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PHASE BEHAVIOR OF COAL FLUIDS:

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DATA FOR CORRELATION DEVELOPMENT

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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 a "scaled-variable-reduced-coordinate" approach was further developed to provide for generalized vapor pressure predictions. Utility of this approach is demonstrated by correlating the vapor pressures of a number of compounds at temperatures from the triple point to the critical point. The new correlation results in precise representation of vapor pressures of diverse chemical species, generally within their experimental uncertainties (%AAD within 0.1) when two adjustable parameters are used to characterize each substance. The proposed model compares favorably with existing correlations, while having 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, 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 vapor pressures, where generalized predictions yield average errors of less than 1.5% over the full saturation range, based on a single experimental measurement.

A UNIFIED FRAMEWORK FOR THE PREDICTION OF SATURATION PROPERTIES:
VAPOR PRESSURE PREDICTIONS

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ABSTRACT

A new framework is proposed for correlating saturation properties using a "scaled-variable-reduced-coordinate" approach. Utility of this approach is demonstrated by correlating the vapor pressures of a number of compounds at temperatures from the triple point to the critical point. The new framework results in precise representation of vapor pressures of diverse chemical species, generally within their experimental uncertainties (%AAD within 0.1) when two adjustable parameters are used to characterize each substance. The proposed model compares favorably with existing correlations, while having 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, 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 vapor pressures, where generalized predictions yield average errors of less than 1.5% over the full saturation range, based on a single experimental measurement.

INTRODUCTION

The saturation properties of pure fluids play a major role in both the theoretical understanding of fluid phase behavior and in 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 to a variety of models and applications.

In previous studies (1,2,3) we have demonstrated a need for precise pure-fluid saturation properties, especially vapor pressure and liquid density, in our overall effort of correlating phase equilibrium data for mixtures. 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 generalized predictions of mixture properties.

The literature contains many correlations (see, e.g., 4,5) for predicting saturation properties. A careful analysis of the existing methods, however, reveals inadequacies for even the prediction of such a basic property as the vapor pressure.

The majority of existing correlations are based on one of two approaches, each offering certain advantages: equations of state (EOS) (5,6,7), or corresponding states theory (CST) (4,8-12). In the present work, we present a unified framework for the correlation of saturation properties which utilizes the CST concepts.

Specifically, we sought to develop a framework for the proper reduction and correlation of pure-fluid saturation properties over a temperature range extending from the triple point to the critical point. The desired characteristics of such a framework are:

- (1) ability to correlate a number of saturation properties (at the desired precision) over the full saturation range,

- (2) ability to satisfy established theoretical limiting behavior for the properties considered,
- (3) ability to predict the behavior of fluids of widely varying chemical nature,
- (4) suitability for generalization to provide a predictive capability, and
- (5) simplicity.

In the present work, we illustrate the utility of our proposed framework for precise representation of saturation properties through the development of a vapor pressure correlation. Similar correlations for liquid density (13) and other saturation properties have been developed, using the same framework and satisfying the characteristics listed above.

MODEL DEVELOPMENT

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

$$\frac{(Y_{\infty}^{\alpha} - Y^{\alpha})}{(Y_{\infty}^{\alpha} - Y_0^{\alpha})} = \Theta(\epsilon) \quad (1)$$

or

$$Y^{\alpha} = Y_0^{\alpha} [1 - \Theta(\epsilon)] + \Theta(\epsilon) Y_{\infty}^{\alpha} \quad (2)$$

where

$$\epsilon = (X_{\infty} - X) / (X_{\infty} - X_0) \quad (3)$$

X = correlating variable

Y = saturation property at given X

Y_{∞} = asymptotic value of saturation property at X_{∞}

Y_0 = initial value of saturation property at X_0

α = scaling exponent

The framework given by Equations (1) - (3) is identical to that which we have used in previous studies to correlate physical properties, where Y included such properties as T_b , T_c , p_c , and w (1,2,14) and, for normal paraffins, θ was expressed as:

$$\theta = \exp(-C_1 X) \quad (4)$$

where C_1 = correlation constant

X = carbon number

$\alpha = 1$

Such a definition has lead to precise correlations for these physical properties of normal paraffins with reasonable extrapolation capability, allowing for predictions of such properties for the heavier members of this homologous series (for which experimental data are unavailable).

VAPOR PRESSURE CORRELATION

Beginning with the general framework given by Equations (1) and (3), we propose the following definitions for θ and α :

$$\theta = \frac{1 - A^{\epsilon B}}{1 - A^{\epsilon}} \quad (5)$$

and

$$\frac{\alpha_c - \alpha}{\alpha_c - \alpha_t} = \frac{\epsilon (1 + C\epsilon)}{1 + C} \quad (6)$$

where,

$$\epsilon = \frac{T_c - T}{T_c - T_t} \quad (7)$$

A, B, C - correlation constants

α_c - the limiting value of α at the critical temperature

α_t - the limiting value of α at the triple point temperature

Thus, recasting Equation (1):

$$Y = (Y_c^\alpha - (Y_c^\alpha - Y_t^\alpha) \Theta)^{1/\alpha} \quad (8)$$

and applying Equations (5), (6), and (7) as definitions for Θ , α and ϵ , respectively, we obtain our proposed model for the correlation of saturated properties, where Y becomes p for vapor pressure, ρ for liquid density, etc.

Figure 1 illustrates the variation of the reduced vapor pressure with reduced temperature for a number of compounds with different degrees of acentricity and polarity. The figure indicates that the reduced vapor pressure is affected by two factors--the temperature and the chemical nature of the substance. Using the proposed framework given by Equation (8), the variations in the vapor pressure with temperature and chemical structure are presented by two simple functions both of which are temperature dependent. The first, given by Equation (5), presents the effect of reduced temperature on the correlating function, Θ , and the second, as shown in Figure 2, depicts the variation of the scaling exponent, α , with reduced temperature, ϵ . As given, the proposed correlation:

- (a) provides for a universal representation for scaled-then-reduced pressure*, 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).

Further evidence for the ability of α_c and α_t to account for effects of variation in the chemical species is given by Figure 3, where values of α_c and

* 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 $(Y_c - Y)/(Y_c - Y_t)$.

α_t show a strong correlation with the reduced triple-point temperature, T_{rt} , which is substance-dependent.

CRITERIA OF EVALUATION

One of the basic requirements for a useful saturation property correlation is accurate representation of data (within experimental uncertainty) over the complete saturation range. Figures 4 and 5 present error plots for ethane and nitrogen in which B , α_c , and α_t in Equations (5) and (6) are treated as substance-specific parameters and A and C as universal constants. The quality of fit produced by the proposed vapor pressure correlation is excellent and compares favorably with the results obtained from the Wagner and Iglesias et al., equations (15, 16).

Quality of the fit aside, several criteria for the development of vapor pressure correlations have been proposed over the years by Riedel (17), Waring (18), Ambrose (19) and Chase (20). While such criteria have evolved from experimental and phenomenological observations, most lack a sound theoretical basis. Accordingly, careful examination of the validity for such criteria is required prior to their adoption.

Scaling theory (15,21,22) places the following requirement for the limiting behavior of the vapor pressure at the critical point

$$\lim_{T \rightarrow T_c} \frac{(d^2 p)}{dT^2} = \infty \quad (9)$$

Our correlation satisfies this scaling law behavior. However, it is at odds with the Riedel-Plank criterion, which requires a zero value for $d\alpha/dT$ ($\alpha = (T/p)(dp/dT)$) at the critical point. Wagner (15) has also concluded that the Riedel-Plank criterion is not suitable for the fluids he considered, but he

stated that it cannot be entirely excluded that both $d\alpha/dT$ and d^2p/dT^2 would become infinite as $T \rightarrow T_c$.

While scaling theory provides a clear assessment for the value of d^2p/dT^2 at the critical point, little information exists regarding the limiting value of dp/dT . The proposed correlation takes the following form as the critical point is approached ($\epsilon \rightarrow 0$):

$$\lim_{\epsilon \rightarrow 0} (dp/dT) = \left(\frac{p_c^{(1-\alpha_c)}}{\alpha_c} \right) (p_c^{\alpha_c} - p_t^{\alpha_c}) \left(\frac{1}{T_c - T_t} \right) \left(\frac{B \ln A}{A - 1} \right) \epsilon^{B-1} \quad (10)$$

Thus, the limiting value of dp/dT at the critical point depends on the value of B . For the majority of fluids considered in this study, we find a value of $B < 1$ to provide the optimum fit to the data. This implies that dp/dT at the critical point is infinite. We found that setting $B=1$ or $B>1$, to force $(dp/dT)_c$ to be either zero or finite, consistently resulted in worsened fits of the experimental data.

Based on the proposed correlation, the approach of dp/dT to infinity as the critical point is approached is rather slow; the value of dp/dT at $\epsilon=10^{-10}$ for ethane was found to be comparable to that obtained using the Wagner equation, which produces a finite limiting value for $(dp/dT)_c$.

The Waring criterion (18) requires a minimum to exist in a $\Delta H/\Delta Z$ vs T_r plot at a reduced temperature of about 0.8 to 0.85. This criterion, in turn, would satisfy Thodos' observation for the existence of an inflection point in $\ln p$ vs $(1/T)$, since

$$\frac{\Delta H}{\Delta Z} = -R \frac{d(\ln p)}{d(1/T)} \quad (11)$$

Figure 6 presents the variation of $\Delta H/\Delta Z$ with reduced temperature for ethane as given by our correlation, which is clearly in agreement with Waring's criterion.

Our discussion thus far has dealt with criteria that apply at temperatures above the normal boiling point. For lower temperatures, $T < 0.6T_c$, comparison of the calculated $\Delta H/\Delta Z$ values with those based on experimental measurements offers a reasonable check on the applicability of a given correlation at low temperatures. Such agreement between the two quantities signifies that the rate of change of pressure with respect to temperature is in accordance with the Clausius-Clapeyron equation expressed by Equation (11). As shown in Figure 6, a favorable comparison exists between our calculated $\Delta H/\Delta Z$ and those based on experimental measurements (deviations within 0.5%).

DATA BASE EMPLOYED

Tables I and II present the data base employed in this study to determine the parameters in the vapor pressure correlation given by Equations 5-8. Table I gives the sources and ranges of the vapor pressures, and Table II presents the critical and triple point properties used.

DATA REDUCTION PROCEDURE

Various strategies have been suggested for the reduction of vapor pressure data (15,23), each trying to reflect the level of confidence placed in the different measurements considered. While highly precise and internally-consistent data are available, special attention is still recommended when dealing with pressures below 1 kPa, since such measurements tend to have relatively larger errors (23).

Ideally, a weighted least squares objective function is desirable, since each data point is assessed an appropriate weight to reflect the uncertainty associated with the measurement. For the systems considered in this study, however, excellent overall fits were obtained using the relative error objective function given below:

$$SS = \sum ((P_{calc} - P_{exp})/P_{exp})^2 \quad (12)$$

where,

P_{exp} - experimental vapor pressure

P_{calc} - calculated vapor pressure

The present model treats both the triple point and critical point vapor pressures as input variables. To avoid the effects of uncertainty in these two end points on the overall quality of fit, both end point vapor pressure values were treated as parameters and allowed to float within the average relative error of each fluid during all parameter regressions.

A Marquart (24) nonlinear regression procedure was employed in the calculations. Definitions of the statistical quantities used are given in the Nomenclature.

MODEL EVALUATION

As indicated by Equations 5-8, the proposed correlation contains five parameters, A , B , C , α_c , and α_t . Our studies, however, have indicated that good precision is retained when some of these parameters are treated as universal constants. Simple values for two of the parameters ($A = 2/3$, $C = 4/3$) were found to be adequate, based on the regression of the data in Table I.

Table III presents the description of specific cases included in our evaluations of the proposed framework. These evaluations are designed to assess two equally important capabilities we seek: first, the ability to correlate different properties within their experimental uncertainty over the full saturation range (making as many of the parameters as necessary substance dependent) and second, the suitability for generalization. Accordingly, a systematic progression from a "correlative" model toward a "predictive" one is evident from the list of cases considered in Table III. Specifically, Cases 1 through 3 are used to investigate the precision in representing the existing

experimental data, and Cases 4 and 5 are employed to evaluate the potential for generalized predictive capability.

Results for two cases dealing specifically with data correlation are presented in Tables IV and V. In "Case 1", A and C are treated as universal constants, while α_c , α_t , and B are substance-specific. In "Case 2", α_c and α_t are treated as substance-specific and B is set to an optimum value of 0.985.

Table IV contains the optimum parameters for each case, while Table V gives the accuracy of the predictions of the vapor pressures. Comparison of the results for the two cases (Table V) 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 each of the fluids considered (RMS = 0.021 bar, and %AAD = 0.057). However, the results of Case 2, a two-constant model, show only minor deterioration in the overall quality of the fit (RMS = 0.022 bar, and %AAD = 0.067).

Table V also presents a comparison of the present work with two correlations which are rated favorably in the literature (23). The results show that Cases 1 and 2 and the correlations of Wagner (a four-constant equation) (15) and Iglesias et al., (a three-constant equation) (16) are generally equivalent in performance (%AAD within 0.1%), with Case 1 and Wagner's equation being slightly superior (%AAD of about 0.05%). However, Wagner's equation requires one or two more substance-specific constants than Case 1 or 2 of this work.

Assessment of the overall value of the present correlation, based on the number of regressed parameters and the potential for simple generalizations, shows it to be highly viable and perhaps superior to others evaluated, especially, since the same framework is applicable to other saturation properties.

Extension of the proposed model to a generalized form, based on data for the compounds given in Table I, follows.

MODEL GENERALIZATION

The ultimate goal of any correlation development is a generalized model that can provide precise and reliable a priori predictions for all systems including those on which no experimental data are available. The ability of Case 2 (in which only α_c and $(\alpha_c - \alpha_t)$ are treated as substance-specific parameters) to provide highly precise predictions for a wide range of chemical species has already been demonstrated. This, along with the observed systematic dependence of α_c and $(\alpha_c - \alpha_t)$ with reduced triple-point temperature, as shown in Figure 3, suggests the possibility for the development of a generalized model based on the generalization of α_c and $(\alpha_c - \alpha_t)$.

The development of a generalized equation for α_c begins with the assumption that α_c can be expressed as,

$$\alpha_c = f_i + f_s + \sum_j \nabla_j \quad (13)$$

in which f_i represents the basic functional dependence of α_c on the reduced initial point temperature (preferably the triple-point temperature) and f_s represents the observed variation of α_c with Z_c for simple fluids.

The ∇_j 's represent other correction terms included to account for variations of α_c with known physical properties. Based on close inspection of Figure 3, three ∇_j corrections were included: the first to account for variation in Z_c from a simple fluid Z_c value of 0.29, the second to account for variations in ω , and the third to account for observed variations in the ratio of ω/Z_c .

Based on regressions of the data set given in Table I, the following form was selected for α_c :

$$\alpha_c = C_1 T_{rt}^{C_2} + C_3 Z_c^{C_4} + [C_3^{(Z_c-0.29)} + C_5^w + C_6^{(3w-w/Z_c)} - 3.0] \quad (14)$$

Similar arguments lead to the following form for $(\alpha_c - \alpha_t)$:

$$(\alpha_c - \alpha_t) = C_1 T_{rt}^{C_2} + C_3 Z_c^{C_4} + (C_1 - 1) T_{rt}^{C_4} + [C_3^{(Z_c-0.29)} - 1.0] C_7 \quad (15)$$

The constants C_1 - C_7 were determined from regressions of the data set given in Table I and are reported in Table VI. In order to test the generality of the relations given in Equations (14) and (15), a data base of 29 additional substances was compiled, as given in Table VII (The data included in this compilation are, in general, less precise than used for model development.) The vapor pressures of all substances shown in Tables I and VII were then predicted (using Equations 14 and 15). Results of three cases based on the generalized equations are given in Table VIII. In Case 3 ($\alpha_c - \alpha_t$) is determined from Equation (15) and α_c is a regressed substance-specific parameter, and in Case 4 both α_c and $(\alpha_c - \alpha_t)$ are calculated from Equations (14) and (15). Case 5 shows the results of using the normal boiling point as the lower vapor pressure point (where T_{rb} is substituted for T_{rt}) along with Equations (14) and (15) to predict vapor pressures between the normal boiling point and the critical point.

The results of Case 3 demonstrate the advantages of a one-parameter model using the proposed framework. The quality of the fit obtained (%AAD = 0.58%) combined with the convenience of only one substance-specific input variable makes this an attractive approach in dealing with complex molecular species for which completely generalized predictions are inadequate.

Table VIII also presents a comparison of Case 4 with the predictions of the Gomez-Thodos model (25) which requires the normal boiling point, T_b , as an input parameter. As shown in Table VIII, Case 4 and Gomez-Thodos (25) are essentially equivalent for normal fluids with Case 4 providing considerably better predictions for polar fluids such as water. For the various fluids included in this comparison, the proposed framework appears to give better predictions as indicated by the overall %AAD of 1.35%, which is about half the value obtained from the Gomez-Thodos method.

In the event that the triple point conditions are not available as input parameters, we have found that the normal boiling point may be used as the lower vapor pressure point (where T_{rb} is substituted for T_{rt}) along with Equations (14) and (15) to predict vapor pressures between the normal boiling point and the critical point with reasonable accuracy. Results using the normal boiling point as the lower end point are shown as Case 5 in Table VIII. Case 5 indicates that for most fluids considered use of the normal boiling point as the lower vapor pressure point results in only minor changes in the quality of vapor pressure predictions (%AAD of 1.35 and 0.83 for Cases 4 and 5, respectively). These results may be attributed to the fact that vapor pressure measurements below atmospheric pressure contain larger uncertainties.

DISCUSSION

The present work, as expressed by Equation (8), suggests that there are advantages in scaling the thermodynamic property prior to normalizing by the reducing coordinates. Most important of these advantages is that such a variable transformation leads to simpler relationships between independent (T) and dependent (p) variables and is a convenient means to account for variation in chemical structure.

Regarding the proposed definitions for α and θ , our definitions correspond, to a first approximation, with the requirements of scaling laws (27, 28). For example, expansion of the proposed correlating function θ , as expressed by Equation (5), produces the following functional form

$$\theta = A_1 \epsilon^B + A_2 \epsilon^{2B} + A_3 \epsilon^{3B} + \dots \quad (16)$$

At the limit, this form is equivalent to that given by scaling laws (28,29). Our optimum value of B used in Equation (5) suggests a scaling law first exponent of 0.985, in comparison to a value of 1.0 which appears in the works of Levelt-Sengers (28). Fortunately, the proposed framework does not preclude other definitions for θ (or α), if the alternative definitions prove to be better or theoretically more acceptable.

The results of our evaluation thus far suggest that while sufficient evidence has been presented in support of the correlative capability of the proposed framework, the limited data base used for parameter generalization makes such generalization preliminary in nature. An expanded compilation of precise experimental data to include the various chemical structures of interest is required for more reliable generalized predictions.

As indicated by Equations (14) and (15), both Z_c and w 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 (56-59), and attempts have been made to overcome such shortcoming. Our present studies on vapor pressures and similar studies involving liquid densities 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 for which Z_c and w characterization is inadequate.

In summary, several advantages can be cited for the proposed framework based on our evaluation of its abilities in correlating vapor pressures (and a number of other saturation properties), including:

1. This method offers a precise and efficient approach for correlating saturation properties over the full saturation range.
2. The present work demonstrates the benefits of scaling the thermodynamic variable prior to reduction as required by the corresponding states principles.
3. The parameters of θ and α can be defined in a manner consistent with theoretical requirements of scaling theory and the desired attributes of phenomenological observations.
4. The model parameters α_c and α_t appear to be suitable for generalization and to have a potential in quantifying the extent of fluid polarity.
5. The proposed approach has provided a reasonably accurate predictive generalized correlation and an effective means to estimate the critical properties of some chemical species, which cannot be measured experimentally.

CONCLUSIONS

A new framework is proposed for correlating saturation properties using a scaled-variable-reduced-coordinate approach. Utility of this framework is demonstrated by correlating vapor pressures of a number of compounds at temperatures from the triple point to the critical point. The new framework results in precise representation of vapor pressures of diverse chemical species within experimental uncertainties (%AAD within 0.1) when two adjustable parameters are used to characterize each substance. In addition, the proposed model compares favorably with the existing correlations and has

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 show an excellent potential for generalized predictions. This is demonstrated by the results given here for vapor pressures, where generalized predictions yield average errors of less than 1.5% over the full saturation range, based on a single experimental measurement.

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NOMENCLATURE

A,B,C	correlation constants
H	enthalpy
P	pressure
T	temperature
X	correlating variable
Y	saturation property
Z	compressibility factor
RMSE	root mean square error
%AAD	average absolute percent deviation
SS	objective function defined by Equation (12)

Greek Symbols

α	correlation scaling exponent
$\Delta\alpha$	$\alpha_c - \alpha_t$
ϵ	reduced variable for property X
Θ	correlating function
ω	acentric factor

Subscripts

c	critical state
t	triple point state
calc	calculated
exp	experimental
r	reduced property
o	lower limiting value of saturation property
∞	upper limiting value of saturation property

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TABLE I
SOURCES OF VAPOR PRESSURE DATA

	Temperature Range, K	Pressure Range, bar	Source	No. of Points
Methane	90.68 - 90.53	0.1174 - 45.957	30	43
	189.90 - 190.39	45.09 - 45.79	31	71
Ethane	90.348 - 305.33	1.131×10^{-5} - 48.714	32	131
Propane	85.47 - 369.80	1.6808×10^{-9} - 42.42	33	54
Argon	83.804 - 150.651	0.6895 - 48.578	15	58
Nitrogen	63.148 - 126.200	0.1252 - 34.002	15	68
Benzene	278.681 - 377.07	0.04782 - 2.000	34	28
	320.00 - 560.00	0.3205 - 47.726	35	13
Carbon	217.113 - 276.165	5.3033 - 37.7152	29	19
Dioxide	269.179 - 304.14	31.3227 - 73.775	28	37
Water	273.16 - 647.13	0.0061173 - 220.55	36	39
Fluorine	53.4811 - 144.31	0.00252 - 52.153	37	123
Butane	134.86 - 425.16	6.736×10^{-6} - 37.960	38	79
Ammonia	195.48 - 405.4	0.06075 - 113.04	40	23
Acetone	259.175 - 508.10	0.04267 - 47.0	41	47
Oxygen	54.36 - 154.581	0.00146 - 50.429	40	21
Decane	268.148 - 490.292	0.00017 - 2.7002	42	34
Hydrogen	13.95 - 33.18	0.072 - 13.13	43	21
Methanol	288.049 - 352.776	0.09815 - 1.78306	44	7
	353.46 - 512.64	1.8300 - 80.971	19	12
Ethanol	292.772 - 362.756	0.05726 - 1.55824	44	12
	373.29 - 513.92	2.2623 - 61.484	19	14
Ethylene	104.11 - 175.84	0.00124 - 1.4551	46	31
	200.00 - 282.15	4.554 - 50.222	47	28

TABLE II
PHYSICAL CONSTANTS OF COMPOUNDS

Substance	T, K	P, bar	Source
----- Critical Point -----			
Methane	190.530	45.957	30
Ethane	305.330	48.714	32
Propane	369.80	42.42	33
Argon	150.86	48.979	16
Nitrogen	126.200	34.002	15
Benzene	562.161	48.898	16
Carbon Dioxide	304.14	73.775	28
Water	647.13	220.55	36
Fluorine	144.31	52.15	37
Butane	425.16	37.960	38
Ammonia	405.4	113.04	40
Acetone	508.10	47.0	41
Oxygen	154.581	50.429	40
n-Decane	617.6	21.076	4
Hydrogen	33.18	13.13	43
Methanol	512.64	80.971	19
Ethanol	513.92	61.484	19
Ethylene	282.34	50.4	48
----- Triple Point -----			
Methane	90.68	0.1174	30
Ethane	90.348	1.131×10^{-5}	32
Propane	85.470	1.6808×10^{-9}	33

Argon	83.804	0.6895	15
Nitrogen	63.148	0.1252	15
Benzene	278.681	0.047823	34
Carbon Dioxide	216.58	5.180	39
Water	273.16	0.0061173	36
Fluorine	53.4811	0.00252	37
Butane	134.86	6.736×10^{-6}	38
Ammonia	195.48	0.06075	40
Acetone	*		
Oxygen	54.36	0.00146	40
n-Decane	*		
Hydrogen	13.95	0.072	43
Methanol	*		
Ethanol	*		
Ethylene	103.986	0.0012	48

* The triple point vapor pressure was not available for this compound. The lowest available data point was used in place of the triple point.

TABLE III

DESCRIPTION OF ALL CASES
STUDIED IN THE PRESENT WORK

Case	Description
1	<p>Three-parameter model. $A = 2/3$, $C = 4/3$. B, α_c, $\Delta\alpha$ regressed as substance-specific parameters.</p>
2	<p>Two-parameter model. $A = 2/3$, $B = 0.985$, $C = 4/3$. α_c, $\Delta\alpha$ regressed as system-specific parameters.</p>
3	<p>One-parameter model. $A = 2/3$, $B = 0.985$, $C = 4/3$, $\Delta\alpha$ from Equation (15). α_c regressed as a single system-specific parameter.</p>
4	<p>Generalized model from triple point to critical point. $A = 2/3$, $B = 0.985$, $C = 4/3$. α_c and $\Delta\alpha$ from Equations (14) and (15), respectively.</p>
5	<p>Generalized model from normal boiling point to critical point. $A = 2/3$, $B = 0.985$, $C = 4/3$. α_c and $\Delta\alpha$ from Equations (14) and (15) with T_t and P_t replaced by T_b and 1.01325 bar.</p>

TABLE IV
CORRELATION PARAMETERS

Substance	Case 1			Case 2	
	B	α_c	$\Delta\alpha$	α_c	$\Delta\alpha$
Methane	0.985563	0.367628	0.076820	0.367095	0.077123
Ethane	0.982571	0.286707	0.118977	0.285817	0.118164
Propane	0.985976	0.253856	0.133578	0.254118	0.133961
Argon	0.987831	0.403972	0.061925	0.406640	0.064018
Nitrogen	0.987541	0.371782	0.073122	0.373573	0.074591
Benzene	0.983012	0.337015	0.078684	0.335910	0.077850
CO ₂	0.985512	0.445291	0.042534	0.446087	0.043218
Water	0.986568	0.274569	0.082424	0.275168	0.082894
Fluorine	0.982217	0.323592	0.102246	0.322449	0.101325
n-Butane	0.990349	0.270732	0.111373	0.272124	0.112467
Ammonia	0.989999	0.312871	0.075813	0.315470	0.077826
Acetone	0.989068	0.312321	0.067950	0.314483	0.069519
Oxygen	0.979662	0.325301	0.107611	0.323157	0.105933
n-Decane	0.987354	0.263208	0.087572	0.264044	0.088207
Hydrogen	0.997330	0.389571	0.061751	0.398497	0.068486
Methanol	0.999291	0.279051	0.057560	0.287404	0.064084
Ethanol	1.006410	0.284439	0.069511	0.296183	0.078389
Ethylene	0.983463	0.315356	0.104812	0.314739	0.104325
Case 1: $A=2/3, C=4/3$					
Case 2: $A=2/3, B=0.985, C=4/3$					

TABLE V
MODEL EVALUATION

	This Work				Literature			
	Case 1		Case 2		Wagner(15)		Iglesias(16)	
	RMS, bar	%AAD	RMS, bar	%AAD	RMS, bar	%AAD	RMS, bar	%AAD
Methane	0.005	0.015	0.005	0.016	0.005	0.015	0.010	0.053
Ethane	0.017	0.054	0.021	0.068	0.017	0.056	0.018	0.065
Propane	0.015	0.065	0.012	0.066	0.010	0.039	0.010	0.063
Argon	0.003	0.017	0.006	0.025	0.002	0.015	0.005	0.024
Nitrogen	0.002	0.016	0.005	0.024	0.002	0.015	0.003	0.030
Benzene	0.006	0.014	0.008	0.019	0.004	0.014	0.014	0.051
CO ₂	0.004	0.007	0.004	0.007	0.008	0.013	0.032	0.043
Water	0.051	0.043	0.034	0.047	0.022	0.022	0.033	0.047
Fluorine	0.007	0.069	0.006	0.072	0.002	0.051	0.010	0.079
Butane	0.037	0.176	0.030	0.184	0.026	0.131	0.032	0.172
Ammonia	0.028	0.031	0.054	0.056	0.026	0.011	0.047	0.048
Acetone	0.017	0.054	0.024	0.055	0.018	0.061	0.016	0.048
Oxygen	0.018	0.084	0.018	0.106	0.006	0.032	0.020	0.127
Decane	0.001	0.057	0.002	0.061	0.001	0.054	0.002	0.142
Hydrogen	0.002	0.056	0.012	0.105	0.005	0.071	0.012	0.196
Methanol	0.040	0.092	0.064	0.169	0.027	0.065	0.037	0.088
Ethanol	0.057	0.154	0.060	0.251	0.038	0.077	0.072	0.157
Ethylene	0.006	0.066	0.009	0.073	0.006	0.063	0.019	0.171
Overall	0.021	0.057	0.022	0.067	0.014	0.045	0.023	0.081

TABLE VI
GENERALIZED CORRELATION PARAMETERS

<u>Parameter</u>	<u>Value</u>
A	2/3
B	0.985
C	4/3
C ₁	0.433
C ₂	1.722
C ₃	0.775
C ₄	0.897
C ₅	0.799
C ₆	0.941
C ₇	2.643

TABLE VII
SOURCES OF VAPOR PRESSURE DATA USED
TO TEST THE GENERALIZED MODEL

	Temperature Range, K	Pressure Range, bar	Source	No. of Points
Neon	24.56 - 44.448	0.43379 - 26.64	40	23
Propylene	87.89 - 365.57	9.5×10^{-9} - 46.646	40	29
*o-Xylene	336.610 - 418.517	0.062742 - 1.03906	49	9
	432.17 - 630.33	1.4644 - 37.318	50	20
*Refrigerant 12	170.0 - 384.95	0.00867 - 41.25	40	23
*Acetic Acid	293.15 - 594.75	0.015373 - 57.84	51	
*Propanol	258.15 - 536.85	0.00133 - 50.55	51	16
*tert-Butanol	304.15 - 356.05	0.07999 - 1.01325	52	5
	356.48 - 508.87	1.01353 - 42.32	53	13
*Hydrogen Cyanide	267.25 - 456.65	0.266 - 50.66	52	11
*Toluene	308.516 - 384.659	0.06357 - 1.03903	49	9
	398.32 - 591.79	1.5049 - 41.066	50	21
*Methyl Isobutyrate	284.9 - 467.5	0.0340 - 11.51	54	22
Acetylene	192.4 - 308.7	1.283 - 62.47	43	14
*Bromine	260.0 - 584.2	0.042 - 103.4	43	17
*Methyl Chloride	180.0 - 416.0	0.0165 - 69.0	43	26
	416.25	66.79	55	1
*Chlorine	233.15 - 417.16	0.7746 - 77.11	43	20
*Carbon Tetrachloride	110.0 - 227.5	0.0286 - 37.45	43	13
Deuterium	18.7 - 38.34	0.1709 - 16.65	43	22
Deuterium Oxide	277.0 - 644.7	0.00668 - 218.4	43	25
*n-Heptane	200.0 - 540.1	2.0×10^{-5} - 27.35	43	27
*Refrigerant 11	200.0 - 471.2	0.0043 - 44.09	43	20

*Refrigerant 113	240.0 - 487.5	0.0233 - 34.11	43	25
*Refrigerant 114	190.0 - 419.0	0.0058 - 32.61	43	24
*Refrigerant 115	199.82 - 353.09	0.1604 - 31.55	43	16
*Refrigerant 13B1	170.0 - 340.2	0.059 - 39.64	43	19
*Refrigerant 22	150.0 - 369.3	0.0017 - 49.89	43	23
*Refrigerant 500	200.0 - 378.6	0.1219 - 44.26	43	19
*Sulfur Dioxide	200.0 - 420.0 430.8	0.02056 - 66.19 77.83	43 4	23 1
Xenon	161.4 - 289.7	0.816 - 58.21	43	14
*Refrigerant 13	91.0 - 302.0	3.817×10^{-6} - 38.70	43	23
*Refrigerant 23	149.82 - 299.09	0.0429 - 48.36	43	16

* Lowest data point is not the fluid triple point.

TABLE VIII
EVALUATION OF GENERALIZED MODEL

	This Work						Literature	
	Case 3		Case 4		Case 5		Gomez (25)	
	RMS, bar	%AAD	RMS, bar	%AAD	RMS, bar	%AAD	RMS, bar	%AAD
Methane	0.049	0.209	0.017	0.346	0.043	0.335	0.021	0.118
Ethane	0.020	0.084	0.018	0.083	0.121	0.499	0.027	0.152
Propane	0.058	0.241	0.044	0.362	0.116	0.478	0.028	0.592
Argon	0.067	0.264	0.064	0.342	0.063	0.323	0.053	0.242
Nitrogen	0.030	0.188	0.030	0.282	0.026	0.363	0.044	0.354
Benzene	0.029	0.072	0.015	0.211	0.060	0.403	0.022	0.541
CO ₂	0.074	0.187	0.096	0.302	0.096	0.302	0.030	0.065
Water	0.150	0.134	0.207	0.590	1.365	2.487	3.594	10.209
Fluorine	0.005	0.066	0.030	0.776	0.099	0.444	0.043	0.553
Butane	0.047	0.265	0.036	0.371	0.157	0.968	0.023	1.461
Ammonia	0.048	0.060	0.091	0.206	0.195	0.474	0.712	3.378
Acetone	0.035	0.195	0.024	0.274	0.084	0.388	0.034	2.517
Oxygen	0.017	0.141	0.057	1.094	0.045	0.337	0.037	1.441
Decane	0.053	0.274	0.002	0.800	0.008	0.378	0.006	1.227
Hydrogen	0.040	0.667	0.032	0.800	0.008	0.161	0.041	3.142
Methanol	0.138	0.765	0.063	0.628	0.742	3.063	0.173	2.866
Ethanol	0.201	1.631	0.257	1.799	0.096	0.291	0.427	2.320
Ethylene	0.096	0.388	0.075	1.510	0.039	0.248	0.055	2.186
Neon	0.053	0.392	0.068	0.602	0.052	0.428	0.108	2.117
Propylene	0.010	0.309	0.061	2.948	0.061	0.384	0.028	1.057
o-Xylene	0.079	0.419	0.144	1.431	0.150	0.823	0.015	0.494

Refrigerant 12	0.024	0.090	0.093	1.454	0.136	0.604	0.013	0.239
Acetic Acid	0.294	1.188	0.515	7.027	0.902	5.222	0.453	9.248
Propanol	0.444	2.090	0.177	3.463	0.138	1.053	0.421	9.240
t-Butanol	0.188	1.338	0.062	1.438	0.104	0.974	0.272	5.648
Hydrogen Cyanide	0.182	0.945	0.397	4.080	0.360	2.196	0.271	3.317
Toluene	0.066	0.301	0.104	0.978	0.123	0.635	0.017	0.321
Methyl Isobutyrate	0.354	2.269	0.187	2.375	0.116	1.910	0.244	3.218
Acetylene	0.393	0.859	0.589	1.613	0.587	1.608	0.395	1.716
Bromine	0.184	0.578	0.416	1.828	0.215	0.252	0.152	1.007
Methyl Chloride	0.411	1.792	0.691	2.798	0.767	1.132	0.665	2.314
Chlorine	0.080	0.255	0.067	0.533	0.067	0.496	0.076	0.570
Carbon Tetrachloride	0.162	1.755	0.182	2.345	0.242	0.784	0.170	3.245
Deuterium	0.053	0.470	0.078	1.218	0.053	0.347	0.116	2.721
Deuterium Oxide	0.078	0.214	0.032	0.440	1.166	1.725	2.597	14.679
n-Heptane	0.067	1.312	0.026	2.500	0.129	0.901	0.005	0.986
Refrigerant 11	0.023	0.141	0.060	1.073	0.130	0.563	0.025	0.469
Refrigerant 113	0.016	0.147	0.019	0.215	0.063	0.522	0.032	0.444
Refrigerant 114	0.066	0.528	0.029	1.606	0.060	0.504	0.065	0.764
Refrigerant 115	0.043	0.296	0.106	1.093	0.058	0.365	0.050	0.284
Refrigerant 13B1	0.025	0.130	0.044	0.724	0.037	0.288	0.074	0.664
Refrigerant 22	0.170	0.869	0.019	1.408	0.115	0.519	0.010	1.280
Refrigerant 500	0.021	0.063	0.112	1.612	0.085	0.888	0.889	21.793
Sulfur Dioxide	0.080	0.842	0.082	0.939	0.138	0.535	0.110	1.610
Xenon	0.062	0.282	0.057	0.576	0.059	0.502	0.117	0.388
Refrigerant 13	0.272	1.524	0.140	2.954	0.034	0.413	0.174	12.943
Refrigerant 23	0.064	0.172	0.150	1.351	0.174	0.603	0.097	1.433
Overall	0.111	0.583	0.125	1.349	0.206	0.832	0.277	2.927

FIGURE 2
EFFECT OF TEMPERATURE ON
SCALING EXPONENT

SOURCE	1	Methane	2	Ethane	3	Propane
	4	Argon	5	Nitrogen	6	Benzene
	7	CO2	8	Water	9	Fluorine
	10	n-Butane	11	Ammonia	12	Acetone
	13	Oxygen	14	n-Decane	15	Hydrogen
	16	Methanol	17	Ethanol	18	Ethylene

FIGURE 3
EFFECT OF REDUCED TRIPLE POINT
TEMPERATURE ON LIMITING VALUES
OF SCALING EXPONENTS

FIGURE 4
COMPARISON OF ETHANE
VAPOR PRESSURE REPRESENTATIONS

FIGURE 5
COMPARISON OF NITROGEN
VAPOR PRESSURE REPRESENTATIONS

FIGURE 6
ETHANE dP/dT VARIATION WITH
TEMPERATURE

- END -

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10 / 31 / 90