP ROUTINE F2R Z,H,F.
CALL TABLE(PR,TR,Z1,F1,FLAG,ZC)
C IF OUT OF RANGE OF TABLE, SKIP TO NEXT DATA POINT
IF(FLAG-1.C)18,13,13
18 PSI(I)=-((1./((1.987*T)))*(H1*TC*DTX)+(1.-Z1)*CPX
FC(I)=F1*EXP(PSI(I))
GO TO(16,17),I
16 I=2
DTX=(2./ALPHA)*(((1.-X1)*A2*A2+X1*A1*A2)/CAX)-(((1.-X1)*((2.*B
12)**3)+X1*((B1+B2)**3))/CBX))
CPX=(2./ALPHA)*(((1.-X1)*A2*A2+(X1)*A1*A2)/CAX)-((1.+ALPHA)*((1.-
1X1)*((2.*B2)**3)+(X1)*((B1+B2)**3)))/CBX)+(1.+ZC2/ZC)
GO TO 18
17 DEV1=((FE1-FC(1))/FE1)*100.
DEV2=((FE2-FC(2))/FE2)*100.
C PRINT RESULTS
CALL PUTPT1 (PTN,T,P,X1,FC,FE1,FE2,DEV1,DEV2,CASE,I2)
CALL PUTPT2 (PTN,TC,PC,X1,TR,PR,Z1,F1,H1,PSI)
I2=C
C GET NEXT POINT
GO TO 13
20 CALL SYSTEM
STOP
END

```

```

SUBROUTINE TABLE(PR,TR,Z1,HI,F1,FLAG,ZC)
DIMENSION TAB(20)
DIMENSION HTR(31,20),HDA(31,20),H(31,20),HDB(31,20),HTS(20),HS(20)
DIMENSION ZTR(31,20),ZDA(31,20),Z(31,20),ZDB(31,20),ZTS(20),ZS(20)
DIMENSION FTR(31,20),FDA(31,20),F(31,20),FDB(31,20),FTS(20),FS(20)
COMMON HTR,HDA,H,HDB,HTS,HS,ZTR,ZDA,Z,ZDB,ZTS,ZS,FTR,FDA,F,FDB,FTS
1,FS
C   TABLE OF PR VALUES
TAB(1)=-.20
TAB(2)=-.30
TAB(3)=-.40
TAB(4)=-.50
TAB(5)=-.60
TAB(6)=-.70
TAB(7)=-.80
TAB(8)=-.90
TAB(9)=1.00
TAB(10)=1.05
TAB(11)=1.10
TAB(12)=1.20
TAB(13)=1.40
TAB(14)=1.60
TAB(15)=1.80
TAB(16)=2.0
TAB(17)=4.0
TAB(18)=6.0
TAB(19)=8.0
TAB(20)=10.0
FLAG=0.0
K=0
C   CHECK PR
IF(PR-TAB(1))1,2,2
2 IF(TAB(20)-PR)1,3,3
C   OUT OF RANGE OF TABLE
1 Z1=0.0
H1=0.0
F1=0.0
FLAG=1.0
GO TO 226
C   GET POINT IN TABLE
3 DO 4 I=1,20
IF(PR-TAB(I))5,6,4
4 CONTINUE
C   DIRECT HIT IF 6
C   INTERPOLATE IF 5
5 J=I-1
K=I
GO TO 7
6 J=I
C   CHECK TO FIND IF DA AND DB FROM TABLE FOUND IS TO BE USED OR IF TO
C   USE LAST DA AND DB OF TABLE PR=1.2
7 IF(I-13)25,9,9
9 ID=12
GO TO 8
25 ID=J
C   IS TR LESS THAN SATURATION PT.
8 IF(TR-HTR(I,J))10,11,11
10 IF(TR-HTS(J))12,13,14
12 FLAG=1.

```

```

G0 T0 226
AT SATURATION POINT
C
13 H1=HS(J)
   IFT(D-12)30,31,31
31 DAH=HDA(1,12)
   DBH=HDB(1,12)
G0 T0 24
30 DAH=HDA(1,J)
   DBH=HDB(1,J)
G0 T0 24
C
   BETWEEN SAT. AND FIRST PT. IN TABLE, INTERPOLATE
C
   TR INTERPOLATION
14 FACT=(HTS(J)-TR)/(HTS(J)-HTR(1,J))
   ANSHO=(H(1,J)-HS(J))*FACT+HS(J)
   IF(K)16,16,15
C
   INTERPOLATE VS PR
15 ANSHO1=(H(1,K)-HS(K))+FACT+HS(K)
   FACT1=(TAB(K)-PR)/(TAB(K)-TAB(J))
   H1=(ANSHO-ANSHO1)*FACT1+ANSHO
   IF(D-12)32,33,33
33 IF(K-13)32,35,35
35 DAH=HDA(1,12)
   DBH=HDB(1,12)
G0 T0 24
32 DAH=(HDA(1,J)-HDA(1,K))*FACT1+HDA(1,K)
   DBH=(HDB(1,J)-HDB(1,K))*FACT1+HDB(1,K)
G0 T0 24
16 H1=ANSHO
   DAH=HDA(1,J)
   DBH=HDB(1,J)
G0 T0 24
C
   POINT IN BODY OF TABLE
11 D0 17 I=1,31
C
   FIND CORRECT PLACEMENT
C
18 INTERPOLATE
C
19 DIRECT HIT
   IF(TR-HTR(1,J))18,19,17
17 CONTINUE
G0 T0 1
18 L=I-1
   N=I
C
   INTERPOLATE VS TR
   FCTR=(HTR(L,J)-TR)/(HTR(L,J)-HTR(N,J))
   ANSH=(H(N,J)-H(L,J))*FCTR+H(L,J)
   IF(K)20,20,21
C
   INTERPOLATE VS PR
21 ANSH1=(H(N,K)-H(L,K))*FCTR+H(L,K)
   PFACT=(TAB(K)-PR)/(TAB(K)-TAB(J))
   H1=(ANSH-ANSH1)*PFACT+ANSH
   IF(D-12)44,43,43
43 IF(K-13)44,45,45
C
   IF PR ABOVE 1.2 USE 1.2 DA AND DB VALUES
45 DAH=(HDA(N,12)-HDA(L,12))*FCTR+HDA(L,12)
   DBH=(HDB(N,12)-HDB(L,12))*FCTR+HDB(L,12)
G0 T0 24
C
   INTERPOLATE DA AND DB
44 DAH=(HDA(N,J)-HDA(L,J))*FCTR+HDA(L,J)
   DBH=(HDB(N,J)-HDB(L,J))*FCTR+HDB(L,J)
   DAH1=(HDA(N,K)-HDA(L,K))*FCTR+HDA(L,K)
   DBH1=(HDB(N,K)-HDB(L,K))*FCTR+HDB(L,K)
   DAH=(DAH-DAH1)*PFACT+DAH

```

```

DBH=(DBH-DBH1)*PFACT+DBH1
G0 T024
20 H1=ANSH
DAH=(HDA(N,J)-HDA(L,J))*FCTR+HDA(L,J)
DBH=(HDB(N,J)-HDB(L,J))*FCTR+HDB(L,J)
G0 T024
19 IF(K)22,22,23
22 H1=H(I,J)
DAH=HDA(I,J)
DBH=HDB(I,J)
G0 T024
C INTERPØLATE VS PR
23 PFACT=(TAB(K)-PR)/(TAB(K)-TAB(J))
H1=(H(I,J)-H(I,K))*PFACT+H(I,K)
DAH=(HDA(I,J)-HDA(I,K))*PFACT+HDA(I,K)
DBH=(HDB(I,J)-HDB(I,K))*PFACT+HDB(I,K)
C GET F VALUES
24 J=J
K=K
DAF=DAF
FACT=FACT
IF(TR-FTR(I,J))110,111,111
110 IF(TR-FTS(J))112,113,114
112 FLAG=1.
G0 T0 226
C AT SATURATION PØINT
113 F1=FS(J)
IF(ID-12)230,231,231
231 DAF=FDA(1,12)
DBF=FDB(1,12)
G0 T0 124
230 DAF=FDA(1,J)
DBF=FDB(1,J)
G0 T0124
C BETWEEN SAT. AND FIRST PT. IN TABLE, INTERPØLATE
C TR INTERPØLATION
114 ANSF0=(F(1,J)-FS(J))*FACT+FS(J)
IF(K)116,116,115
115 ANSF01=(F(1,K)-FS(K))*FACT+FS(K)
C INTERPØLATE VS PR
F1=(ANSF0-ANSF01)*FACT1+ANSF01
IF(ID-12)232,233,233
233 IF(K-13)232,235,235
235 DAF=FDA(1,12)
DBF=FDB(1,12)
G0 T0124
232 DAF=(FDA(1,J)-FDA(1,K))*FACT1+FDA(1,K)
DBF=(FDB(1,J)-FDB(1,K))*FACT1+FDB(1,K)
G0 T0 124
116 F1=ANSF0
DAF=FDA(1,J)
DBF=FDB(1,J)
G0T0124
C PØINT IN BØDY ØF TABLE
111 IF(TR-FTR(I,J))118,119,117
117 CØNTINUE
G0 T0 124
C INTERPØLATE VS TR
118 ANSF=(F(N,J)-F(L,J))*FCTR+F(L,J)
IF(K)120,120,121
121 ANSF1=(F(N,K)-F(L,K))*FCTR+F(L,K)

```

```

C INTERPOLATE VS PR
F1=(ANSF-ANSF1)*PFACT+ANSF1
IF(ID-12)244,243,243
243 IF(K-13)244,245,245
C IF PR ABOVE 1.2 USE 1.2 DA AND DB VALUES
245 DAF=(FDA(N,12)-FDA(L,12))*FCTR+FDA(L,12)
DBF=(FDB(N,12)-FDB(L,12))*FCTR+FDB(L,12)
GO TO 124
C INTERPOLATE DA AND DB
244 DAF=(FDA(N,J)-FDA(L,J))*FCTR+FDA(L,J)
DBF=(FDB(N,J)-FDB(L,J))*FCTR+FDB(L,J)
DAF1=(FDA(N,K)-FDA(L,K))*FCTR+FDA(L,K)
DBF1=(FDB(N,K)-FDB(L,K))*FCTR+FDB(L,K)
DBF=(DBF-DBF1)*PFACT+DBF1
DAF=(DAF-DAF1)*PFACT+DAF1
GO TO 124
120 F1=ANSF
DAF=(FDA(N,J)-FDA(L,J))*FCTR+FDA(L,J)
DBF=(FDB(N,J)-FDB(L,J))*FCTR+FDB(L,J)
GO TO 24
119 IF(K)122,122,123
122 F1=F(I,J)
DAF=FDA(I,J)
DBF=FDB(I,J)
GO TO 124
C INTERPOLATE VS PR
123 F1=(F(I,J)-F(I,K))*PFACT1+F(I,K)
DAF=(FDA(I,J)-FDA(I,K))*PFACT1+FDA(I,K)
DBF=(FDB(I,J)-FDB(I,K))*PFACT1+FDB(I,K)
C GET Z VALUES
124 J=J
K=K
IF(TR-ZTR(I,J))210,211,211
210 IF(TR-ZTS(J))212,213,214
212 FLAG=1.
GO TO 226
C AT SATURATION POINT
213 Z1=ZS(J)
IF(ID-12)130,131,131
131 DAZ=ZDA(1,12)
DBZ=ZDB(1,12)
GO TO 224
130 DAZ=ZDA(1,J)
DBZ=ZDB(1,J)
GO TO 224
C BETWEEN SAT. AND FIRST PT. IN TABLE, INTERPOLATE
C TR INTERPOLATION
214 ANSZ0=(Z(1,J)-ZS(J))*FACT+ZS(J)
IF(K)216,216,215
215 ANSZ01=(Z(1,K)-ZS(K))*FACT+ZS(K)
C INTERPOLATE VS PR
Z1=(ANSZ0-ANSZ01)*FACT1+ANSZ01
IF(ID-12)132,133,133
133 IF(K-13)132,135,135
135 DAZ=ZDA(1,12)
DBZ=ZDB(1,12)
GO TO 224
132 DAZ=(ZDA(1,J)-ZDA(1,K))*FACT1+ZDA(1,K)
DBZ=(ZDB(1,J)-ZDB(1,K))*FACT1+ZDB(1,K)
GO TO 224
216 Z1=ANSZ0

```



```

      DAZ=ZDA(I,J)
      DBZ=ZDB(I,J)
      GO TO 224
211 IF(TR-7TR(I,J))218,219,217
217 CONTINUE
      GO TO 224
C     POINT IN BODY OF TABLE
C     INTERPOLATE VS TR
218 ANSZ=(Z(N,J)-Z(L,J))*FCTR+Z(L,J)
      IF(K)220,220,221
221 ANSZ1=(Z(N,K)-Z(L,K))*FCTR+Z(L,K)
C     INTERPOLATE VS PR
      Z1=(ANSZ-ANSZ1)*PFACT+ANSZ1
      IF(ID-12)144,143,143
143 IF(K-13)144,145,145
C     IF PR ABOVE 1.2 USE 1.2 DA AND DB VALUES
145 DAZ=(ZDA(N,12)-ZDA(L,12))*FCTR+ZDA(L,12)
      DBZ=(ZDB(N,12)-ZDB(L,12))*FCTR+ZDB(L,12)
      GO TO 224
C     INTERPOLATE DA AND DB
144 DAZ=(ZDA(N,J)-ZDA(L,J))*FCTR+ZDA(L,J)
      DBZ=(ZDB(N,J)-ZDB(L,J))*FCTR+ZDB(L,J)
      DAZ1=(ZDA(N,K)-ZDA(L,K))*FCTR+ZDA(L,K)
      DBZ1=(ZDB(N,K)-ZDB(L,K))*FCTR+ZDB(L,K)
      DAZ=(DAZ-DAZ1)*PFACT+DAZ1
      DBZ=(DBZ-DBZ1)*PFACT+DBZ1
      GO TO 224
220 Z1=ANSZ
      DAZ=(ZDA(N,J)-ZDA(L,J))*FCTR+ZDA(L,J)
      DBZ=(ZDB(N,J)-ZDB(L,J))*FCTR+ZDB(L,J)
      GO TO 224
219 IF(K)222,222,223
222 Z1=Z(I,J)
      DAZ=ZDA(I,J)
      DBZ=ZDB(I,J)
      GO TO 224
C     INTERPOLATE VS PR
223 Z1=(Z(I,J)-Z(I,K))*PFACT1+Z(I,K)
      DAZ=(ZDA(I,J)-ZDA(I,K))*PFACT1+ZDA(I,K)
      DBZ=(ZDB(I,J)-ZDB(I,K))*PFACT1+ZDB(I,K)
C     CHECK ZC FOR DA OR DB CORRECTION
224 IF(ZC-.27)227,226,225
226 RETURN
C     USE DA FOR CORRECTION
225 Z1=Z1+DAZ*(ZC-0.27)
      H1=H1+DAH*(ZC-0.27)
      F1=F1*10.**(DAF*(ZC-0.27))
      GO TO 226
C     USE DB FOR CORRECTION
227 Z1=Z1+DBZ*(ZC-0.27)
      H1=H1+DBH*(ZC-0.27)
      F1=F1*10.**(DBF*(ZC-0.27))
      GO TO 226
      END

```

```

SUBROUTINE SUBPT1 (PT1,T,P,X1,FC,FE1,FE2,DEV1,DEV2,CASE,IZ)
DIMENSION FC(2)
NPT=XFIX(PT1)
ICASE = XFIX(CASE)
IF(IZ)17,17,9
9 PRINT 7
7 FORMAT(1H3,33X,9HTABLE ONE,7X,21HFUGACITY COEFFICIENTS)
8 GO TO(1,2,3,4,5,6),ICASE
1 PRINT 10
10 FORMAT(1H0,33X,6HSYSTEM,4X,13HCO2 - METHANE)
GO TO 16
2 PRINT 11
11 FORMAT(1H0,33X,6HSYSTEM,4X,16HMETHANE - ETHANE)
GO TO 16
3 PRINT 12
12 FORMAT(1H0,33X,6HSYSTEM,4X,12HCO2 - BUTANE)
GO TO 16
4 PRINT 13
13 FORMAT(1H0,33X,6HSYSTEM,4X,17HMETHANE - PENTANE)
GO TO 16
5 PRINT 14
14 FORMAT(1H0,33X,6HSYSTEM,4X,28HMETHANE - BUTANE (SATURATED))
GO TO 16
6 PRINT 15
15 FORMAT(1H0,33X,6HSYSTEM,4X,30HMETHANE - BUTANE (SUPERHEATED))
GO TO 16
16 IF(IZ)17,17,18
18 PRINT 19
19 FORMAT(1H0,53X,17HFUGACITY COEFF. 1,11X,17HFUGACITY COEFF. 2/1H ,
110X,7HPT. NO.,4X,7HIENP. K,3X,10HPRESS. ATM,4X,2HX1,6X,22HCALC
2EXP PCI DEV,6X,22HCALC EXP PCI DEV)
LNCT=0
17 IF(LNCT-49)21,21,22
22 LN=1
GO TO 9
21 PRINT 20,NPT,T,P,X1,FC(1),FE1,DEV1,FC(2),FE2,DEV2
20 FORMAT(1H 10X,16,5X,F7.2,4X,F7.3,3X,F6.3,1X,F7.3,3X,F7.3,4
1X,F6.3,1X,F7.3,3X,F7.3)
LNCT=LNCT+1
RETURN
END

```

```
SUBROUTINE OUTPI2 (PTN,TC,PC,X1,TR,PR,Z1,F1,H1,PSI)
DIMENSION PSI(2)
CASE=CASE+1.
NPT=XFIX(PTN)
IF(CASE-1.)1,1,2
1 WRITE OUTPUT TAPE 6,3
3 FORMAT(1H3,33X,9H-TABLE TWO,3X,22HPROPERTIES OF MIXTURES/1H0,10X,2H
1PT. NO.,4X,7HTC, K,3X,10HPC, ATM.,4X,2HX1,7X,2HTR,6X,2HPR,6X,1
2HZ,8X,6H(F/P)N,5X,1HH,7X,5HPSI 1,7X,5HPSI 2//)
LNCT=0
2 WRITE OUTPUT TAPE 6,4,NPT,TC,PC,X1,TR,PR,Z1,F1,H1,PSI(1),PSI(2)
4 FORMAT(1H, 6X,16,3X,F7.2,4X,F7.2,3X,F7.3,3X,F6.3,1X,F7.3,
16X,F6.3,1X,F7.3,5X,F7.3,5X,F7.3)
LNCT=LNCT+1
IF(LNCT-45)6,6,5
5 CASE=C.
6 RETURN
END
```

### Nomenclature for Computer Program

The nomenclature used attempted to conform insofar as possible to common terminology with certain exceptions. Because of the rules and limitations of the FORTRAN language, not all mathematical symbols and terms are directly usable, and must therefore be modified. For example, there are no lower case letters in FORTRAN. In addition, certain terms such as fugacity coefficient were named so as to conform with the work of Mazzei, *op. cit.*, in order to make the comparison with the Pitzer method clearer to the reader. In particular, the table headings in Tables 1 and 2 use the same nomenclature, where applicable, as Mazzei's work.

NOMENCLATURE FOR COMPUTER PROGRAM

ALPHA	$\alpha = 1.0 + \exp \left[ -10 \frac{P}{(x_1 P_{c1} + x_2 P_{c2}) - 1} \right]^2$
A1, A2	$a_{1,2} = \left[ \frac{Z_c T_c}{P_c} \alpha + 1 \right]_{1,2}^{1/2}$
B1, B2	$b_{1,2} = \frac{1}{2} \left[ \frac{Z_c T_c}{P_c} \right]_{1,2}^{1/3}$
CAX	$(x_1 a_1 + x_2 a_2)^2$
CBX	$x_1^2 (2b_1)^3 + 2x_1 x_2 (b_1 + b_2)^3 + x_2^2 (2b_2)^3$
DAZ, DBZ	Da and Db correction terms for Z table.
DAF, DBF	Da and Db correction terms for (f/p) table.
DAH, DBH	Da and Db correction terms for (H*-H) / Tc' table.
DEV1, 2	$\frac{(f/py)_{exp.} - (f/py)_{calc.}}{(f/py)_{exp.}} \times 100\%$
DTX1, 2	$\frac{1}{T_c'} \left[ \frac{\partial T_c'}{\partial x_{1,2}} - \sum_{i=1}^c x_i \frac{\partial T_c'}{\partial x_i} \right]$
DPX1, 2	$\frac{1}{P_c'} \left[ \frac{\partial P_c'}{\partial x_{1,2}} - \sum_{i=1}^c x_i \frac{\partial P_c'}{\partial x_i} \right]$
F	Fugacity coefficient.
F1, (F/P)M	Table value of fugacity coefficient
FC1, 2	Calculated fugacity coefficient for components 1 or 2.
FDA, FDB	Equivalent to DAF, DBF.
FE1, 2	Experimental fugacity coefficient for components 1 or 2.
FLAG	Variable used to determine if a point is out of range of tables.
FS	Saturation value of fugacity coefficient.

FTR	Reduced temperature in F table.
FTS	Saturation temperature in F table.
H	Ideal gas enthalpy departure term, $\frac{(H^*-H)}{Tc'}$
H1	Table value of enthalpy departure.
HDA, HDB	Equivalent to DAH, DBH.
HS	Saturation value of enthalpy departure term.
HTR	Reduced temperature in H table.
HFS	Saturation temperature in H table.
NPT	Point number.
OUTPT1,2	Subroutines for printing results of calculations.
P	Pressure.
PC	Pseudocritical pressure.
PC1,2	Pure component critical pressure.
PR	Reduced Pressure.
PSI1,2	$\Psi_{1,2} = \frac{1}{RT} \left( \frac{H^*-H}{Tc'} \right) \left( \frac{\partial Tc'}{\partial x_{1,2}} - \sum_{i=1}^c x_i \frac{\partial Tc'}{\partial x_i} \right) Tc'$ $+ (1-z) \left( \frac{\partial Pc'}{\partial x_{1,2}} - \sum_{i=1}^c x_i \frac{\partial Pc'}{\partial x_i} \right)$
T	Temperature
TAB(I)	Table of values of F, H, or Z against reduced temperature at a constant reduced pressure.
TC	Pseudocritical temperature.
TC1,2	Pure component critical temperature.
TR	Reduced temperature.
TS	Saturation temperature.
X1	Mole fraction component 1, $x_1$ .
Z	Compressibility factor.
Z1	Table value of compressibility factor.

ZC	Pseudocritical compressibility factor, $Z_c'$ .
ZC <sub>1,2</sub>	Pure component compressibility factor.
ZDA, ZDB	Equivalent to DAZ, DAB.
ZS	Saturation value of compressibility factor.
ZTR	Reduced temperature in Z table.
ZTS	Saturation temperature in Z table.

TABLE ONE FUGACITY COEFFICIENTS

PT. NO.	TEMP. K	PRESS. ATM	X1	FUGACITY COEFF. 1			FUGACITY COEFF. 2		
				CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
1	344.27	100.CC	0.204	1.020	1.003	-1.742	0.729	0.721	-1.105
5	344.27	200.CC	0.204	1.075	1.096	1.952	0.547	0.520	-5.253
6	344.27	200.CC	0.406	0.978	0.945	-3.469	0.568	0.560	-1.482
8	344.27	200.CC	0.847	0.884	0.863	-2.453	0.641	0.638	-0.449
9	344.27	300.CC	0.204	1.098	1.102	0.321	0.438	0.431	-1.691
11	344.27	300.CC	0.605	0.913	0.880	-3.703	0.511	0.503	-1.630
13	344.27	400.CC	0.204	1.117	1.117	0.017	0.390	0.392	0.392
14	344.27	400.CC	0.406	0.991	0.964	-2.817	0.423	0.424	0.141
15	344.27	400.CC	0.605	0.921	0.894	-3.038	0.469	0.459	-2.096
17	344.27	500.CC	0.204	1.156	1.158	0.141	0.375	0.373	-0.547
18	344.27	500.CC	0.406	1.020	1.002	-1.815	0.404	0.406	0.402
25	415.94	100.CC	0.204	1.017	1.016	-0.128	0.864	0.853	-1.333
29	415.94	200.CC	0.204	1.055	1.063	0.754	0.761	0.737	-3.238
31	415.94	200.CC	0.605	0.977	0.963	-1.489	0.787	0.783	-0.534
32	415.94	200.CC	0.847	0.963	0.954	-0.956	0.794	0.802	1.039
33	415.94	300.CC	0.204	1.095	1.114	1.723	0.684	0.663	-3.222
35	415.94	300.CC	0.847	0.963	0.959	-0.379	0.729	0.748	2.494
36	415.94	400.CC	0.204	1.137	1.175	3.674	0.639	0.620	-3.129
37	415.94	400.CC	0.406	1.031	1.035	0.434	0.650	0.655	0.729
39	415.94	400.CC	0.847	0.961	0.977	-0.436	0.693	0.723	4.094
40	415.94	500.CC	0.204	1.175	1.235	5.172	0.625	0.601	-3.940
48	310.94	100.CC	0.204	1.044	1.230	15.121	0.608	0.575	-5.810
51	310.94	100.CC	0.847	0.898	0.869	-3.288	0.711	0.733	2.999
52	310.94	200.CC	0.204	1.094	1.421	23.045	0.404	0.351	-14.966
53	310.94	200.CC	0.406	0.941	1.018	7.581	0.430	0.392	-9.776
55	310.94	200.CC	0.847	0.830	0.781	-6.224	0.518	0.586	11.557
56	310.94	300.CC	0.204	1.082	1.408	23.136	0.303	0.281	-7.889
57	310.94	300.CC	0.406	0.920	0.945	2.674	0.332	0.311	-6.625
59	310.94	300.CC	0.847	0.799	0.743	-7.502	0.430	0.502	14.385
60	310.94	400.CC	0.204	1.076	1.417	24.043	0.266	0.252	-5.663
61	310.94	400.CC	0.406	0.920	0.970	5.133	0.292	0.279	-4.569
63	310.94	400.CC	0.847	0.800	0.738	-8.334	0.393	0.478	17.841
64	310.94	500.CC	0.204	1.106	1.468	24.680	0.255	0.238	-7.002
65	310.94	500.CC	0.406	0.944	0.996	5.264	0.276	0.263	-4.792



TABLE ONE FUGACITY COEFFICIENTS

SYSTEM METHANE - ETHANE

PT. NO.	TEMP. K	PRESS. ATM	X1	FUGACITY COEFF. 1			FUGACITY COEFF. 2		
				CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
79	294.27	136.C9	0.556	0.921	0.838	-9.872	0.374	0.340	-10.069
82	294.27	187.12	0.556	0.867	0.773	-12.164	0.278	0.275	-1.267
85	294.27	238.16	0.556	0.834	0.720	-15.836	0.248	0.245	-1.183
95	294.27	170.11	0.738	0.830	0.739	-12.302	0.350	0.322	-8.776
98	294.27	221.15	0.738	0.795	0.695	-14.349	0.294	0.274	-7.382
107	294.27	136.C9	0.893	0.841	0.791	-6.274	0.476	0.372	-27.985
110	294.27	187.12	0.893	0.792	0.741	-6.919	0.371	0.285	-30.139
113	294.27	238.16	0.893	0.769	0.708	-8.639	0.332	0.239	-38.803
119	310.94	102.C7	0.319	1.071	1.049	-2.052	0.474	0.451	-5.157
121	310.94	136.C9	0.319	1.058	1.060	0.217	0.406	0.361	-12.529
124	310.94	187.12	0.319	1.012	0.983	-2.931	0.314	0.298	-5.263
127	310.94	238.16	0.319	0.971	0.918	-5.792	0.282	0.271	-4.025
135	310.94	136.C9	0.556	0.941	0.861	-9.283	0.451	0.340	-32.786
138	310.94	187.12	0.556	0.906	0.828	-9.368	0.351	0.275	-27.552
141	310.94	238.16	0.556	0.879	0.770	-14.216	0.315	0.245	-28.574
149	310.94	136.C9	0.738	0.896	0.817	-9.635	0.504	0.452	-11.415
152	310.94	187.12	0.738	0.860	0.773	-11.205	0.399	0.365	-9.314
155	310.94	238.16	0.738	0.840	0.735	-13.659	0.360	0.321	-12.228
164	310.94	153.10	0.893	0.859	0.812	-5.816	0.516	0.404	-27.814
167	310.94	204.14	0.893	0.827	0.775	-6.673	0.437	0.328	-33.334
169	310.94	238.16	0.893	0.813	0.758	-7.247	0.409	0.296	-38.130
181	327.60	204.14	0.319	1.031	0.941	-9.566	0.368	0.358	-2.902
193	327.60	170.11	0.556	0.945	0.850	-11.144	0.456	0.430	-5.966
196	327.60	221.15	0.556	0.924	0.814	-13.490	0.396	0.379	-4.536
206	327.60	153.10	0.738	0.907	0.832	-9.033	0.538	0.488	-10.257
209	327.60	204.14	0.738	0.884	0.798	-10.746	0.459	0.414	-10.879
211	327.60	238.16	0.738	0.874	0.780	-12.031	0.433	0.384	-12.836
223	327.60	204.14	0.893	0.856	0.815	-5.009	0.506	0.386	-31.168
225	327.60	238.16	0.893	0.842	0.800	-5.269	0.476	0.351	-35.432
236	344.27	187.12	0.319	1.054	0.950	-10.906	0.453	0.439	-3.096
239	344.27	238.16	0.319	1.034	0.903	-14.500	0.414	0.401	-3.247
248	344.27	187.12	0.556	0.960	0.878	-9.362	0.497	0.529	6.141
251	344.27	204.14	0.556	0.956	0.848	-12.760	0.480	0.460	-4.334
253	344.27	238.16	0.556	0.949	0.830	-14.313	0.456	0.434	-5.159
261	344.27	136.C9	0.738	0.932	0.867	-7.465	0.631	0.584	-8.090
264	344.27	187.12	0.738	0.910	0.837	-8.699	0.541	0.498	-8.602
267	344.27	238.16	0.738	0.896	0.814	-10.031	0.498	0.445	-11.865
279	344.27	204.14	0.893	0.885	0.847	-4.436	0.571	0.435	-31.211
281	344.27	238.16	0.893	0.876	0.836	-4.738	0.541	0.399	-35.638
295	360.94	238.16	0.319	1.051	0.936	-12.244	0.479	0.461	-3.800
306	360.94	187.12	0.556	0.973	0.876	-11.017	0.562	0.545	-3.138
309	360.94	238.16	0.556	0.971	0.854	-13.731	0.517	0.498	-3.819
320	360.94	187.12	0.738	0.926	0.861	-7.564	0.600	0.559	-7.264
323	360.94	238.16	0.738	0.914	0.842	-8.519	0.556	0.507	-9.676
332	360.94	153.10	0.893	0.929	0.896	-3.643	0.689	0.563	-22.398
335	360.94	204.14	0.893	0.910	0.877	-3.811	0.626	0.489	-27.934

TABLE ONE FUGACITY COEFFICIENTS

PT. NO.	TEMP. K	PRESS. ATM	X1	FUGACITY COEFF. 1			FUGACITY COEFF. 2		
				CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
337	360.94	238.16	0.893	0.904	0.869	-4.044	0.597	0.453	-31.837
346	377.60	153.10	0.319	1.060	0.977	-8.516	0.638	0.606	-5.207
349	377.60	204.14	0.319	1.068	0.966	-10.529	0.565	0.544	-3.782
351	377.60	238.16	0.319	1.065	0.955	-11.496	0.543	0.518	-4.800
361	377.60	170.11	0.556	0.981	0.897	-9.346	0.642	0.627	-2.367
364	377.60	221.15	0.556	0.974	0.880	-10.706	0.588	0.573	-2.602
371	377.60	102.07	0.738	0.970	0.919	-5.521	0.780	0.752	-3.662
374	377.60	153.10	0.738	0.954	0.894	-6.667	0.702	0.661	-6.161
378	377.60	204.14	0.738	0.940	0.876	-7.291	0.639	0.597	-7.067
380	377.60	238.16	0.738	0.936	0.869	-7.725	0.613	0.566	-8.356
392	377.60	204.14	0.893	0.937	0.898	-3.799	0.671	0.535	-25.462
394	377.60	238.16	0.893	0.927	0.892	-3.975	0.645	0.501	-28.683
403	394.27	153.10	0.319	1.053	0.981	-7.376	0.685	0.655	-4.509
406	394.27	204.14	0.319	1.064	0.975	-8.704	0.618	0.596	-3.757
408	394.27	238.16	0.319	1.064	0.975	-9.129	0.597	0.571	-4.592
417	394.27	153.10	0.556	0.988	0.915	-7.988	0.712	0.700	-1.646
420	394.27	204.14	0.556	0.982	0.901	-8.975	0.649	0.643	-0.970
422	394.27	238.16	0.556	0.978	0.895	-9.283	0.624	0.616	-1.374
429	394.27	119.08	0.738	0.975	0.921	-5.876	0.787	0.755	-4.184
432	394.27	170.11	0.738	0.963	0.902	-6.741	0.719	0.684	-5.150
435	394.27	221.15	0.738	0.956	0.890	-7.467	0.672	0.633	-6.186
447	394.27	187.12	0.893	0.951	0.921	-3.219	0.721	0.599	-20.317
450	394.27	238.16	0.893	0.946	0.914	-3.479	0.684	0.548	-24.762

TABLE ONE FUGACITY COEFFICIENTS

PT. NO.	TEMP. K	PRESS. ATM	FUGACITY COEFF. 1				FUGACITY COEFF. 2		
			XI	CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
452	31C.94	13.61	0.286	0.761	0.759	-0.280	0.975	0.966	-0.934
453	31C.94	17.01	0.235	0.715	0.717	0.331	0.957	0.946	-1.177
454	31C.94	20.41	0.202	0.669	0.673	0.600	0.941	0.927	-1.523
455	31C.94	23.82	0.178	0.626	0.634	1.260	0.925	0.909	-1.711
456	31C.94	27.22	0.160	0.583	0.597	2.277	0.909	0.893	-1.752
457	31C.94	30.62	0.145	0.543	0.564	3.736	0.893	0.878	-1.696
458	31C.94	34.02	0.133	0.503	0.532	5.413	0.878	0.865	-1.487
460	31C.94	47.63	0.100	0.342	0.415	17.610	0.823	0.802	-2.601
461	31C.94	54.44	0.090	0.256	0.351	27.086	0.799	0.772	-3.485
462	31C.94	61.24	0.075	0.173	0.313	44.687	0.772	0.740	-4.383
463	31C.94	68.05	0.056	0.071	0.300	76.339	0.755	0.710	-6.303
464	31C.94	71.45	0.051	0.059	0.271	78.215	0.734	0.699	-5.000
465	31C.94	74.51	0.060	0.051	0.191	73.412	0.717	0.701	-2.341
466	31C.94	71.52	0.050	0.060	0.271	78.023	0.730	0.698	-4.558
467	31C.94	74.37	0.054	0.054	0.215	75.066	0.715	0.696	-2.776
469	344.27	11.91	0.723	0.801	0.800	-0.170	1.021	1.011	-1.003
472	344.27	20.41	0.464	0.709	0.698	-1.545	0.999	1.001	0.225
474	344.27	27.22	0.365	0.639	0.644	0.704	0.968	0.963	-0.501
476	344.27	34.02	0.306	0.575	0.594	3.251	0.943	0.937	-0.602
478	344.27	47.63	0.246	0.435	0.488	10.891	0.909	0.889	-2.211
480	344.27	61.24	0.220	0.264	0.367	31.751	0.912	0.856	-6.515
481	344.27	68.05	0.216	0.165	0.336	51.004	0.959	0.847	-13.250
482	344.27	74.85	0.222	0.134	0.281	52.303	0.934	0.850	-9.902
484	344.27	80.56	0.287	0.110	0.191	42.433	0.940	0.923	-1.793
485	344.27	69.41	0.216	0.158	0.326	51.452	0.952	0.847	-12.455
487	377.60	20.41	0.850	0.745	0.730	-2.117	1.111	1.142	2.699
489	377.60	27.22	0.687	0.675	0.668	-0.988	1.074	1.089	1.371
491	377.60	34.02	0.589	0.608	0.614	0.912	1.057	1.056	-0.099
492	377.60	40.83	0.520	0.543	0.569	4.523	1.044	1.021	-2.282
493	377.60	47.63	0.476	0.469	0.522	10.133	1.057	1.009	-4.803
495	377.60	61.24	0.432	0.319	0.425	25.006	1.133	1.005	-12.740
496	377.60	68.05	0.432	0.275	0.371	25.772	1.142	1.030	-10.861
497	377.60	71.45	0.448	0.247	0.336	26.369	1.177	1.070	-10.029
499	415.94	30.62	0.981	0.719	0.684	-5.082	1.244	1.464	15.051
500	415.94	34.02	0.923	0.683	0.646	-5.696	1.257	1.460	13.904
501	415.94	37.42	0.876	0.644	0.614	-4.955	1.311	1.443	9.139
503	415.94	44.23	0.809	0.572	0.557	-2.780	1.393	1.435	2.925
504	415.94	47.63	0.790	0.538	0.528	-1.808	1.429	1.470	2.809
505	415.94	51.03	0.795	0.500	0.490	-2.016	1.504	1.639	8.224
506	415.94	51.59	0.812	0.489	0.476	-2.822	1.573	1.810	13.107
507	415.94	49.26	0.788	0.521	0.519	-0.305	1.449	1.525	5.000

TABLE ONE FUGACITY COEFFICIENTS

PT. NO.	TEMP. K	PRESS. ATM	FUGACITY COEFF. 1			FUGACITY COEFF. 2			
			X1	CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
508	31C.94	13.61	0.894	0.987	0.990	0.254	0.871	0.741	-17.564
509	31C.94	20.41	0.920	0.979	0.979	0.020	0.820	0.675	-21.420
510	31C.94	27.22	0.932	0.971	0.965	-0.653	0.745	0.620	-20.166
511	31C.94	40.83	0.943	0.959	0.944	-1.553	0.569	0.509	-11.822
512	31C.94	54.44	0.946	0.947	0.926	-2.278	0.454	0.412	-10.176
514	31C.94	85.06	0.946	0.917	0.890	-2.984	0.335	0.258	-29.726
515	31C.94	102.21	0.941	0.903	0.873	-3.487	0.272	0.196	-38.774
516	31C.94	119.08	0.933	0.895	0.880	-1.688	0.216	0.152	-41.865
517	31C.94	136.09	0.920	0.890	0.841	-5.819	0.164	0.114	-43.837
518	31C.94	153.10	0.897	0.891	0.831	-7.253	0.114	0.082	-38.483
519	31C.94	167.05	0.822	0.951	0.875	-8.189	0.055	0.046	-19.520
522	344.27	20.41	0.819	0.991	0.998	0.691	0.820	0.711	-15.398
523	344.27	27.22	0.849	0.987	0.990	0.300	0.762	0.645	-18.203
524	344.27	40.83	0.879	0.981	0.979	-0.255	0.617	0.550	-12.120
526	344.27	68.05	0.894	0.967	0.957	-1.031	0.491	0.388	-26.611
527	344.27	85.06	0.893	0.961	0.943	-1.933	0.409	0.310	-32.094
528	344.27	102.21	0.887	0.956	0.939	-1.847	0.349	0.231	-51.042
530	344.27	136.09	0.856	0.968	0.931	-3.991	0.221	0.148	-49.497
531	344.27	153.10	0.814	1.004	0.959	-4.694	0.150	0.105	-42.764
532	344.27	159.09	0.766	1.064	1.012	-5.123	0.110	0.081	-35.671
534	377.60	20.41	0.614	1.029	1.038	0.876	0.781	0.706	-10.622
535	377.60	27.22	0.685	1.029	1.030	0.143	0.722	0.649	-11.267
536	377.60	40.83	0.757	1.014	1.018	0.405	0.617	0.564	-9.486
537	377.60	54.44	0.788	1.022	1.009	-1.250	0.547	0.493	-10.868
538	377.60	68.05	0.798	1.014	1.012	-0.204	0.510	0.421	-21.192
539	377.60	85.06	0.801	1.017	1.019	0.203	0.435	0.347	-25.386
541	377.60	119.08	0.758	1.066	1.047	-1.830	0.291	0.216	-34.645
542	377.60	136.09	0.742	1.091	1.054	-3.466	0.235	0.184	-27.813
543	377.60	141.60	0.675	1.197	1.154	-3.688	0.176	0.142	-24.129
544	415.94	13.61	0.058	1.301	1.038	-25.291	0.806	0.785	-2.714
546	415.94	27.22	0.429	1.116	1.131	1.306	0.705	0.650	-8.501
547	415.94	40.83	0.602	1.074	1.038	-3.435	0.628	0.624	-0.588
548	415.94	54.44	0.614	1.105	1.120	1.329	0.553	0.483	-14.502
550	415.94	85.06	0.642	1.141	1.143	0.167	0.425	0.340	-25.043
552	415.94	109.55	0.510	1.434	1.439	0.332	0.269	0.199	-35.236
553	444.27	27.22	0.094	1.535	1.469	-4.759	0.682	0.657	-3.799
554	444.27	40.83	0.279	1.726	1.241	-39.084	0.685	0.547	-25.241
555	444.27	54.44	0.356	1.416	1.257	-12.643	0.503	0.458	-9.911
556	444.27	68.05	0.337	1.676	1.504	-11.460	0.402	0.374	-7.446
557	444.27	69.75	0.295	1.917	1.725	-11.120	0.367	0.328	-12.025

TABLE ONE FUGACITY COEFFICIENTS

PT. NO.	TEMP. K	PRESS. ATM	X1	FUGACITY COEFF. 1			FUGACITY COEFF. 2		
				CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
559	294.27	13.61	0.809	0.988	0.990	0.202	0.855	0.673	-27.100
561	294.27	34.02	0.898	0.962	0.954	-0.863	0.619	0.441	-40.294
563	294.27	40.83	0.907	0.948	0.944	-0.421	0.563	0.392	-43.514
565	294.27	68.05	0.920	0.918	0.895	-2.552	0.401	0.256	-56.754
568	294.27	95.26	0.909	0.890	0.852	-4.463	0.266	0.169	-57.477
579	310.94	20.41	0.783	0.985	0.991	0.590	0.795	0.581	-36.832
582	310.94	40.83	0.862	0.964	0.963	-0.094	0.591	0.389	-51.970
584	310.94	68.05	0.881	0.945	0.924	-2.266	0.441	0.262	-68.359
587	310.94	95.26	0.865	0.930	0.899	-3.494	0.300	0.174	-72.668
591	310.94	119.08	0.835	0.934	0.880	-6.154	0.211	0.124	-70.524
598	327.60	20.41	0.678	1.003	0.995	-0.834	0.789	0.624	-26.431
599	327.60	27.22	0.739	0.998	0.988	-1.011	0.727	0.545	-33.357
602	327.60	54.44	0.819	0.982	0.962	-2.045	0.510	0.336	-51.846
605	327.60	85.06	0.827	0.967	0.934	-3.586	0.381	0.215	-77.187
607	327.60	102.21	0.815	0.969	0.925	-4.765	0.309	0.177	-79.491
609	327.60	115.68	0.786	0.986	0.929	-6.181	0.249	0.135	-84.752
612	327.60	125.89	0.729	1.044	0.900	-16.000	0.186	0.100	-86.038
613	327.60	127.65	0.622	1.215	1.135	-7.016	0.131	0.071	-84.367
614	344.27	10.21	0.172	1.112	1.004	-10.710	0.835	0.809	-3.197
620	344.27	54.44	0.745	1.012	0.982	-3.056	0.526	0.361	-45.753
622	344.27	81.67	0.759	1.009	0.977	-3.316	0.409	0.237	-72.380
624	344.27	95.26	0.753	1.019	0.974	-4.586	0.347	0.195	-78.149
628	344.27	119.08	0.683	1.097	1.027	-6.842	0.234	0.119	-96.661
630	344.27	123.16	0.616	1.203	1.127	-6.700	0.191	0.095	101.508
631	360.94	13.61	0.111	1.200	1.010	-18.768	0.808	0.780	-3.577
637	360.94	68.05	0.672	1.060	1.007	-5.289	0.479	0.319	-50.046
640	360.94	95.26	0.610	1.173	1.121	-4.678	0.309	0.182	-69.722
644	360.94	115.54	0.550	1.288	1.212	-6.297	0.233	0.128	-82.334
657	377.60	103.43	0.472	1.385	1.331	-4.072	0.283	0.193	-46.516
658	394.27	27.22	0.142	1.304	1.038	-25.657	0.711	0.697	-2.037
659	394.27	34.02	0.265	1.239	1.071	-15.682	0.660	0.621	-6.203
664	394.27	81.67	0.410	1.417	1.390	-1.918	0.375	0.287	-30.664
666	394.27	86.01	0.360	1.592	1.593	0.046	0.336	0.255	-31.650

TABLE ONE FUGACITY COEFFICIENTS  
SYSTEM METHANE - BUTANE (SUPERHEATED)

PT. NO.	TEMP. K	PRESS. ATM	X1	FUGACITY COEFF. 1			FUGACITY COEFF. 2		
				CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
670	294.27	27.22	0.894	0.969	0.964	-0.503	0.711	0.497	-42.967
675	294.27	40.83	0.912	0.948	0.934	-1.457	0.567	0.395	-43.433
678	294.27	85.06	0.912	0.895	0.865	-3.958	0.309	0.208	-48.734
682	294.27	204.14	0.912	0.796	0.739	-7.670	0.094	0.062	-51.872
686	294.27	34.02	0.970	0.954	0.941	-1.434	0.698	0.519	-34.486
689	294.27	68.05	0.970	0.909	0.887	-2.478	0.459	0.295	-55.548
691	294.27	102.07	0.970	0.870	0.838	-3.808	0.320	0.180	-77.998
693	294.27	170.11	0.970	0.806	0.765	-5.301	0.167	0.083	101.342
694	294.27	204.14	0.970	0.783	0.739	-5.951	0.135	0.063	114.300
697	310.94	27.22	0.845	0.981	0.980	-0.053	0.728	0.505	-44.183
704	310.94	68.05	0.894	0.941	0.920	-2.336	0.455	0.278	-63.692
707	310.94	136.09	0.894	0.893	0.841	-6.176	0.228	0.130	-75.029
709	310.94	204.14	0.894	0.850	0.786	-8.081	0.134	0.080	-67.572
713	310.94	34.02	0.912	0.966	0.953	-1.401	0.705	0.526	-34.047
716	310.94	68.05	0.912	0.936	0.909	-2.942	0.472	0.312	-51.256
719	310.94	136.09	0.912	0.884	0.834	-6.034	0.244	0.142	-71.931
721	310.94	204.14	0.912	0.841	0.782	-7.507	0.147	0.084	-74.428
726	310.94	40.83	0.970	0.956	0.942	-1.523	0.684	0.488	-40.219
729	310.94	85.06	0.970	0.910	0.886	-2.762	0.452	0.255	-77.315
732	310.94	170.11	0.970	0.841	0.805	-4.505	0.235	0.103	127.773
733	310.94	204.14	0.970	0.821	0.784	-4.736	0.196	0.081	141.534
737	327.60	34.02	0.845	0.981	0.971	-1.002	0.702	0.516	-36.050
740	327.60	68.05	0.845	0.968	0.944	-2.540	0.482	0.311	-55.109
743	327.60	136.09	0.845	0.940	0.885	-6.254	0.254	0.152	-67.245
745	327.60	204.14	0.845	0.910	0.840	-8.309	0.157	0.098	-59.992
750	327.60	40.83	0.894	0.969	0.958	-1.155	0.673	0.493	-36.510
753	327.60	85.06	0.894	0.942	0.915	-2.937	0.447	0.282	-58.490
757	327.60	204.14	0.894	0.882	0.825	-6.945	0.194	0.115	-68.910
761	327.60	34.02	0.912	0.972	0.962	-1.032	0.752	0.566	-32.931
764	327.60	68.05	0.912	0.948	0.926	-2.361	0.543	0.355	-53.035
769	327.60	204.14	0.912	0.873	0.821	-6.321	0.209	0.115	-81.388
775	327.60	54.44	0.970	0.955	0.939	-1.701	0.637	0.418	-52.498
778	327.60	102.07	0.970	0.917	0.892	-2.800	0.465	0.235	-97.836
781	327.60	204.14	0.970	0.853	0.823	-3.679	0.261	0.104	150.797
786	344.27	40.83	0.845	0.981	0.968	-1.334	0.689	0.499	-38.135
788	344.27	68.05	0.845	0.972	0.948	-2.582	0.548	0.351	-56.041
791	344.27	136.09	0.845	0.952	0.907	-5.016	0.325	0.185	-75.428
793	344.27	204.14	0.845	0.932	0.875	-6.474	0.216	0.120	-80.123
798	344.27	40.83	0.894	0.974	0.964	-1.089	0.724	0.515	-40.548
801	344.27	85.06	0.894	0.953	0.928	-2.740	0.513	0.315	-62.729
804	344.27	170.11	0.894	0.915	0.873	-4.759	0.296	0.169	-75.292
805	344.27	204.14	0.894	0.902	0.858	-5.083	0.255	0.142	-79.412
809	344.27	34.02	0.912	0.978	0.969	-0.880	0.789	0.580	-36.003
812	344.27	68.05	0.912	0.960	0.939	-2.231	0.602	0.387	-55.468
815	344.27	136.09	0.912	0.925	0.888	-4.160	0.387	0.218	-77.558
817	344.27	204.14	0.912	0.893	0.853	-4.745	0.272	0.147	-84.821

TABLE ONE FUGACITY COEFFICIENTS  
SYSTEM METHANE - BUTANE (SUPERHEATED)

PT. NO.	TEMP. K	PRESS. ATM	X1	FUGACITY COEFF. 1			FUGACITY COEFF. 2		
				CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
822	344.27	40.83	0.970	0.973	0.962	-1.168	0.764	0.532	-43.555
825	344.27	85.06	0.970	0.946	0.925	-2.217	0.581	0.322	-80.309
828	344.27	170.11	0.970	0.897	0.871	-2.980	0.374	0.163	129.185
833	360.94	34.02	0.845	0.985	0.976	-0.949	0.789	0.592	-33.333
836	360.94	68.05	0.845	0.979	0.955	-2.473	0.605	0.400	-51.211
839	360.94	136.09	0.845	0.962	0.923	-4.246	0.391	0.230	-69.867
841	360.94	204.14	0.845	0.945	0.902	-4.712	0.277	0.158	-75.234
846	360.94	40.83	0.894	0.980	0.970	-1.017	0.764	0.554	-37.868
849	360.94	85.06	0.894	0.964	0.941	-2.469	0.572	0.359	-59.267
851	360.94	136.09	0.894	0.945	0.913	-3.458	0.434	0.253	-71.452
853	360.94	204.14	0.894	0.920	0.886	-3.841	0.318	0.180	-76.568
860	360.94	68.05	0.912	0.970	0.950	-2.071	0.654	0.422	-54.947
863	360.94	136.09	0.912	0.941	0.908	-3.614	0.451	0.258	-74.951
865	360.94	204.14	0.912	0.916	0.881	-3.917	0.335	0.184	-82.217
869	360.94	34.02	0.970	0.982	0.974	-0.815	0.841	0.609	-38.162
873	360.94	85.06	0.970	0.959	0.939	-2.170	0.634	0.355	-78.459
877	360.94	204.14	0.970	0.911	0.885	-2.896	0.388	0.168	131.248
886	377.60	102.07	0.845	0.978	0.948	-3.204	0.537	0.346	-55.210
889	377.60	204.14	0.845	0.955	0.925	-3.216	0.338	0.198	-70.718
895	377.60	54.44	0.894	0.982	0.986	0.407	0.727	0.515	-41.107
899	377.60	136.09	0.894	0.958	0.929	-3.148	0.496	0.300	-65.220
901	377.60	204.14	0.894	0.939	0.910	-3.219	0.381	0.224	-70.164
907	377.60	54.44	0.912	0.981	0.967	-1.465	0.736	0.514	-43.167
913	377.60	204.14	0.912	0.936	0.905	-3.459	0.395	0.223	-77.344
921	377.60	85.06	0.970	0.971	0.950	-2.255	0.684	0.394	-73.578
925	377.60	204.14	0.970	0.932	0.909	-2.507	0.440	0.206	113.830
932	394.27	68.05	0.845	0.991	0.969	-2.262	0.700	0.493	-41.892
937	394.27	204.14	0.845	0.968	0.936	-3.402	0.399	0.244	-63.667
943	394.27	54.44	0.894	0.988	0.973	-1.518	0.760	0.551	-37.916
946	394.27	102.07	0.894	0.979	0.954	-2.626	0.625	0.399	-56.634
949	394.27	204.14	0.894	0.958	0.930	-2.969	0.438	0.267	-64.060
955	394.27	54.44	0.912	0.988	0.973	-1.530	0.767	0.547	-40.205
959	394.27	136.09	0.912	0.969	0.941	-2.967	0.562	0.344	-63.380
961	394.27	204.14	0.912	0.955	0.926	-3.101	0.450	0.265	-69.728
966	394.27	40.83	0.970	0.980	0.980	10.213	0.750	0.611	-22.674
970	394.27	102.07	0.970	0.971	0.955	-1.689	0.681	0.388	-75.488
973	394.27	204.14	0.970	0.947	0.930	-1.782	0.484	0.246	-96.646
978	310.94	20.43	0.784	0.985	0.991	0.601	0.795	0.583	-36.404
986	327.60	34.02	0.784	0.994	0.980	-1.436	0.658	0.488	-34.908
990	344.27	25.80	0.608	1.021	1.002	-1.892	0.736	0.593	-24.105
997	344.27	34.02	0.707	1.010	0.990	-2.064	0.675	0.517	-30.616
1005	344.27	85.06	0.784	0.997	0.964	-3.458	0.416	0.246	-68.949
1008	344.27	170.11	0.784	0.986	0.936	-5.345	0.204	0.114	-79.308
1016	360.94	34.02	0.608	1.034	1.006	-2.787	0.685	0.550	-24.555
1023	360.94	68.05	0.707	1.037	0.990	-4.713	0.501	0.333	-50.600
1028	360.94	204.14	0.707	1.057	0.967	-9.299	0.185	0.107	-73.067

TABLE ONE FUGACITY COEFFICIENTS  
 SYSTEM METHANE - BUTANE (SUPERHEATED)

PT. NO.	TEMP. K	PRESS. ATM	X1	FUGACITY COEFF. 1			FUGACITY COEFF. 2		
				CALC	EXP	PCT DEV	CALC	EXP	PCT DEV
1040	360.94	204.14	0.784	0.989	0.928	-6.614	0.231	0.133	-73.887
1041	377.60	25.30	0.287	1.162	1.039	-11.876	0.721	0.656	-9.856
1044	377.60	40.15	0.475	1.112	1.068	-4.149	0.610	0.517	-18.037
1053	377.60	102.07	0.608	1.148	1.095	-4.846	0.362	0.249	-45.314
1055	377.60	204.14	0.608	1.171	1.053	-11.234	0.194	0.142	-36.925
1062	377.60	204.14	0.707	1.066	0.966	-10.397	0.242	0.155	-56.217
1069	377.60	204.14	0.784	0.997	0.941	-5.954	0.294	0.172	-70.706
1071	394.27	27.22	0.287	1.140	1.032	-10.504	0.740	0.668	-10.838
WEF									
UNLOAD									
REMARK									

END OF FILE



TABLE TWO PROPERTIES OF MIXTURES

PT	TC, K	PC, ATM.	X1	TR	PR	Z	(F/P)M	H	PSI 1	PSI 2
1	278.65	66.82	C.204	1.236	1.497	0.717	0.781	2.584	0.268	-0.069
5	278.43	66.77	C.204	1.236	2.995	0.632	0.628	4.671	0.537	-0.138
6	254.35	60.99	C.406	1.354	3.279	0.741	0.708	3.900	0.322	-0.220
8	206.32	49.46	C.847	1.669	4.043	0.876	0.842	2.569	0.049	-0.273
9	278.43	66.77	C.204	1.236	4.493	0.680	0.529	5.918	0.731	-0.187
11	231.92	55.61	C.6C5	1.484	5.395	0.864	0.726	4.019	0.229	-0.351
13	278.43	66.77	C.204	1.236	5.991	0.804	0.484	6.349	0.837	-0.214
14	254.35	60.99	C.406	1.354	6.558	0.887	0.598	5.325	0.505	-0.345
15	231.92	55.61	C.6C5	1.484	7.193	0.962	0.705	4.333	0.267	-0.409
17	278.43	66.77	C.204	1.236	7.489	0.935	0.472	6.447	0.896	-0.230
18	254.35	60.99	C.406	1.354	8.198	1.007	0.589	5.444	0.550	-0.376
25	278.65	66.82	C.204	1.493	1.497	0.886	0.894	1.445	0.130	-0.033
29	278.43	66.77	C.204	1.494	2.995	0.830	0.813	2.709	0.260	-0.067
31	231.92	55.61	C.605	1.793	3.597	0.913	0.897	1.941	0.085	-0.131
32	206.32	49.46	C.847	2.016	4.043	0.954	0.935	1.751	0.030	-0.164
33	278.43	66.77	C.204	1.494	4.493	0.831	0.753	3.673	0.374	-0.096
35	206.32	49.46	C.847	2.016	6.065	0.996	0.923	2.262	0.042	-0.235
36	278.43	66.77	C.204	1.494	5.991	0.891	0.718	4.175	0.455	-0.116
37	254.35	60.99	C.406	1.635	6.558	0.956	0.784	3.426	0.274	-0.187
39	206.32	49.46	C.847	2.016	8.087	1.074	0.930	2.514	0.053	-0.294
40	278.43	66.77	C.204	1.494	7.489	0.981	0.711	4.318	0.503	-0.129
48	278.65	66.82	C.204	1.116	1.497	0.534	0.679	3.773	0.430	-0.110
51	206.32	49.46	C.847	1.507	2.022	0.855	0.866	1.844	0.036	-0.197
52	278.43	66.77	C.204	1.117	2.995	0.500	0.495	6.137	0.794	-0.203
53	254.35	60.99	C.406	1.222	3.279	0.620	0.591	5.093	0.465	-0.318
55	206.32	49.46	C.847	1.507	4.043	0.819	0.772	3.391	0.072	-0.398
56	278.43	66.77	C.204	1.117	4.493	0.622	0.393	7.256	1.013	-0.260
57	254.35	60.99	C.406	1.222	4.919	0.707	0.502	6.150	0.606	-0.414
59	206.32	49.46	C.847	1.507	6.065	0.900	0.726	4.051	0.095	-0.525
60	278.43	66.77	C.204	1.117	5.991	0.772	0.354	7.550	1.112	-0.285
61	254.35	60.99	C.406	1.222	6.558	0.850	0.465	6.488	0.682	-0.466
63	206.32	49.46	C.847	1.507	8.087	1.020	0.717	4.242	0.109	-0.602
64	278.43	66.77	C.204	1.117	7.489	0.921	0.344	7.580	1.169	-0.300
65	254.35	60.99	C.406	1.222	8.198	0.995	0.454	6.572	0.731	-0.500
79	243.46	47.86	C.556	1.209	2.843	0.601	0.617	4.673	0.400	-0.501
82	243.46	47.86	C.556	1.209	3.909	0.617	0.524	5.862	0.504	-0.631
85	243.46	47.86	C.556	1.209	4.976	0.706	0.487	6.231	0.539	-0.675
95	222.26	47.25	C.738	1.324	3.600	0.714	0.662	4.415	0.226	-0.637
98	222.26	47.25	C.738	1.324	4.680	0.751	0.613	5.050	0.260	-0.733
107	203.89	46.49	C.893	1.443	2.928	0.807	0.791	2.902	0.061	-0.508
110	203.89	46.49	C.893	1.443	4.025	0.787	0.730	3.847	0.081	-0.678
113	203.89	46.49	C.893	1.443	5.123	0.838	0.703	4.218	0.090	-0.751
119	270.44	48.27	C.319	1.150	2.114	0.493	0.615	4.536	0.554	-0.260
121	270.44	48.27	C.319	1.150	2.819	0.529	0.551	5.318	0.652	-0.305
124	270.44	48.27	C.319	1.150	3.876	0.582	0.456	6.491	0.798	-0.374
127	270.44	48.27	C.319	1.150	4.933	0.678	0.418	6.843	0.842	-0.395

TABLE TWO PROPERTIES OF MIXTURES

PT	TC, K	PC, ATM.	XI	TR	PR	Z	(F/P)M	H	PSI 1	PSI 2
135	243.46	47.86	C.556	1.277	2.843	0.680	0.679	4.026	0.326	-0.408
138	243.46	47.86	C.556	1.277	3.909	0.672	0.594	5.175	0.421	-0.527
141	243.46	47.86	C.556	1.277	4.976	0.743	0.557	5.574	0.456	-0.571
149	222.26	47.25	C.738	1.399	2.880	0.785	0.770	3.125	0.151	-0.425
152	222.26	47.25	C.738	1.399	3.960	0.765	0.703	4.141	0.201	-0.566
155	222.26	47.25	C.738	1.399	5.040	0.816	0.673	4.532	0.222	-0.625
164	203.89	46.49	C.893	1.525	3.293	0.638	0.814	2.740	0.054	-0.455
167	203.89	46.49	C.893	1.525	4.391	0.839	0.772	3.399	0.068	-0.569
169	203.89	46.49	C.893	1.525	5.123	0.867	0.755	3.642	0.074	-0.614
181	270.44	48.27	C.319	1.211	4.229	0.641	0.512	6.009	0.701	-0.328
193	243.46	47.86	C.556	1.346	3.554	0.731	0.683	4.197	0.324	-0.405
196	243.46	47.86	C.556	1.346	4.620	0.761	0.634	4.851	0.376	-0.471
206	222.26	47.25	C.738	1.474	3.240	0.816	0.791	2.981	0.137	-0.385
209	222.26	47.25	C.738	1.474	4.320	0.815	0.744	3.716	0.172	-0.483
211	222.26	47.25	C.738	1.474	5.040	0.846	0.727	3.958	0.184	-0.518
223	203.89	46.49	C.893	1.607	4.351	0.868	0.809	2.952	0.056	-0.469
225	203.89	46.49	C.893	1.607	5.123	0.892	0.792	3.189	0.061	-0.510
236	270.44	48.27	C.319	1.273	3.876	0.669	0.593	5.189	0.575	-0.270
239	270.44	48.27	C.319	1.273	4.933	0.738	0.554	5.609	0.623	-0.292
248	243.46	47.86	C.556	1.414	3.909	0.773	0.716	3.984	0.293	-0.367
251	243.46	47.86	C.556	1.414	4.265	0.785	0.704	4.157	0.306	-0.383
253	243.46	47.86	C.556	1.414	4.976	0.819	0.686	4.398	0.325	-0.407
261	222.26	47.25	C.738	1.549	2.880	0.855	0.841	2.339	0.102	-0.287
264	222.26	47.25	C.738	1.549	3.960	0.834	0.794	3.110	0.136	-0.384
267	222.26	47.25	C.738	1.549	5.040	0.872	0.768	3.482	0.154	-0.433
279	203.89	46.49	C.893	1.688	4.391	0.892	0.844	2.587	0.047	-0.391
281	203.89	46.49	C.893	1.688	5.123	0.913	0.832	2.819	0.051	-0.430
295	270.44	48.27	C.319	1.335	4.933	0.773	0.615	5.053	0.536	-0.251
306	243.46	47.86	C.556	1.483	3.909	0.807	0.762	3.473	0.243	-0.305
309	245.77	47.91	C.536	1.469	4.971	0.841	0.725	3.979	0.293	-0.338
320	222.26	47.25	C.738	1.624	3.960	0.862	0.826	2.726	0.114	-0.321
323	222.26	47.25	C.738	1.624	5.040	0.894	0.802	3.086	0.130	-0.367
332	203.89	46.49	C.893	1.770	3.293	0.912	0.899	1.858	0.032	-0.266
335	203.89	46.49	C.893	1.770	4.391	0.913	0.875	2.319	0.040	-0.335
337	203.89	46.49	C.893	1.770	5.123	0.932	0.865	2.542	0.044	-0.370
346	270.44	48.27	C.319	1.396	3.171	0.777	0.750	3.428	0.346	-0.162
349	270.44	48.27	C.319	1.396	4.229	0.773	0.692	4.289	0.434	-0.203
351	270.44	48.27	C.319	1.396	4.933	0.809	0.673	4.528	0.459	-0.215
361	243.46	47.86	C.556	1.551	3.554	0.843	0.813	2.814	0.188	-0.236
364	243.46	47.86	C.556	1.551	4.620	0.857	0.779	3.335	0.224	-0.281
371	222.26	47.25	C.738	1.699	2.160	0.913	0.916	1.442	0.057	-0.161
374	222.26	47.25	C.738	1.699	3.240	0.896	0.880	2.015	0.080	-0.226
378	222.26	47.25	C.738	1.699	4.320	0.893	0.850	2.520	0.101	-0.285
380	222.26	47.25	C.738	1.699	5.040	0.914	0.838	2.747	0.111	-0.312
352	203.89	46.49	C.893	1.852	4.391	0.931	0.900	2.117	0.035	-0.293
394	203.89	46.49	C.893	1.852	5.123	0.949	0.892	2.326	0.039	-0.325

TABLE TWO PROPERTIES OF MIXTURES

PT	TC, K	PC, ATM.	X1	TR	PR	Z	(F/P)M	H	PSI 1	PSI 2
403	270.44	48.27	C.319	1.458	3.171	0.809	0.785	3.034	0.794	-0.137
406	270.44	48.27	C.319	1.458	4.229	0.804	0.735	3.816	0.370	-0.173
408	270.44	48.27	C.319	1.458	4.933	0.835	0.718	4.053	0.393	-0.184
417	243.46	47.86	C.556	1.619	3.199	0.873	0.854	2.277	0.146	-0.183
420	243.46	47.86	C.556	1.619	4.265	0.868	0.817	2.858	0.184	-0.230
422	243.46	47.86	C.556	1.619	4.976	0.891	0.801	3.088	0.199	-0.249
429	222.26	47.25	C.738	1.774	2.520	0.924	0.922	1.476	0.056	-0.159
432	222.26	47.25	C.738	1.774	3.600	0.909	0.892	1.997	0.076	-0.215
435	222.26	47.25	C.738	1.774	4.680	0.921	0.872	2.396	0.092	-0.260
447	203.89	46.49	C.893	1.934	4.025	0.940	0.923	1.866	0.030	-0.247
450	203.89	46.49	C.893	1.934	5.123	0.964	0.914	2.159	0.035	-0.290
452	342.91	57.35	C.286	0.907	C.237	0.872	0.908	0.728	-0.177	0.071
453	336.24	59.59	C.235	0.925	0.285	0.854	0.894	0.842	-0.224	0.069
454	331.89	61.15	C.202	0.937	0.334	0.836	0.878	0.979	-0.272	0.069
455	328.73	62.34	C.178	0.946	0.382	0.817	0.863	1.112	-0.321	0.069
456	326.38	63.27	C.160	0.953	0.430	0.795	0.846	1.254	-0.372	0.071
457	324.46	64.08	C.145	0.958	0.478	0.774	0.831	1.397	-0.425	0.072
458	322.98	64.76	C.133	0.963	0.525	0.751	0.815	1.554	-0.482	0.074
460	319.45	66.82	C.100	0.973	0.713	0.639	0.754	2.393	-0.790	0.088
461	318.60	67.52	C.090	0.976	C.806	0.555	0.721	3.064	-1.036	0.102
462	316.71	68.47	C.075	0.982	0.894	0.445	0.690	3.960	-1.383	0.112
463	313.80	69.59	C.056	0.991	0.978	0.211	0.661	6.308	-2.232	0.132
464	312.98	69.89	C.051	0.993	1.022	0.195	0.645	6.781	-2.392	0.129
465	314.45	69.36	C.060	0.989	1.074	0.209	0.612	7.388	-2.489	0.159
466	312.81	69.94	C.050	0.994	1.028	0.204	0.644	6.749	-2.381	0.125
467	313.45	69.71	C.054	0.992	1.067	0.216	0.622	7.143	-2.451	0.140
469	395.69	43.39	C.723	0.870	0.274	0.815	0.857	0.848	-0.067	0.175
472	365.52	50.74	C.464	0.942	0.402	0.803	0.852	1.201	-0.184	0.159
474	353.50	54.27	C.365	0.974	0.502	0.776	0.832	1.399	-0.263	0.151
476	346.60	56.70	C.306	0.993	0.600	0.749	0.810	1.646	-0.343	0.151
478	340.59	59.67	C.246	1.010	0.798	0.662	0.758	2.406	-0.556	0.181
480	339.29	61.20	C.220	1.015	1.001	0.466	0.694	3.973	-0.966	0.273
481	338.78	61.39	C.216	1.016	1.108	0.328	0.656	5.931	-1.382	0.381
482	338.92	60.98	C.222	1.016	1.227	0.274	0.607	6.687	-1.511	0.431
484	346.21	57.84	C.287	0.994	1.393	0.237	0.508	8.125	-1.530	0.616
485	338.70	61.38	C.216	1.016	1.131	0.319	0.646	6.055	-1.407	0.388
487	409.79	40.50	C.850	0.921	0.504	0.711	0.791	1.743	-0.060	0.339
489	392.57	44.39	C.687	0.962	0.613	0.694	0.780	1.948	-0.146	0.320
491	382.51	47.17	C.589	0.987	C.721	0.665	0.763	2.283	-0.227	0.325
492	375.87	49.43	C.520	1.005	0.826	0.622	0.743	2.648	-0.314	0.340
493	372.01	51.04	C.476	1.015	0.933	0.548	0.718	3.255	-0.426	0.387
495	367.45	52.66	C.432	1.028	1.163	0.387	0.655	5.254	-0.720	0.548
496	366.32	52.50	C.432	1.031	1.296	0.337	0.618	5.978	-0.808	0.614
497	367.26	51.80	C.448	1.028	1.379	0.294	0.585	6.726	-0.961	0.699
499	423.48	37.85	C.981	0.982	0.809	0.576	0.726	2.980	-0.010	0.538
500	418.34	39.06	C.923	0.994	0.871	0.533	0.716	3.230	-0.047	0.563

TABLE The PROPERTIES OF MIXTURES

PT	TC, K	PC, ATM.	X1	TR	PR	Z	(F/P)M	H	PSI 1	PSI 2
501	414.17	40.10	C.876	1.004	0.933	0.476	0.704	3.749	-0.088	0.622
503	408.11	41.68	C.809	1.019	1.061	0.426	0.678	4.880	-0.170	0.719
504	406.22	42.13	C.790	1.024	1.130	0.385	0.660	5.346	-0.205	0.772
505	406.38	41.98	C.795	1.024	1.216	0.320	0.627	6.047	-0.226	0.876
506	407.87	41.55	C.812	1.020	1.242	0.291	0.610	6.510	-0.219	0.948
507	405.92	42.17	C.788	1.025	1.168	0.360	0.647	5.583	-0.217	0.807
508	227.09	45.42	C.894	1.369	0.300	0.969	0.974	0.225	0.013	-0.112
509	218.81	45.66	C.920	1.421	0.447	0.958	0.965	0.315	0.014	-0.163
510	215.93	45.97	C.932	1.440	0.592	0.945	0.954	0.456	0.018	-0.247
511	216.44	46.94	C.943	1.437	0.870	0.925	0.931	0.783	0.030	-0.492
512	213.55	46.56	C.946	1.456	1.169	0.900	0.910	1.154	0.040	-0.696
514	209.59	45.69	C.946	1.484	1.862	0.857	0.868	1.814	0.054	-0.953
515	211.28	45.67	C.941	1.472	2.238	0.835	0.842	2.165	0.071	-1.130
516	213.98	45.63	C.933	1.453	2.609	0.818	0.813	2.575	0.095	-1.328
517	218.34	45.57	C.920	1.424	2.987	0.796	0.777	3.075	0.135	-1.556
518	226.00	45.43	C.897	1.376	3.370	0.758	0.721	3.775	0.212	-1.848
519	250.43	44.80	C.822	1.242	3.729	0.642	0.573	5.351	0.507	-2.343
522	252.40	44.95	C.819	1.364	0.454	0.949	0.958	0.377	0.034	-0.155
523	245.13	45.68	C.849	1.404	0.596	0.940	0.949	0.501	0.039	-0.219
524	242.94	47.45	C.879	1.417	0.861	0.921	0.928	0.812	0.056	-0.409
526	227.68	45.54	C.894	1.512	1.494	0.893	0.900	1.349	0.072	-0.605
527	227.33	45.40	C.893	1.514	1.874	0.869	0.877	1.723	0.091	-0.762
528	229.31	45.36	C.887	1.501	2.253	0.849	0.853	2.041	0.114	-0.894
530	239.46	45.11	C.856	1.438	3.017	0.802	0.783	3.026	0.213	-1.264
531	252.99	44.72	C.814	1.361	3.424	0.745	0.705	3.956	0.354	-1.548
532	268.13	44.20	C.766	1.284	3.599	0.680	0.625	4.798	0.531	-1.739
534	315.76	42.49	C.614	1.196	0.480	0.909	0.925	0.632	0.106	-0.169
535	299.12	44.12	C.685	1.262	0.617	0.903	0.920	0.794	0.111	-0.242
536	288.15	46.90	C.757	1.310	0.871	0.884	0.899	1.035	0.120	-0.375
537	269.91	45.92	C.788	1.399	1.185	0.878	0.895	1.337	0.133	-0.493
538	258.76	44.67	C.798	1.459	1.523	0.871	0.883	1.547	0.139	-0.548
539	257.12	44.59	C.801	1.469	1.908	0.845	0.859	1.923	0.169	-0.680
541	270.62	44.11	C.758	1.395	2.700	0.785	0.779	3.000	0.314	-0.985
542	275.57	43.92	C.742	1.370	3.099	0.758	0.734	3.571	0.396	-1.138
543	295.91	43.07	C.675	1.276	3.288	0.675	0.642	4.557	0.622	-1.293
544	456.88	34.12	C.058	0.910	0.359	0.774	0.829	1.411	0.450	-0.028
546	373.40	40.41	C.429	1.114	0.674	0.824	0.859	1.240	0.262	-0.197
547	336.85	44.66	C.602	1.235	0.914	0.836	0.867	1.361	0.214	-0.323
548	321.27	43.23	C.614	1.295	1.259	0.815	0.846	1.777	0.267	-0.425
550	305.70	42.63	C.642	1.361	1.995	0.769	0.801	2.564	0.353	-0.634
552	343.40	40.74	C.510	1.211	2.689	0.600	0.632	4.562	0.820	-0.853
553	451.71	34.87	C.094	0.984	0.781	0.606	0.736	2.777	0.737	-0.077
554	415.32	38.34	C.279	1.070	1.065	0.618	0.887	3.000	0.666	-0.258
555	387.23	38.72	C.356	1.147	1.406	0.626	0.727	3.074	0.666	-0.368
556	389.51	38.17	C.337	1.141	1.783	0.501	0.650	4.251	0.947	-0.481
557	400.15	37.55	C.295	1.110	1.858	0.431	0.598	5.009	1.165	-0.487

TABLE TWO PROPERTIES OF MIXTURES

PT	TC, K	PC, ATM.	X1	TR	PR	Z	(F/P)M	H	PSI 1	PSI 2
559	242.64	45.57	C.809	1.213	0.299	0.949	0.961	0.311	0.028	-0.117
561	222.93	46.69	C.898	1.320	0.729	0.904	0.920	0.875	0.045	-0.397
563	222.58	47.15	C.907	1.322	0.866	0.889	0.903	0.981	0.049	-0.473
565	213.50	45.99	C.920	1.378	1.480	0.836	0.859	1.753	0.066	-0.761
568	216.02	45.88	C.909	1.362	2.076	0.770	0.797	2.600	0.110	-1.097
579	250.02	45.55	C.783	1.244	0.448	0.927	0.940	0.489	0.047	-0.168
582	236.86	47.42	0.862	1.313	0.861	0.886	0.901	0.996	0.067	-0.421
584	224.11	45.94	0.881	1.387	1.481	0.841	0.863	1.721	0.091	-0.671
587	227.80	45.78	0.865	1.365	2.081	0.772	0.799	2.592	0.153	-0.978
591	235.73	45.67	C.835	1.319	2.607	0.725	0.731	3.432	0.245	-1.241
598	276.86	44.86	C.678	1.183	0.455	0.910	0.929	0.586	0.077	-0.163
599	263.94	45.73	C.739	1.241	0.595	0.901	0.919	0.759	0.083	-0.234
602	246.35	46.82	C.819	1.330	1.163	0.848	0.872	1.486	0.118	-0.536
605	237.84	45.64	C.827	1.377	1.864	0.797	0.823	2.265	0.161	-0.771
607	240.98	45.58	C.815	1.359	2.242	0.764	0.784	2.791	0.212	-0.932
609	248.51	45.43	C.786	1.318	2.546	0.725	0.735	3.379	0.294	-1.081
612	263.09	45.08	C.729	1.245	2.793	0.642	0.654	4.295	0.467	-1.257
613	289.65	44.23	C.622	1.131	2.886	0.509	0.523	5.696	0.842	-1.386
614	390.70	39.44	C.172	0.881	0.259	0.837	0.877	0.790	0.737	-0.049
620	266.22	46.44	C.745	1.293	1.172	0.828	0.857	1.616	0.167	-0.487
622	255.46	45.28	C.759	1.348	1.804	0.780	0.812	2.337	0.218	-0.687
624	256.98	45.24	C.753	1.340	2.106	0.750	0.781	2.788	0.266	-0.810
628	274.63	44.74	C.683	1.254	2.662	0.652	0.672	4.079	0.490	-1.055
630	291.10	44.17	C.616	1.183	2.788	0.570	0.594	4.932	0.706	-1.132
631	403.22	38.75	C.111	0.895	0.351	0.792	0.844	1.185	0.351	-0.044
637	277.92	44.74	C.672	1.299	1.521	0.779	0.817	2.181	0.261	-0.534
640	292.56	44.12	C.610	1.234	2.159	0.624	0.697	3.724	0.521	-0.814
644	306.94	43.56	C.550	1.176	2.653	0.557	0.597	4.870	0.769	-0.940
657	325.17	42.77	C.472	1.161	2.418	0.525	0.599	4.798	0.839	-0.750
658	399.31	39.34	C.142	0.987	0.692	0.688	0.775	2.083	0.520	-0.086
659	378.70	41.33	C.265	1.041	0.823	0.700	0.779	2.158	0.463	-0.167
664	339.29	42.11	C.410	1.162	1.939	0.520	0.647	4.195	0.784	-0.545
666	350.45	41.57	C.360	1.125	2.069	0.447	0.588	4.993	0.996	-0.560
670	221.66	46.19	C.894	1.328	0.589	0.925	0.938	0.646	0.033	-0.277
675	220.96	47.11	C.912	1.332	0.867	0.892	0.906	0.964	0.045	-0.469
678	215.21	45.88	C.912	1.367	1.854	0.790	0.819	2.296	0.094	-0.973
682	215.21	45.88	C.912	1.367	4.449	0.765	0.659	4.604	0.188	-1.946
686	200.64	46.16	0.970	1.467	0.737	0.941	0.946	0.604	0.009	-0.304
689	199.59	45.92	0.970	1.474	1.482	0.880	0.891	1.431	0.021	-0.663
691	199.37	45.87	0.970	1.476	2.225	0.837	0.844	2.130	0.030	-0.969
693	199.37	45.87	0.970	1.476	3.708	0.808	0.768	3.350	0.047	-1.526
694	199.37	45.87	0.970	1.476	4.450	0.822	0.743	3.741	0.053	-1.705
697	235.34	46.15	C.845	1.321	0.590	0.924	0.936	0.662	0.046	-0.251
704	220.60	45.97	C.894	1.410	1.480	0.853	0.872	1.638	0.077	-0.650
707	220.05	45.85	C.894	1.413	2.968	0.791	0.772	3.125	0.145	-1.222
709	220.05	45.85	C.894	1.413	4.452	0.793	0.699	4.227	0.196	-1.651

TABLE TWO PROPERTIES OF MIXTURES

PT	TC, K	PC, ATM.	X1	TR	PR	Z	(F/P)M	H	PSI 1	PSI 2
713	218.68	46.62	C.912	1.422	0.730	0.932	0.940	0.657	0.028	-0.287
716	215.70	45.99	C.912	1.442	1.480	0.867	0.881	1.536	0.060	-0.624
719	215.21	45.88	C.912	1.445	2.966	0.807	0.790	2.931	0.113	-1.174
721	215.21	45.88	C.912	1.445	4.449	0.807	0.721	3.982	0.154	-1.593
726	201.54	46.37	C.970	1.543	0.881	0.948	0.947	0.636	0.010	-0.325
729	199.37	45.87	C.970	1.560	1.854	0.887	0.892	1.577	0.021	-0.679
732	199.37	45.87	C.970	1.560	3.708	0.843	0.810	2.874	0.038	-1.239
733	199.37	45.87	C.970	1.560	4.450	0.854	0.787	3.226	0.043	-1.391
737	238.72	46.81	C.845	1.372	0.727	0.919	0.931	0.752	0.052	-0.283
740	233.74	45.83	C.845	1.402	1.485	0.850	0.869	1.672	0.108	-0.589
743	233.10	45.71	C.845	1.405	2.977	0.787	0.768	3.183	0.203	-1.105
745	233.10	45.71	C.845	1.405	4.466	0.790	0.693	4.294	0.273	-1.486
750	226.77	47.25	C.894	1.445	0.864	0.928	0.932	0.767	0.039	-0.326
753	220.06	45.85	C.894	1.489	1.855	0.860	0.870	1.792	0.079	-0.666
757	220.05	45.85	C.894	1.489	4.452	0.827	0.752	3.650	0.160	-1.353
761	218.68	46.62	C.912	1.498	0.730	0.948	0.950	0.561	0.023	-0.234
764	215.70	45.99	C.912	1.519	1.480	0.896	0.903	1.316	0.049	-0.508
769	215.21	45.88	C.912	1.522	4.449	0.840	0.770	3.438	0.126	-1.305
775	201.01	46.25	C.970	1.630	1.177	0.942	0.943	0.836	0.012	-0.392
778	199.37	45.87	C.970	1.643	2.225	0.897	0.898	1.612	0.020	-0.659
781	199.37	45.87	C.970	1.643	4.450	0.891	0.823	2.808	0.036	-1.150
786	242.10	47.47	C.845	1.422	0.860	0.922	0.929	0.803	0.055	-0.298
788	233.74	45.83	C.845	1.473	1.485	0.879	0.890	1.449	0.089	-0.485
791	233.10	45.71	C.845	1.477	2.977	0.823	0.806	2.753	0.167	-0.910
793	233.10	45.71	C.845	1.477	4.466	0.823	0.743	3.749	0.226	-1.235
798	226.77	47.25	C.894	1.518	0.864	0.945	0.944	0.656	0.032	-0.266
801	220.06	45.85	C.894	1.564	1.855	0.888	0.893	1.568	0.066	-0.555
804	220.05	45.85	C.894	1.564	3.710	0.845	0.812	2.854	0.119	-1.008
805	220.05	45.85	C.894	1.564	4.452	0.856	0.789	3.204	0.134	-1.130
809	218.68	46.62	C.912	1.574	0.730	0.960	0.959	0.493	0.019	-0.196
812	215.70	45.99	C.912	1.596	1.480	0.920	0.921	1.161	0.041	-0.426
815	215.21	45.88	C.912	1.600	2.966	0.872	0.857	2.196	0.077	-0.794
817	215.21	45.88	C.912	1.600	4.449	0.868	0.805	3.005	0.105	-1.086
822	201.54	46.37	C.970	1.708	0.881	0.970	0.966	0.504	0.007	-0.235
825	199.37	45.87	C.970	1.727	1.854	0.931	0.932	1.216	0.015	-0.473
828	199.37	45.87	C.970	1.727	3.708	0.896	0.874	2.182	0.026	-0.850
833	238.72	46.81	C.845	1.512	0.727	0.950	0.952	0.549	0.034	-0.187
836	233.74	45.83	C.845	1.544	1.485	0.904	0.908	1.274	0.075	-0.407
839	233.10	45.71	C.845	1.548	2.977	0.852	0.837	2.416	0.140	-0.762
841	233.10	45.71	C.845	1.548	4.466	0.850	0.781	3.301	0.190	-1.037
846	226.77	47.25	C.894	1.592	0.864	0.957	0.954	0.575	0.026	-0.223
849	220.06	45.85	C.894	1.640	1.855	0.911	0.912	1.385	0.055	-0.467
851	220.05	45.85	C.894	1.640	2.968	0.884	0.870	2.065	0.082	-0.696
853	220.05	45.85	C.894	1.640	4.452	0.880	0.822	2.825	0.113	-0.950
860	215.70	45.99	C.912	1.673	1.480	0.936	0.937	1.026	0.035	-0.359
863	215.21	45.88	C.912	1.677	2.966	0.894	0.882	1.942	0.065	-0.670

TABLE TWO PROPERTIES OF MIXTURES

PT	TC, K	PC, ATM.	X1	TR	PR	Z	(F/P)M	H	PSI 1	PSI 2
865	215.21	45.88	C.912	1.677	4.449	0.890	0.838	2.658	0.088	-0.916
869	200.64	46.16	C.970	1.799	0.737	0.982	0.977	0.360	0.305	-0.150
873	199.37	45.87	C.970	1.810	1.854	0.946	0.948	1.084	0.012	-0.403
877	199.37	45.87	C.970	1.810	4.450	0.924	0.888	2.223	0.026	-0.826
886	233.10	45.71	C.845	1.620	2.233	0.891	0.892	1.680	0.093	-0.507
889	233.10	45.71	C.845	1.620	4.466	0.874	0.813	2.922	0.161	-0.877
895	224.74	46.83	C.894	1.680	1.163	0.951	0.951	0.755	0.032	-0.269
899	220.05	45.85	C.894	1.716	2.968	0.904	0.894	1.830	0.070	-0.589
901	220.05	45.85	C.894	1.716	4.452	0.901	0.854	2.508	0.096	-0.806
907	219.30	46.75	C.912	1.722	1.164	0.957	0.957	0.712	0.025	-0.262
913	215.21	45.88	C.912	1.755	4.449	0.510	0.868	2.386	0.076	-0.786
921	199.37	45.87	C.970	1.894	1.854	0.958	0.961	0.959	0.011	-0.340
925	199.37	45.87	C.970	1.894	4.450	0.942	0.911	2.044	0.022	-0.727
932	233.74	45.83	C.845	1.687	1.485	0.939	0.939	1.009	0.054	-0.294
937	233.10	45.71	C.845	1.691	4.466	0.895	0.844	2.602	0.137	-0.748
943	224.74	46.83	C.894	1.754	1.163	0.960	0.961	0.686	0.028	-0.234
946	220.05	45.85	C.894	1.792	2.226	0.931	0.934	1.301	0.048	-0.401
949	220.05	45.85	C.894	1.792	4.452	0.920	0.881	2.272	0.083	-0.699
955	219.30	46.75	C.912	1.798	1.164	0.966	0.966	0.653	0.022	-0.231
959	215.21	45.88	C.912	1.832	2.966	0.930	0.924	1.573	0.048	-0.497
961	215.21	45.88	C.912	1.832	4.449	0.928	0.894	2.176	0.066	-0.686
966	201.54	46.37	C.970	1.956	0.881	0.988	0.876	0.375	0.005	-0.156
970	199.37	45.87	C.970	1.978	2.225	0.962	0.961	1.013	0.011	-0.344
973	199.37	45.87	C.970	1.978	4.450	0.958	0.928	1.912	0.020	-0.651
978	249.76	45.56	C.784	1.245	0.448	0.927	0.941	0.488	0.046	-0.168
986	256.24	46.74	C.784	1.279	0.728	0.890	0.909	0.948	0.089	-0.323
990	296.45	44.61	C.608	1.161	0.578	0.876	0.898	0.847	0.128	-0.199
997	277.36	46.38	C.707	1.241	0.734	0.874	0.898	1.001	0.118	-0.285
1005	249.03	45.42	C.784	1.382	1.873	0.800	0.826	2.254	0.189	-0.686
1008	249.03	45.42	C.784	1.382	3.745	0.756	0.702	4.089	0.340	-1.234
1016	302.94	45.59	C.608	1.191	0.746	0.850	0.880	1.111	0.161	-0.250
1023	269.23	45.02	C.707	1.341	1.512	0.808	0.838	1.978	0.213	-0.513
1028	268.63	44.92	C.707	1.344	4.545	0.755	0.634	4.860	0.510	-1.231
1040	249.03	45.42	C.784	1.449	4.494	0.811	0.723	3.973	0.314	-1.140
1041	369.36	41.08	C.287	1.022	0.616	0.775	0.827	1.481	0.341	-0.137
1044	337.75	44.55	C.475	1.118	0.901	0.756	0.812	1.808	0.315	-0.285
1053	293.04	44.10	C.608	1.289	2.314	0.698	0.730	3.386	0.453	-0.702
1055	293.04	44.10	C.608	1.289	4.629	0.725	0.579	5.390	0.704	-1.092
1062	268.63	44.92	C.707	1.406	4.545	0.794	0.691	4.329	0.434	-1.048
1069	249.03	45.42	C.784	1.516	4.494	0.840	0.766	3.495	0.264	-0.958
1071	370.40	41.20	C.287	1.064	0.661	0.794	0.838	1.406	0.308	-0.124