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PROJECT TITLE: Phase Behavior of Coal Fluids: Data for Correlation
                 Development

REPORT PERIOD: August 15, 1989 to October 15, 1989

SUMMARY

During the present report period, our framework for correlating
saturation properties using the scaled-variable-reduced-coordinate approach
was used to develop a correlation for saturated liquid densities of pure
fluids at temperatures from the triple point to the critical point. The new
correlation results in precise representation of liquid densities of diverse
chemical species with average errors of 0.12% when two adjustable parameters
are used to characterize each substance. In addition, the proposed model
compares favorably with the modified Rackett and the Hankinson-Thomson
correlations with the added advantages of covering the full saturation range
and obeying scaling-law behavior in the near-critical region. Although the
approach is essentially empirical, the results obtained suggest an underlying
physical significance for the model parameters and show an excellent potential
for generalized predictions. This is demonstrated by the results given here
for saturated liquid densities where fully generalized predictions yield
average errors of less than 1.0%.

DISCLAIMER

PHASE BEHAVIOR OF COAL FLUIDS:

DATA FOR CORRELATION DEVELOPMENT

Report for the Period
August 15, 1989 to October 15, 1989

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PHASE BEHAVIOR OF COAL FLUIDS:
DATA FOR CORRELATION DEVELOPMENT

ABSTRACT

The effective design and operation of processes for conversion of coal to fluid fuels requires accurate knowledge of the phase behavior of the fluid mixtures encountered in the conversion process. Multiple phases are present in essentially all stages of feed preparation, conversion reactions and product separation; thus, knowledge of the behavior of these multiple phases is important in each step. The overall objective of the author's work is to develop accurate predictive methods for representation of vapor-liquid equilibria in systems encountered in coal conversion processes. The objectives of the present project include:

(1) Measurements of binary vapor-liquid phase behavior data for selected solute gases (e.g. CO_2 and C_2H_6) in a series of heavy hydrocarbon solvents to permit evaluation of interaction parameters in models for phase behavior. Both solubilities of the gases in the liquid phase and of the heavy solvents in the gas phase will be determined.

(2) Measurements on ternary systems in which high-melting-point solvents are dissolved in more volatile aromatics to provide mixed solvents; this will facilitate measurements at lower temperatures than would be possible in the pure high-melting-point aromatic solvents, which would be solid at operating conditions.

(3) Evaluation of existing equations-of-state and other models for representation of phase behavior in systems of the type studied experimentally; development of new correlation frameworks as needed.

(4) Generalization of the interaction parameters for the solutes studied to a wide spectrum of heavy solvents; presentations of final results

in formats useful in the design/optimization of coal liquefaction processes.

During the present report period, our framework for correlating saturation properties using the scaled-variable-reduced-coordinate approach was used to develop a correlation for pure fluid saturated liquid densities at temperatures from the triple point to the critical point. The new correlation results in precise representation of the saturated liquid densities of diverse chemical species with average errors of 0.12% when two adjustable parameters are used to characterize eac ı substance. In addition, the proposed model compares favorably with the modified Raokett and the Hankinson-Thomson correlations with the added advantages of covering the full saturation range and obeying scaling-law behavior in the near-critical region.

Although the approach is essentially empirical, the results obtained suggest an underlying physical significance for the model parameters and show an excellent potential for generalized predictions. This is demonstrated by the results given here for saturated liquid densities where fully generalized predictions yield average errors of less than 1.0%.

INTRODUCTION

Saturated pure fluid properties play a major role in both the theoretical understanding of phase behavior and the design and operation of a multitude of industrial processes. Such properties are essential both when used directly in calculations or when used as input variables in a variety of models and applications.

In previous studies (1-3) we have demonstrated a need for precise pure-fluid saturation properties, especially vapor pressure and liquid density, in our overall effort to develop accurate correlations for phase equilibrium behavior of coal fluids. Such data have been used to estimate the

input variables (e.g. T_c, P_c, ω) for a number of generalized-parameter equations of state that we have developed to facilitate prediction of mixture properties.

The literature contains several correlations for predicting saturated liquid densities (4-8). A careful analysis of the existing methods, however, reveals limitations in terms of their range of applicability and/or lack of suitablity for generalization.

The majority of the existing correlations are based on one of two approaches, each offering certain advantages: equations of state (EOS) (9-11), or corresponding states theory (CST) (12-15). We have recently developed a unified framework for the correlation of saturation properties which utilizes CST concepts (16). The merits of the proposed approach were demonstrated in our previous work dealing with vapor pressure predictions. The present work is a continuation of our efforts to provide correlations for other saturation properties. Specifically, we sought to use the general framework presented earlier (16) to develop a correlation for pure-fluid saturated liquid densities. The desired characteristics of such a correlation are:

(1) ability to correlate the saturated liquid density with high precision over the full saturation range,

(2) ability to satisfy establish.d theoretical limiting behavior in the near-critical region,

(3) suitability for generalization to provide predictive capability,

(4) ability to predict the behavior of fluids of widely varying chemical nature, and

(5) simplicity.

MODEL DEVELOPMENT

We define a function $\Theta(\epsilon)$ such that (16):

$$(Y_\infty^\alpha - Y^\alpha)/(Y_\infty^\alpha - Y_o^\alpha) = \Theta(\epsilon) \tag{1}$$

or

$$Y^\alpha = Y_\infty^\alpha[1 - \Theta(\epsilon)] + \Theta(\epsilon)Y_o^\alpha \tag{2}$$

where

$$\epsilon = (X_\infty - X)/(X_\infty - Y_o) \tag{3}$$

X = correlating variable

Y = saturation property at given X

Y_∞ = asymptotic value of saturation property at X_∞

Y_o = initial value of saturation property at X_o

α = scaling exponent

In the present study, we selected the initial condition as the fluid triple point and the upper asymptotic limit as the critical point. However, the definitions for $\Theta(\epsilon)$ and ϵ are general and any two well defined limits could be used.

For the liquid densities, we use the same definition for Θ as previously proposed for correlation of vapor pressure (16),

$$\Theta = (1 - A^{\epsilon^B})/(1 - A) \tag{4}$$

and introduce a new form for α ,

$$\frac{\alpha_c - \alpha}{\alpha_c - \alpha_t} = (1-A^\epsilon)/(1-A) \tag{5}$$

where,

$$\epsilon = (T_c-T)/(T_c-T_t) \tag{6}$$

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A,B — model parameters

α_c — the value of α at the critical temperature

α_t — the value of α at the triple point temperature

Thus, recasting Equation (1) as:

$$Y = \left(Y^{\alpha}_c - (Y^{\alpha}_c - Y^{\alpha}_t)\,\Theta\right)^{(1/\alpha)} \tag{7}$$

and applying Equations (4), (5), and (6) as definitions for Θ, α, and ϵ, respectively, one would obtain our proposed model for the correlation of saturated liquid densities, where Y becomes ρ_L.

Figure 1 illustrates the variation of the scaled densities with scaled temperature, ϵ, for a number of compounds with different degrees of acentricity and polarity. The figure indicates that the reduced density depends on both the temperature and the chemical structure of the substance.

Using the proposed framework given by Equation (7), the variations in the liquid density with temperature and chemical structure are represented in terms of two simple functions (Θ and α) both of which are temperature dependent. The first, as shown in Figure 2, presents the effect of reduced temperature on the correlating function, Θ, and the second, as shown in Figure 3, depicts the variation of the scaling exponent, α, with reduced temperature, ϵ. Inspection of Figures 2 and 3 reveals that the proposed correlation:

(a) provides for a universal representation for scaled-then-reduced densities*, Θ, in terms of the reduced temperature, ϵ, and

(b) accounts for variation due to the chemical structure through the limiting values of the scaling exponent (α_c and α_t).

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* In the context of this work, a scaled variable is one which is raised to a power, e.g., Y^{α}, and a reduced variable is one divided by the critical property or the adjusted critical, i.e., Y/Y_c or $(Y_c-Y)/(Y_c-Y_t)$.

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CRITERIA OF EVALUATION

One of the desired features of the saturation property correlation is accurate representation of experimental data (within their uncertainty) over the complete saturation range. Figures 4A and 4B illustrate the ability of the proposed correlating framework, as shown for ethane. While regression of the three model parameters (A, α_c, α_t) of the proposed liquid density correlation certainly fits the experimental data within their precision, the quality of fit produced by regressing only one model parameter remains excellent and compares favorably with the results obtained from the Hankinson-Thomson (6) and the modified Rackett (4) equations within the range of application deemed most appropriate for these two correlations (0.25 < T_r < 0.95).

Scaling-law behavior provides a constraint on the behavior of density near the critical point (17). In the immediate vicinity of the critical point, coexisting densities should be described by

$$\frac{\rho - \rho_c}{\rho_c} = \pm \, C \, \left| \frac{T - T_c}{T_c} \right|^{\beta} \tag{8}$$

where β is a universal scaling exponent and C is a system dependent coefficient. Accordingly, to satisfy our stated requirement of obeying the theoretical limits of behavior at the critical point, our proposed model must, in an expanded form, yield a leading term with the appropriate scaling-law exponent (18). Further, it must describe the critical point anomaly given by the following derivatives:

$$\lim_{T \to T_c} \left(\frac{d\rho}{dT} \right) = \infty \tag{9}$$

and

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$$\lim_{T \to T_c} \left(\frac{d^2 \rho}{dT^2}\right) = \infty \tag{10}$$

In an expanded form, our model can be written as,

$$\rho = \rho_c + a_1 \, \epsilon^B + a_2 \, \epsilon^{2B} + \dots \tag{11}$$

Thus, the model meets both of the requirements stated above and provides the correct behavior in the near-critical region, since $B < 1$. The currently accepted value for β, as predicted by three-dimensional Ising models, is 0.325 (18). This is the value that we have adopted for B in Equation (4).

Following the works of Charoensombut-amon and Kobayashi (19) and our previous work correlating mixture phase properties (20), one can extend the range of usefulness of Equation (8) to lower temperatures by coupling the order parameter equation

$$\phi_+ - \phi_- = \sum_{i=o}^{N} b_i(\tau)^{\beta + i\Delta} \tag{12}$$

and the rectilinear diameter equation

$$(\phi_+ + \phi_-)/2 = \phi_c + a_0(\tau)^{1-\bar{\alpha}} + \sum_{j=1}^{M} a_j(\tau)^j \tag{13}$$

to develop the following expression for the correlation of coexisting phase densities.

$$\phi_+ = \phi_c + a_0(\tau)^{1-\bar{\alpha}} + \sum_{j=1}^{M} a_j \, (\tau)^j \pm \frac{1}{2} \sum_{i=0}^{N} b_i(\tau)^{\beta + i\Delta} \tag{14}$$

where $\qquad \tau = (T_c - T)/T_c$

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ϕ — order parameter (+/- for the liquid and vapor phase, respectively)

$\bar{\alpha}, \beta$ — universal scaling-law exponents

N,M — number of expansion terms

a,b — system-specific constants

The leading term (i=0) of Equation (12) is the limiting scaling-law behavior of the order parameter, ϕ, and the subsequent terms in the summation are the Wegner corrections (21) to the limiting scaling behavior. While such an extension is capable of precise correlation of phase densities for both pure fluids and mixtures (using scaling pressure as a correlating variable), several parameters are required (a_i's and b_i's) and difficulty in generalizing these parameters deters further development. However, comparison of Equations (11) and (14) suggests that the proposed model produces a functional form similar to that obtained from extended scaling with an added advantage of being a closed-form equation.

DATA BASE EMPLOYED

Tables I and II present the data base employed in this study. Listed in Table I are the sources and ranges of data taken from the literature. Table II presents the critical and triple point properties used, along with their sources.

DATA REDUCTION PROCEDURE

The following least squares objective function, SS, was used in all model evaluations:

$$SS = \Sigma((\rho_{calc} - \rho_{exp})/\rho_{exp})^2 \tag{15}$$

where,

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ρ_{exp} = experimental density

ρ_{calc} = calculated density

A Marquart (22) nonlinear regression procedure was employed in the calculations. Definitions of the statistical quantities used to evaluate the results are given in the Nomenclature.

MODEL EVALUATION

As indicated by Equations (4) and (5), the proposed correlation contains four parameters, A, B, α_c and α_t. Our studies, however, have indicated that a good level of precision may be obtained by treating some of the parameters as universal constants that apply to all fluids.

Four specific cases were studied and results are presented in Tables III and IV. In Case 1, B is treated as a universal constant, while α_c, α_t and A are substance-specific. In Case 2, only α_c and α_t are treated as substance-specific. In Case 3, $\Delta\alpha$, (α_c - α_t), comes from a generalized equation and only α_c is treated as substance-specific. In case 4, the model is completely generalized; that is, no substance-specific parameters are used.

Comparison of the results for the four cases indicates that for the most accurate representation of experimental data, the flexibility offered by a three constant equation is desirable and leads to precise representation of the experimental data for the various fluids considered (RMSE = 1.14 kg/m3 and % AAD = 0.11). By comparison, the results of Case 2, where we have a two-constant model, show only minor deterioration in the overall quality of the fit (RMSE = 1.42 kg/m3, % AAD = 0.12). Possibly more significant from a correlation point of view, however, is the distribution of error for a given fluid, where (as expected) Case 1 produces better error distribution as shown in Figure 4A for ethane.

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Case 3 presents the results of a one parameter model, where α_c was retained as a system-specific parameter and advantage was taken of the observed relation between $\Delta\alpha$ and T_{rt}. Figure 5 shows this relation between $\Delta\alpha$ and T_{rt}, where values shown for α_c and α_t were obtained from the regressions for the two-parameter model. A linear relation was established between $\Delta\alpha$ and T_{rt} for simple fluids (those with Z_c values near 0.285).

$$\Delta\alpha = C_1 + C_2 \, T_{rt} \tag{16}$$

The variations exhibited by other fluids were accounted for by an exponential relation such that

$$\Delta\alpha = C_1 + C_2 \, T_{rt}^{(C_3 + C_4 Z_c)} \tag{17}$$

While the form of Equation (17) was merely a depiction of the observed variation of $\Delta\alpha$ with T_{rt} for simple fluids, the exponential term was selected to account for deviation from simple behavior through the value of Z_c. As shown in Table IV, the overall quality of the fit remains reasonable (RMS = 4.71 kg/m3, %AAD = 0.28), however, individual fluids such as water, show significant deviations.

Our one-parameter model as represented by Case 3 compares very favorably with the one-parameter models of the modified Rackett equation (4) and the Hankinson-Thomson correlation (6). As shown by the results given in Table IV, using the same data base and constrained to their recommended range of application, both the modifed Rackett correlation (RMSE = 10.24 kg/m3, %AAD = 0.63) and the Hankinson-Thomson correlation (RMSE = 9.04 kg/m3, %AAD = 0.53) produce about twice the error obtained from the present correlation. Perhaps more importantly, the new model covers the full saturation range, while the literature models were evaluated only over the range of $0.25 < T_r < 0.95$.

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Case 4 presents the results of a completely generalized model in which the following form for α_c (developed on the similar arguments given above for $\Delta\alpha$) along with the above relation for $\Delta\alpha$ was used:

$$\alpha_c = C_5 + C_6 T_{rt}^{(C_7 + C_8\omega)} \tag{18}$$

Values for the constants C_1 through C_8 were obtained from regressions based on data for the first 14 compounds listed in Table I and are listed in Table V. The remaining eight compounds in Table I were used as checks on the generalized model and the errors shown are for predictions based on the parameters in Table V. As shown in Table IV, the only fluid which shows a significant deviation is water with a %AAD $-$ 6.2%. This may be attributed to the strong hydrogen-bonding nature of water.

The results of both the model evaluation (Cases 1-3) and the parameter generalization (Case 4) reveal the viability of the proposed model for the purposes of data reduction and generalized predictions. Comparison of the overall accuracy of the present model (%AAD $-$0.59) to similar generalization given by Hankinson and Thomson (6) and Thodos and coworkers (5) for a wide spectrum of chemical species confirms our conclusion, especially since the present model is developed from a multi-property framework.

As indicated by Equations (17) and (18), both Z_c and ω were employed for parameter generalization. The inadequacy of either parameter to fully characterize variation in molecular structure of anormal fluids has been documented in the past by several investigators (43-46), and attempts have been made to overcome such shortcoming. Our present studies on liquid densities and similar studies involving vapor pressures indicate a realistic possibility exists for the development of a meaningful indexing parameter for variation in molecular structure based on α_c. Perhaps such an undertaking will

facilitate generalized predictions for highly demanding molecular structures such as water.

CONCLUSIONS

A framework for correlating saturation properties using our scaled-variable-reduced-coordinate approach was used to develop a correlation for saturated liquid densities of pure fluids at temperatures from the triple point to the critical point. The new correlation results in precise representation of liquid densities of diverse chemical species with average errors of 0.12% when two adjustable parameters are used to characterize each substance. In addition, the proposed model compares favorably with the modified Rackett and the Hankinson-Thomson correlations with the added advantages of covering the full saturation range and obeying scaling-law behavior in the near critical region.

Although the approach is essentially empirical, the results obtained suggest an underlying physical significance for the model parameters and show an excellent potential for generalized predictions. This is demonstrated by the results given here for saturated liquid densities where fully generalized predictions yield average errors of less than 1.0%.

NOMENCLATURE

A,B	correlation constants
a,b	parameters in equations 12-14
N,M	number of expansion terms
T	temperature
Z	compressibility factor
X	correlating variable
Y	any saturation property
RMSE	root mean square error
%AAD	average absolute percent deviation
SS	objective function (defined by Equation (15))

Greek Symbols

α	correlation scaling exponent
α	scaling-law exponent

$\Delta\alpha$ $\alpha_c - \alpha_t$

β scaling-law exponent

ϵ reduced variable for property X

Θ correlating function

ρ saturated density

τ reduced temperature, $(T_c - T)/T_c$

ϕ order parameter

ω acentric factor

Subscripts

c   critical state

t   triple point state

calc   calculated

exp   experimental

L   liquid

r   reduced property

o   lower limiting value of saturation property

∞ upper limiting value of saturation property

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TABLE I

SOURCES OF LIQUID DENSITY DATA

Substance	Temperature Range, K			Density Range, kg/m3			Source	No. of Points
Methane	90.68	-	190.555	160.43	-	451.56	23	61
Ethane	90.348	-	305.33	204.48	-	651.92	24	60
Propane	85.47	-	369.80	218.69	-	732.78	25	121
n-Butane	134.86	-	425.16	227.85	-	735.27	26	73
Benzene	278.68	-	561.75	304.64	-	896.51	27	60
Nitrogen	63.15	-	126.26	314.10	-	869.70	28	33
Fluorine	53.481	-	144.31	573.80	-	1704.77	29	48
Argon	83.78	-	150.86	535.62	-	1414.8	30	70
Carbon Dioxide	216.58	-	304.14	467.72	-	1178.12	31	23
Ammonia	195.48	-	405.40	235.00	-	733.86	32	68
Methanol	175.4	-	512.7	274.73	-	904.98	33	37
Acetic Acid	293.15	-	594.75	350.60	-	1049.1	34	16
Acetone	329.25	-	508.15	273.00	-	750.00	35	10
Hydrogen Fluoride	189.58	-	461.15	290.00	-	1193.0	36	30
Water	273.16	-	647.13	322.00	-	999.78	37	39
Hydrogen	13.95	-	33.18	31.43	-	77.04	33	21
Propylene	87.89	-	365.57	223.00	-	768.85	38	30
Neon	24.56	-	44.448	483.00	-	1249.3	38	22
Oxygen	54.36	-	154.581	436.10	-	1306.8	38	12
Freon-12	170.00	-	384.95	558.00	-	1686.1	38	14
Decane	243.5	-	617.55	236.00	-	671.10	33	33
Cyclohexane	310.93	-	510.93	509.06	-	759.44	39	7
	288.15	-	313.15	759.67	-	783.31	40	5

TABLE II

PHYSICAL CONSTANTS OF COMPOUNDS

Substance	Critical Point		Triple Point		Source
	T, k	Density, kg/m^3	T, K	Density, kg/m^3	
Methane	190.555	160.43	90.68	451.56	23
Ethane	305.33	204.48	90.348	651.92	24
Propane	369.80	218.69	85.47	732.78	25
n-Butane	425.16	227.85	134.86	735.27	26
Benzene	561.75	304.64	278.68	896.51	27
Nitrogen	126.26	314.10	63.15	869.70	28
Fluorine	144.31	573.80	53.481	1704.77	29
Argon	150.86	535.62	83.78	1414.8	30
Carbon Dioxide	304.14	467.72	216.58	1178.12	31
Ammonia	405.40	235.00	195.48	733.86	32
Methanol	512.70	274.73	175.4	904.98	33
Acetic Acid	594.75	350.60	289.80	1052.87*	34,41
Acetone	508.15	273.00	178.20	947.32*	35,41
Hydrogen Fluoride	461.15	290.00	189.58	1193.0	36
Water	647.13	322.00	273.16	999.78	37
Hydrogen	33.18	31.43	13.95	77.04	33
Propylene	365.57	223.00	87.89	768.85	38
Neon	44.448	483.00	24.56	1249.3	38
Oxygen	154.581	436.10	54.36	1306.8	38
Freon-12	384.95	558.00	115.40	1829.29*	38,41
Decane	617.55	236.00	243.5	671.10	33
Cyclohexane	553.4	273.25	279.7	794.1*	41

* Triple point density regressed from three-parameter model

TABLE III

CORRELATION PARAMETERS

Substance	Case 1			Case 2		Case 3
	A	αc	Δα	αc	Δα	αc
Methane	1.192820	0.531302	0.079238	0.636918	0.066552	0.428392
Ethane	1.499230	0.672254	0.236881	0.572687	0.239784	0.380519
Propane	2.500740	1.068950	0.327583	0.552945	0.318268	0.365692
n-Butane	1.019980	0.355471	0.275795	0.581717	0.276026	0.373070
Benzene	0.278548	-0.849345	0.236635	0.557609	0.177584	0.348263
Nitrogen	5.423500	1.925250	-0.005172	0.537057	0.082804	0.315621
Fluorine	0.599509	-0.183069	0.097075	0.542442	0.054689	0.359816
Argon	0.398247	-0.735/35	0.009843	0.497804	-0.059298	0.293106
CO_2	0.621126	-0.200521	0.055424	0.620479	0.003598	0.376696
Ammonia	0.798606	0.095204	0.039926	0.542884	0.007054	0.401351
Methanol	0.264131	-0.511160	0.398588	0.798240	0.337027	0.620.77
Acetic Acid	0.639147	0.037820	0.176344	0.699849	0.132466	0.534503
Acetone	0.351800	-0.483746	0.660580	0.549669	0.836002	0.251259
HF	1.971120	0.760770	0.561794	0.489317	0.524031	0.353058
Water	5.490110	2.158090	-4.221360	0.860980	-1.777520	1.035930
Hydrogen	0.200381	-1.528160	-0.408874	0.585346	-0.811727	0.547744
Propylene	1.703880	0.706117	0.356525	0.509943	0.346465	0.322376
Neon	0.408403	-0.676931	-0.112287	0.558500	-0.255802	0.383015
Oxygen	0.675935	-0.088861	0.146368	0.523311	0.127753	0.329442
Freon-12	4.196760	1.522980	0.341602	0.557729	0.313227	0.350733
Decane	2.360260	1.046950	-0.143442	0.559018	-0.053490	0.423197
Cyclohexane	3.777440	1.614490	0.516924	0.637913	0.443701	0.323319

Case 1	B=0.325
Case 2	A=4/3, B=0.325
Case 3	A=1.07068, B=0.325, Δα from generalized model

TABLE IV

COMPARATIVE EVALUATION OF PRESENT WORK AND EXISTING METHODS FOR PREDICTION OF SATURATED LIQUID DENSITIES

| | This Work | | | | | | | | Literature | | | |
| Substance | Case 1 | | Case 2 | | Case 3 | | Case 4 | | Rackett (4) | | Hankinson-Thomson (6) | |
	RMSE, Kg/m³	%AAD	RMSE, Kg/m³	%AAD	RMSE, Kg/m³	%AAD	RMSE, Kg/m³	%AAD	RMSE, Kg/m³	%AAD	RMSE, Kg/m³	%AAD
Methane	0.64	0.14	0.63	0.14	0.64	0.15	1.84	0.63	0.37	0.09	0.58	0.13
Ethane	0.73	0.08	0.72	0.08	0.85	0.13	1.01	0.16	1.33	0.19	0.95	0.12
Propane	0.42	0.05	0.42	0.05	0.53	0.08	0.51	0.08	1.99	0.25	1.29	0.16
Butane	0.30	0.04	0.30	0.04	0.64	0.09	0.76	0.10	1.37	0.18	0.76	0.10
Benzene	1.52	0.25	1.77	0.29	2.19	0.33	2.38	0.35	1.38	0.14	1.95	0.19
Nitrogen	0.75	0.09	0.97	0.12	0.96	0.12	2.57	0.31	2.83	0.36	1.89	0.24
Fluorine	0.22	0.01	0.49	0.03	1.44	0.10	1.39	0.10	2.34	0.13	0.76	0.04
Argon	1.43	0.10	1.65	0.12	1.72	0.12	5.04	0.43	3.79	0.28	1.64	0.12
Carbon Dioxide	0.44	0.04	0.55	0.05	0.63	0.05	3.54	0.35	2.57	0.21	2.85	0.24
Ammonia	0.17	0.02	0.22	0.03	1.66	0.26	2.81	0.41	1.30	0.18	3.97	0.56
Methanol	2.80	0.33	2.88	0.36	2.75	0.34	2.74	0.34	19.37	2.38	15.80	1.91
Acetic Acid	0.69	0.06	0.73	0.07	1.68	0.18	6.36	0.68	19.93	2.03	7.41	0.73
Acetone	1.07	0.13	1.41	0.18	6.09	0.76	12.67	1.53	9.22	1.09	12.05	0.78
Hydrogen Fluoride	1.20	0.11	1.21	0.12	1.93	0.21	2.03	0.23 *	28.27	3.01	33.0	2.83
Water	2.93	0.29	4.50	0.40	21.07	2.24	54.87	6.23	31.67	3.07	23.73	2.10
Hydrogen	0.17	0.22	0.22	0.29	0.49	0.64	0.90	1.19	1.07	1.42	1.51	1.98
Propylene	0.38	0.05	0.41	0.06	0.87	0.11	2.70	0.44	4.30	0.54	3.85	0.48
Neon	0.84	0.07	1.08	0.09	2.68	0.23	3.32	0.30	3.51	0.29	5.08	0.38
Oxygen	0.54	0.04	0.61	0.05	0.57	0.05	2.52	0.23	3.08	0.23	1.25	0.08
Freon-12	1.32	0.08	1.62	0.09	3.17	0.19	3.88	0.25	6.42	0.26	5.31	0.22
Decane	0.86	0.11	0.90	0.11	3.28	0.50	3.19	0.51	2.44	0.26	2.76	0.37
Cyclohexane	1.03	0.12	1.14	0.13	3.00	0.39	3.57	0.41	2.08	0.24	2.04	0.24
Overall:	1.14	0.11	1.42	0.12	4.71	0.28	11.81	0.59	10.24	0.63	9.04	0.53

*Last eight compounds used as checks on the generalized model.

TABLE V

GENERALIZED CORRELATION PARAMETERS

Parameter	Value
A	1.07068
B	0.325
C_1	3.63493
C_2	-3.73713
C_3	0.32786
C_4	-0.90951
C_5	0.36141
C_6	2.95802
C_7	16.4993
C_8	-25.4640

FIGURE 1
LIQUID DENSITY VARIATION WITH TEMPERATURE

SOURCE

	Methane	Ethane	Propane	n-Butane
	Benzene	Nitrogen	Fluorine	Argon
	CO2	Ammonia	Methanol	Acetic Acid
	Acetone	HF	Water	
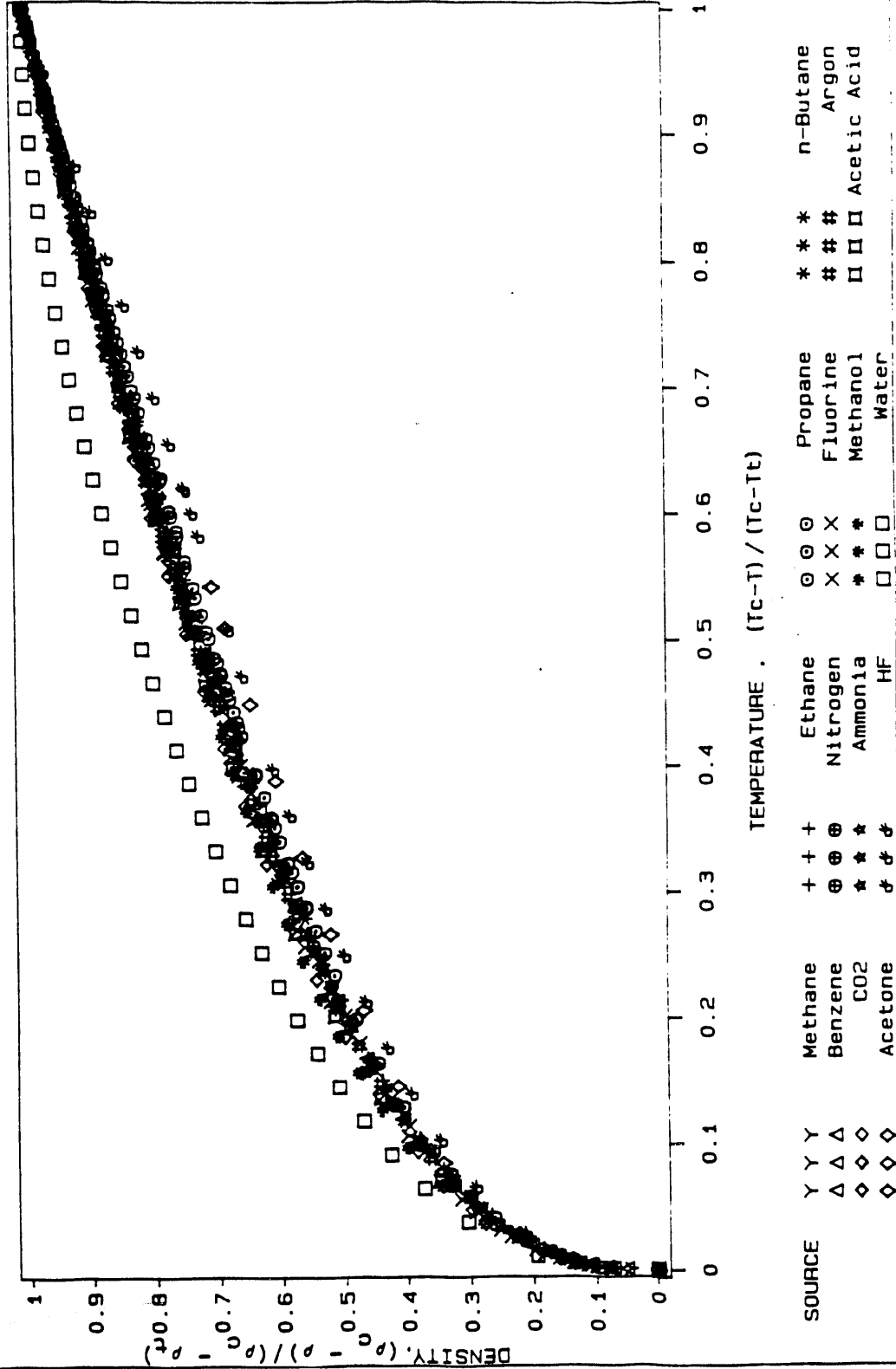
FIGURE 2
EFFECT OF TEMPERATURE ON
UNIVERSAL CORRELATING FUNCTION, θ

$\theta = (1 - A^{e^B})/(1 - A)$

A = 1.0707

B = 0.325

CORRELATING FUNCTION, θ

TEMPERATURE, $(Tc-T)/(Tc-Tt)$
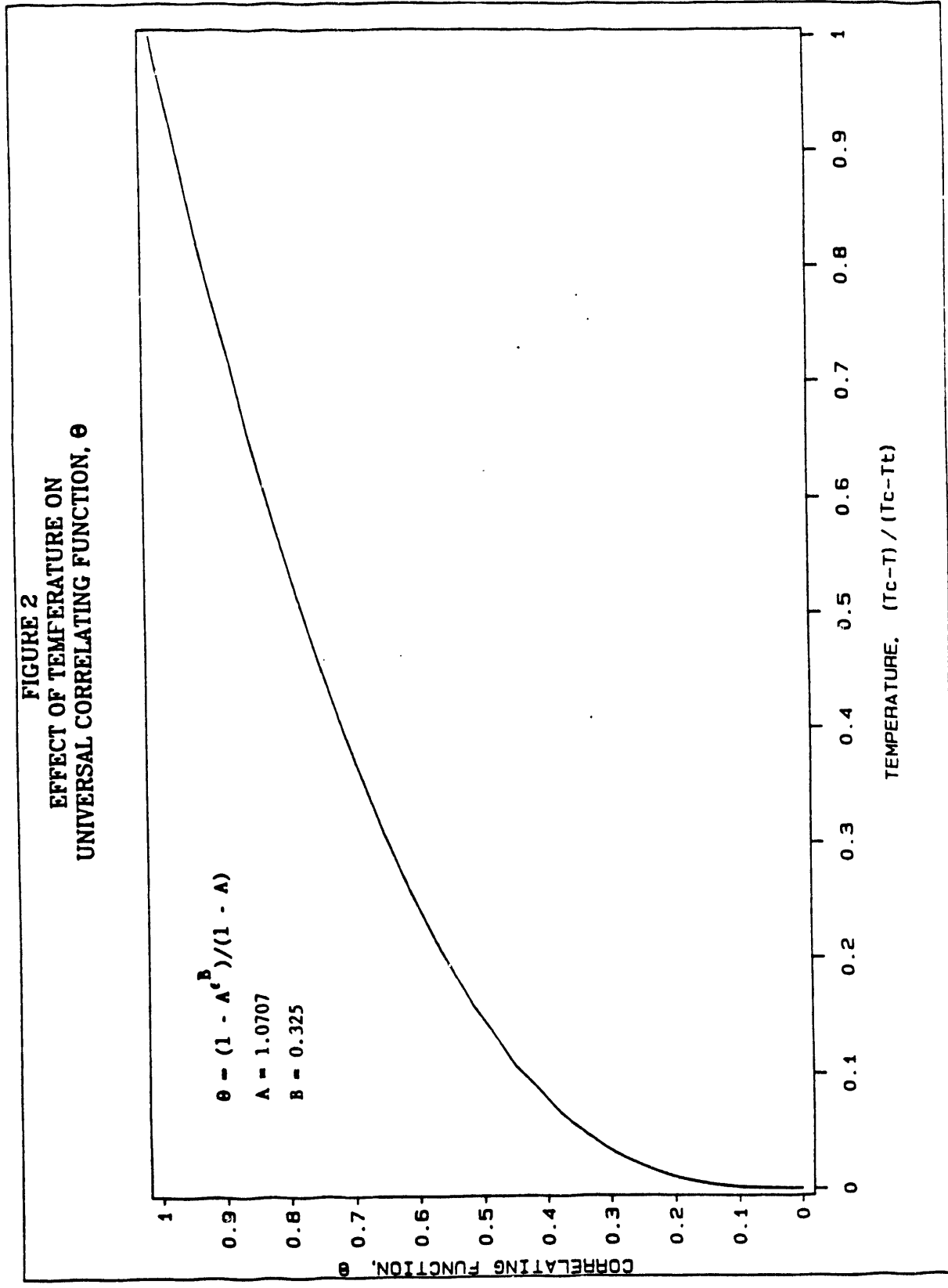
FIGURE 3
EFFECT OF TEMPERATURE ON
SCALING EXPONENT

FIGURE 4A
COMPARISON OF ETHANE
LIQUID DENSITY REPRESENTATIONS

% DEVIATION

TEMPERATURE . (Tc-T) / (Tc-Tt)

SOURCE ⊕ ⊕ ⊕ 3 Constants   □ □ □ 2 Constants   △ △ △ 1 Constant
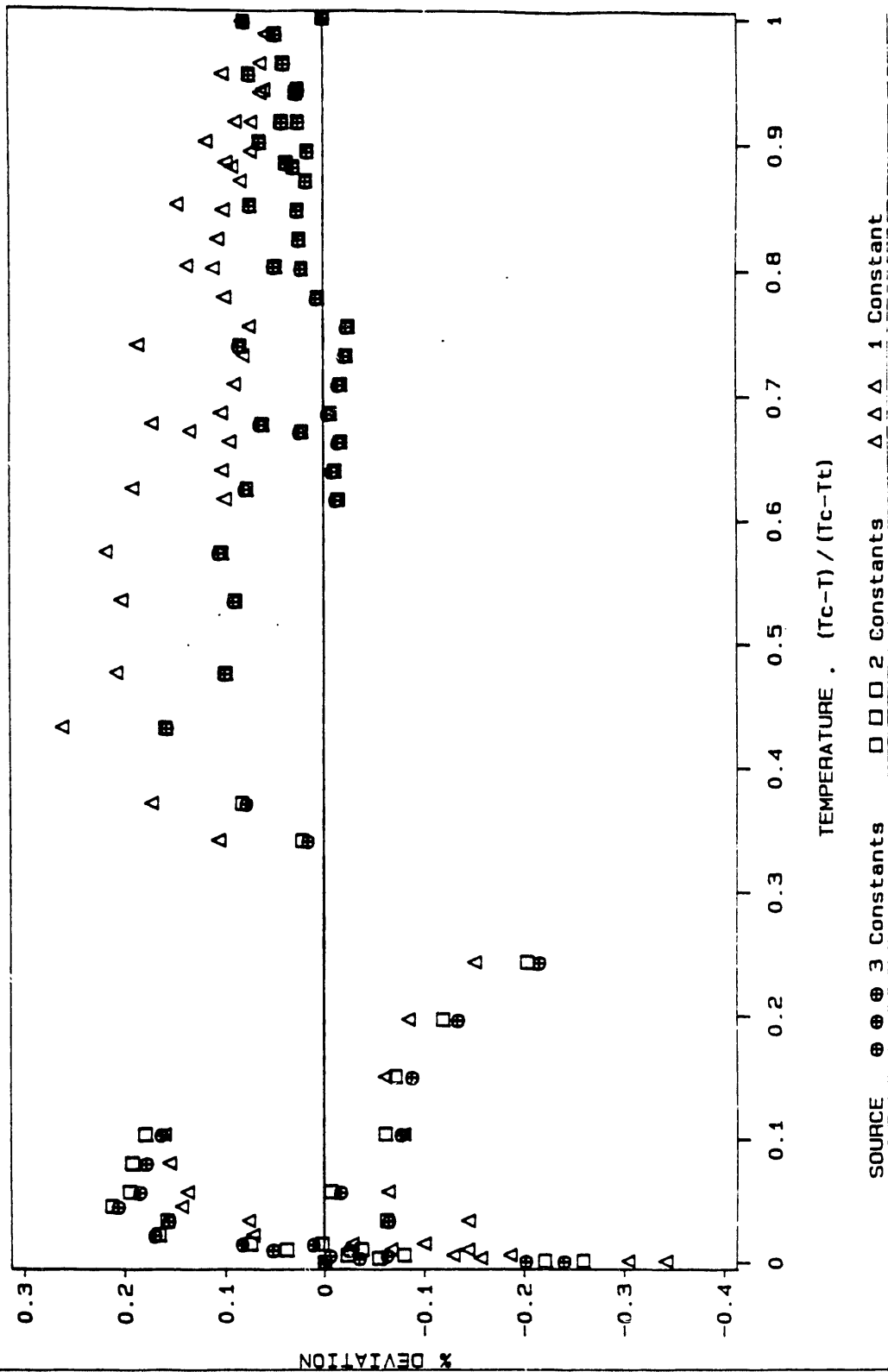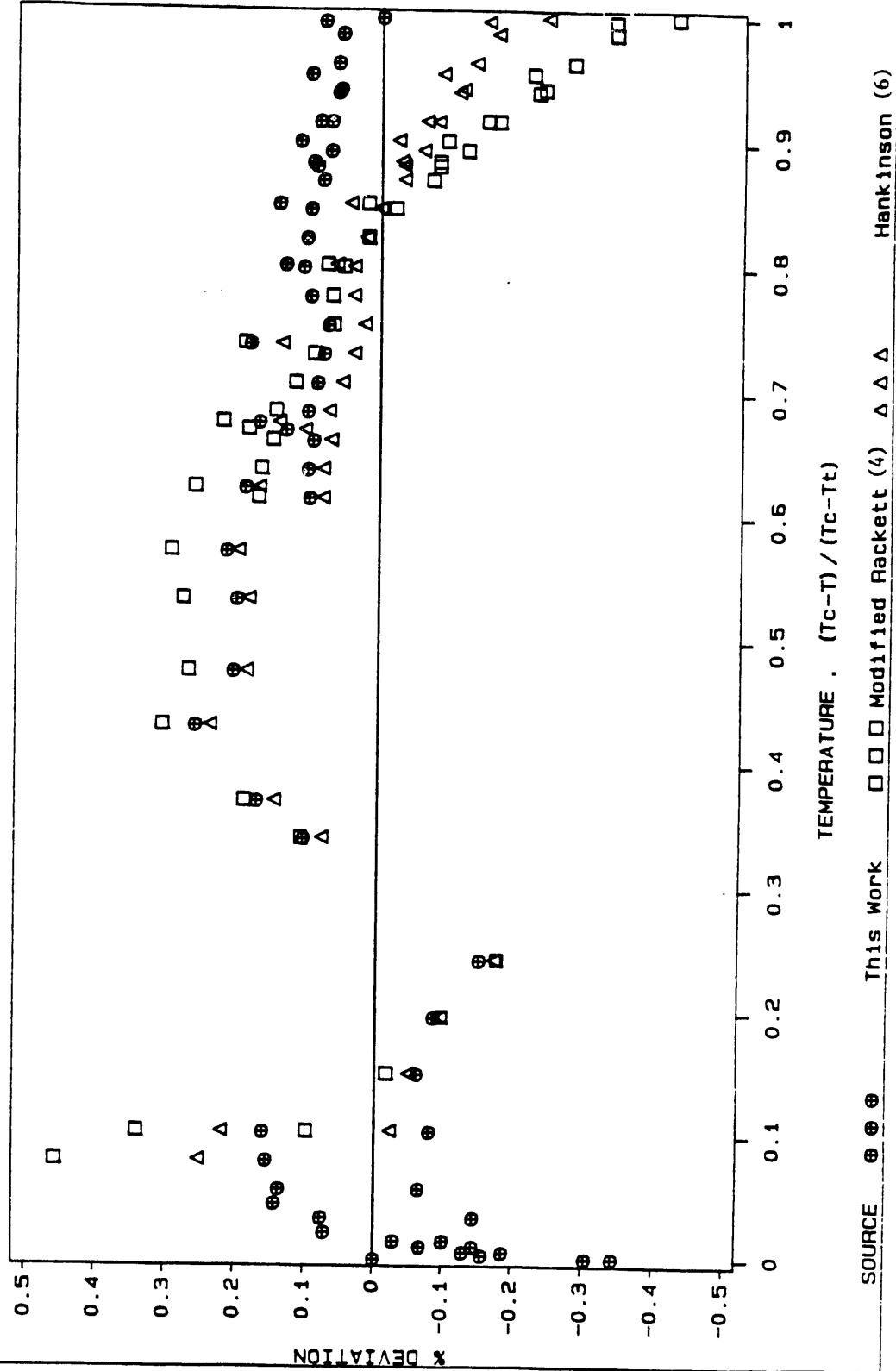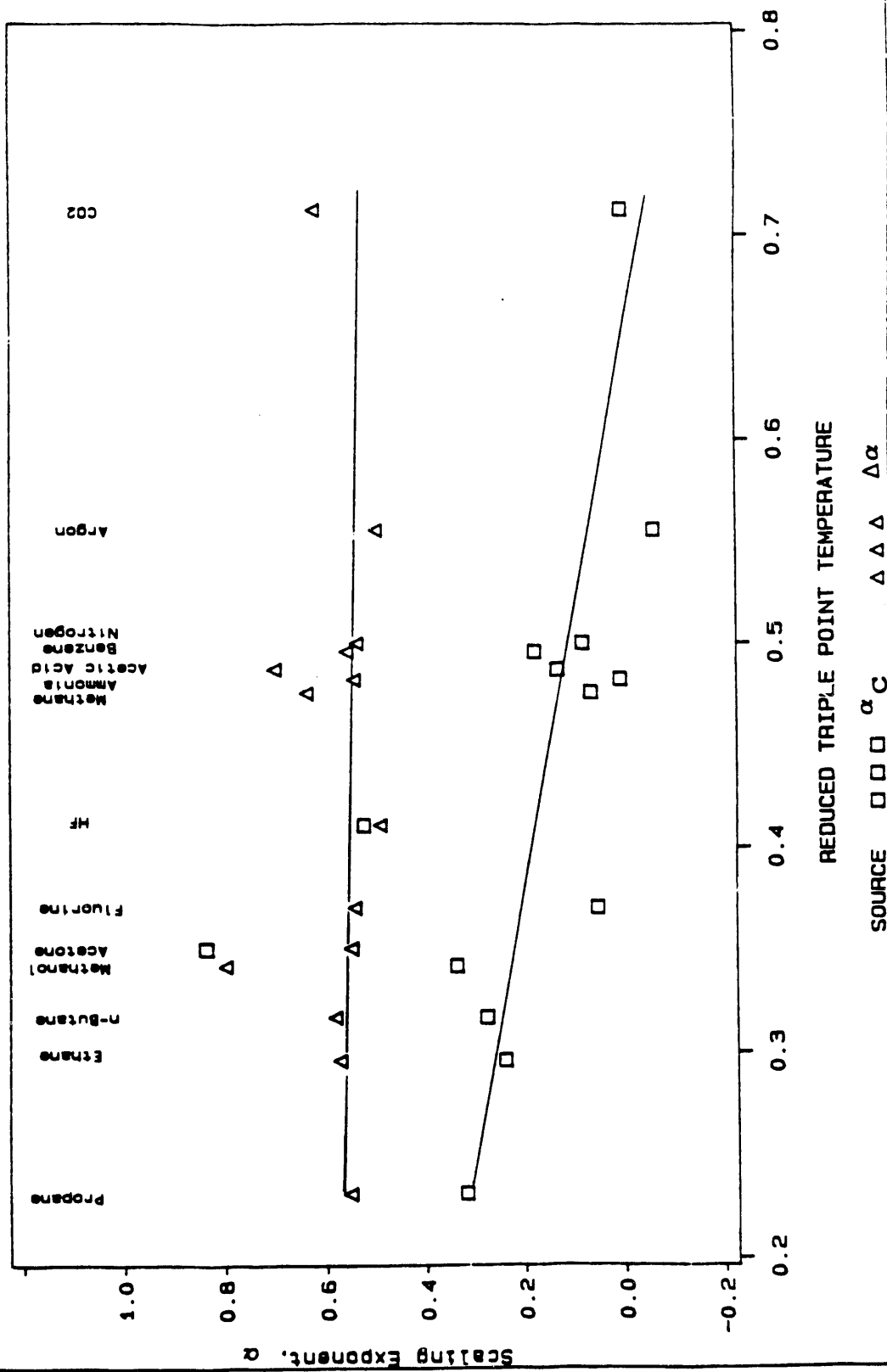
FIGURE 4B
COMPARISON OF ETHANE
LIQUID DENSITY REPRESENTATIONS

FIGURE 5
EFFECT OF REDUCED TRIPLE POINT TEMPERATURE
ON LIMITING VALUES OF SCALING EXPONENT

END

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2/04/92

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