Predicting Vapor-Liquid Equilibrium Over the Entire Two-Phase Region Using Wagner Equation with Only Limited VLE Data

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Authorization to Submit Dissertation

This dissertation of Todd T. Nichols, submitted for the degree of Doctorate of Philosophy with a Major in Chemical Engineering and titled "Predicting Vapor-Liquid Equilibrium Over the Entire Two-Phase Region Using Wagner Equation with Only Limited VLE Data," has been reviewed in final form. Permission, as indicated by the signatures and dates below, is now granted to submit final copies to the College of Graduate Studies for approval.

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Abstract

The predictive error relative to analytic values of entire-curve Wagner constants is studied for the reduced vapor pressures predicted by Wagner constants that are parameterized from a limited data interval. An algebraic solution for the fully-determined case based on only four data points is used to estimate the limited-data Wagner constants. First, seventy-two species are used to assess the impact of the location of the two interior points and the location and width of the limited-data interval upon the error in predicted $P_{v,r}$ due to data imprecision. Hydrogen, helium, R152a, and water are used to assess error due to Wagner imperfection and compare predictive capability of the algebraic fully-determined and regressed over-determined approaches. Second, the repeatability/reproducibility of VLE data in the literature is studied by comparing reduced pressures calculated from Antoine constants applicable to a limited temperature interval with the entire-curve Wagner analytic values over the same limited-data interval. The entire-curve Wagner analytics are treated as "true" or "best" values and the Antoine analytic values as surrogate experimental data. Wagner constants for fifty-five species are subsequently estimated from the Antoine analytics for the fully-determined case, from which reduced vapor pressures below and above the interval are predicted and compared with the entire-curve Wagner analytics to estimate the ability of limited VLE data to be used to accurately represent the entire two-phase curve. The predictive capability of such limited-data Wagner constants is compared with that of the semi-theoretical Riedel and the empirical Ambrose-Walton equations. Lastly, reduced vapor pressures predicted from the standard and modified forms of the Riedel and Ambrose-Walton equations are used to parameterize the Wagner equation, again using the algebraic, fully-determined solution. The predictive power of such Wagner constants is compared to that of the underlying source correlations themselves. This is the first time the error of limited-data Wagner constants is segmented by interval location and width, between that due to data imprecision vs. equation imperfection, and fully- vs. over-determined solutions. Neither using a four-point, fully-determined solution rather than over-determination, nor using predictive correlations to supply "data" to a Wagner parameterization are instinctive approaches, and hence their novelty.

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Dedication

My family has paid a significant price for this academic pursuit. Long work days and long commutes unfortunately resulted in less family time when I would have to attend to my academic studies after arriving home from work. My wife Kerry, of course, felt my absence the most. Kerry and our children have unlimited confidence in my abilities, and they spurred me on during the hardest times. Wanting to be worthy of that biased faith that my family seems to always exhibit helped me to not quit. Pursuing a PhD part-time is an arduous task, not just for the student, but just as much, if not more so, for the student's family. I dedicate this research to my wife Kerry, and our six children, Bradley, Travis, Stacey, Megan, Spencer, and Lane. It is as much their degree as it is mine.

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Nomenclature

a, b, c, d	Wagner constants, defined by Eq. [1]
$f^{(0)}, f^{(1)}, f^{(2)}$	Ambrose-Walton equation coefficients, Eqs. [10a-10c]
h	Riedel equation parameter, Eq. [11g]
t^*	The t* test statistic
A%Err	Absolute value of error percentage
A, B, C	Antoine equation coefficients, Eq. [9]
A^+, B^+, C^+, D^+	Riedel equation coefficients, Eq. [11a]
F	Function used to estimate Wagner constants, defined by Eqs. [2a] – [2d] *[AA]* indicates calculations use raw data; *[RD]* indicates calculations use raw data; *[WA]* indicates calculations use analytic data points determined by entire-curve Wagner constants; Definition of seven other bracketed terms are given in Ch. 3 text and summarized in Table D.1
H	Hypothesis for t* test statistic
K	Riedel equation parameter, defined by Eqs. [11e-11f] for organic acids and alcohols, equal to 0.0838 otherwise
P	Pressure; unit is specifically bar for the Antoine equation (Eq. [9])
Q	Riedel equation parameter, defined by Eq. [11b]
S	The t* test statistic, sample variance
T	Absolute temperature; specifically ^{0}K for the Antoine equation (Eq. [9])
$\overline{X}$	The t* test statistic, sample average

Greek Letters

α_c	Riedel equation parameter, Eq. [11c]
ΔH	Heat of vaporization

$\Delta \text{Log } P_{v,r}$	Antoine equation, Log ($P_{v,r}$ @$T_{r,min}$) - Log $P_{v,r,f}$ Ambrose-Walton equation, Log ($P_{v,r}$ @T_r=0.7) - Log $P_{v,r,f}$ Riedel equation, Log $P_{v,r,b}$ - Log $P_{v,r,f}$
ΔT_r	Antoine equation, $T_{r,min}$ - $T_{r,f}$ Ambrose-Walton equation, 0.7- $T_{r,f}$ Riedel equation, $T_{r,b}$ - $T_{r,f}$
ΔZ	Difference in compressibility factors of vapor and liquid
ε	Parameters used to calculate η coefficients, defined in Table 1.4. Subscripts are unique identifiers and are not meant to correspond to specific Wagner constants or data points.
η	Coefficients in F function, defined in Table 1.4
μ	Population mean of an average error in t* test statistic
τ	1 - T_r
ψ	Riedel equation parameter, Eq. [11d] for standard form and Eq. [12a] for modified form
ω	Acentric Factor

Subscripts

0	Refers to null hypothesis in t* test statistic
0.7	Pertains to the reduced temperature of 0.7
1, 2	H (t* test statistic), refers to alternative hypothesis; η, T_r, and τ, indicates the data point
3	η, T_r, and τ, indicates the data point
4	μ, “quarter” point distribution; η, T_r, and τ, indicates the data point
8	“Eighth” point distribution
a	Pertains to Wagner constant a in F function and η
b	T , P, and ψ, pertains to normal boiling point; F function and η, pertains to Wagner constant b
c	T and P, pertains to critical point; F function and η, pertains to Wagner constant c

d	Pertains to Wagner constant d
e	"Even" point distribution
f	Pertains to normal fusion point
i	Index notation for the four data points used by F function and η
j	Index notation for Wagner constants in F function and η
min	Pertains to the lower bound of the Antoine temperature interval
max	Pertains to the upper bound of the Antoine temperature interval
r	Reduced, relative to the critical point
t	Pertains to triple point
v	P, vapor pressure t* test statistic, degrees of freedom
w	Indicates F function is used to estimate Wagner constants
SA	Modified Riedel equation, pertains to the second anchor point ($T_r = 0.7$)
T_{r1}, T_{r2}, T_{r3}, T_{r4}	Indicates the corresponding reduced temperature for $Ln\ P_{v,r}$ variables of the F function, Eqs. [2, 2a-2d]
α	Probability of type I error for t* test statistic. Value is 0.05.

Superscripts

(0)	Ambrose –Walton coefficient f, zero-order in terms of ω
(1)	Ambrose –Walton coefficient f, 1st order in terms of ω; F function, data inputs pertain to reduced temperature point distribution of 0.6, 0.7, 0.8 and 0.9
(2)	Ambrose –Walton coefficient f, 2nd order in terms of ω; F function, data inputs pertain to reduced temperature point distribution of 0.3, 0.6, 0.7 and 0.95
(3)	F function, data inputs pertain to reduced temperature point distribution of 0.2, $T_{r,b}$, 0.7 and 0.9

Introduction

I.1 Objectives

The goal of this work is to develop an easy, universal approach that will provide improved Vapor-Liquid Equilibrium (VLE) prediction over the entire two-phase region for pure substances using Corresponding States Principle (CSP) and the well-known four-parameter Wagner vapor-pressure equation. The resulting methodology is expected to allow one to fill in VLE knowledge gaps while requiring only the knowledge and simple tools available to engineering practitioners.

The primary hypothesis is the following:

> *Hypothesis I: Only four reduced VLE points of good precision from commonly found limited-data intervals are required to predict VLE accurately along the entire two-phase region for pure species.*

Assuming that the functional form of the Wagner equation allows for the accurate definition of the entire VLE curve of a pure substance, Hypothesis I, if true, allows four accurate vapor pressures to transform the Wagner equation from being merely correlative over the limited-data interval to instead being predictive over the entire two-phase range. This leads one to subsequently consider whether or not the VLE data and predictive correlations regressed from data by different researchers in the literature as a whole have accuracy and self-consistency sufficient to allow the Wagner equation to become predictive. Thus, the following hypothesis is made:

> *Hypothesis II: The accuracy of VLE data available in peer-reviewed technical literature and their consistency between different researchers is by and large of high enough degree to allow such limited data/correlations to be used to estimate Wagner constants capable of accurately predicting VLE over the entire two-phase curve for pure species.*

For species lacking a range of VLE data, or if it is found that the second hypothesis does not have strong support, the assessment of the subsequent hypothesis becomes important:

> *Hypothesis III: Vapor pressure estimations from a set of source predictive correlations may be used to parameterize the Wagner equation that will have greater predictive power than the source correlations themselves.*

The above three hypotheses will be tested, with the objective of developing an improved approach to entire-curve VLE prediction.

I.2 Roadmap

The results of this research are presented in three parts, with each part focused primarily upon one hypothesis. For most species, the normal fusion point is close to the triple point. Because many more species have their normal fusion point listed in the literature than their triple point, the range from the normal fusion point to the critical point is referred to in this work as the entire two-phase VLE curve.

Chapter 1 addresses Hypothesis I. It presents the results of Wagner constants estimated from least-squares regression of entire-curve VLE data from *NIST* (Lemmon et al., 2011) for argon, hydrogen, helium, R152a, and water. The last four species are used to compare the roles of data imprecision and equation imperfection to predictive error and to compare the four-point fully-determined approach and over-determined regression. The entire-curve Wagner constants of the five *NIST* species and those of another sixty-seven species from the literature are used to investigate the dependency of predictive error upon the width of a limited-data interval and its location on the VLE curve. The results are relevant to those researching methods to leverage limited VLE data of good precision to predict the VLE curve above and below the source data's interval. The results provide the justification for using a fully-determined approach in such research. The equations and property data common to all three chapters are presented.

Chapter 2 subsequently addresses Hypothesis II and investigates the net contribution of data repeatability/reproducibility to the predictive power of limited vapor-liquid equilibrium (VLE) data by comparing reduced pressures calculated from Antoine constants applicable to a limited temperature interval with the entire-curve Wagner analytic values over the same limited-data interval. The concept of extrapolation burden is expanded upon. The results provide insight into how well limited VLE data given in the literature, or correlations based on limited data, may compare with assumed best values determined by another researcher using thermodynamic data from the entire two-phase curve. The predictive power of Wagner constants estimated from Antoine analytic data are compared with the predictive capability of the semi-theoretical Riedel and the empirical Ambrose-Walton equations. The results are relevant to engineers tasked with assessing the feasibility of predicting VLE over the entire two-phase curve when only data or correlation of limited applicability is available.

The results presented in Chapter 2 cause one to consider the validity of Hypothesis III. For many species only the critical and normal boiling points and acentric factor are given in technical handbooks. Consequently, Chapter 3 addresses using VLE predictions from standard and modified forms of the Riedel and Ambrose-Walton equations to estimate Wagner constants. The results of this chapter are relevant to the research of predictive correlation development in general and to engineers tasked with predicting VLE for a species when only the stated three data points are available.

I.3 Significance of the Research

The importance of the results of this research stems from the broad need for accurate VLE data of pure substances, the current lack of a successful universal approach for VLE prediction, and the difficulty of obtaining accurate experimental measurements at low and high temperatures.

I.3.1 Need for Accurate VLE Data

Accurate VLE data are fundamental to the development of many thermodynamic/physical property models and theoretical frameworks, such as equations of state (EOS), vapor-phase association experiments, and aerosol chemical and growth kinetics.

Some EOSs require partial or the entire two-phase region vapor pressure data. For example, Hirschfelder et al. (1958) used explicit formulas for vapor pressure in their generalized EOS, and Span et al. (1998) used vapor pressure calculations from a correlation for their reference EOS for nitrogen. Golobic & Gaspersic (1994) required a species' saturation pressure at the reduced temperatures of 0.7 and 0.75 in functions for their third and fourth parameters. Nasrifar et al. (2000) require saturation pressures in their model for liquid densities, so they used a generalized form of the Riedel vapor pressure correlation. Hatami et al. (2011) compared VLE predictions of five cubic EOSs and showed the necessity of having the critical point used in the EOS be compatible with the subcritical vapor pressure data.

Vapor phase association constants can be estimated from experimental P-V-T data (Prausnitz et al., 1999), and the calculations require the saturation pressures of the targeted species. Miyamoto et al. (1999), for example, used the Antoine equation to estimate the saturation vapor pressure in their experimental determination of the association constant for monocarboxylic acids.

Condensation of vapor species is one of the primary mechanisms for aerosols to change size and composition. Adsorption of gases onto atmospheric aerosols is often described in terms of a partition coefficient defined in part by the saturation vapor pressure of the adsorbed species (Seinfeld & Pandis, 2006).

More accurate entire-curve VLE predictions from limited data, or improved VLE predictions when only the critical and normal boiling points and acentric factor are available, can contribute to the ongoing research efforts focused on such thermodynamic/physical property model development.

I.3.2 Lack of Successful Universal Approach to VLE Prediction

CSP holds that all substances will exhibit the same behavior when they have the same values of suitable dimensionless properties. In reality, the numbers of species that closely satisfy the hypothesis of corresponding states, known as “perfect” or “simple” fluids, are relatively few. The two dimensionless properties used most commonly in CSP are reduced temperature and reduced pressure, where the adjective “reduced” means divided by the corresponding critical property. Pitzer and his associates (Pitzer, 1955; Pitzer, Lippmann, Curl Jr, Huggins, & Petersen, 1955) found that the increase in the slope of the vapor pressure curve, and similarly the increase in the entropy of vaporization, over that of a simple or perfect fluid could be quantified in what has become the well known acentric factor, ω, whose value is related to the reduced vapor pressure at the reduced temperature of 0.7.

The acentric factor accounts for deviation from perfection due to molecular size (large, globular) and shape (elongation). Theoretically, all species with the same value of the acentric factor have the same shape for their intermolecular potential curve, and subsequently will exhibit the same behavior at the same reduced temperature and reduced pressure. Fluids for which this theory reasonably applies have been classified as “normal.” Non-normal fluids are those whose imperfections affect the intermolecular potential curve in ways significantly different than do a molecule's shape and size. Quantum mechanics, polarity, hydrogen-bonding, and self-association are examples of non-normal affects not reliably accounted for in a ω-based CSP theory.

Vetere (2006), in his comparison of several CSP-based universal correlations as part of his study of the Riedel equation, highlights the difficulty of trying to predict entire-range VLE with the normal boiling point or ω as the only data point besides the critical point. Predicting VLE at lower temperatures is particularly problematic for a universal approach like CSP because the intermolecular forces for non-spherical molecules can deviate significantly from those of "simple" molecules. The effect of molecular shape increases with decreasing temperature, e.g., quantum effects are significant for low-molecular-weight gases at low temperatures, and boiling points of isomers decrease as the amount of branching increases. Hydrogen bonding causes substances (e.g., acids, alcohols, and amines) to strongly associate (Prausnitz et al., 1999), which association increases in the liquid phase as temperature decreases. Dipole interactions of some associating substances, such as alcohols, increase at low temperatures (Vetere, 2006).

Consequently, in order to achieve the desired accuracy, especially at lower temperatures, some developers of CSP-based theoretical VLE correlations utilize reference fluids, require more saturation points than just the critical point, incorporate a species-specific parameter, or limit their work to a specific type of substance or homologous series. Ambrose & Patel (1984) showed that two reference fluids could be used to predict vapor pressures better than one reference fluid. Sorner & Strom (2002) expanded to 3 reference fluids, and Rozhnov et al. (2008) used 16 reference fluids to improve accuracy. In some cases the reference species need to be from the targeted species' family (Armstrong, 1981; Teja et al., 1981).

Rogdakis & Lolos (2006) require the triple point or normal fusion point in addition to the critical point. Velasco et al. (2008) require the triple, normal boiling, and critical points. Halm & Stiel (1967), on the other hand, introduced a new species-specific parameter, the polar factor, to help account for the deviations from normality experienced by polar fluids. An & Yang (2012) modified the Lee-Kesler equation by adding a species-dependent constant and limited their equation to organic substances.

The universal approach resulting from the research presented here - accurate entire-curve VLE predictions from limited data or improved VLE predictions when only the critical and normal boiling points and acentric factor are available - can contribute to the ongoing research efforts focused on such thermodynamic/physical property model development.

Unlike some of the approaches to predict VLE discussed above, the approach presented here does not require appropriate reference fluids, does not require a new deviation parameter, nor does it require a data range so extensive as to include the triple/fusion point vapor pressure. The universal approach developed here has the potential to offer better predictive power with less complexity and effort.

I.3.3 Difficulty Obtaining Accurate Experimental VLE Data

Experimentally measuring VLE in the low-temperature region can be difficult because of the very low vapor pressures sometimes involved. According to Rossiter & Baetzold (1992), pressure uniformity within the measuring apparatus is more difficult to maintain at three or more orders of magnitude below atmospheric pressure due to several factors, e.g., effects of chemical reactions, gas adsorption, metal degassing, gas leakage, and deformation of mechanical components. Albright (2009) asserts that measurement accuracy for pressure is 1-10% at best below 10 Pa (10^{-4} bar) for the Knudsen method, a static technique commonly used for low-pressure measurements. Weber (1992) has even less regard for static methods, concluding that only 26 ppm of air in the gas sample can introduce an error of 0.4 kPa (0.004 bar) in static pressure measurements of refrigerants in the 10-210 kPa (0.1-2.1 bar) range, which corresponds to an error of 4% at his low-pressure end and 0.1% at his upper end. Weber asserts that very high sample purity (only 1 ppm air) is required with static techniques to produce pressure measurements with the same accuracy as his more accurate dynamic measurement technique.

Rossiter & Baetzold (1992), although holding to the opinion that accurate pressure measurement is more difficult several decades below atmospheric, do assert that national standards laboratories can measure pressures of inert gases with 1% accuracy down to 10^{-4} Pa (10^{-9} bar) with static methods, while stressing, however, the importance of proper materials of construction and the experimenter's knowledge/skill in their discussion of pressure measurement using static methods. Similarly, Ruzicka et al. (2008) claim to have developed a static-method apparatus capable of measuring the pressure of organic compounds down to 0.1 Pa (10^{-6} bar) with an accuracy of 0.05%. Although some researchers such as Rossiter & Baetzold (1992) and Ruzicka et al. (2008) do claim accurate measurements at relatively low pressures, their apparatuses are tailor-designed for specific species and require significant experimental rigor, and the VLE curve for many substances still extend several decades lower than the "accurate" range claimed by these researchers. The analytic saturation pressure at the normal fusion point for some substances studied in this work extends down to the 10^{-12} decade.

Consequently, researchers have developed methods of using low-temperature thermal data (e.g., heat capacity and heats of vaporization) to extrapolate higher-temperature VLE data down to the low-temperature region (Ambrose, Counsell, & Hicks, 1978; Ambrose & Davies, 1980; Hogge et al., 2016; King & Al-Najjar, 1974; Poling, 1996; K. Ruzicka & Majer, 1994). The extrapolated low-temperature VLE behavior is forced to be thermodynamically consistent with the thermal data.

Because measuring vapor pressure at high temperatures can also be difficult, many researchers attempt to interpolate from the atmospheric region up to the critical point by enforcing fit-of-form constraints. Two constraints have been developed for the same curve feature that is believed to be generally applicable to all substances. Thodos (1950), in his study of saturated aliphatic hydrocarbons, found that an inflection point in the $Ln\ P$ vs. $1/T$ curve existed, and it occurred at a higher temperature than the normal boiling point. Waring (1954) showed that because of the thermodynamically exact relationship $\Delta H_\mathrm{v}/\Delta Z_v = -\mathrm{R}\ d(Ln\ P)/d(1/T)$, a minimum in the $\Delta H_\mathrm{v}/\Delta Z_v$ vs. T_r curve is required to occur at this inflection point. ΔH_v and ΔZ_v represent differences in the enthalpies and compressibility factors, respectively, of vapor and liquid at saturation. For most substances, Waring concluded that this minima resides in the reduced-temperature interval 0.8 - 1.0. Waring recommended this criterion as a qualitative fit-of-form test.

Ambrose et al. (1978) attempted to quantify the constraint more by restricting the $\Delta H_\mathrm{v}/\Delta Z_v$ minimum to the 0.8-0.9 reduced temperature range and by showing that the inflection point in the $Ln\ P_v$ vs. $1/T$ curve is ensured by requiring that the vapor pressure at the reduced temperature of 0.95 take on a value within a specified range. The specified range is an approximation, based in part on the general properties of the VLE curve for the type of substances being studied. The authors developed the approximate specified range for non-associated substances and specifically stated that it did not apply to alcohols, for example. Thus, neither the qualitative $\Delta H_v/\Delta Z_v$ minimum of Waring nor its approximate family-dependent Ambrose extension at T_r=0.95 are sufficiently quantitative and general to provide an easy universal method of verification of VLE interpolation to the high-temperature end.

In summary, some of the tools researchers use try to overcome the deficiency of accurate vapor pressure at low and high temperatures are the following: 1) complex curve fitting/regression of data; 2) ancillary low-temperature thermal data/approximations for extrapolation of VLE to the lower region; and/or 3) attempt to transform qualitative fit-of-form tests such as the Waring criterion into a quantitative constraints in the high-temperature region. The universal method resulting from the research presented here, however, is a simple algebraic framework, in which the above three commonly used elements are absent.

I.4 Broader Impacts of the Proposed Work

There are phenomena of which VLE is a part, such as aerosol creation and growth. Inorganics and several hundred organic compounds have been identified in atmospheric aerosols (Seinfeld & Pandis, 2006). VLE is mathematically coupled to other thermodynamic properties. Improved VLE predictive approaches, such as the one presented here, can contribute to the generation of more accurate analytic VLE data for species for which there are sparse experimental data. Such analytic data could contribute to improved modeling of broader phenomena like aerosol development or multi-property thermodynamic models.

An artificial neural network (ANN) is a viable solution approach for a problem characterized by "a high-dimensional problem space; complex, unknown, or mathematically intractable interactions between problem variables" (Schalkoff, 1997), which describes molecular thermodynamics well. Additionally, ANNs require much data – they are for problems that are data rich and model poor. On the longer-term horizon, perhaps accurate analytic data from improved VLE predictive methods will be used to train ANN-based thermodynamic models.

I.5 Novelty with the Approach

Others who study the Wagner equation compare its predictive power relative to experimental VLE data or best values estimated from the simultaneous regression of thermal and VLE data, their parameterization of the Wagner equation is an over-determined solution of experimental data, when the VLE data is from a limited interval the VLE extension is unidirectional, and they do not perform a segmented error analysis. The approach in this work differs from these other researchers on all of these fronts, and more.

In Chapter 1, the roles of error due to data imprecision and error due to imperfection of the Wagner equation are compared, and the dependency of predictive error upon the data interval's width and location are investigated. This researcher is not aware of such a segmented error analysis of the Wagner equation's parameterization being reported anywhere else in the literature.

Using Antoine analytics to represent a limited-data interval and entire-curve Wagner analytics to represent "best values" for the entire two-phase curve is a unique method to provide a broad indication of data disagreement in the literature. Generally, researchers compare several available data sets to determine the degree of data consistency for a targeted substance. Such an in-depth analysis does provide a thorough look at an individual species, but the novel approach used in Chapter 2 provides a good, quick, overall indication of the level of data consistency and precision that a practitioner can expect to find in the literature. The new concept of "extrapolation burden," more fully developed in Chapter 2, is a novel quotient created to quantify the relative difficulty a researcher or practitioner may experience when trying to extrapolate a species' VLE downward to the triple point.

To use the most accurate data possible is the most natural and logical path to follow when trying to parameterize a predictive correlation. The concept of using a set of source predictive correlations to provide the "data" with which another predictive correlation is parameterized is counter intuitive, and therein lays its novelty. This researcher is not aware of any other work in the literature postulating, let alone providing strong evidence for, the hypothesis that Wagner equation parameterized from VLE predictions can have better predictive power than the source correlations themselves. The approach presented in Chapter 3 has the potential to be modified and improved to provide more avenues for increased predictive VLE for species with sparse experimental data.

There are two novel elements that run through all three chapters. The primary novel element is the use of an easy algebraic, fully-determined solution to estimate the Wagner constants. Using a four-point fully-determined solution rather than an over-determined solution may again be counter intuitive, and again, therein lays its novelty. That so much valuable technical insight and predictive success can arise from a relatively simple, algebraic parameterization of the Wagner equation is remarkable.

The second element regards the breadth of predictive extension. Other researchers look at extending VLE predictability in one direction, either upward to the critical point or extrapolation down to the triple point. This work is unique in that it addresses extending VLE both above and below the limited data interval, and it provides a look at predictive power over the entire two-phase curve in aggregate. This work also only uses VLE data, whereas other researchers generally rely upon thermal data when extending down to the triple point.

I.6 Common Elements of Implementation

All calculations are performed in Microsoft EXCEL. Two other elements common to the entire work are discussed below - calculation round off and error statistics.

I.6.1 Calculation Round Off

An important element of any correlative analysis, overlooked by many correlators, is that of round off used during calculations. It was chosen to let general data accuracies reported in the literature determine the round off used in this work. Accuracy is defined as the closeness of a given value (either measured or analytic) to the true value. Accuracy of measured or analytic data is defined here in terms of significant digits. For example, most temperature values in Kelvin in the literature, both low and high, are given to five significant digits; consequently, reduced temperature and τ (1 minus the reduced temperature) values in this work are rounded off to five significant digits when used as inputs to calculations or generated outputs.

Accuracy of a pressure measurement can vary significantly depending upon the pressure's true value, the experimental technique, and the understanding/competence of the experimenter, as discussed previously. However, for this work what constitutes good pressure accuracy is defined by the measurement range most commonly found in the literature. Measuring pressure is considered relatively easy in the 1-200 kPa (0.01-2 bar) range, and high quality measurements around atmospheric pressure have error less than 0.01% (Ruzicka et al., 2008).

An error of 0.01% of atmospheric corresponds to the 10^{-4} decade in bar, which is consistent with the previously discussed observation of Albright (2009) that measurement accuracy, for the static Knudsen method at least, decreases as one goes below the 10^{-4} decade. The true value of atmospheric pressure assumed in this work is the generally accepted value of 1.01325 bars. Five significant digits in the mantissa of the natural logarithm of reduced pressure ($Ln\ P_{v,r}$) provide the six-significant-digit accuracy of 1.01325. Five significant digits in pressure, or four digits in the mantissa of $Ln\ P_{v,r}$, correspond to a 10^{-4} bar accuracy in pressure. Such significant digits define what constitutes good accuracy for pressure.

The far majority of species with Antoine-constants given in Poling et al. (2001) has a stated minimum pressure not less than 0.02 bar. The stated maximum pressure for most of them is 2 bar. Thus, the far majority of Antoine equations used in this work lay in the relatively "easy-" and "accurate-to-measure" range. Consequently, the round off used for pressure in this work corresponds to that defined for good accuracy.

Interestingly, most values for the acentric factor, which is logarithm based, are reported with only three significant digits. This may be because many values are based on extrapolations rather than interpolation or a direct measurement. For consistency sake, however, the $Ln\ P_{v,r}$ values for the reduced temperature of 0.7 calculated from acentric factors are rounded off to four digits in the mantissa.

The precision of temperature and pressure data, in Kelvin and bar, respectively, provided in Poling et al. (2001) is not greater than two significant digits right of the decimal point. *NIST* (Lemmon et al., 2011), however, can provide output data results with more significant digits. For the work in Chapter 1, absolute temperature and pressure inputs for the five *NIST* species have more significant digits than that of Poling et al. (2001) - only the reduced forms were rounded off as inputs. However, the Antoine equation, which is used in Chapters 2 & 3, is not in reduced form, and a consistent round off for absolute values is required as well. Consequently, absolute temperature and pressure inputs are rounded off to two digits right of the decimal point for the work in Chapters 2 and 3. This nuance has small influence on reduced vapor pressures predicted by the Wagner equation and its impact is limited to the five *NIST* species because their critical temperature and pressure inputs are not rounded off to two digits right of the decimal point in Chapter 1.

No inherent accuracy is assumed for *NIST* data (Lemmon et al., 2011) or VLE analytic values from Antoine constants and entire-curve Wagner constants. However, a reasonable round off level has to be fixed for temperature and vapor pressure values to force the emergence of imprecision error and to enforce calculation consistency. Rounding off is not done for internal calculations, but rounding off to the precision summarized in Table I.1 is performed when parameters are used as inputs to calculations and when generated as final outputs. Parameters listed in Table I.1 are defined as they are introduced in the subsequent narrative.

I.6.2 Error Statistics

Accuracy of reduced vapor pressures relative to a reference value are given in terms of absolute percent error: A%Err: = |100*(Reference - Calculated)/Reference|. The "Reference" value generally refers to an entire-curve Wagner analytic value, and "Calculated" generally indicates an Antoine analytic or a predicted value.

Average error can sometimes be misleading. Many correlations have been found to have good average errors while having a relatively high maximum error. Low error at the high-temperature end can result in an impressive average error while masking significantly larger error at the low-temperature end. Unintended error masking can also occur if data points have unequal weights. Consequently, in this work, all points have the same weight when calculating an average error, both average and maximum errors are presented, and error statistics for different reduced temperature segments are provided.

Chapter 1: Error Dependency Upon Data Interval & Fully-Determined Case

1.1 Abstract

The predictive error in vapor pressure of limited-data Wagner constants relative to that of entire-curve constants is studied for eleven data intervals. Good precision is assumed for data inputs, four digits in the mantissa of $Ln\ P_{v,r}$ and five digits for T_r. An algebraic solution for the fully-determined case based on four data points is used to estimate Wagner constants. Seventy-two species are used to assess the impact of the location of the two interior points and the location and width of the limited-data interval upon the error in predicted $P_{v,r}$ due to data imprecision. Hydrogen, helium, R152a, and water are used to assess error due to Wagner imperfection and compare predictive capability of the algebraic fully-determined and regressed over-determined cases. The results indicate that limited VLE data of good precision from reduced temperature intervals with a width ≥ 0.1 and a lower bound ≤ 0.6 can generally provide reasonable VLE predictions for pure substances, with average entire-curve error of approximately 1%. It is shown that the algebraic fully-determined solution presented is a viable tool for investigating the extensibility of limited-data Wagner constants.

1.2 Introduction

The Wagner equation has been shown to be successful at accurately representing phase equilibrium along the entire co-existence curve for many substances (Ambrose, 1986; Poling, 1996; Poling et al., 2001; Vetere, 2006; J. T. Wu & Liu, 2005). It is generally not considered to be predictive because the constants are not known *apriori*; being unique for each substance, the four constants are determined by data regression. The work presented here explores the ability of the Wagner equation to become predictive for the entire two-phase region by estimating the constants from limited VLE data.

Since Wagner (1973) developed his original vapor pressure equation with species-dependent constants, slightly different forms have been used by researchers, some with an additional term, and some with different exponents. Poling (1996), for example, concluded that when higher-temperature VLE data was combined with simultaneous regression of low-temperature heat capacity data, the entire two-phase region VLE for nine hydrocarbon species was accurately described by a four-term form using τ exponents of 1, 1.5, 3, and 6, but the VLE for ethanol and isopropanol was fit better with a five-term form using the τ exponents of 1, 1.5, 2.5, 5, and 6. The form of the Wagner equation used in this work is

[1] $$Ln\, P_{v,r} = (a\tau + b\tau^{1.5} + c\tau^{2.5} + d\tau^{5})/T_r.$$

Ln refers to natural logarithm, *P* refers to pressure, and *T* represents absolute temperature. The subscript *v* indicates the pressure corresponds to the vapor-liquid equilibrium curve, and *r* indicates that the parameter is reduced with respect to the critical point (i.e., $T_r = T/T_c$ and $P_r = P/P_c$, where the subscript *c* refers to the critical point). The parameter τ equals $1\text{-}T_r$. The four-term form given in Eq. [1] is chosen because a fifth term is not justified except in the cases of a few species (Ambrose, 1986), and it is recommended (Poling et al., 2001) for general application.

1.3 Investigative Approach

Constants for the Wagner equation applicable to the entire two-phase VLE curve for many pure substances are reported in the literature. These are referred to here as “entire-curve” constants, and vapor pressures calculated using such constants are referred to as “entire-curve analytic” data. Entire-curve constants for sixty-seven substances are taken from *The Properties of Gases and Liquids* (Poling et al., 2001).

Additionally, *NIST* data (Lemmon et al., 2011) is used with least-squares regression to determine the entire-curve Wagner constants for helium, hydrogen, argon, water, and R152a. Hydrogen and helium are added to include quantum gases, to which the molecular theory of corresponding states is not generally considered to be applicable without using "effective" critical parameters (Prausnitz et al., 1999). Many researchers, including Poling et al. (2001), use τ^3 and τ^6 instead of $\tau^{2.5}$ and τ^5, respectively, for water, so constants corresponding to the Eq. [1] form of Wagner's equation need to be determined for water. Constants for argon are determined because, as a heavy noble gas, it is one of the few species strictly considered to be a "simple" molecule. R152a is added to include a refrigerant.

Several researchers have used limited VLE data to estimate Wagner constants that were then used to extend VLE predictions. In some cases only VLE data is used (Ambrose, 1978; McGarry, 1983; G. & J., 2011), and in other cases researchers use thermal data in the intervals where VLE data are lacking and simultaneously regress thermal property and VLE models in an attempt to extend the range of VLE prediction into the temperature and pressure range of the thermal data (Ambrose et al., 1978; Ambrose & Davies, 1980; Hogge et al., 2016; King & Al-Najjar, 1974; Poling, 1996; K. Ruzicka & Majer, 1994). The extension from limited VLE data is generally in one direction, either above or below the original data interval. The leveraging of thermal data is usually used when trying to extrapolate VLE down towards the triple point. Researchers such as these use non-linear, over-determined regression algorithms to parameterize the Wagner equation.

Because the Wagner equation has four species-specific constants, accurate values of these constants can be calculated algebraically from any four VLE data points provided: 1) the Wagner equation's functional form allows for perfect characterization of the species' VLE over the entire two-phase curve, and 2) the four data points have perfect precision. Neither of these two conditions is ever satisfied completely. Consequently, when using the Wagner equation to correlate VLE data, there will exist some level of equation imperfection error corresponding to the degree to which condition one is not satisfied and some level of data imprecision error corresponding to the degree to which condition two is not satisfied. Naturally, researchers using the Wagner equation try to maximize the data precision and the number of data points in an attempt to mitigate error due to imperfection and imprecision.

Although correlative power within the data interval from which a correlation is parameterized is usually proportional to the number of data points used, a dependency of similar strength upon the number of points does not necessarily exist for the predictive power when using the correlation to extrapolate outside the data interval. That is because extrapolation can involve considerable error (Smith, 1979), and an increase in the amount of parameterization points within the data interval itself may not lessen the extrapolation error. The Antoine equation is a good example of this behavior because it is a quasi-linear approximation to a nonlinear vapor pressure curve. It is well known that the Antoine equation is unreliable for extrapolation of vapor pressure outside the data range from which it is parameterized (Poling et al., 2001). Increasing the number of data points within the parameterization interval will not necessarily increase its predictive power outside the interval.

Because the curvature of the vapor pressure curve is not constant, even robust nonlinear equations such as Wagner can experience the dangers of extrapolation, where the predictive error outside the interval has diminished dependency upon the amount of regressed data points. Such extrapolation error for a given interval can be influenced by both data imprecision and equation imperfection. Consequently, it is hypothesized that a fully-determined parameterization of the Wagner equation can be a useful error assessment tool when extending predictions of the Wagner equation beyond the data interval from which it is parameterized. Four data points, i.e., a fully-determined solution, are used to algebraically estimate limited-data Wagner constants in a controlled and methodical manner to estimate the dependency of the imperfection and imprecision errors upon the parameterization interval's width and location on the VLE curve. The goal is to determine the validity of Hypothesis I.

The work presented in this chapter is unique from other researchers in several ways. First, a relatively simple, algebraic, fully-determined solution using only four points is used instead of complex, over-determined regression. Second, only VLE data is used to extend predictive capability to the entire two-phase curve, no thermal data is utilized to bridge gaps. Third, the extension is bi-directional, both extrapolating down towards the critical point and interpolating upward to the critical point. Fourth, an error segmentation is presented that has never before been attempted – error due to data imprecision and equation imperfection is separated, and the dependency of predictive error upon the data interval's width and location is assessed. The research literature is largely silent on these elements of Wagner parameterization and predictive power.

Wagner constants estimated from the fully-determined case using four of the entire-curve Wagner analytics from a limited-data interval are used to predict VLE. The contribution of imprecision error is estimated by comparing these predictions along the entire two-phase curve with the entire-curve Wagner analytics.

Since the limited-data constants are based upon four entire-curve analytics, the difference between their predictions over the entire two-phase curve and the entire-curve analytics is primarily due to round-off error, or imprecision error. A reliable point distribution is determined from a statistical analysis of the imprecision error of three distributions. An assessment of the impact of data interval width and location upon imprecision error is then performed using the selected point distribution.

Subsequently, Wagner constants are algebraically determined for four species (hydrogen, helium, R152a, and water) for which the data used to generate the entire-curve Wagner constants are known. The constants are estimated using four underlying data points from a limited interval. The predictions from the limited-data constants over the entire two-phase curve are compared with the entire-curve Wagner analytics. The imprecision error is subtracted from this total error to estimate the imperfection error for several data intervals for the four species. Lastly, these same four species are used to compare the predictive capability of the fully-determined case vs. that of the over-determined case (using more than four points).

Regression algorithms for an over-determined system can involve characteristics that will influence the results and whose influence may be species-dependent (e.g., data spacing, data weighting, method for estimating initial values of the constants, and the error minimization scheme employed). Using a consistent algebraic method independent of species and regression algorithm characteristics allows for accurate relative error comparisons.

1.4 Discussion

1.4.1 Regressing Wagner Constants for Five Species Using NIST Data

The results of the regression of entire-curve Wagner constants for helium, hydrogen, argon, water, and R152a are shown in Table 1.1. The table shows the normal boiling point and critical properties from *NIST*, the number of analytic points used for each regression, the regressed constants, the average and maximum absolute percentage errors for reduced pressure, and the reduced temperature at which the maximum error occurs are shown.

The value of the normal boiling point corresponding to the regressed constants is also indicated in Table 1.1. Using the *NIST* critical property values, 1.01325 bar for normal atmospheric pressure, and the regressed Wagner constants shown in the table, the normal reduced boiling point is determined for each of the five species using the *SOLVER* routine in *EXCEL*. Rounding the solved reduced boiling point to five significant digits and rounding the *NIST* critical temperature to 2 digits right of the decimal point, the normal boiling point temperature is calculated and also rounded to 2 digits right of the decimal point. That is the value of T_b shown in the "Regression" section of the table, and it is the normal boiling point corresponding to the VLE curve represented by the regressed Wagner constants.

Except for argon, all the maximum errors occur in the low-temperature region, very close to the normal fusion point. One can see that helium and water have worse maximum error than the others. The inclusion of the fifth τ^6 term does reduce the errors for helium and water (not shown here), but their errors using the 4-term form are still sufficiently low to be acceptable. When rounded off to five significant digits, the temperature of the normal boiling point for helium determined from the Wagner equation is the same as that of *NIST*, (although *NIST* differs by 0.07 °K relative to that of Sec. A of Appendix A of Poling et al. (2001), and that of water is 0.01 higher than that of *NIST*.

The detailed results for every analytic point used in each regression are presented in Appendix A.

1.4.2 Entire-Curve Wagner Constants and Physical Properties

The literature values for the entire-curve Wagner constants for the seventy-two species are given in Table 1.2. The physical properties used are shown in Table 1.3. Although the dipole moment is not used as a mathematical input in this work, it is included in the table to provide an indication of polarity. The normal boiling point for each species is determined by inserting the atmospheric pressure, 1.01325 bars, into the Wagner equation and solving for the saturation temperature. The value of the acentric factor is also calculated from the Wagner equation. Thus, the Riedel and Ambrose-Walton equations will have their anchor points for each species consistent with the species' Wagner equation when error comparisons are made in Chapters 2 and 3. Rounding off absolute values of critical temperature and pressure as inputs to two digits right of the decimal point is reflected in Table 1.3.

The critical properties corresponding to the Wagner constants given in Section D of Appendix A of Poling et al. (2001) differed from those given in Section A of the same appendix for several species. The data from Section A of Appendix A of Poling et al. (2001) for the species with entire-curve Wagner constants are shown here in Table B.1 of Appendix B. The critical constants of the Wagner equations that are different from those in Section A of Poling et al. (2001), the calculated normal boiling points and acentric factors determined from the Wagner constants, and any absolute difference relative to Section A of Poling et al. (2001) are detailed here in Table B.2 of Appendix B.

1.4.3 Estimating Wagner Constants Algebraically (Fully-Determined Case)

The fully-determined solution to the Wagner equation requires only four data points, and algebra allows each Wagner constant to be represented by an $F_{w,j}$ function given by

$$F_{w,j} = \eta_{j1} Ln\, P_{v,r,T_{r1}} + \eta_{j2} Ln\, P_{v,r,T_{r2}} + \eta_{j3} Ln\, P_{v,r,T_{r3}} + \eta_{j4} Ln\, P_{v,r,T_{r4}}\ , \tag{2}$$

where the subscript *j* refers to the Wagner constant (*a*, *b*, *c*, or *d*). The reduced temperature subscript on $Ln\ P_{v,r}$ and the value of the "*i*" subscript in the η_{ji} terms indicate the corresponding data point of the four selected VLE data points. The only arguments of the universal $F_{w,j}$ function are a species' four $Ln\ P_{v,r}$ values. The sixteen η_{ji} coefficients (4 for each of the 4 Wagner constants) only depend upon the four reduced temperatures; thus, they are the same for all species for any fixed set of four reduced temperatures. The values of the η_{ji} coefficients are rounded off to seven significant digits right of the decimal point to ensure the assumed precision of the Wagner constants.

Eq. [2] for each of the four Wagner constants is

$$a = F_{w,a} = \eta_{a1} Ln\, P_{v,r,T_{r1}} + \eta_{a2} Ln\, P_{v,r,T_{r2}} + \eta_{a3} Ln\, P_{v,r,T_{r3}} + \eta_{a4} Ln\, P_{v,r,T_{r4}}, \tag{2a}$$

$$b = F_{w,b} = \eta_{b1} Ln\, P_{v,r,T_{r1}} + \eta_{b2} Ln\, P_{v,r,T_{r2}} + \eta_{b3} Ln\, P_{v,r,T_{r3}} + \eta_{b4} Ln\, P_{v,r,T_{r4}}, \tag{2b}$$

$$c = F_{w,c} = \eta_{c1} Ln\, P_{v,r,T_{r1}} + \eta_{c2} Ln\, P_{v,r,T_{r2}} + \eta_{c3} Ln\, P_{v,r,T_{r3}} + \eta_{c4} Ln\, P_{v,r,T_{r4}}, \tag{2c}$$

and

$$d = F_{w,d} = \eta_{d1} Ln\, P_{v,r,T_{r1}} + \eta_{d2} Ln\, P_{v,r,T_{r2}} + \eta_{d3} Ln\, P_{v,r,T_{r3}} + \eta_{d4} Ln\, P_{v,r,T_{r4}}. \tag{2d}$$

1.4.3.1 Derivation of $F_{w,j}$ Functions

The $F_{w,j}$ functions are derived by inverting the Wagner equation to express each constant in terms of one point on the saturation curve and the other constants, as given below:

$$a = \frac{(Ln\, P_{v,r,1})T_{r,1}}{\tau_1} - b\tau_1^{0.5} - c\tau_1^{1.5} - d\tau_1^{4} \tag{3}$$

$$b = \frac{(Ln\, P_{v,r,2})T_{r,2}}{\tau_2^{1.5}} - \frac{a}{\tau_2^{0.5}} - c\tau_2 - d\tau_2^{3.5} \tag{4}$$

$$c = \frac{(Ln\, P_{v,r,3})T_{r,3}}{\tau_3^{2.5}} - \frac{a}{\tau_3^{1.5}} - \frac{b}{\tau_3} - d\tau_3^{2.5} \tag{5}$$

[6] $$d = \frac{(Ln\, P_{v,r,4})T_{r,4}}{\tau_4^5} - \frac{a}{\tau_4^4} - \frac{b}{\tau_4^{3.5}} - \frac{c}{\tau_4^{2.5}}\,.$$

Substituting Eq. [3] into [4] for *a* gives

[4a] $$b = \frac{\frac{(Ln\, P_{v,r,2})T_{r,2}}{\tau_2^{1.5}} - \frac{(Ln\, P_{v,r,1})T_{r,1}}{\tau_1 \tau_2^{0.5}} + c\left(\frac{\tau_1^{1.5}}{\tau_2^{0.5}} - \tau_2\right) + d\left(\frac{\tau_1^4}{\tau_2^{0.5}} - \tau_2^{3.5}\right)}{1 - \left(\frac{\tau_1}{\tau_2}\right)^{0.5}}\,.$$

Inserting [4a] into [3] for *b* results in

[3a] $$a = \frac{(Ln\, P_{v,r,1})T_{r,1}}{\tau_1}\left\{1 + \frac{\tau_1^{0.5}}{\tau_2^{0.5}\left[1 - \left(\frac{\tau_1}{\tau_2}\right)^{0.5}\right]}\right\} - \left(Ln\, P_{v,r,2}\right)T_{r,2}\frac{\tau_1^{0.5}}{\tau_2^{1.5}\left[1 - \left(\frac{\tau_1}{\tau_2}\right)^{0.5}\right]}$$
$$-c\left[\tau_1^{1.5} + \frac{\tau_1^{0.5}\left(\frac{\tau_1^{1.5}}{\tau_2^{0.5}} - \tau_2\right)}{1 - \left(\frac{\tau_1}{\tau_2}\right)^{0.5}}\right] - d\left[\tau_1^4 + \frac{\tau_1^{0.5}\left(\frac{\tau_1^4}{\tau_2^{0.5}} - \tau_2^{3.5}\right)}{1 - \left(\frac{\tau_1}{\tau_2}\right)^{0.5}}\right].$$

The coefficients dependent upon τ in Eqs. [3a] & [4a] were replaced with ε parameters to avoid algebraic errors in the subsequent iterative substitutions, resulting in

[3b] $$a = \varepsilon_{a2}\left(Ln\, P_{v,r,1}\right)T_{r,1} - \varepsilon_{a3}\left(Ln\, P_{v,r,2}\right)T_{r,2} - c\varepsilon_{a4} - d\varepsilon_{a5}$$

and

[4b] $$b = -\varepsilon_{b1}\left(Ln\, P_{v,r,1}\right)T_{r,1} + \varepsilon_{b2}\left(Ln\, P_{v,r,2}\right)T_{r,2} + c\varepsilon_{b3} + d\varepsilon_{b4}\,,$$

where the definitions for the ε parameters are given in Table 1.4.

Substituting Eqs. [3b] & [4b] for *a* and *b*, respectively, into Eq. [5] produces the following for the Wagner constant *c*,

[5a] $$c\left(1 + \frac{\varepsilon_{b3}}{\tau_3} - \frac{\varepsilon_{a4}}{\tau_3^{1.5}}\right) = \left(\frac{\varepsilon_{b1}}{\tau_3} - \frac{\varepsilon_{a2}}{\tau_3^{1.5}}\right)\left(Ln\, P_{v,r,1}\right)T_{r,1} + \left(\frac{\varepsilon_{a3}}{\tau_3^{1.5}} - \frac{\varepsilon_{b2}}{\tau_3}\right)\left(Ln\, P_{v,r,2}\right)T_{r,2} +$$
$$+ \frac{(Ln\, P_{v,r,3})T_{r,3}}{\tau_3^{2.5}} + d\left(\frac{\varepsilon_{a5}}{\tau_3^{1.5}} - \frac{\varepsilon_{b4}}{\tau_3} - \tau_3^{2.5}\right).$$

Replacing the coefficients dependent upon ε parameters and τ in the above equation allows the simplification to

[5b] $$c = \varepsilon_{c2}\left(Ln\, P_{v,r,1}\right)T_{r,1} + \varepsilon_{c3}\left(Ln\, P_{v,r,2}\right)T_{r,2} + \varepsilon_{c1}\left(Ln\, P_{v,r,3}\right)T_{r,3} + d\varepsilon_{c4}\,,$$

where the various new ε_c parameters are also defined in Table 1.4.

Eq. [5b] is now substituted for *c* in Eqs. [3b] & [4b], yielding

[3c] $$a = (\varepsilon_{a2} - \varepsilon_{a4}\varepsilon_{c2})\left(Ln\ P_{v,r,1}\right)T_{r,1} - (\varepsilon_{a3} + \varepsilon_{a4}\varepsilon_{c3})\left(Ln\ P_{v,r,2}\right)T_{r,2}$$
$$-\varepsilon_{a4}\varepsilon_{c1}\left(Ln\ P_{v,r,3}\right)T_{r,3} - d(\varepsilon_{a5} + \varepsilon_{a4}\varepsilon_{c4})$$

and

[4c] $$\mathrm{b} = (\varepsilon_{b3}\varepsilon_{c2} - \varepsilon_{b1})\left(Ln\ P_{v,r,1}\right)T_{r,1} - (\varepsilon_{b3}\varepsilon_{c3} + \varepsilon_{b2})\left(Ln\ P_{v,r,2}\right)T_{r,2}$$
$$+\varepsilon_{b3}\varepsilon_{c1}\left(Ln\ P_{v,r,3}\right)T_{r,3} - d(\varepsilon_{b3}\varepsilon_{c4} + \varepsilon_{b4}).$$

Substituting Eqs. [3c], [4c], and [5b] for *a*, *b*, and c, respectively, into Eq. [6] results in

[6a] $$d\varepsilon_d = \varepsilon_{d1}\left(Ln\ P_{v,r,1}\right)T_{r,1} + \varepsilon_{d2}\left(Ln\ P_{v,r,2}\right)T_{r,2} + \varepsilon_{d3}\left(Ln\ P_{v,r,3}\right)T_{r,3} +$$
$$\left(\frac{1}{\tau_4^5}\right)\left(Ln\ P_{v,r,4}\right)T_{r,4}\ ,$$

where the ε$_d$ terms are given by

[6a-i] $$\varepsilon_d = 1 - \frac{\varepsilon_{a5} + \varepsilon_{a4}\varepsilon_{c4}}{\tau_4^4} + \frac{\varepsilon_{b3}\varepsilon_{c4} + \varepsilon_{b4}}{\tau_4^{3.5}} + \frac{\varepsilon_{a4}}{\tau_4^{2.5}}\ ,$$

[6a-ii] $$\varepsilon_{d1} = -\frac{\varepsilon_{a2} - \varepsilon_{a4}\varepsilon_{c2}}{\tau_4^4} - \frac{\varepsilon_{b3}\varepsilon_{c2} - \varepsilon_{b1}}{\tau_4^{3.5}} - \frac{\varepsilon_{c2}}{\tau_4^{2.5}}\ ,$$

[6a-iii] $$\varepsilon_{d2} = \frac{\varepsilon_{a3} + \varepsilon_{a4}\varepsilon_{c3}}{\tau_4^4} - \frac{\varepsilon_{b3}\varepsilon_{c3} + \varepsilon_{b2}}{\tau_4^{3.5}} - \frac{\varepsilon_{c3}}{\tau_4^{2.5}}\ ,$$

and

[6a-iv] $$\varepsilon_{d3} = \frac{\varepsilon_{a4}\varepsilon_{c1}}{\tau_4^4} - \frac{\varepsilon_{b3}\varepsilon_{c1}}{\tau_4^{3.5}} - \frac{\varepsilon_{c1}}{\tau_4^{2.5}}\ .$$

Subsequently dividing Eq. [6a] by ε$_d$ gives the following for Wagner constant *d*,

[6b] $$d = \frac{\varepsilon_{d1}}{\varepsilon_d}\left(Ln\ P_{v,r,1}\right)T_{r,1} + \frac{\varepsilon_{d2}}{\varepsilon_d}\left(Ln\ P_{v,r,2}\right)T_{r,2} + \frac{\varepsilon_{d3}}{\varepsilon_d}\left(Ln\ P_{v,r,3}\right)T_{r,3} + \frac{1}{\tau_4^5\varepsilon_d}\left(Ln\ P_{v,r,4}\right)T_{r,4}\ .$$

Eq. [6b] is substituted for *d* into the equations for the other constants (Eqs. [3c], [4c], and [5b]) to finally produce equations for all four constants with the four vapor pressure points as arguments, as given previously in Eqs. [2a]-[2d]. All the ε and η parameters are defined in Table 1.4**.**

1.5 Results

1.5.1 Predictive Error Due to Imprecision of Limited Data

Analytic $Ln\ P_{v,r}$ values predicted from entire-curve Wagner constants from eleven limited-reduced-temperature intervals are rounded-off to the fourth significant digit in the mantissa. The analytic data are then used to estimate “limited-data” Wagner constants using Eqs. [2a] - [2d]. Such a function is referred to as $F_{w,j}[WA]$, where “[WA]” has been added to indicate that the four $Ln\ P_{v,r}$ values used are entire-curve Wagner analytic values. The difference between the reduced pressures predicted from these limited-data constants over the entire two-phase curve relative to the entire-curve analytics isolates the part of the predictive error of the Wagner equation that is due primarily to imprecision of the limited data (the rounding off stated in Table I.1).

The imprecision error is first used to help determine a reasonable point distribution, after which, the selected point distribution is used to assess the self-consistency of imprecision error, the influence of interval width and location, and the resulting errors in estimated Wagner constants.

1.5.1.1 Determination of Reasonable Point Distribution

Eleven limited-data intervals with reduced-temperature widths ranging from 0.05 to 0.4 are selected. The intervals are representative of the applicable temperature ranges for the Antoine and Extended-Antoine equations provided in Poling et al. (2001).

An interval is defined by the lowest and the highest points used in the calculation of the Wagner constants. There are an infinite number of possible arrangements for the remaining two internal data points. The three following distributions for the two internal points are investigated: 1) the “even” distribution where the interval is divided into thirds, and the two points are equally spaced within the interval at 1/3 and 2/3 of the interval width; 2) the "quarter" distribution where the interval is divided into fourths, and the two internal data points are located at the 1/4 and 3/4 positions; and 3) the "eighth" distribution, dividing the interval into eighths, and the two internal data points are located at the 1/8 and 7/8 positions. The four reduced temperatures for each interval and point distribution combination are shown in Table B.3 of Appendix B. The values of the η parameters for each interval and point distribution combination are shown in Tables B.4 through B.8.

The absolute percent error (A%Err) of the predicted $P_{v,r}$ relative to the analytic values for the various intervals are calculated for each species at the normal fusion point, normal boiling point, and for all points at 0.05 reduced temperature increments from $T_r = 0.95$ down to the normal fusion point. A%Err represents 100 * | ($P_{v,r}$ analytic – $P_{v,r}$ predicted)/ $P_{v,r}$ analytic |. For each interval|distribution combination, the average error for all seventy-two species in aggregate is calculated at the normal fusion and boiling points and for three temperature segments: 1) the lower region, the "$T_r \leq 0.6$" segment, contains all the reduced temperature values ranging from 0.6 down to the normal fusion point, calculated in 0.05 reduced temperature increments; 2) the upper region, the "$T_r > 0.6$" segment, contains the points from 0.65 up to and including 0.95, also calculated in 0.05 reduced temperature increments; and 3) the entire two-phase curve is represented by the "All T_rs" segment and includes all the calculated points from the normal fusion point up to the reduced temperature of 0.95. The normal boiling point is included in the “All T_rs” rather than the other two segments. Propane is the only species with $T_{r,f} < 0.25$, and its $T_{r,f}$ value of 0.23 is sufficiently close to 0.25 such that the data point for $T_\mathrm{r} = 0.25$ is not included in the error statistics for propane.

Because not all species have the same number of points in each segment, for any given interval the average error for a segment is the average of all the points for all species in that segment rather than the average of species-specific segment averages. Similarly, the maximum error for a segment is the largest error of all the points for all 72 species in that segment. The error at each of an interval's four data points used in the $F_{w,j}[WA]$ function is zero by algebraic definition; consequently, such points are excluded from the error statistics to avoid skewing the average error values and giving an artificial advantage or disadvantage to an interval. Obviously, the most statistically significant aggregate error is for "All T_rs" because it involves the most points.

The population variances of the average error for the three distributions (“even,” “quarter” and “eighth”) for a given interval are treated as unknown and unequal. The well-known t^* test statistic with ν degrees of freedom is used to compare the means of two populations, where t_0^* and ν are given by (Hines & Montgomery, 1980)

$$[7] \qquad t_0^* = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}}$$

and

$$[8] \qquad \nu = \frac{\left(\frac{S_1^2}{n_1}+\frac{S_2^2}{n_2}\right)^2}{\frac{\left(\frac{S_1^2}{n_1}\right)^2}{n_1+1}+\frac{\left(\frac{S_2^2}{n_2}\right)^2}{n_2+1}} - 2\ .$$

The sample means are indicated by $\bar{X}$, sample variances by S, and the sample sizes by n.

Lumley et al. (2002) showed that even with a highly skewed population, sample sets as small as 65 result in the sample means having a near-normal distribution, thus satisfying the general conditions of the Central Limit Theorem and permitting the use of the t-test, whether or not the variances of the two populations are assumed equal (i.e., whether the t or the t^* test is used). Hines & Montgomery (1980) give the crude rule of thumb that a sample size of 100 or more is satisfactory to satisfy the general conditions of the Central Limit Theorem even for such an ill-behaved population that has most of its distribution in the tails. In this study, the sample sizes for each intra-interval point distribution are 69-72 for $T_{r,f}$ and $T_{r,b}$, greater than 200 for each of the two reduced temperature segments $T_r \leq 0.6$ and $T_r > 0.6$, and over 600 for the entire-curve (All T_rs). Consequently, the general conditions of the Central Limit Theorem should be satisfied and allow a statistical comparison of the error of different intra-interval point distributions.

The null hypotheses and corresponding alternative hypotheses tested are

	μ_e vs. μ_4	μ_e vs. μ_8	
H_0:	$\mu_e = \mu_4$	$\mu_e = \mu_8$	
H_1:	$\mu_e > \mu_4$	$\mu_e > \mu_8$	if $t_0^* > t_{\alpha,\nu}$
H_2:	$\mu_e < \mu_4$	$\mu_e < \mu_8$	if $t_0^* < -t_{\alpha,\nu}$

where the population mean of an average error is indicated by μ, and the subscripts "e," "4," and "8" indicate the "even," "quarter," and "eighth" distribution, respectively. The value of 0.05 is used for α, the probability of type I error. The value of $t_{0.05,120}$ is 1.658, and the value of $t_{0.05,\infty}$ is 1.645. There are no cases where $1.645 \leq t_0^* < 1.658$; consequently, the value of 1.658 is used for $t_{\alpha,\nu}$ for all values of $\nu \geq 120$ in the automated formula for the hypothesis testing.

The value of ν is rounded off to an integer, and the $\bar{X}$ values are rounded off to the nearest 0.0001%. All other statistical inputs are not rounded off. The t_0^* test is performed for the two null hypotheses H_0: $\mu_e = \mu_4$ and H_0: $\mu_e = \mu_8$. The results of the two t_0^* tests for each of the eleven intervals for five average A%Errs - $T_{r,f}$, $T_{r,b}$, $T_r \leq 0.6$, $T_r > 0.6$, and "All T_rs" - are shown in Table 1.5. The accepted one-sided alternative hypothesis is indicated when the null hypothesis is rejected. Absence of an alternative hypothesis means the corresponding null hypothesis is not rejected.

The accepted alternative hypotheses shown in Table 1.5 that pertain to the "eighth" distribution are in normal font. The null hypothesis H_0: $\mu_e = \mu_8$ cannot be rejected for twenty-seven of the cells in the table. For the remaining twenty-eight cells, the H_2: $\mu_e < \mu_8$ alternative hypothesis is accepted for twenty-seven while only one cell ($T_{r,f}$ in the 0.5-0.9 interval) shows the H_1: $\mu_e > \mu_8$ alternative hypothesis being accepted; the "eighth" distribution provides an advantage for only one out of the fifty-five cells in the table. Consequently, a point distribution heavily favoring the ends doesn't appear to provide an advantage over the "even" distribution.

The **H_2: $\mu_e < \mu_4$** entries in Table 1.5 are in bold-face font, and the font for *H_1: $\mu_e > \mu_4$* entries are italicized. The null hypothesis (H_0: $\mu_e = \mu_4$) cannot be rejected for twenty-one of the fifty-five cells, while the remaining cells are split evenly between the *H_1: $\mu_e > \mu_4$* and the **H_2: $\mu_e < \mu_4$** alternative hypotheses at seventeen apiece.

Looking at the Summary section of Table 1.5, one can see that the *H_1: $\mu_e > \mu_4$* alternative hypothesis is accepted twice as often as **H_2: $\mu_e < \mu_4$** at $T_{r,f}$, and subsequently in the $T_r \leq 0.6$ and "All T_rs" segments. The "even" distribution makes up the difference in the $T_r > 0.6$ segment. The differences in average errors between the "even" and "quarter" distributions when an alternative hypothesis is accepted is in the hundredths of percent.

The averages for the different interval | distribution combinations are shown in Appendix B in Tables B.9 through B.13. Averages where **H_2: $\mu_e < \mu_4$** is accepted are displayed in bold face font, and those where *H_1: $\mu_e > \mu_4$* is accepted are italicized. The maximum A%Err and t^* test statistical details for each interval are given in Tables B.14 through B.24, where "S-S Test Result" indicates results for the single-sided hypothesis testing.

The error for which hypothesis testing is performed in this exercise is not total predictive error but solely that due to the chosen data imprecision. Equation imperfection will subsequently be seen to generally exert a greater influence upon total error than data imprecision, diminishing potential differences between the “even” and “quarter” point distributions. Consequently, the intuitively appealing “even” distribution is used in the rest of this work.

1.5.1.2 Error Dependency Upon Interval Width and Location

The error statistics of the predicted $P_{v,r}$ relative to the entire-curve analytic values for the various intervals are displayed in Table 1.6 for the “even” distribution, sorted by ascending order in the average A%Err at the normal fusion point. Maximum error is not shown for the $T_r \leq 0.6$ and “All T_rs” segments because it is the same as that for the normal fusion point.

Looking at the $T_{r,f}$ and $T_r \leq 0.6$ columns of Table 1.6, one can see that the error at the low-temperature end of the VLE curve increases as the interval width decreases and as the interval location moves up the reduced temperature scale. The $T_r > 0.6$ column shows that the error in the upper portion of the VLE curve also increases as the interval decreases, but the error decreases instead of increasing as the interval location moves up the reduced temperature scale. One can see that the average entire-curve (“All T_rs”) error due to data imprecision does not exceed 1% until the interval width approaches 0.05.

These trends are more easily seen in Table 1.7 where the lower end point of the interval is given vertically and the interval width is listed horizontally (3-D contours for the average errors are displayed in Figures B.1 and B.2 in Appendix B). For every row (lower bound) with multiple cells, the average and maximum errors at the normal fusion point decrease with increasing interval width. In every column (width) with multiple cells, the errors decrease as the interval location moves down the VLE curve. These two trends are logical. The maximum and average errors are strongly tied and follow the same trends.

For example, the gray highlight in the maximum error section suggests that the maximum error at the normal fusion point would be 6% if one restricted himself to the shaded intervals. The corresponding cells in the average error section indicate that the average error would be less than 1% if one restricted himself to those same intervals.

Moving to the average and maximum errors for the $T_r > 0.6$ segment, one can see that the errors in every row with multiple cells decrease as the interval width increases, just as in the low-temperature region. However, contrary to that of the low region, the errors decrease as the interval location moves up the VLE curve. Again, these two trends are logical, and the maximum and average errors are strongly tied because they both follow the same trends. The gray highlight in the maximum error section of this segment's results indicate the location-width combinations for which these two trends suggest that both the maximum and average errors would be less than 1%. Essentially, for most intervals given in the literature with temperature and vapor pressure data of the precision given in Table I.1, relatively little error will be produced from data imprecision when extending up the VLE curve as long as the reduced temperature width is not less than 0.1.

It is obvious from Table 1.7 that the error reduction in the low-temperature region is more than an order of magnitude greater than the error increase in the upper region as the interval location is moved down the VLE curve. The error analysis thus far is strictly applicable to only when the Wagner equation can be assumed to provide a perfect fit, and when the temperature and vapor pressure data precision corresponds to that given in Table I.1. However, Table 1.7 shows quantitatively, in relative terms, the disproportionate impact the interval width and location have when extrapolating below the interval down towards the triple point compared to interpolation above the interval towards the critical point. It also suggests that the predictive error due to data imprecision increases significantly once the interval width gets smaller than 0.1.

Returning to Table 1.6, the importance of reducing the error at the low-temperature end in order to decrease that for the entire two-phase curve in aggregate is shown. One can see that the average error for the $T_r \leq 0.6$ segment follows the same ascending order as the average error at the normal fusion point. The error for the entire two-phase region ("All T_rs") follows the same trend, the one exception being the 0.55-0.7 interval, where error is less than that for the 0.5-0.6 interval. This reinforces the intuitive assumption that the extrapolation error at the very-low-temperature end of the VLE curve is sufficiently larger than the predictive error over the rest of the VLE curve, to such an extent that the very-low-end errors dominate the statistics in aggregate to the overall VLE curve.

The statistics in Table 1.7 are averages for the entire set of 72 species; however, such trends evidenced by the averages cannot be assumed to strictly apply to every species. This is shown in Table 1.8 for hydrogen, R152a, helium, and water. The “even” distribution will rarely be exactly met with experimental data, so four reduced temperatures for selected intervals are chosen from the data originally downloaded from *NIST* that are closest to the “even” distribution. To ensure interval membership, the bottom reduced temperature value was the minimum value that was greater than or equal to the interval's bottom, and the top reduced temperature value was the maximum value that was less than or equal to the interval's top. Because the previous point-distribution assessment indicated that the "quarter" distribution in general may have a slight advantage to that of the "even" with respect to imprecision error, the internal points erred in favor of the "quarter" distribution; in other words, the lower internal point was the maximum reduced temperature that was less than or equal to that dictated by the "even" distribution, and the upper internal point was the minimum reduced temperature that was greater than or equal to that dictated by the "even" distribution

The $F_{w,j}[WA]$ function is used to estimate Wagner constants for four intervals; although the four reduced temperatures are dictated by this *NIST* download, the four reduced vapor pressures are still entire-curve Wagner analytics. Two intervals with large widths and the same lower bound of 0.5, as well as two other intervals with small widths having the same lower bound of 0.6, are selected to see how the error trends for individual species compare with those trends represented by interval averages in Table 1.7. The normal fusion point for argon is at a reduced temperature greater than 0.55, so it is not included in this analysis.

Table 1.8 shows the error in Wagner constants and for reduced vapor pressure at the three temperature segments for the four species. Cells shaded indicate deviations from the average trends displayed in Table 1.7. One can see that for helium the average error in the reduced vapor pressure for the low-temperature region and entire curve in aggregate is smaller for the 0.5-0.7 interval than for the 0.5-0.9 interval. Having the same lower bound of 0.50086, the errors would be expected to be greater for the smaller width interval of 0.5-0.7.

The 0.5-0.7 interval is an exception for hydrogen as well, the vapor pressure in the low-temperature region being less than that in the wider 0.5-0.9 interval. The VLE curves for both helium and hydrogen encompass a very small temperature range, less than 4° K and 20° K, respectively. Perhaps the average location and width trends for imprecision error are less applicable for species whose entire-curve reduced temperature range occurs over a small absolute temperature range, i.e., have small values for the difference $T_c - T_t$.

Except for the two instances discussed above, the error in reduced vapor pressure increases with decreasing interval width, consistent with the interval averages shown in Table 1.7. Similarly, the width of 0.1 appears to be a cliff point for these four species. The error in vapor pressure for hydrogen, R152a, and helium increases by about an order of magnitude when going from the width of 0.1 down to 0.05, and the small-width interval of 0.60-0.65 is where the average vapor pressure percent error for the temperature segments increases from tenths of percent into single digits. The cliff, however, is less pronounced for water. The data in Tables 1.7 and 1.8 suggest that vapor pressure predictive error due to data imprecision exhibits consistent trends with respect to interval width and location. Unless one is focused on solely minimizing error in the upper region, one should generally try to use a data interval with the lowest temperature possible and of reduced width of at least 0.1 to reduce imprecision error.

1.5.1.3 Self-Consistency of Predictive Error Upon Data Imprecision

Several trends were noted during the discussion of Table 1.7, and below the interval average errors for singular points and temperature segments are plotted in a manner that reveals a self-consistency of the error statistics that transcends interval width and location. It was mentioned that the error at the very-low-temperature end of the VLE curve is sufficiently larger than that over the rest of the VLE curve to cause the very-low-end errors to dominate the statistics for the low-temperature end and the overall VLE curve. The influence of the error at the very-low-temperature end is clearly visible in Figures 1.1 and 1.2, where it can be seen that the relationships between the error at the normal fusion point and that of the $T_r \leq 0.6$ segment and entire-curve are linear on the logarithmic scale. Thus, the error at the normal fusion point (i.e., the very-low-temperature end) can accurately predict an interval's average error in the low-temperature-region and for the overall curve, independent of the interval’s width and location.

One can see from Table 1.6, however, that the error of the $T_r > 0.6$ segment does not track closely to error at either $T_{r,f}$ or $T_{r,b}$. This is graphically displayed in Figures 1.3 and 1.4 with the interval averages. It is obvious that other factors, such as the interval location and width as indicated in Table 1.7, significantly influence the error at the high-temperature end.

Because normal boiling points are known for many substances, it would be desirable to be able to use the boiling point to predict a species' error in the low-temperature end of its VLE curve. The influence of the error at $T_{r,b}$ upon the error at $T_{r,f}$ and the $T_r \leq 0.6$ segment is displayed in Figures 1.5 and 1.6, respectively. The form of the scatter plots in Figures 1.5 and 1.6 are similar to that of Figure 1.3 and indicates that error at the normal boiling point is not able to provide reasonable estimates of error in the low-temperature region.

It was previously mentioned that the maximum error at the normal fusion point follows the same ascending order as the average error; this tracking tendency is graphically displayed in Figure 1.7. Figure 1.8 shows the average vs. maximum plot at the normal boiling point; although less linear than that of Figure 1.7, the maximum error at the normal boiling point appears to track reasonably well to that of the average error. Figures 1.7 and 1.8 indicate a consistency between average and maximum errors at the normal fusion and boiling points.

Figures 1.1 through 1.8 indicate the following for vapor pressure predictive error due to data imprecision: 1) the error at $T_{r,f}$ is a reasonable indicator of average error in the low-temperature segment of the curve and for the average error of the entire two-phase curve; 2) the average error in the upper-temperature segment cannot be predicted from the error at the normal fusion and boiling points; 3) the average error for the lower-temperature segment and for the entire two-phase curve in aggregate cannot be predicted from the error at the normal boiling point because there isn't a consistent relationship between the error at $T_{r,f}$ and that at $T_{r,b}$; and 4) despite previous conclusion #3, predictive error of VLE extensions from limited data due to data imprecision reveals much self-consistency along the two-phase curve that transcends the influence of interval width and location.

1.5.1.4 Error in Estimated Wagner Constants

The average and maximum errors of the predicted Wagner constants for the eleven intervals are shown in Table 1.9, listed in the same order as in Table 1.6 (ascending order of average $T_{r,f}$ error). Immediately evident from Table 1.9 is the lack of strong dependency of Wagner-constant error, either average or maximum, upon the error at $T_{r,f}$. This lack of tracking is particularly surprising for *d* because that constant exerts its greatest influence in the Wagner equation at low T_r (high τ values).

Comparing the errors in Table 1.6 and those in Table 1.9 quickly reveals two characteristics. First, that the error in predicted reduced vapor pressure is generally significantly less than that in predicted Wagner constants. The interval with the largest reduced vapor pressure error, 0.6-0.65 for example, produces average $P_{r,f}$ error of 17% but average errors in *b*, *c*, and *d* of 101%, 102%, and 193%, respectively, and the maximum error in *d* is over 7,000%.

The species with the maximum error in *d* for all eleven intervals is hydrogen, but hydrogen was never the species with maximum error in P_r. The large error in hydrogen's *d* and its inordinately small influence in the error of predicted P_r occur because the analytic value of *d* is a small 0.053125. The value of τ for hydrogen at the normal fusion point is 0.59089, which taken to the fifth power is 0.072. A *d* value of 0.5 and 0.1, a difference of 100% in *d*, results in values for the product $\tau^5 d$ of 0.0036 and 0.0072, respectively. Such differences in the third and fourth digits of the mantissa will not produce differences of 100% in the predicted $P_{r,f}$.

Formic acid has the maximum error for *b* and *c* in the 0.6-0.65 interval, 880% and 1,363%, respectively, while exhibiting error in the predicted P_r of only 4.2% at the normal fusion point and 3.5% at T_r=0.95. Formic acid's analytical values for *b* and *c* are 0.44255 and -0.35558, respectively. In contrast, the species with the largest maximum error (204%) for this interval is 2-butanol rather than hydrogen or formic acid, with *a*, *b*, *c*, and *d* values of -8.09820, 1.64406, -7.4900, and -5.27355, respectively, and errors of 16.6%, 229%, 62.5%, and 109%, respectively. Double-digit and triple-digit error of such relatively large Wagner constants have a greater chance of producing large error in predicted vapor pressures on the low-temperature end.

The second characteristic of the relationship between predicted vapor pressure error and predicted Wagner constant error that is quickly apparent when comparing the errors in Table 1.6 and those in Table 1.9 is how relatively easy it is to predict vapor pressure at the high-temperature end. Despite having triple-digit percent errors in *b*, *c*, and *d*, the intervals 0.55-0.6 and 0.6-0.65 have maximum reduced vapor pressure errors of 5.8% and 4.2%, respectively, in the $T_r > 0.6$ segment. Relatively poor estimates of Wagner constants, although resulting in triple-digit A%Err in the $Tr \leq 0.6$ segment, can produce only single-digit

A%Err in the $T_r > 0.6$ segment. The ability of only four data points from an interval only 0.05 reduced temperature units wide to predict vapor pressure within 6% at the high-temperature end highlights the difference in difficulty between predicting vapor pressure at the low- and high-temperature ends of the VLE curve.

The Wagner constant error statistics are sorted by average error in the constant a in Table 1.10. Three trends are evident from the table. First, it is clear that the average error of b, and to a large degree that of c, track closely to that of a. Second, the errors of the constants a, b, and c are strongly influenced by the interval width, the errors increasing as the width decreases. Surprisingly, at the same interval width, the errors in a, b, and c increase as the interval location moves down the reduced temperature scale, just the opposite than for error in reduced vapor pressure. Third, the error of the constant d tracks neither to the error of predicted P_r nor with the error of the other constants.

Referring back to Table 1.8, the error between the Wagner constants estimated from the limited-data intervals and their entire-curve counter parts displayed in the table affirms two of the points discussed above. First, differences in percent error of Wagner constants between species cannot be used to estimate their relative capability for predicting vapor pressure. Both R152a and helium have similar vapor pressure errors for the 0.60-0.65 interval, but the percent errors in Wagner constants a, c, and d for helium are several times those for R152a. Second, even for a single species, differences in error in Wagner constants will not always indicate corresponding differences in vapor pressure predictive capability. The absolute percent errors for all four Wagner constants for hydrogen, for example, are larger for the 0.5-0.7 interval than for the 0.5-0.9 interval, but the average error in reduced vapor pressure for the $T_r \leq 0.6$ segment using the 0.5-0.7 interval is less than that of the 0.5-0.9 interval.

Although it will be shown in the next section that error due to imperfection of the Wagner equation is generally a greater contributor to total predictive error, the error assessment given thus far provides valuable insight into the role of data imprecision error when estimating Wagner constants.

After performing this assessment of error due to data imprecision, it was found that an erroneous value for the literature entire-curve Wagner constant a for two species had been used in the calculations. A value of $-9.490\underline{5}4$ instead of the correct $-9.490\underline{3}4$ had been used for 1-hexanol, and -10.033664 had been used instead of the correct -10.03664 for hexadecane. This discrepancy in the a values for these two species is minor, 0.002% and 0.03%, respectively, and it would not affect the results of the statistics and hypothesis testing for the seventy-two species in aggregate. The correct values of a for 1-hexanol and hexadecane are used in all subsequent investigations reported in Chapters 2 and 3 and are properly reflected in Tables 1.2, 1.3, and B.2.

1.5.2 Predictive Error Due to Imperfection of Wagner's Functional Form

The previous exercise with hydrogen, R152a, helium, and water, for which the results were shown in Table 1.8, is repeated, but the four vapor pressures used to estimate Wagner constants are taken from the data originally downloaded from *NIST* rather than using entire-curve Wagner analytic vapor pressures. The raw data used are from the data set used to regress the entire-curve Wagner constants, which are given in the tables of Appendix A. "[RD]" is added to the $F_{w,j}$ function name to indicate that raw data is used rather than entire-curve analytic values of $Ln\ P_{v,r}$. If precision of data is perfect, and the functional form of the Wagner equation is perfect, the VLE predictions of Wagner constants estimated by the limited-data $F_{w,j}[RD]$ function would exactly match the entire-curve Wagner analytic values. This ideal total error of zero would be a consequence of the four raw data points used in each limited-data interval being part of the full-range data set used to regress the entire-curve Wagner constants.

The actual total error, however, between the VLE predictions using the $F_{w,j}[RD]$ function and the entire-curve Wagner analytics is the sum of the error due to data imprecision and the error due to imperfection of the Wagner equation. Having already estimated the imprecision error, the equation imperfection error can be estimated by subtracting the imprecision error from the total error. This exercise does not provide statistical inferences because only four species are used, but it does provide quantitative examples of the error due to imperfection of the Wagner equation and its dependency upon the interval width and location. The results for VLE predictions of the $F_{w,j}[RD]$ function are shown in Table 1.11. The same reduced temperature points are used as for the $F_{w,j}[WA]$ function exercise for Table 1.8. Consequently, the "4 Points" and "Width" columns are not shown in Table 1.11 because they are the same as shown in Table 1.8.

The A%Err in predicted reduced vapor pressures at several reduced temperatures for the $F_{w,j}[RD]$ function compared to the analytic values calculated from the entire-curve Wagner constants is shown in Table 1.11. The intervals in the table are sorted in ascending order of error per the previous analytic assessment described in Table 1.6. The cells where the values differ from ascending order are highlighted in gray. 0.7 is the only reduced temperature where the ascending order from the previous analytic assessment is maintained. However, although all four species have cases where the ascending order is broken, the majority of cases involve small differences and/or small values; when dealing with singular points, it is hard to claim that 0% and 0.01% errors, for example, are meaningfully different. Water, however, does have breaks that involve relatively large differences that can't be assumed to be un-meaningful.

There are fewer breaks in the ascending order for the temperature segment average errors shown at the far right of the table. The "$T_r > 0.6$" segment, with 7 points for each species, mirrors the ascending order of the analytic assessment. The "All T_rs" average, with 13 points for each species, only breaks the order for helium and water, and again, it would be hard to argue statistically that the helium break, 0.227% dropping to 0.206% rather than increasing, is really meaningful. A similar argument can be made for the breaks in the "$T_r \leq 0.6$" segment, involving 5 points per species, for hydrogen and R152a. For all four species, the temperature segment errors for the smallest interval (0.6-0.65) are greater than those for the larger 0.5-0.7 and 0.5-0.9 intervals, generally consistent with the trend of data imprecision error vs. interval width. A prominent inconsistency, however, is that water doesn’t exhibit the cliff between the 0.6-0.7 and 0.6-0.65 intervals.

The average errors for the four species in aggregate are displayed in the Summary section of Table 1.11. The breaks in the analytic ascending order are again highlighted. With four points for each reduced temperature, the average errors do mirror the ascending order of the analytic assessment for seven reduced temperatures. Similarly, the average errors of the temperature segments show greater consistency with the analytic ascending order. The "$T_r >$ 0.6" and "All T_rs" segment average errors, based on increasingly a greater number of points, 28 and 52 respectively, mirror the analytic ascending order shown in Table 1.6 determined by several hundred points for the temperature segments. Only the "$T_r \leq 0.6$” segment average error for the 0.5-0.7 interval breaks from the analytic order. The results of Table 1.11 suggest that when expanded to the aggregate scale, the ascending order of interval average errors based on raw data is the same as that resulting from using Wagner analytic data. Consistent with Table 1.6, the average total “All T_rs” error for all four species combined does not exceed 1% until the interval width gets below 0.1, and the average for a single species does not exceed 2% until the interval width approaches 0.05.

Logically, one would expect the total error represented by the $F_{w,j}[RD]$ function to be less consistent than data imprecision error because the $F_{w,j}[RD]$ function incorporates Wagner imperfection, and imperfection error can be species-dependent. Despite less consistency, the results of Table 1.11 suggest that limited raw data of good precision from intervals of 0.1 or greater in reduced temperature width have the potential to provide reasonable VLE predictions outside of the interval.

Given that the error in predicted reduced vapor pressures shown in Table 1.8 for the $F_{w,j}[WA]$ function represents an estimate of the error due to data imprecision, the data due to Wagner imperfection is estimated as the error of the $F_{w,j}[WA]$ function subtracted from the total error represented by the $F_{w,j}[RD]$ function shown in Table 1.8. That difference, and its ratio to the data imprecision error, is shown in Table 1.12. The average errors for the $F_{w,j}[RD]$ and $F_{w,j}[WA]$ functions are included in the table for reference.

One can see that in several cases the average A%Err error due to Wagner imperfection has a negative value, i.e., the error from Wagner imperfection partially cancels out that due to data imprecision. These cells are shaded, and their absolute values represent the magnitude of the total percent error reduction caused by the cancellation effect. Hydrogen shows a value of zero for Wagner imperfection error for all three temperature segments for the 0.6-0.7 interval because in that case the raw vapor pressures are equal to those of the entire-curve analytic values (when rounded off to four digits in the mantissa of $Ln\ P_{v,r}$) for the four reduced temperatures, causing both the $F_{w,j}[RD]$ and $F_{w,j}[WA]$ functions to calculate the same values for the four Wagner constants, which results in the $F_{w,j}[RD]$ function not introducing any error above that of the $F_{w,j}[WA]$ function. Of the nine cells where Wagner imperfection reduces total error, seven correspond to the small interval 0.6-0.65. The interval with the largest Wagner imperfection errors is also 0.6-0.65, for R152a. Perhaps the greatest impact of

Wagner imperfection occurs with data intervals of small width, either helping to cancel out error or adding to total error.

The last three columns of Table 1.12 show the ratio of the Wagner imperfection error to that of data imprecision. The absolute value of negative ratios, also shaded, represent the fraction of the data imprecision error canceled out by opposing Wagner imperfection error. Not a single shaded cell has a ratio even in single digits; their absolute values are all less than 1, i.e., the error due to Wagner imperfection cancels out only a part of the error due to imprecision. In comparison, of the thirty-nine ratio cells with non-negative values, i.e., Wagner imperfection adds to total error, one cell is undefined because data imprecision error is zero, three cells have a value of zero, six cells have a non-zero ratio of less than 1.0, while twenty cells have ratios in single digits, and nine have ratios in double digits.

In other words, based on this sample of four species, error due to Wagner imperfection generally adds to vapor pressure predictive error much more frequently and in greater magnitude than it diminishes total error. As is total error (i.e., error of the $F_{w,j}[RD]$ function), Table 1.12 shows that Wagner imperfection error is less consistent and more species-dependent than data imprecision error. These characteristics of imperfection error relative to imprecision error - 1) being generally much larger, 2) displaying less consistent dependency upon the interval, and 3) being more species-dependent – suggest that small differences in imprecision error between point distributions have only minor impact to total predictive error.

1.5.3 Fully- vs. Over-Determined Solution

The same four species are used to perform a preliminary study of the influence of the number of parameterization points upon the predictive error when extending outside the interval. Using raw data, the predictive capability of the algebraic fully-determined case and the regressed over-determined case are compared. The over-determined case involves least-squares regression of all the data points originally downloaded from *NIST* that fall within the data intervals. These data points are subsets of the data given in Appendix A and were used to regress the entire-curve Wagner constants shown in Table 1.1.

The 0.5-0.7 and 0.6-0.65 intervals are selected to allow for any potential dependency upon interval width to be revealed. The number of data points used in the over-determined cases is not meant to imply experimental feasibility. For example, the entire two-phase curve for helium spans only 3.05 degrees Kelvin ($T_f = 2.15$, $T_c = 5.20$), but sixty-six points are used for its over-determined case in the 0.5 - 0.7 reduced temperature interval alone, which number of points would not be possible experimentally, but such a number of points is possible when downloading *NIST* data.

The results are shown in Table 1.13. For all four species, the over-determined cases are consistent with the general trend of error increasing as interval width decreases displayed by the $F_{w,j}[WA]$ function, i.e., errors for the smaller 0.6-0.65 interval are greater than those for the 0.5-0.7. Over-determined cells in bold font have greater error than their $F_{w,j}[RD]$ counterpart while those shaded gray have less error. For most points and temperature segments, the errors of the fully- and over-determined cases are similar in magnitude. One exception is the 0.60-0.65 interval for hydrogen, where the over-determined case is better by an order of magnitude; 11.5% error reduced to 1.4% at the normal fusion point, for example.

Looking at the three columns to the far right of the table containing the segment averages, there are 24 cells for the over-determined case. Comparing the over-determined error with that of the fully-determined case, one can see that 15 of the 24 cells for the over-determined case are shaded gray and result in less average segment error, while 9 cells have bold font and show greater error, equating to 62.5% and 37.5% of the 24 cells, respectively. Table 1.13 shows that although over-determined regression generally results in less error than the fully-determined case, using many high-precision points in a limited-data interval does not guarantee better vapor pressure predictability outside the interval than using only four points.

Two other general patterns are evident from these 24 cells. One, the magnitude of the difference in error between the two methods for the four species diminishes as the interval width increases – the differences for the 0.5-0.7 interval are generally in hundredths of percent, while differences for the 0.6-0.65 interval are in the tens of percent or single digit percentage points. Second, with the small interval 0.6-0.65, the over-determined solution has split results – it produces less error for half of the species (hydrogen and helium) and greater error for the other half (R152a and water).

Continuing to look at the 24 cells of the average error for the temperature segments, eight of the nine cells where regression has greater error belong to R152a and water. The only two cells for “All T_rs” with bold face font again belong to the over-determined case for these two species at the 0.6-0.65 interval. Hydrogen and helium showed interesting behavior for the 0.5-0.7 interval for imprecision error (Table 1.8). As noted previously, besides being quantum gases, hydrogen and helium have small temperature ranges between their triple and critical points. Besides being polar, R152a and water, on the other hand, have hundreds of degrees Kelvin separating their triple points from their critical points.

The new term "extrapolation burden" is now introduced to normalize differences in temperature spread on the bottom portion of the two-phase curve. When logarithmic vapor pressure is plotted versus the reciprocal thermodynamic temperature, Thodos (1950) showed that the curvature for a pure species generally changes at the normal boiling point. Consequently, in this chapter, it is decided to focus on the portion of the saturation curve below the normal boiling point to define what is referred to in this work as "extrapolation burden." The difference between the logarithm base 10 of the reduced vapor pressure at the normal fusion and boiling points quantifies the extent of vapor pressure downward extrapolation in decades required below the normal boiling point ($\Delta Log\ P_{v,r} = Log\ P_{v,r,b} - Log\ P_{v,r,f}$). The difference between the reduced temperature of the normal fusion and boiling points quantifies the reduced temperature range over which the vapor pressure extrapolation spans ($\Delta T_r = T_{r,b} - T_{r,f}$). The ratio of the decades of reduced pressure divided by the reduced temperature span ($\Delta Log\ P_{v,r} / \Delta T_r$) provides a quantitative estimate of the extrapolation burden of a species, using the normal boiling point as the starting point for the downward extrapolation.

For example, the difference in the reduced temperatures of the normal fusion and boiling points for helium is 0.4, but the breadth of the reduced vapor pressures between these two points is only 1.35 decades. Water, on the other hand, only has a 0.15 reduced temperature span that has to account for 2.22 decades in reduced vapor pressure. The extrapolation burden ratio is 3.4 and 6.0 for helium and hydrogen, respectively, but 12.9 and 14.4 for R152a and water, respectively. Because the Wagner equation is in reduced form, perhaps the extrapolation burden influences the importance that the number of parameterization points may have when extending VLE prediction outside of the parameterization interval.

1.6 Summary

The investigation of imprecision error involves seventy-two species. The investigation of total error, imperfection error, and the role the number of parameterization points plays in the predictive error outside the parameterization interval involves four species. There is ample room for more exhaustive study of these themes; however, the results presented in this chapter provide solid support for the following five propositions regarding the power of Wagner constants estimated from only limited VLE data to predict VLE outside of the parameterization interval, when the data is of good precision: 1) the predictive power of the VLE extension is dependent upon the parameterization interval's width and location; 2) the contribution of equation imperfection to total error is generally larger than that due to data imprecision; 3) the difference in the average predictive error between the fully- and over-determined parameterizations diminish as the interval width increases, approaching a tenth of one percent for an interval width of 0.2; 4) the over-determined solution has equal chance of producing either less or more error than the fully-determined approach when the interval is small (e.g., 0.05 width); and 5) the last two conclusions suggest that the relatively simple $F_{w,j}$ function can be a valuable tool for investigating the extensibility of limited-data Wagner constants. Conclusion #1 in quantitative terms is: limited VLE data of good precision from reduced temperature intervals with a width ≥ 0.1 and a lower bound ≤ 0.6 can generally provide reasonable VLE predictions for pure substances, with an average "All T_rs" error around 1%.

It is additionally concluded that a self-consistency in the imprecision error exists that transcends interval characteristics and allows the error at $T_{r,f}$, to be a reliable indicator of the average error in the $T_r \leq 0.6$ segment and for the entire two-phase curve. Unfortunately, the predictive error at $T_{r,b}$ is not a good indicator of the predictive error at points outside of the limited-data interval.

The work reported in this chapter supports Hypothesis I, with the qualifier that the interval width be ≥ 0.1 and the lower bound be ≤ 0.6. The trends and comparisons of the error statistics presented here should have general qualitative applicability to any VLE data of good precision. These results are relevant to those researching methods to leverage limited VLE data of good precision to predict the VLE curve above and below the source data's interval.

The applicability of the approach presented in this chapter to analyze and segment predictive error is not confined to the Wagner equation. Researchers continue to develop new CSP vapor pressure correlations involving species-specific parameters. Park (2010) developed a correlation incorporating three species-specific parameters to describe the VLE over the entire co-existence curve. Sanjari (2013) developed a four-term equation that when applied to 75 species produced less error than the Wagner equation. One could use a fully-determined solution and algebraically determine universal functions, similar to $F_{w,j}$, for the corresponding species-specific parameters of their equations, for example, and test the predictive power of different limited-data intervals and segment the error between that due to data imprecision and that due to equation imperfection.

Chapter 2: Critical Point & Four Antoine Analytic Points

2.1 Abstract

Entire-curve Wagner analytics are treated as “true” or “best” values, and Antoine analytic values are used as surrogate experimental data. Limited-data Wagner constants are estimated from Antoine analytics for the fully-determined case for fifty-five species, from which reduced vapor pressures below and above the interval are predicted and compared with the entire-curve Wagner analytics to estimate the ability of limited VLE data to be used to accurately represent the entire two-phase curve**.** The Antoine intervals have a pressure range of 0.02-2 bars for most species, an average reduced temperature interval width of 0.20, and an average lower bound reduced temperature of 0.53. The Wagner constants estimated from Antoine analytics have an average entire-curve error of 4.8%, with the majority of the error occurring when extending down towards the triple point (9.55%), compared to 1.36% average error when extending up to the critical point. Such limited-data Wagner constants produce less predictive error for alcohols, while the semi-theoretical Riedel equation has the advantage for organic acids, and the empirical Ambrose-Walton equation produces less error for the remaining species. A comparison of Wagner and Antoine analytic values over the Antoine interval for fifty-fives species indicate that repeatability/reproducibility of VLE data in the literature averages around 2% but varies considerably between species. Data repeatability by itself is not found to be a strong indicator of predictive power of the limited-data Wagner constants; however, it is found to be a discriminator of performance relative to that of Riedel and Ambrose-Walton for some polar species. It is found that both the $F_{w,j}[AA]$ function and Riedel equation treat all substance types with respect to extrapolation burden in a more consistent manner than does the Ambrose-Walton equation.

2.2 Introduction

Data sources for many process engineers are restricted to a few technical handbooks, and when data for a species of interest is found in such sources, it may be given in terms of a correlation rather than experimental data, may be of unknown precision, and it is usually limited in range. The broad intent of the work presented here in this dissertation is to provide the practitioner with a qualitative and quantitative assessment of using limited VLE data, either experimental or analytic from a correlation, to predict VLE for a pure substance over the entire two-phase curve.

Several researchers have used limited data to estimate Wagner constants that were then used to extend VLE predictions in one direction, either interpolation upward to the critical point or extrapolation downward to the triple point. Ambrose (1978), Ambrose, Counsell, and Hicks (1978), McGarry (1983), and Forero G. & Velasquez J. (2011) are representative of efforts to interpolate between a limited data set and the critical point. Ambrose (1978) treated the triple point and critical point vapor pressures as unknowns and used a fitting algorithm to determine them along with the four Wagner constants. Ambrose et al. (1978) and McGarry (1983) showed that applying three specific constraints in the 0.5 – 0.95 reduced temperature range could reduce the predictive error for non-associating species. Forero G. & Velasquez J. (2011) used analytic values predicted from the Antoine equation to regress Wagner constants which were then used to extend above the intervals up to the critical point. Excluding alcohols, which associate and were found to be problematic, these researchers reported average predictive error generally less than 1%.

When attempting to extrapolate downward, researchers generally combine low-pressure thermal data with atmospheric-range VLE data and use simultaneous model regressions to estimate analytic VLE in the lower region, from which they then regress VLE correlations applicable for the atmospheric range down to the triple point (Ambrose et al., 1978; Ambrose & Davies, 1980; Hogge et al., 2016; King & Al-Najjar, 1974; Poling, 1996; K. Ruzicka & Majer, 1994). Ambrose & Davies (1980) found that the differences between the extrapolated predictions and the analytic “best” values to be 0-20%, 0-10%, and 0-5% at pressures of 1, 10, and 100 Pa, respectively, significantly greater than the predictive error found by researchers interpolating upward. They also found that the two alcohols included in their study, ethanol and propan-2-ol, responded differently to their fitting approach than did the other species.

The extended predictions in such studies were generally coupled to the reference data set, or ‘best” values; i.e., the extended predictions were compared back to the limited data itself and/or to data of which the limited data was a subset. Using data of good precision, researchers such as those discussed above have generally concluded that their approaches to

VLE extension from a limited VLE data set result in reasonable and acceptable predictive error.

Because the curvature varies as one travels along the two-phase curve, extension error for a VLE correlation parameterized from limited data may depend upon the interval's location and width and the number of parameterization points. Chapter 1 studied the error segmentation when parameterizing the Wagner equation from limited VLE data using a four-point fully-determined solution. The results indicate that limited VLE data of good precision from reduced temperature intervals with a width ≥ 0.1 and a lower bound ≤ 0.6 can generally provide reasonable VLE predictions over the entire two-phase curve for pure substances.

Although correlative power within the data interval from which a correlation is parameterized can be dependent upon the number of data points used, a dependency of similar strength does not necessarily exist for the predictive power when using the correlation to extend outside the data interval. That is because extrapolation can involve considerable error (Smith, 1979), and an increase in the amount of parameterization points within the data interval itself does not guaranteed a lowering of the predictive error outside of the interval. The more nonlinear the true function is, the greater can be the inherent tendency for extension error, and similarly the lesser the chance can be that more parameterization points will decrease the predictive power outside the interval.

Chapter 1 compared the four-point fully-determined solution with over-determined regression using hydrogen, helium, water, and R152a. It was found that the over-determined solution has equal chance of producing either less or more error than the fully-determined approach when the interval is small, and the difference in average predictive error between the two parameterizations diminishes as the interval width increases, approaching less than a tenth of one percent for an interval width of 0.2. For the fifty-five species studied here in Chapter 2, the average reduced temperature interval width is 0.20, and the average interval lower bound is 0.53, suggesting that the fully-determined approach is appropriate for the study of parameterizing the Wagner equation using four Antoine analytics.

Unlike the work of the previous researchers discussed in the preceding paragraphs, this paper addresses the situation when the data used to estimate the Wagner constants are neither part of the reference data nor are they used to generate the reference data to which the predicted VLE are compared. It is found in this work several cases that the limited data used to generate the Wagner constants and the reference set differ significantly and are not consistent with each other, and consequently, good data precision cannot be assumed. The problem of poor data repeatability/reproducibility is not uncommon. Mandel & Paule (1970) discussed the statistical complications involved with trying to determine “best” values from multiple experimental data sources, including proper data weighting. Armstrong (1981) studied the VLE data for chlorine available in the literature, which covered the reduced temperature range of 0.41 – 1.0. He found that data from two sources differed by 1-5% and concluded that the only reliable data fell in the 0.41-0.65 interval.

More problematic, Ambrose & Ghiassee (1987) found in their study of alkanoic acids C_1 to C_{10} that much of the experimental data was fragmentary, of poor accuracy, and lacked good agreement with each other. They chose to develop VLE correlations using more than just statistical curve fitting, utilizing criteria of reasonableness of curve form and discarding some data judged to be outliers. The predictions of the entire-curve Wagner equations they developed varied by several percent in some cases with the experimental data of other researchers.

The engineering practitioner, unlike the researcher, generally has neither the resources nor the inclination to obtain several data sources for a species of interest, perform a detailed error analysis, and determine the “best” or “true” VLE for available data intervals, let alone assess the applicability of fitting constraints and the reliability of potential extension outside of the limited data interval. Consequently, the aim of Chapter 2 is to investigate the potential disagreement one may encounter in practice between a species’ “best” VLE values and experimental values, and to assess how such disagreement may affect the predictive power of Wagner constants estimated from the experimental values.

In other words, the goal of the work discussed in this chapter is to determine the validity of Hypothesis II. The results are relevant to engineers tasked with assessing the feasibility of predicting VLE over the entire two-phase curve when only data/correlation of limited applicability is available.

2.3 Investigative Approach

The Antoine equation, not in reduced form, is given by

[9] $$Log\ P_v = A - \frac{B}{T+C-273.15},$$

where *Log* indicates base 10 logarithm. For values of Antoine constants used in this work, degrees Kelvin and bars are the units for temperature and pressure, respectively.

The Antoine equation is known to accurately represent experimental VLE data over a limited temperature range from which its constants have been regressed (Felder & Rousseau, 1978; Poling et al., 2001). Consequently, Antoine analytics are used as surrogates for experimental data. Fifty-five species that have both entire-curve Wagner constants and limited-range Antoine constants available in the literature are studied. The methodology is simple. Entire-curve Wagner analytics are used to represent the "best" values. Analytic vapor pressure values from Antoine constants are used to estimate limited-data Wagner constants. The vapor pressure predictions of these limited-data Wagner constants over the entire two-phase curve are compared with the entire-curve Wagner analytics.

Several errors may contribute to differences in vapor pressures predicted from the limited-data Wagner constants and the entire-curve Wagner analytics. Obviously, neither the Wagner nor Antoine equations represent data perfectly over the Antoine intervals, so both will have some equation imperfection error. Also, both data sets used by their respective correlators will have had some level of imprecision error. Because errors can sometimes cancel each other, the deviation between the entire-curve Wagner analytics and the Antoine analytics over the Antoine interval is treated as estimates of the net contribution of repeatability/reproducibility disagreement. Large deviation between the Antoine and entire-curve Wagner analytics within an Antoine interval itself suggests poor data reproducibility/repeatability for a given species. Of course, such intra-interval deviations will introduce errors when using the interval's Antoine analytic data to subsequently estimate Wagner constants for extension to regions outside the interval.

Poling et al. (2001) concluded that the applicability of Wagner constants can be extended down to a reduced temperature of 0.5 reliably. In the absence of an accurate vapor pressure data/correlation for a temperature interval of interest, they recommend the Riedel or Ambrose-Walton methods be used to predict VLE at low temperatures and a two-reference-fluid or Riedel method for polar substances in the reduced temperature range 0.5-1.0. Consequently, the semi-theoretical Riedel and empirical Ambrose-Walton equations are chosen as the primary predictive-method comparators to this fully-determined approach using Antoine analytics.

2.3.1 Novelty of Approach

The approach taken in this chapter has several novel elements. First, using Antoine analytics to represent a limited-data interval and entire-curve Wagner analytics to represent "best values" is a novel way to assess the level of VLE data disagreement in the literature. Other researchers generally compare the predictive power of their parameterization with the data from which the parameterization was made and many times do not address issues of data reproducibility. However, comparing one researcher's Antoine analytics with another researcher's entire-curve Wagner analytics provides a good, quick, overall indication of the level of VLE data consistency and precision that a practitioner can expect to find in the literature.

Second, other researchers using a limited VLE data interval study extending VLE predictability in one direction, either upward to the critical point or extrapolation down to the triple point. Downward extrapolation usually involves thermal data. This work is unique in that it addresses extending VLE both above and below the limited data interval, providing a look at predictive power over the entire two-phase curve in aggregate, and it does not use ancillary thermal data. The goal here is to assess the likelihood of a practitioner being able to use only limited VLE data to predict vapor pressures over the entire two-phase curve that are reasonably close to "best" values.

The third novel element is the use of an easy algebraic, fully-determined solution to estimate the Wagner constants rather than a significantly more laborious and complex nonlinear over-determined solution. Lastly, the concept of "extrapolation burden" is more fully developed and provides a quantitative method to normalize the relative difficulty a researcher or practitioner may experience when trying to extrapolate a species' VLE downward to the triple point.

2.3.2 Ambrose-Walton Equation (ω-Based CSP)

CSP is reasonable for primarily normal fluids. The group of fifty-five species studied in this chapter includes thirteen alcohols, six organic acids, six other polar species, one quantum gas, and 29 normal substances.

An often used ω-based CSP equation for VLE prediction is that of Ambrose-Walton, whose form used in this work is given by (Ambrose & Walton, 1989; Poling et al., 2001)

[10] $Ln\ P_{v,r} = f^{(0)} + \omega f^{(1)} + \omega^2 f^{(2)}$, where

[10a] $f^{(0)} = \frac{-5.97616\tau + 1.29874\tau^{1.5} - 0.60394\tau^{2.5} - 1.06841\tau^{5}}{T_r}$,

[10b] $f^{(1)} = \frac{-5.03365\tau + 1.11505\tau^{1.5} - 5.41217\tau^{2.5} - 7.46628\tau^{5}}{T_r}$, and

[10c] $f^{(2)} = \frac{-0.64771\tau + 2.41539\tau^{1.5} - 4.26979\tau^{2.5} + 3.25259\tau^{5}}{T_r}$.

2.3.3 Riedel Equation

Riedel (as cited in Poling et al., 2001) developed a CSP theory for vapor pressure for normal fluids, and his parameter for the slope of the vapor pressure curve is tied to a substance's normal boiling point rather than the reduced temperature of 0.7. The Riedel equation is given by

[11] $Ln\ P_{v,r} = A^{+} - \frac{B^{+}}{T_r} + C^{+}\ LnT_r + D^{+}\ T_r^{6}$,

where

[11a] $A^{+} = -35Q$; $B^{+} = -36Q$; $C^{+} = 42Q + \alpha_c$; $D^{+} = -Q$,

[11b] $Q = K\,(3.758 - \alpha_c)$,

[11c] $\propto_c = \frac{3.758\ K\ \psi_b - Ln\ P_{v,r,b}}{K\psi_b - Ln\ T_{r,b}}$, and

[11d] $\psi_b = -35 + \frac{36}{T_{r,b}} + 42\ Ln\ T_{r.b} - T_{r,b}^{6}$.

The subscript b on ψ indicates that the parameter is based on the reduced temperature of the normal boiling point. Riedel originally had 0.0838 as the value of K, but it has been proposed that K should be a variable instead of a constant, dependent upon the family to which the species belongs (Vetere, 1991b). Vetere developed a linear relationship for K for five families: non-polar compounds, acids, alcohols, glycols, and other polar compounds. The relationships for acids and alcohols were

[11e] $K = -0.120 + 0.025\ h$ and

[11f] $K = 0.373 - 0.030\,h$, respectively, where

[11g] $h = -T_{r,b}\frac{Ln\,P_{v,r,b}}{1-T_{r,b}}$.

Nine different K relationships have been subsequently investigated by Vetere (2006): 1) saturated and branched hydrocarbons, 2) olefins, 3) aromatics, 4) alcohols, 5) ethylene, glycol, phenol, and m-cresol, 6) ketones, 7) esters, 8) acids, and 9) refrigerants and organic polar compounds. Vetere concluded that predictive power of the Riedel equation with a variable K was not significantly improved over other models for some families, such as ketones and esters. The specialized values of the K constant for alcohols and organic acids are used with the Riedel equation in the work presented here.

2.3.4 Applying $F_{w,j}$ Function to Antoine Analytic Data

The quantitative concept of "extrapolation burden" was briefly introduced in Chapter 1. The temperature at which extrapolation downward begins is that which corresponds to the lowest vapor pressure used by the predictive method. For the Riedel and Ambrose-Walton equations, this temperature corresponds to their lower anchor points, the normal boiling point and the reduced temperature of 0.7, respectively. In the case of the Antoine equation, the lower bound of the applicable temperature range represents the point below which extrapolation begins. The reduced temperature distance between the normal fusion point and the commencement of extrapolation is represented by the term ΔT_r. The difference between the base 10 logarithm of the reduced vapor pressures at these two temperatures is represented by $\Delta Log\ P_{v,r}$, and the reduced vapor pressures are the "best" values (entire-curve Wagner analytics). The $\Delta Log\ P_{v,r} / \Delta T_r$ ratio is the decades of reduced vapor pressure divided by the corresponding reduced temperature difference. This ratio estimates the extent of vapor pressure downward extrapolation required by the method predicting VLE relative to the available temperature range over which the extrapolation has to occur, and this ratio is given the term "extrapolation burden."

There are five species for which the Antoine lower bound temperature is slightly less than that of the used normal fusion point, i.e., ΔT_r is negative. There is one species for which the lower bound temperature is less than 0.0001 reduced temperature units greater than the normal fusion point, in which case round off error can exaggerate the value of the $\Delta Log\ P_{v,r} / \Delta T_r$

calculation. Consequently, there is no real extrapolation burden for these six species (tert-butanol, argon, nitrogen, ammonia, water, and hydrogen) with the Antoine equation, in which case the $\Delta Log\ P_{v,r}\ /\Delta T_r$ ratio is given the value of zero. The extrapolation burden for the Antoine, Riedel, and Ambrose-Walton equations are shown in Table 2.1.

The larger the value of the extrapolation burden, the greater the difficulty a species would be expected to experience when extending VLE down to its triple point. Thodos (1950) showed that for a pure species the plot of logarithmic vapor pressure versus the reciprocal thermodynamic temperature generally experiences a curvature change at the normal boiling point. Consequently, the Riedel extrapolation burden, based on the normal boiling point, perhaps may provide a good generic estimate of the downward burden a VLE correlation may experience for a species. The Riedel extrapolation burden for the seventy-two species has an average value of 19.9 for alcohols, 16.0 for organic acids, and 14.4 for the remaining species (the majority of which are normal). These numbers are consistent with the fact that most predictive VLE methods based on reduced temperature and pressure find normal species to be the easiest and alcohols to be among the most problematic. Extrapolation burden is further explored later in this chapter.

The Antoine constants and their applicable temperature and pressure ranges are shown in Table 2.2 , all from Poling et al. (2001). Although Antoine constants are given for helium in Poling et al. (2001), the maximum temperature of its given Antoine range was higher than the *NIST* critical temperature used to regress the entire-curve Wagner constants, resulting in reduced temperatures greater than one in the Antoine range, so helium was not included in this analysis.

The $F_{w,j}$ function using the Antoine analytic data is referred to as $F_{w,j}[AA]$, the "[AA]" being added to indicate that the four input points used are analytic calculations using Antoine constants. The four reduced temperatures and pressures from the “even” distribution used for each species are shown in Table C.1 of Appendix C. The η parameters calculated from the four reduced temperatures are shown in Tables C.2 through C.5. The Wagner constants calculated from the four reduced pressures and sixteen η parameters are given in Table C.6, along with their absolute percent errors relative to the entire-curve constants shown in Table 1.2.

2.4 Discussion and Results

2.4.1 $F_{w,j}$ [AA] vs. Antoine Extrapolated

It is well understood that the Antoine equation itself is not reliable when used to extrapolate VLE outside its applicable temperature interval (Poling et al., 2001). Consequently, it is first necessary to confirm that the VLE predictions of the $F_{w,j}[AA]$ function will be different and better than those merely obtained by extrapolating the Antoine equation. Given that predictive VLE error is greater in the lower-temperature region, the predictive errors at the normal fusion point are used for this comparison and are shown in Table 2.3. Error is given as the absolute value of the percent error (A%Err), which is equal to 100*|(reference $P_{v,r}$ – predicted $P_{v,r}$) / reference $P_{v,r}$|, and the reference $P_{v,r}$ refers to the entire-curve Wagner analytic value. The incremental error for the $F_{w,j}[AA]$ function over that of the extrapolated Antoine is also shown. One can see from Table 2.3 that the $F_{w,j}[AA]$ error is greater, i.e., incremental error is positive, for only seven species, and the error is significantly larger for only one species, 3-methyl butanoic acid. For the majority of the cases the $F_{w,j}[AA]$ error is significantly less than that for the extrapolated Antoine equation. The fact that a few analytic points from a three-coefficient equation can be used to parameterize the four-coefficient Wagner equation that many times results in lower predictive error than the original three-coefficient equation is a testament to the robustness and VLE curve characterization capability of the Wagner equation’s functional form. It also shows that it is possible to use VLE predictions from one correlation to parameterize another, more robust correlation that produces less predictive error than the original source correlation.

The incremental error from Table 2.3 is plotted vs. the extrapolation burden in Figure 2.1. The VLE predictions at the normal fusion point of the $F_{w,j}[AA]$ function and extrapolated Antoine begin to significantly differ once the extrapolation burden reaches a value of 20, suggesting that the $F_{w,j}[AA]$ may be a viable predictive VLE function over the entire two-phase curve for alcohols and “Others” that have a significant extrapolation burden.

To compare the $F_{w,j}[AA]$ function with Riedel and Ambrose-Walton correlations, reduced vapor pressures are calculated in increments of 0.025 reduced temperature units from T_r = 0.95 down to the normal fusion point. Average errors are calculated for three temperature segments: $T_r \leq 0.6$, $T_r > 0.6$, and “All T_rs.” Data points have equal weight when calculating average errors. The normal fusion point for all species studied fall in the $T_r \leq 0.6$ segment. The normal boiling points are included in the lower- or upper-temperature segment to which they belong. Both the normal fusion and boiling points are included in the average for the entire curve, “All T_rs.”

The error statistics of the Fw,j[AA] function for the fifty-five species are shown in Table 2.4. The impact of the error at the normal fusion point upon the Tr ≤ 0.6 segment and “All Trs” is evident. The averages and maximums shown in the Data Summary for the temperature segments are based upon the averages for the individual species.

The summary statistics in Table 2.4 indicate that, as with most CSP-based approaches, the $F_{w,j}[AA]$ function has a harder time with alcohols and organic acids. One can see that the results are consistent with those of the VLE extensions of other researchers discussed earlier (Ambrose, 1978; Ambrose & Davies, 1980; Forero G. & Velasquez J., 2011; McGarry, 1983) - the error in the downward extrapolation (approximately indicated by the $T_r \leq 0.6$ segment) is significantly larger than that for the upward interpolation (approximated by the $T_r > 0.6$ segment), and alcohols are erratic. The magnitudes of the average and maximum errors for this set of fifty-five species appear to be larger than those of the other researchers, which is not surprising given that the limited data sets for the species used here are not partial subsets of the data used to generate the “best” or reference values used for comparison.

Table 2.5 summarizes the comparison data between the three predictive methods, showing the number of species with the lowest and highest errors for different substance categories, further broken down by temperature segment. The general indication from Table 2.5 is that predictive error for the entire two-phase VLE curve is minimized for organic acids by Riedel, minimized for alcohols by the $F_{w,j}[AA]$ function, and minimized for “Others” by Ambrose-Walton.

For all fifty-five species as a group over the entire curve, the Ambrose-Walton appears to perform the best because it provides the least error for the most number of species (27), followed by the $F_{w,j}[AA]$ function. Riedel appears to have the poorest performance, having the least number of “lowest” designations and the most “highest.”

The lowest error/highest error record, however, can be misleading because all lows are not equivalent, nor are all highs. The three methods can be more quantitatively compared by using incremental error relative to the lowest error. This is shown for the normal fusion point in Table 2.6.

For the first entry in Table 2.6, acetic acid, the $F_{w,j}[AA]$ function has the lowest error, 0.36%, while the Riedel and Ambrose-Walton equations result in additional errors of 19.37% and 35.02% , respectively, above the base 0.36%. The species for which the $F_{w,j}[AA]$ function has the lowest error are shown at the top of the table, sorted by substance type and sub-sorted by A%Err. The same sorting is used for the subsequent species for which Riedel and Ambrose-Walton have the lowest error. One can see that the greatest error increase for not knowing *apriori* that the $F_{w,j}[AA]$ function has the lowest error occurs with the Ambrose-Walton equation for 2-octanol, an incremental error of 1,563%. Similarly, the largest error increase for not knowing *apriori* that the Riedel has the lowest error is again the Ambrose-Walton equation, for 1-pentanol with an incremental error of 819%. The largest error increase for not knowing *apriori* that the Ambrose-Walton has the lowest error occurs with the $F_{w,j}[AA]$ function for 2-methyl propanoic acid, an incremental error of 78%. There are eight species with an incremental error greater than 100%; all are alcohols, the highest error in all cases occurs with Ambrose-Walton, the lowest error is achieved by the $F_{w,j}[AA]$ function for six species and by Riedel for two species.

One can see that the lowest predictive error can be relatively high at the normal fusion point because extension downward involves extrapolation rather than interpolation. Table 2.6 shows that using the $F_{w,j}[AA]$ function at the normal fusion point avoids the largest errors but results in the lowest error for only a minority of species. The Ambrose-Walton equation, on the other hand, produces the lowest error for the majority of species, but the incremental errors of the other two methods in such cases are not relatively large. Additionally, the Ambrose-Walton produces extremely large incremental errors for several species, primarily alcohols.

Referring to the Data Summary of Table 2.6, the average error for a method for a substance type is equal to the addition of its average incremental error shown in the summary section of the table with that of the average for the “Lowest A%Err” column; obviously, the method with the least incremental average error has the smallest average predictive error. Note, however, that the maximum error for a method is not equal to the addition of its maximum incremental with that of the maximum shown in the "Lowest A%Err" column because both maximum values don't necessarily correspond to the same species.

The Data Summary section of Table 2.6 quantitatively supports three of the four general trends suggested by Table 2.5 - Riedel's advantage with organic acids, the advantage of the $F_{w,j}[AA]$ function for alcohols, and the advantage of Ambrose-Walton with "Others." However, the fourth trend indicated by Table 2.5 - that Ambrose-Walton is best for all fifty-five species as a group - is not quantitatively supported. Despite Ambrose-Walton having the most species with the lowest error at the normal fusion point, the $F_{w,j}[AA]$ function has the smallest average incremental error for all fifty-five species as a group, largely because of its superior relative performance with alcohols.

The summary data of the incremental error for all the temperature segments are presented in Table 2.7. The statistics from Table 2.6 have been included for reference. The trends indicated for the normal fusion point are generally repeated in the $T_r \leq 0.6$ segment and "All T_rs." The average incremental errors shown in Table 2.7 suggest that if an accurate value of the acentric factor is not known, the $F_{w,j}[AA]$ function may have the advantage for "Others" (e.g., normal species) in the $T_r \leq 0.6$ segment and "All T_rs," while Riedel may have the advantage for the $T_r > 0.6$ segment.

2.4.2 Error Dependency Upon the Reduced Temperature Interval

In Chapter 1 the limited data used for inputs to the $F_{w,j}$ function, the experimental entire-curve data, and the "best" values were closely coupled, and dependency of the predictive error upon interval width and location was seen. In the work described here for the $F_{w,j}[AA]$ function, however, the limited data and "best" value set are decoupled, and the interval width and location are not found to be discriminating factors for predictive error of the $F_{w,j}[AA]$ function. The average A%Err of "All Trs" is plotted versus the interval width and location in Figures C.1 and C.2, respectively, in Appendix C.

2.4.3 Error Dependency Upon Data Repeatability/Reproducibility

The repeatability/reproducibility disagreement of the limited data has the potential to be a significant contributor to the predictive error. The repeatability/reproducibility for a species in this case is estimated by the disagreement between the Antoine analytics and the "best" values represented by the entire-curve Wagner analytics. The %Err of the Antoine analytic values relative to their entire-curve Wagner analytic counterparts within their Antoine intervals are shown in Table 2.8 for 0.05 reduced temperature increments. The spread between the high and low analytic percentage errors for a species, Δ%Err, is also displayed and represents an approximation of the repeatability/reproducibility disagreement over the entire Antoine interval. The methods having the lowest and highest predictive error for the entire two-phase curve ("All T_rs") are included for reference. The fourth entry in Table 2.8, 3-methyl butanoic acid, for example, has consistently negative analytic error at all the discrete reduced temperatures except 0.75. The disagreement of 3-methyl butanoic acid's Antoine analytic values, which are used by the $F_{w,j}[AA]$ function, have a spread of 14.939% (2.088-[-12.851]).

The large range in degree-of-consistency in the Antoine-Wagner analytics of the fifty-five species and the inclusion of several substance types allow the $F_{w,j}[AA]$ function to be used to gain insight into the entire-curve predictive capability of available limited VLE data. The deviation between the Antoine and Wagner analytic data shown in Table 2.8 highlights the fact that an engineer doesn't know *apriori* how consistent a limited data set found in the literature is with an entire-curve "best" representation of a species' VLE.

Ambrose & Ghiassee (1987) in their study of alkanoic acids made specific mention of all six acids used in the research presented here. They considered experimental measurements for acetic acid to be reliable, but the other five species were unstable at high temperatures, and thus, the measurements of their critical properties were considered to be poor. The authors also noted that alcohols, unlike organic acids, generally have reliable measurements up to the critical point; thus, one might expect that alcohols should generally experience less error in the Antoine-Wagner analytics than acids. The average Δ%Err in the Antoine-Wagner analytics shown in the Data Summary of Table 2.8 supports that expectation – an average of 5.99% for acids compared to 1.57% for alcohols.

One might expect that the more experimentally problematic a species is, the less likely it is that a single set of experimental measurements (or a set of Antoine constants regressed from said experiment) will be representative of the true vapor-liquid equilibrium over that limited range. Subsequently, one might think it less likely that their $F_{w,j}[AA]$ functions would accurately extrapolate VLE below and interpolate above the interval. The data in Table 2.8, however, does not strongly support such reasoning. The majority of species have a value of Δ%Err less than 2%, and the A%Err of such species range from 0.03% to 98.5%. It appears that the predictive capability of the $F_{w,j}[AA]$ function has no more of a definitive relationship with the Antoine analytic error than it has with interval width and location when the limited data is decoupled from the "best" value set.

Table 2.8, however, does indicate that there may be a relationship between the Δ%Err levels and the ability of the $F_{w,j}[AA]$ function to have less predictive error than Riedel and Ambrose-Walton for a few substance types. The two columns on the far right of the Data Summary of the table show the number of species for which the A%Err of the $F_{w,j}[AA]$ function is the lowest and the number for which it is not the lowest, along with the corresponding subset average Δ%Err. The relatively small number of species involved in each subset doesn't permit statistical inferences. The average Δ%Err for the two organic acids for which the $F_{w,j}[AA]$ function achieves the lowest predictive error is 0.58%, compared to 8.70% for the four acids for which the function does not achieve the lowest predictive error.

The dipole moments for the 13 alcohols range from 1.6 to 2.0 debye, so they all can be considered to be polar. Applying the law of corresponding states to non-normal species, such as polar compounds, is generally done cautiously, and equations based solely on the acentric factor in particular, such as the Ambrose-Walton method, are considered to be less reliable for strongly polar species. One can see in Table 2.8 that the Ambrose-Walton achieves the lowest VLE predictive error for only a single alcohol, while Riedel achieves the lowest for only three. Just as important as having the lowest predictive error for the remaining nine alcohols is the fact that the $F_{w,j}[AA]$ function does not have the highest predictive error for any of the 13 alcohols. Interesting to note is that the $F_{w,j}[AA]$ function has the lowest predictive error for isopropyl alcohol, 2-octanol, and 1-nonanol despite appreciable difference between the Antoine and Wagner analytics. The overall superior performance of the $F_{w,j}[AA]$ function apparently has nothing to do with Δ%Err and is probably due to the general difficulty that Riedel and Ambrose-Walton equations have with alcohols. The $F_{w,j}[AA]$ function achieves the lowest predictive error for ten "Others," four of which are polar. Treating a dipole moment greater than 1 debye to imply polarity (Prausnitz et al., 1999), six of the "Others" can be considered to be polar, and their results are consistent with those for the organic acids. The $F_{w,j}[AA]$ function has the lowest predictive error for the strongly polar ammonia, water, and acetone, and for the less polar diethyl ether; dipole moments being 1.5, 1.8, 2.9, and 1.3 debye, respectively. However, note that the extrapolation burden for ammonia and water is zero for the $F_{w,j}[AA]$ function, which gives it a significant advantage over the Riedel and Ambrose-Walton.

The average spread in the Antoine-Wagner analytics for these four species is 0.84%. The $F_{w,j}[AA]$ function has the highest predictive error, on the other hand, for the strongly polar methyl isobutyl ketone (μ=2.8 debye) and R152a (μ=2.3 debye), whose spread in the Antoine-Wagner analytics are higher, 2.52% and 9.60%, respectively.

The six normal species for which the $F_{w,j}[AA]$ function achieves the lowest predictive error have a range 0.260-1.066% for the average analytic Δ%Err, which range also encompasses most of the normal species for which the $F_{w,j}[AA]$ function does not achieve the lowest predictive error. Thus, the Δ%Err doesn't appear to discriminate the relative performance between the $F_{w,j}[AA]$ function and the other two methods for normal species.

The average Δ%Err is 0.75% for the two acids and four polar "Others" for which the $F_{w,j}[AA]$ function achieves the lowest predictive error. The results shown in Tables 2.9 and 2.10 suggest the following hypothetical selection rules: 1) use the $F_{w,j}[AA]$ function for alcohols; 2) use the $F_{w,j}[AA]$ function for polar species other than alcohols that have an average Δ%Err less than 0.75%; 3) use Riedel for organic acids that don't satisfy the thresh hold of rule #2; and 4) use Ambrose-Walton for polar species other than alcohols and organic acids that don't satisfy the thresh hold of rule #2, and for normal species.

The incremental error for "All T_rs" using the four above hypothetical rules is compared with those of the three methods in Table 2.9. One can see that rules two through four results in a decrease in the predictive error for organic acids, "Others," and all fifty-five species in aggregate. Obviously, the Δ%Err is not known before hand for a set of limited data, and subsequently any thresh hold is not for practical application. However, the rules are applied in Table 2.9 to reinforce the effect that data repeatability/disagreement can have and to illustrate that, for a predictive method applied to a particular substance type, such data imprecision may exhibit an influence upon the predictive error that is sufficiently consistent to allow for the quantitative determination of a comparative thresh hold, such as the 0.75% indicated here.

Excluding the thresh hold since analytic Δ%Err for a data set is not known *apriori*, the trends discussed in previous sections provide the preliminary practical recommendations for predicting VLE for the entire two-phase curve for a species when only limited VLE data is available: 1) use the $F_{w,j}[AA]$ function for alcohols, 2) use Riedel for organic acids, and 3) use Ambrose-Walton for other species, unless an accurate value of the acentric factor is not known, in which case use the $F_{w,j}[AA]$ function.

2.4.4 The Waring Test

The heat of vaporization is thermodynamically tied to the saturation curve, and Waring (1954) noted that the general shape of the saturation curve requires that the $\Delta H/\Delta Z$ curve plotted against reduced temperature has a minima, where ΔH is the enthalpy of vaporization, and ΔZ is the difference in the compressibility factors of vapor and liquid. Adherence to the Waring minima is implicit in the Riedel equation (Ambrose & Ghiassee, 1987; Velasco, White, Srinivasan, & Dutta, 2012), and the Ambrose-Walton equation has been shown to accurately predict the location and value of the minima for a broad range of pure substances (Velasco et al., 2012). The minima for most substances fall in the reduced temperature range 0.8-0.9, but Ambrose & Ghiassee (1987) found that it occurs closer to the critical point (around 0.95) for alcohols, and Mejbri & Bellagi (2005) has found the minima at reduced temperatures lower than 0.8 for some species. Ambrose & Ghiassee (1987) showed that the existence of a minimum in the $\Delta H/\Delta Z$ vs. T_r curve requires that the Wagner constants b and c have different signs. McGarry (1983) noted that substances with a normal boiling point less than 50 K, however, do not exhibit this minima – subsequently, b and c would not be of opposite sign. One can see from the literature values of the entire-curve Wagner constants shown in Table 1.2 that in all cases b and c have opposite sign, except for hydrogen, whose normal boiling point is below 50 K. Consistent with this 50 K temperature thresh hold, Mejbri & Bellagi (2005) determined that helium, hydrogen, and deuterium do not show a minimum in the $\Delta H_v/\Delta Z_v$ vs. T_r curve when calculated from the *NIST Chemistry WebBook* (Lemmon et al., 2005) enthalpy and compressibility saturation data.

Waring (1954) proposed that the existence of the minima be used as a qualitative test for VLE equations. Thus, the relative signs of b and c are a necessary, albeit insufficient, qualitative fit-of-form test. One can see from Table C.6 that the $F_{w,j}[AA]$ function fails the Waring test for six substances: methanol, 1-heptanol, 1-hexanol, methane, and ammonia had *b* and *c* constants of the same sign, while the two constants of hydrogen, which should have the same sign, had opposite sign. As previously mentioned, Forero G. & Velasquez J. (2011) regressed Wagner constants from analytic values calculated from Antoine constants that they had regressed from limited data. They applied their approach to two hundred fifty-seven species. Unmentioned by the authors, the *b* and *c* constants of one substance studied, bromodifluoromethane, failed the Waring sign test. Their species set included four of the above six substances: methane, methanol, 1-heptanol, and 1-hexanol. The level of consistency between their Antoine constants and those used here from Poling et al. (2001) is unknown. They used non-linear, over-determined regression to estimate the Wagner constants rather than a four-point fully-determined approach. Additionally, for alcohols, (e.g., methanol, 1-heptanol, and 1-hexanol) they used the entire-curve Wagner constants from Poling et al. (2001) as initial guesses for inputs to their regressions, which would pre-dispose the resulting values of their Wagner constants to satisfy the Waring sign test.

The test failure of methane, ammonia, and hydrogen has no practical consequence since the preliminary selection rule #3 recommends the Ambrose-Walton. Preliminary selection rule #1, however, recommends the $F_{w,j}[AA]$ function to be used for the three failing alcohols, and the function does have the lowest predictive error over the entire two-phase curve for methanol and 1-heptanol (see Table 2.6 for their relative advantage at the normal fusion point). It was previously pointed out that Riedel is significantly better than Ambrose-Walton for alcohols (Table 2.6). Consequently, one could choose to use Riedel for an alcohol for which the $F_{w,j}[AA]$ function fails the Waring fit-of-form test if the high-temperature region is of primary concern, or one could choose to use the $F_{w,j}[AA]$ function and trade off less form fit at the high end for better accuracy in the low-temperature region.

2.4.5 Error Dependency Upon Extrapolation Burden

The predictive error at the normal fusion point in logarithmic scale for the three methods are plotted vs. the extrapolation burden quantified by the $\Delta Log\ P_{v,r} / \Delta T_r$ ratio in Figures 2.2-2.4.

In Figure 2.2 for the $F_{w,j}[AA]$ function, the predictive error is not zero for the six species with no extrapolation burden because there are still error contributions from the repeatability/reproducibility disagreement and equation imperfection. The burden of the remaining species ranges between 10 and 34. Except for a few “Others” with a burden around 23, all species fall upon a discernible pattern. The predictive VLE error exhibits a general dependency upon the extrapolation burden regardless of substance type.

The results for Riedel, displayed in Figure 2.3, shows an alcohol extreme outlier with a burden of 23.51 and error of 0.39% (1-pentanol), but a dependency upon the extrapolation burden is evident. Figure 2.4, on the other hand, shows that the Ambrose-Walton has appreciably less consistent dependency. The burden range 13-20, comprised of mostly “Others,” displays a wide spread in vapor pressure predictive error, and all species with a predictive error greater than 79% are alcohols, and they extend over the relatively broad burden range 17-26. There is much more scatter in the Ambrose-Walton plot than in those for the $F_{w,j}[AA]$ function and Riedel.

2.5 Summary

The overall superior performance of the $F_{w,j}[AA]$ function compared to mere extrapolation of the Antoine equation below its applicable temperature interval shows that predictions from a less robust correlation can be used to estimate Wagner constants that can result in significantly better predictive power than the original source correlation. A difference in the functional form between the Wagner and Antoine equations is obviously one factor that allows such improvement to be possible in this specific instance.

The deviation between the Antoine and entire-curve Wagner analytic data, Δ%Err, exhibited by the fifty-five species average approximately 2% but varies considerably between species and highlights the fact that a practitioner doesn’t know *apriori* how consistent a limited data set found in the literature may be with an entire-curve “best” representation of a species’ VLE. Unlike the conditions studied by other researchers and in Chapter 1, the results here suggest that the VLE data available in the literature to an engineering practitioner in many cases may deviate significantly from “best” values, and thus, be judged to be well outside what one would consider good precision.

Neither interval width, interval location, nor analytic Δ%Err exhibit pronounced first-order effects upon the predictive power of the $F_{w,j}[AA]$ function. However, the analytic Δ%Err does appear to exert an influence of sufficient consistency upon polar species other than alcohols such that a preliminary thresh hold is found to discriminate $F_{w,j}[AA]$ function performance relative to that of Riedel and Ambrose-Walton. Based on the results presented thus far, and excluding the thresh hold since analytic Δ%Err for a data set is not known beforehand, the following recommendations are given regarding the three methods investigated for predicting VLE over the entire two-phase curve for a species when only limited VLE data is available: 1) use the limited data to estimate Wagner constants for alcohols, 2) use the Riedel equation for organic acids, and 3) use the Ambrose-Walton equation for other species, unless an accurate value of the acentric factor is not known, in which case use the limited data to estimate Wagner constants. When #1 or #3 recommends using limited data, and the resulting Wagner constants b and c fail the Waring fit-of-form test, one can choose to use Riedel if the high-temperature region is of more concern than minimizing predictive error in the low-temperature region.

The Wagner constants estimated from Antoine analytics have an average entire-curve error of 4.8% for the fifty-five species studied, with error predominately occurring in the region of downward extrapolation, compared to the approximate 1% error of the $F_{w,j}[RD]$ function in Chapter 1. The results only weakly support Hypothesis II, considering that the $F_{w,j}[AA]$ function exhibits better aggregate predictive power for neither all substance categories nor for both reduced temperature segments.

It is found that both the $F_{w,j}[AA]$ function and Riedel equation treat all substance types with respect to extrapolation burden in a more consistent manner than does the Ambrose-Walton equation. The predictive error vs. extrapolation burden plot for the latter exhibits much scatter and reveals that the predictive error may be more related to substance type than to the extrapolation burden imposed by an individual species.

Chapter 3: Critical and Normal Boiling Points & Acentric Factor

3.1 Abstract

Entire-curve Wagner constants are used to generate “true” or “best” reduced vapor pressure values that are compared with those generated by Wagner constants estimated for the fully-determined case from VLE predictions based solely on the critical and normal boiling points and acentric factor. Besides using the standard forms of the Riedel and Ambrose-Walton equations, a modified form of Riedel is created by forcing the value of *K* to provide zero error at the reduced temperature of 0.7, and a modified form of Ambrose-Walton is created by using a pseudo acentric factor that provides zero error at the normal boiling point. It is shown that Wagner constants estimated from VLE predicted from such correlations can provide better VLE predictive power than the underlying source correlations themselves.

3.2 Introduction

One goal of the work presented in this chapter is to provide the practitioner with better approaches to predict entire-curve VLE for pure substances with as little required data as possible. The results detailed in Chapter 1 suggest that a single set of four VLE points of good precision from limited data can be used to estimate Wagner constants that have the potential to reasonably predict vapor pressure both below and above the original data interval.

Chapter 2 investigates the impact of data repeatability/reproducibility disagreement by using entire-curve Wagner analytics for 55 species to represent the “best” values and Antoine analytics to represent single sets of limited-range experimental data. The results lead to several conclusions: 1) VLE data in the literature can deviate significantly from “best” values; 2) Wagner constants estimated from analytic values from another correlation of different form can have greater predictive power than that of the source correlation; 3) the fully-determined approach to estimate Wagner constants from Antoine analytics fail the qualitative Waring fit-of-form test for several species; and 4) Wagner constants estimated from Antoine analytics generally have superior predictive power for alcohols, the Riedel equation is best for organic acids, and the Ambrose-Walton equation has least error for the remaining species (mostly normal and a few polar).

The presence of the Waring inflection point is implicit in the Riedel equation (Ambrose & Ghiassee, 1987), and the Ambrose-Walton equation has good success at predicting its location

(Velasco et al., 2012). Given the relative good performance of Riedel and Ambrose-Walton equations for species other than alcohols, their ability to satisfy the Waring fit-of-form test, and their functional form being different from that of the Wagner equation, the goal of this paper is to determine if Wagner constants estimated using predictions from the Riedel and Ambrose-Walton correlations, and modifications thereof, can result in superior predictive power while also satisfying the qualitative Waring fit-of-form test. In other words, the goal is to prove Hypothesis III, with the additional condition that the Waring test be satisfied.

The results of using predicted VLE values from standard and modified versions of the Riedel and Ambrose-Walton equations to estimate Wagner constants are presented. The predictive error of these Wagner constants is compared first with that of the source equations and second with that of the Wagner constants estimated from limited-range Antoine analytics in Chapter 2. For many species only the critical and normal boiling points and acentric factor are given in technical handbooks – thus, the benefit of using Riedel and Ambrose-Walton as the source correlations. This chapter presents a new approach for using only these three known vapor pressure data points to predict VLE over the entire two-phase curve. The results presented here are relevant to the research of predictive correlation development and to engineers tasked with predicting VLE for a species when only these three data points are available.

The fully-determined case is used here for several reasons. First, the fully-determined approach is unhampered by variables involved with an over-determined solution, e.g., differences in data-weighting schemes and error minimization algorithms. The fully-determined solution provides the quickest way to obtain a preliminary determination of success. Although further analysis will probably follow, the quick determination from the fully-determined approach can define the aim of any subsequent analysis, either more error reduction or more definitive results. Second, if success is achieved, the field practitioner has a relatively easy method to implement now for a targeted species that is absent of the time and resources required by more complex analysis. Third, the fully-determined case is used to be consistent with the work described in the previous chapters, allowing comparison between the results.

3.3 Investigative Approach

There are two novel elements of the approach presented in this chapter that are noteworthy. First, using a four-point, fully-determined solution rather than a complex over-determined solution may be counter intuitive, but therein lays its novelty. That significant predictive success can arise from a relatively simple, algebraic parameterization of the Wagner equation may be surprising to some.

Second, this researcher is not aware of any other work in the literature hypothesizing, let alone proving, that the Wagner equation parameterized from VLE predictions can have better predictive error than the source correlations themselves. To use the most accurate data possible is the most natural and logical path to follow when trying to parameterize a predictive correlation. Although the concept of using a set of source predictive correlations to provide the "data" with which another predictive correlation is parameterized appears to be counter intuitive, the concept proves to be very insightful.

The group of 72 species studied in this chapter is the same set as studied in Chapter 1; it includes 22 alcohols, 9 organic acids, 6 other polar species, and 35 normal substances (hydrogen and helium, although quantum gases, are included in the count of normal substances). As in the previous chapter, reduced vapor pressures calculated from entire-curve Wagner constants are referred to as "entire-curve analytic" data and are used as the reference standard, the "best" values, for error comparison.

3.3.1 Modification of Riedel Equation

The standard Riedel equation, given by Eq. [11] uses the normal boiling point as an anchor point, but any other saturation point can become a secondary anchor by using it to back calculate the value of *K*. Inverting Eq. [11] and substituting Eqs. [11a] and [11b] for A^+, B^+, C^+, D^+, and *Q* gives a substance-specific relationship for *K* based upon an additional saturation point,

$$[12] \quad K = \frac{Ln\, P_{v,r,SA} - \alpha_c\, Ln\, T_{r,SA}}{(3.758 - \alpha_c)\psi_{SA}}.$$

The subscript "*SA*" has been added to indicate that a variable or parameter pertains to the secondary anchor point. The parameter ψ_{SA} has the same functional form as that of ψ_b and is given by

[13] $$\psi_{SA} = -35 + \frac{36}{T_{r,SA}} + 42\, Ln\, T_{r,SA} - T_{r,SA}^{6}.$$

The parameter α_c is dependent upon *K*, so Eq. [11c] has to be substituted for α_c into Eq. [12] to arrive at the final relationship for the substance-dependent *K*,

[12a] $$K = \frac{(Ln\, P_{v,r,b})(Ln\, T_{r,SA}) - (Ln\, P_{v,r,SA})(Ln\, T_{r,b})}{3.758[(Ln\, T_{r,SA})\psi_b - (Ln\, T_{r,b})\psi_{SA}] + (Ln\, P_{v,r,b})\psi_{SA} - (Ln\, P_{v,r,SA})\psi_b}\,.$$

Using the reduced temperature of 0.7 for the secondary anchor point, Eq. [12a] has the potential to result in a negative value for *K* because of round off error if the normal boiling point reduced temperature is very close to 0.7 (the acentric factor has only three significant digits right of the decimal point). Such is the situation for only one of the 72 species, butanoic acid, where the difference between $T_{r,b}$ and 0.7 is only 0.00011, in which case the Vetere value of *K* given by Eq. [11e] is retained.

The name Riedel(ω), or the short hand R(ω), is used to represent using Eq. [12a] and the acentric factor to determine the value of *K*: the value calculated from Eq. [12a] is used if positive, and the Vetere (2006) value of *K* is used if the value calculated from Eq. [12a] is negative, in which case the standard Riedel and R(ω) are equivalent. It is hypothesized that R(ω) will provide more reliable vapor pressure estimates than the standard Riedel for the part of the two-phase equilibrium curve containing the additional anchor point. For the case where the normal boiling reduced temperature is below 0.7, R(ω) is expected to have better predictive accuracy above the normal boiling point. Conversely, R(ω) is expected to have better accuracy below the normal boiling point when $T_{r,\mathrm{b}} > 0.7$.

3.3.2 Modification of Ambrose-Walton Equation

Unlike the Riedel equation with its *K* parameter, the standard Ambrose-Walton relationship given by Eq. [10], with its twelve coefficients, doesn't have a single parameter that can be methodically adjusted to provide an additional universal anchor point. It was decided to swap the normal boiling point with the reduced temperature of 0.7 as the anchor point. The anchor point can be changed by simply using the acentric factor estimated from the normal boiling point. The Ambrose-Walton is quadratic in the acentric factor; thus, the acentric factor can be estimated from any saturation point by

[14] $$\omega = \frac{-f^{(1)} \pm \sqrt{\left(f^{(1)}\right)^2 - 4f^{(2)}\left(f^{(0)} - Ln\, P_{v,r}\right)}}{2f^{(2)}}.$$

Using the normal boiling point, values calculated from Eq. [14] using the negative square root in the numerator are compared with the acentric factor values given in Poling et al. (2001) for 313 species. The produced acentric values have an average absolute deviation from the values in Poling et al. (2001) of 0.004, with 10 species having a deviation greater than 0.02. The name Ambrose-Walton(T_b), or the short hand A-W(T_b), is used to represent using in Eq. [10] the value of the acentric factor given by Eq. [14] using the normal boiling point and the negative square root. Although Poling et al. (2001) note that for most species the ω^2 term in the Ambrose-Walton equation is negligible when using it to estimate the acentric factor from the normal boiling point vapor pressure, the quadratic is chosen because it is easy to calculate and it removes any potential error arising from a linear estimate. It is expected that A-W(T_b) will have better predictive accuracy than the standard Ambrose-Walton at lower temperatures for species with a normal boiling point reduced temperature below 0.7 and better accuracy for upper temperatures for species having a normal boiling point reduced temperature above 0.7.

3.4 Discussion

The expected performance of the modified correlations relative to their standard counter parts are summarized in Table 3.1. It is hypothesized that the different anchor point in the modified forms will improve the predictive accuracy on the part of the two-phase VLE curve in which the new anchor point resides. It is unclear whether or not the different anchor point will improve predictive accuracy for the part of the two-phase VLE curve in which the anchor point does not reside, thus, the question marks in Table 3.1. With a second anchor point at the reduced temperature of 0.7, Riedel(ω) is expected to perform better than the standard Riedel below the normal boiling point for the case when $T_{r,b} > 0.7$ and above the normal boiling point when $T_{r,b} < 0.7$. Alternatively, with the acentric factor defined by the normal boiling point, A-W(T_b) is expected to perform better than the standard Ambrose-Walton below the normal boiling point for the case when $T_{r,b} < 0.7$ because the anchor point is lower down the VLE curve than is the reduced temperature 0.7. Similarly, A-W(T_b) is expected to perform better than the standard Ambrose-Walton above the normal boiling point for the case when

$T_{r,b}$ > 0.7 because the anchor point is higher up the VLE curve than is the reduced temperature 0.7.

3.4.1 Determining Best Correlation for Below and Above the Normal Boiling Point

A comparison of the predictive error of the standard Riedel and Ambrose-Walton equations and their modified forms at the normal fusion point is shown in Table 3.2. The reduced temperature of the normal fusion and boiling points are given for each species, along with the difference between 0.7 and the reduced normal boiling point temperature. The absolute percent error (A%Err) relative to the entire-curve Wagner analytics are shown for each correlation. The correlation with the least error when the standard Riedel and Ambrose-Walton go head-to-head is indicated, and that with the least error of all four correlations is also indicated ("All Four" column).

We look first at the species where 0.7 is below the normal boiling point reduced temperature, i.e., the value of 0.7-$T_{r,b}$ is negative. R(ω) is expected to be more accurate than Riedel below the normal boiling point, e.g., at the normal fusion point, for such species, and consequently, it is expected that R(ω) will outperform all four correlations for a species where Riedel has less error than Ambrose-Walton. Riedel has less error than Ambrose-Walton for one "Others", helium, and for five organic acids. One can see that the expectation is met for helium and for three of the five qualifying organic acids. However, R(ω) outperforms all the other correlations for only two of the nine alcohols where Riedel has lower error than Ambrose-Walton. The Summary section of Table 3.2 shows that when averaged over each substance type, the modified Riedel does meet expectations for organic acids - Riedel outperformed Ambrose-Walton, and R(ω) has the least error of all correlations. However, R(ω) does not meet expectations for alcohols with $T_{r,b}$ > 0.7; it does not have the least error of all four correlations despite Riedel outperforming Ambrose-Walton.

It is unclear regarding what to expect for the A-W(T_b) modification for species where 0.7-$T_{r,b}$ is negative. The standard Ambrose-Walton might be better because its anchor point would be lower down that part of the two-phase curve, while the modified form might perform better because it provides a more accurate representation of the two-phase curve at the higher-temperature normal boiling point where curvature changes. Ambrose-Walton has less error than Riedel for a single organic acid, 2-methyl propanoic acid, and for four alcohols. One can see that the modified Ambrose-Walton has the least absolute percent error of all four correlations for the single qualifying organic acid and for all four qualifying alcohols. However, A-W(T_b) does not perform better for any of the thirteen "Others" where the standard Ambrose-Walton is superior to Riedel. Consequently, it appears that the modified Ambrose-Walton may offer an advantage when $T_{r,b} > 0.7$ for organic acids and alcohols while providing no advantage for "Others."

We now look at the case where $T_{r,b} < 0.7$, i.e., the value of $0.7\text{-}T_{r,b}$ is positive. There are no expectations for R(ω) because it is unknown whether or not the extra anchor point above the normal boiling point would improve predictive accuracy below the normal boiling point. R(ω) has the least error of all correlations for eleven species, seven of which correspond to species where Riedel performs better than Ambrose-Walton, and Ambrose-Walton performs better than Riedel for the other four species. Additionally, there are nine species for which Riedel has less error than Ambrose-Walton but R(ω) does not have the least error of all the correlations. Consequently, the modified Riedel can provide improved predictive accuracy for some species where $T_{r,b} < 0.7$, but its performance appears to be independent of the predictive power of the standard Riedel.

A-W(T_b) is expected to perform better than its standard counterpart on the low-temperature end for species where $T_{r,b} < 0.7$ because the anchor point of the modified form is at a lower reduced temperature than 0.7. One can see in Table 3.2 that the modified form does not appear to provide an advantage for organic acids and alcohols, but it does appear to provide a clear advantage for five normal "Others" and 1 polar "Others." There are ten "Others" where the error of Ambrose-Walton and A-W(T_b) are the same, and only three "Others" for which the Ambrose-Walton error is lower than both Riedel and A-W(T_b) (pentafluorobenzene, toluene, and hydrogen). Consequently, one would be better off using A-W(T_b) for estimating the normal fusion point of "Others" when $T_{r,b} < 0.7$.

The Ambrose-Walton equation and its modified form show an interesting behavior for alcohols with $T_{r,b} > 0.7$. The predictive error at the normal fusion point is parabolic vs. the value of $0.7\text{-}T_{r,b}$. Only the errors for 1-octanol and 1-heptanol, which sandwich the parabola's inflection point at 2-ethyl-1-hexanol, deviate slightly from the parabolic form. The

A%Err increases as the value of $0.7\text{-}T_{r,b}$ gets smaller in magnitude until reaching -0.01471 for 2-ethyl-1-hexanol, after which the error decreases as the $0.7\text{-}T_{r,b}$ difference approaches zero. The correlation with the least error for this subset switches between A-W(T_b) and Riedel at some $0.7\text{-}T_{r,b}$ value between -0.076 and -0.047. It appears that Ambrose-Walton and its modified form have appreciably less predictive error than Riedel and its modified form for the few alcohols with a value of $0.7\text{-}T_{r,b}$ more negative than -0.076, but the error of the Ambrose-Walton and its modified form quickly turn horrendous as the value of $0.7\text{-}T_{r,b}$ becomes more positive than -0.047.

Comparing all four correlations to each other, the Summary section of Table 3.2 shows that R(ω) results in lowest error for organic acids, Riedel for alcohols, Ambrose-Walton for "Others" with $T_{r,b} > 0.7$, and A-W(T_b) for "Others" with $T_{r,b} < 0.7$. The "All Four" entries in the Summary section that match the hypotheses are in italic font, that which contradicts a hypothesis is shaded in gray, and the cells with normal font and no shading are cases for which there are no expectations. Organic acids with $T_{r,b} < 0.7$ is one such cell having no expectations, for which R(ω) has the least average predictive error. Restricting the comparison to just modified vs. standard forms, one can see that the R(ω) correlation has better predictive power than the standard Riedel only for organic acids. The A-W(T_b), however, is superior to its standard counterpart for all substance types with $T_{r,b} < 0.7$.

The normal fusion point generally has the largest error along the entire two-phase curve, thus, it tends to dominate when included in averages of equally weighted points. Table 3.3 shows the results for the equally-weighted average absolute percent errors for the parts of the two-phase VLE curve, both below and above the normal boiling point. The sorting is the same as in Table 3.2. One can see that the parabolic relationship between error and the value of $0.7\text{-}T_{r,b}$ seen at the normal fusion point for alcohols is maintained for Ambrose-Walton and its modified form in the $T_r < T_{r,b}$ segment of the VLE curve.

The average for a subset shown in the Summary section of Table 3.3 is not the average of all the corresponding species' averages in that subset, but rather it is the sum of the individual A%Err values for the VLE points of all species in that subset divided by the number of total points in the subset. This is done because the number of points above and below the normal boiling point varies for each species given that the value of the normal boiling point varies. The normal boiling point itself is not included in either of the two temperature segments.

Helium and hydrogen are the only quantum gases represented (included in normal "Others"), and it appears the R(ω) correlation performs the best for helium in the low-temperature segment and the best for hydrogen over the entire two-phase curve. One can see that the "All Four" entries in the Summary section of the table for the $T_r < T_{r,b}$ segment are the same as those for the single normal fusion point shown in Table 3.2, except that the standard Riedel is superior to the standard Ambrose-Walton in their head-to-head competition for the 6 polar "Others" when $T_{r,b} < 0.7$. There are no polar "Others" with $T_{r,b} > 0.7$ for comparison in this work's sample pool of 72 species.

The Summary section of Table 3.3 shows the correlation that has the least predictive error for each substance subset in the "All Four" column, segregated further by location of the normal boiling point. One can see that only one subset of species has results contrary to the expectations shown in Table 3.1, alcohols with $T_{r,b} > 0.7$, which cells are shaded in gray; R(ω) is expected to be best performer of "All Four" below the normal boiling point, and A-W(T_b) above. The "All Four" entries of the other subsets are consistent with the expectations and are shown in italic font. There are no expectations regarding several, shown in normal font without shading. Note that R(ω) has the least predictive error for the $T_r > T_{r,b}$ segment for all substance subsets except "Others" with $T_{r,b} > 0.7$.

Because the error at low temperatures tend to dominate the entire-curve statistics when points are equally weighted, the entries in the "All Four" column in the Summary section of Table 3.3 for the $T_r < T_{r,b}$ segment also apply to the entire curve, i.e., the correlation that has the least error for a species subset at the low-temperature end of the curve ends up also having the least error in aggregate over the entire curve when the four correlations are compared head-to-head. The $F_{w,j}$ function, however, will be shown to provide a method to combine the best correlations below and above the normal boiling point to reduce the average error over the entire two-phase curve.

The Summary section of Table 3.3 suggests the correlations to combine via the $F_{w,j}$ function. First, R(ω) appears to be best for the entire two-phase co-existence curve for organic acids, and yet there is still significant predictive error, so four R(ω) points are used to estimate

Wagner constants to assess whether or not the $F_{w,j}$ function can improve upon the R(ω) correlation. The Wagner constants estimated by Eq. [2] from such combinations are denoted by $F_{w,j}[R(\omega)]$. Second, it is hypothesized that the predictive error over the entire curve for alcohols can be decreased by combining Riedel points below the normal boiling point with R(ω) points above the normal boiling point, and the Wagner constants estimated by Eq. [2] from such combinations are denoted by $F_{w,j}[R|R(\omega)]$. Third, the standard Ambrose-Walton cannot be out-performed in aggregate for "Others" with $T_{r,b} > 0.7$ either below or above the normal boiling point, and the average errors are sufficiently small such that only minimal benefit could potentially be achieved by $F_{w,j}$ functions based on vapor pressure predictions of the Ambrose-Walton. Thus, this subset of species is not targeted by $F_{w,j}$ functions. Fourth, it is hypothesized that error can be reduced for "Others" with $T_{r,b} < 0.7$ by using A-W(T_b) points below the normal boiling point and R(ω) points above, and the equations for the estimated Wagner constants for such combinations are denoted by $F_{w,j}[A\text{-}W(T_b)|R(\omega)]$.

Three different point distributions are used. Because of the general characteristics of the S shape of the log P_v vs. $1/T$ curve, it is desired to capture the best predictions from both below and above the normal boiling point. A reduced temperature ≥ 0.9 is included to try to incorporate the region around the upper inflection point. The vapor pressure at the reduced temperature of 0.6 has been shown to significantly increase the prediction of VLE and other thermodynamic properties for polar fluids when combined with the acentric factor (Halm & Stiel, 1967, 1970; Wu & Stiel, 1985). The predictive error of the four correlations involved generally increases as the saturation temperature decreases, with the error increasing significantly at reduced temperatures lower than 0.6. Although the predictions of the four correlations being used are not what would be considered good precision compared to actual data, the four saturation points at the reduced temperatures of 0.6, 0.7, 0.8, and 0.9 are initially chosen for use in the $F_{w,j}$ function because it represents an interval of decent width and located in the part of the VLE curve with the least predictive error by the four correlations. The superscript "(1)" is used to indicate this point distribution for $F_{w,j}$ functions comprised of points from two correlations.

However, that set of points can exclude the standard Riedel and A-W(T_b) being used if the normal boiling point's reduced temperature is less than 0.6. Consequently, the set of reduced temperatures 0.3, 0.6, 0.7, and 0.95 are used to extend the interval below any reasonable normal boiling point and extend the interval further upward into the area of the upper inflection point. The reduced temperatures of 0.6 and 0.7 are chosen to help establish the middle of the VLE curve with accurate data since standard Riedel and A-W(T_b) have the normal boiling point as an anchor and R(ω) has the acentric factor as an additional anchor. The superscript "(2)" is used to indicate this point distribution

The third set of points includes the reduced temperatures 0.2, $T_{r,b}$, 0.7, and 0.95. The low end of the interval is lowered to 0.2 to account for those species where the below-T_b correlation is accurate, and the normal boiling point is used to enforce zero error at this known point, thereby providing good representation for the below-T_b segment of the two-phase VLE curve for such species. The normal boiling point pressure, 1.01325 bars, is used for $T_{r,b}$. The superscript "(3)" is used to indicate this point distribution.

The temperature of the triple point (or normal fusion point) is not always known, thus, the lowest reduced temperature of the four-point distributions used is fixed rather than being tied to a species-dependent lower bound. Additional implementation specifics are given below for some $F_{w,j}$ functions.

3.4.1.1 $F_{w,j}[R(\omega)]$

R(ω) predictions at the four reduced temperatures of 0.6, 0.7, 0.8, and 0.9 are used with this function.

3.4.1.2 $F_{w,j}^{(3)}[R|R(\omega)]$

The reduced vapor pressure at T_r=0.7 is from R(ω) since it should be accurate at that reduced temperature and be consistent with the Riedel value for T_r=0.2 given that both correlations have the normal boiling point as an anchor and both have similar functional form.

3.4.1.3 $F_{w,j}^{(3)}[A\text{-}W(T_b)|R(\omega)]$

Unlike for $F_{w,j}^{(3)}[R|R(\omega)]$, the vapor pressure for T_r=0.7 in $F_{w,j}^{(3)}[A\text{-}W(T_b)|R(\omega)]$ is calculated using the A-W(T_b) if 0.7 is below the normal boiling point reduced temperature and R(ω) if it is above because R(ω) and A-W(T_b) do not share a similar functional form.

The point distributions for the three fully-determined cases, and the corresponding values of the η parameters, used in this study to calculate Wagner constants from the seven $F_{w,j}$ functions are summarized in Table D.1 of Appendix D.

3.5 Results

When discussing statistics for predicted VLE points, the "All T_rs" term is used here to indicate the entire two-phase curve, including the normal boiling point. The error at the normal boiling point will not always be zero because not all of the correlations and functions have the normal boiling point as an anchor.

The results of the various $F_{w,j}$ functions are compared in Table 3.4 for "All T_rs." The types of $F_{w,j}$ function suggested by the Summary results of Table 3.3 are also indicated in the Summary section of Table 3.4. The cell of the function having the least average error for a substance subset is shaded in gray. A comparison indicates that some $F_{w,j}$ functions with the least subset error are not consistent with the correlations that have the least subset errors of the below-T_b and above-T_b curve segments. For example, $F_{w,j}^{(3)}[R|R(\omega)]$ has the minimum average error for organic acids rather than $F_{w,j}[R(\omega)]$, and $F_{w,j}[R(\omega)]$ has less error than the $F_{w,j}\ [A\text{-}W(T_b)|R(\omega)]$ functions for polar "Others" with $T_{r,b} < 0.7$. On the other hand, consistent with the Summary results in Table 3.3 are the $F_{w,j}[R|R(\omega)]$ functions having the least average error for alcohols and the $F_{w,j}^{(3)}[A\text{-}W(T_b)|R(\omega)]$ function having the minimum average error for the twenty-seven "Others" and the twenty-one normal "Others" with $T_{r,b} < 0.7$.

One can see that error can be disproportionately increased when using an $F_{w,j}\ [A\text{-}W(T_b)|R(\omega)]$ function for alcohols. 2-ethyl-1-hexanol and 2-butanol, for example, have very high predictive error with Ambrose-Walton for the below-T_b segment, and they have horrendous entire-curve error with the $F_{w,j}\ [A\text{-}W(T_b)|R(\omega)]$ functions. Several other alcohols have error percentages in the thousands when using the $F_{w,j}\ ^{(1)}[A\text{-}W(T_b)|R(\omega)]$ function. Thus, no $F_{w,j}$ function using points from Ambrose-Walton or A-W(T_b) is recommended with alcohols. Despite the $F_{w,j}^{(1)}[A\text{-}W(T_b)|R(\omega)]$ function having the lowest errors for alcohols with $T_{r,b} > 0.76$ (1-eicosanol, 1-octadecanol, 1-heptadecanol, and 1-hexadecanol), the A-W(T_b) correlation instead would be preferable in practice for such alcohol species because its low-temperature error does not have the compounding effect that can potentially be induced with a $F_{w,j}$ function. The primary target of the $F_{w,j}\ [A\text{-}W(T_b)|R(\omega)]$ functions is "Others", and their horrendous performance with alcohols is a stark reminder of how error can be compounded when using a poor source correlation for low-temperature prediction inputs.

Not surprisingly, the $F_{w,j}$ *[R(ω)]* and $F_{w,j}$ *[R|R(ω)]* functions perform best for polar species while $F_{w,j}[A\text{-}W(T_b)|R(\omega)]$ functions have the advantage with normal species. As mentioned previously, no attempt is made to design an $F_{w,j}$ function to outperform the Ambrose-Walton correlation for normal species that have $T_{r,b} > 0.7$, but the $F_{w,j}$ function with the least error for this subset is indicated by gray shading in the Summary of Table 3.4 for reference.

The average A%Err for the segments is given in Appendix D, Tables D.2 and D.3, respectively. Looking at the Summary section of the two tables, one can see that the functions with the least subset average errors for the $T_r < T_{r,b}$ segment are the same as for "All Trs" (Table 3.4), but those for the $T_r < T_{r,b}$ segment are not.

3.5.1 Minimum Possible Entire-Curve Average Error & Levels of Success

The minimum possible entire-curve total A%Err for a given species using the four correlations is the sum of the minimum error below the normal boiling point with that above. This total "All T_rs" error is then divided by the number of calculated points plus 1 to arrive at the minimum possible average A%Err for the entire VLE curve. The error at the normal boiling point is zero for a species in this hypothetical minimum error because the vapor pressure of 1.01325 bars is known; thus, the total number of points has to be increased by one because the normal boiling point is excluded from the $T_r < T_{r,b}$ and $T_r > T_{r,b}$ temperature segments. The minimum possible errors are shown in Table D.4 of Appendix D. The specifics of the calculation for helium are given at the bottom of the table as an example. The general disparity between the predictive error below and that above the normal boiling point is readily apparent.

The minimum possible average error for a species is the best that can be expected using any combination of the four correlations for the two temperature segments $T_r < T_{r,b}$ and $T_r > T_{r,b}$. This minimum possible error is the most stringent test because the final Wagner constants chosen for a species would have to blend well the functional form of the best correlation for the $T_r < T_{r,b}$ segment with that of the best correlation for the $T_r < T_{r,b}$ segment, while accurately predicting the normal boiling point pressure. A less stringent test is having an entire-curve average A%Err less than all of the four correlations. The least stringent test is having an entire-curve average A%Err less than just the Riedel and Ambrose-Walton equations. A set of Wagner constants that can predict better than or equal to the standard

Riedel and Ambrose-Walton is considered a satisfactory success since those two correlations are the primary tools available and recommended for use when VLE data is sparse. A set of Wagner constants is considered to have superior success if it can also match or beat the additional R(ω) and A-W(T_b) correlations introduced here since it has been shown that they can perform better than their standard counterparts in many cases. Ultimate success is achieved when the estimated Wagner constants can meet or beat the minimum possible error; a methodology than can on average incorporate the best predictive powers of the four correlations would be remarkable.

3.5.2 Comparison to Minimum Possible Entire-Curve Average Error

Table 3.5 shows subset least average entire-curve errors for several comparators. The minimum possible average A%Err from Table D.4 is displayed here for reference, given that it is the criterion for Ultimate success. The minimum possible errors indicate a dependency upon relative position of the normal boiling point to the reduced temperature of 0.7, and the dependency for normal “Others” is reverse of that for organic acids and alcohols. The large average minimum entire-curve errors (19.65 and 8.93%) for alcohols indicate that none of the four correlations can describe them well, and one might conclude the same for organic acids with $T_{r,b} > 0.7$, whose average minimum possible error is 3.93%.

To the right of the minimum possible error is displayed the least average error one could achieve if one knew *apriori* which would have the lowest error in head-to-head competition between the standard Riedel and Ambrose-Walton correlations for each individual species. Similarly, the next column over displays the least average error one could achieve knowing *apriori* which of the four correlations provides the least entire-curve predictive error for each species. The next column shows the least average error possible if one knew which $F_{w,j}$ function was best for each species. The subsequent columns to the right indicate the average errors obtained when the best subset method is applied to every member of the substance subset. The best subset $F_{w,j}$ functions and their corresponding average errors are taken from Table 3.4, except for “Others” with $T_{r,b} < 0.7$, in which case the average is based upon the results of the subset best methods for normal and polar species combined. The subset of normal “Others” species with $T_{r,b} > 0.7$ is included for reference as in Table 3.4, but it is excluded from the following discussion regarding the results of Table 3.5 since that subset is not targeted.

Looking at the averages of the species-specific least errors, the $F_{w,j}$ functions produce less error than do the four correlations, which in turn result in less error than when limited to only the standard Riedel and Ambrose-Walton. Interestingly, the $F_{w,j}$ functions result in less average error than the minimum possible error for every species subset, whereas, the four correlations do not. In other words, four vapor pressures predicted by two of the four correlations can be used via the $F_{w,j}$ functions to result in less error than the individual correlations themselves produce over the entire curve and also less than when the entire-curve error is minimized for a species by splitting the VLE curve at the normal boiling point and using the best correlation for each temperature segment. The fact that a fully-determined formulation such as the $F_{w,j}$ function based on vapor pressure predictions can outperform the source correlations is a testament to the robustness of the Wagner equation and indicates that the fully-determined case can improve VLE predictive error if used wisely. These results reinforce the conclusion from Chapter 2 that Wagner constants estimated from predictions can perform better than the source correlations.

As shown in Tables 3.3 and 3.4, however, no single correlation or $F_{w,j}$ function results in the least error for all species, let alone for each member of a subset of species. Indeed, individual correlations and $F_{w,j}$ functions perform very poorly for some species. Thus, benefit to the practitioner can result only if subset best methods can perform well relative to the minimum possible error. This comparison is made with the “Average Using Subset Best Method” columns. In every case the subset best $F_{w,j}$ function has less average predictive error than the subset best correlation. The last column of the table shows the success level of the subset best $F_{w,j}$ function. The success level is less than satisfactory for only alcohols with $T_{r,b} < 0.7$. Although $F_{w,j}^{(2)}[R|R(\omega)]$, the best $F_{w,j}$ function for this subset of alcohols (17.24%), does have slightly less error than the subset best correlation, standard Riedel (17.59%), it is greater than the error obtainable if one knows *apriori* for each species the best of all four correlations (9.22%) or the best between just the standard Riedel and Ambrose-Walton (13.37%). The subset best $F_{w,j}$ functions achieve either satisfactory or ultimate success for the other substance subsets. One can see that there is no “Superior” entry in the “Success” column - if the subset best $F_{w,j}$ function can outperform the species-specific “All Four” average error, then it also ends up beating the minimum possible error and achieving Ultimate success.

Table 3.5 overall shows that subset best $F_{w,j}$ functions have better predictive power than subset best correlations, except for “Others” with $T_{r,b} > 0.7$ (all normal species except for helium), which is not a targeted species subset. The subset best $F_{w,j}$ functions achieve ultimate success in aggregate for 30 of the 72 species.

The data shown in Table 3.5 for alcohols is especially interesting. First, the species-specific $F_{w,j}$ functions produce much less error than the minimum possible (8.95% vs. 19.65% and 7.80% vs. 8.93%), indicating that improvement in predictive error can be achieved by combining predicted VLE from two of the four correlations for individual species; however, neither a single correlation for either the below- and above-T_b segments nor $F_{w,j}$ function for the entire VLE curve describe the alcohol subset well enough for one to be confident of which to use for a given alcohol *apriori*.

Second, for alcohols with $T_{r,b} < 0.7$, the subset best $F_{w,j}$ function is only slightly better than the subset best correlation, 17.24 and 17.59%, respectively. Consequently, one may decide to use the Riedel correlation instead of the more algebraically cumbersome $F_{w,j}^{(2)}[R|R(\omega)]$ function for alcohols with $T_{r,b} < 0.7$. The nine alcohols in this subset share three different species-specific correlation winners at the normal fusion point (see Table 3.2) and six different $F_{w,j}$ function winners for the entire two-phase curve (see Table 3.4). The lack of a correlation that can consistently describe the VLE below the normal boiling point accurately for these alcohols results in the large entire-curve minimum possible error of 8.93% and subsequently prohibits a single correlation or $F_{w,j}$ function from being successful. Consequently, the results for the underlying four correlations used in this work do not strongly recommend any predictive method for this species subset.

Third, although the subset best function $F_{w,j}^{(1)}[R|R(\omega)]$ is significantly better than the subset best correlation Riedel for alcohols with $T_{r,b} > 0.7$ and approaches closely the minimum possible error of 19.65%, it unfortunately still has a large error of 20.46%. It was mentioned when discussing the results shown in Tables 3.3 & 3.4 that the A-W(T_b) correlation and the $F_{w,j}^{(1)}[A\text{-}W(T_b)|R(\omega)]$ function perform significantly better than the subset best methods for the four alcohols with $T_{r,b} > 0.76$ (e.g., 1-eicosanol, 1-octadecanol, 1-heptadecanol, and 1-

hexadecanol). The actual appropriate reduced temperature threshold may be lower, but the limited sample pool in this analysis suggests a value near 0.76.

Table 3.6 shows the average errors when the $T_{r,b} > 0.7$ subset is divided further for alcohols to account for the 0.76 threshold. The two new distinct species subsets are shaded in gray. The best $F_{w,j}$ function for the two new alcohol subsets achieve Ultimate success while only Satisfactory success is achieved by the aggregate $T_{r,b} > 0.7$ segment best function $F_{w,j}^{(1)}[R|R(\omega)]$.

It was mentioned during the discussion of Table 3.4, however, that the $F_{w,j}\ [A\text{-}W(T_b)|R(\omega)]$ function can exhibit disproportionate errors for other alcohols because of the poor predictive behavior of Ambrose-Walton at low reduced temperatures for alcohols in general, which poor predictive power is compounded when its low–temperature prediction is used as one of the four points. Consequently, the A-W(T_b) correlation is recommended for alcohols with $T_{r,b} > 0.76$ because it doesn't induce the compound effect. One can see from Table 3.6 that some error reduction is lost by using A-W(T_b) instead of $F_{w,j}\ ^{(1)}[A\text{-}W(T_b)|R(\omega)]$ (average error of 15.86% compared to 12.95%) for this species subset, but the goal of minimizing maximum error and not just minimizing average error drives this recommendation.

Table 3.7 shows the average incremental errors for the recommended correlations and $F_{w,j}$ functions, relative to the minimum possible entire-curve error. By definition, every negative incremental error for a subset corresponds to an aggregate ultimate success level. The average entire-curve error reduction of 13.22% for some alcohols and the 1.06% reduction for polar "Others" are strong evidence of the flexibility of the Wagner equation and the utility of the fully-determined method employing the $F_{w,j}$ function for substance subsets.

3.5.3 Waring Test

All six $F_{w,j}$ functions shown in Table 3.5 pass the qualitative Waring fit-of-form test for all species in their corresponding substance subset – the constants b and c had opposite signs for all species, except helium and hydrogen, whose normal boiling points are below 50 K. The Wagner constants corresponding to the subset best $F_{w,j}$ functions indicated in Table 3.5, and the corresponding Extrapolation Burdens, are displayed in Appendix D, Table D.5. Consistent with the definition of extrapolation burden, that corresponding to the Riedel equation is used for those species with $T_{r,b} < 0.7$, and that corresponding to the Ambrose-Walton equation is used for species where $T_{r,b} > 0.7$.

3.5.4 Error Dependency Upon Extrapolation Burden

The A%Err at the normal fusion point for the subset $F_{w,j}$ functions recommended in Table 3.7 is plotted vs. extrapolation burden in Figure 3.1. Although sufficient error spread exists to preclude a reliable correlation between the error and burden, there is a discernible dependency of the error upon the burden. This is not surprising given that all of the subset $F_{w,j}$ functions recommended in Table 3.7 are based upon the modified Riedel correlation, and only one of the functions involves Ambrose-Walton. The plots for the five individual subset $F_{w,j}$ functions for the species for which they are recommended are shown in Appendix D, Figures D.1 through D.5. One can see in Figure D.5 that the spread between 0 and 10% error at values of extrapolation burden less than 10 comes, not surprisingly, from the $F_{w,j}^{(3)}[A\text{-}W(T_b)|R(\omega)]$ function.

3.5.5 Comparison with $F_{w,j}[AA]$ Function

The use of the $F_{w,j}$ function using analytic predictions from Antoine constants was discussed in Chapter 2; these functions were referred to as $F_{w,j}[AA]$, where the "AA" indicates that the four data points are Antoine analytics. Table 3.8 compares the average and incremental errors of the subset recommended predictive methods with those of the $F_{w,j}[AA]$ function for the 55 species used in that study. None of the alcohols had a normal boiling point reduced temperature above 0.76. Using analytic data from Antoine constants (a surrogate for limited-range experimental data) provides significantly better VLE prediction for the six alcohols with $T_{r,b} < 0.7$ (cell shaded in gray) and has only slightly greater error for the seven alcohols with $T_{r,b} > 0.7$. There is one caveat with the performance of the $F_{w,j}[AA]$ function for alcohols: the function failed the Waring test for three members of this subset - methanol ($T_{r,b} < 0.7$), and 1-heptanol and 1-hexanol (both with $T_{r,b} > 0.7$). Consequently, one may prefer to use the $F_{w,j}[AA]$ function for alcohols where $T_{r,b} < 0.7$, unless the function fails the Waring test, in which case one could choose to use Riedel or the $F_{w,j}^{(2)}[R|R(\omega)]$ function. The recommended predictive methods result in less error than the $F_{w,j}[AA]$ function for all the remaining substance subsets.

3.6 Potential Modifications

The approach presented here to estimate Wagner constants could be modified in several ways. Replacing the fully-determined $F_{w,j}$ functions with an over-determined solution algorithm could minimize error-compounding effects resulting from using predictions as inputs rather than accurate data, especially when one or more of the four predictions are of particularly poor accuracy. An over-determined approach might also better blend predictions from two correlations that have different functional form, such as Riedel and Ambrose-Walton. Utilizing quantitative fitting constraints, as did McGarry (1983), is another possible modification.

Although Waring (1954) showed that a fourth parameter is necessary to accurately describe VLE over the entire two-phase curve, Vetere (1991a) concluded that the presence of the Wagner d constant is mostly inconsequential to predictive error when data of lower accuracy is used. He mathematically tied the values of the remaining three Wagner constants to the critical and normal boiling points, with the defining relationships dependent upon the species type. He concluded that the three-constant predictive Wagner equation was generally superior to other predictive correlations (including the original Riedel using $K = 0.0838$) while noting that it did perform significantly worse for a few species. Vetere (1991b, 2006) subsequently attempted to improve the Riedel predictive method by making the K parameter dependent upon species type. Given that VLE from predictive correlations will generally be of lower accuracy relative to actual data, a potential modification to the approach presented here would be to use predictive correlations to provide VLE inputs into the parameterization of a three-parameter Wagner equation rather than the full four-parameter form.

Obviously, one is not limited to just the four predictive correlations used in this work - developing predictive VLE correlations is an on-going focus of research in the literature, providing a wide array of possible source correlations. Nor does one have to limit the base required experimental data to the critical and normal boiling points and acentric factor. For example, Rogdakis & Lolos (2006) and Velasco et al. (2008) developed VLE correlations that require the triple or normal fusion point vapor pressure and temperature; however, requiring an anchor point at the lower bound of the VLE curve can be a significant practical disadvantage. One could add a species-specific correction factor, as did An & Yang (2012) for organics with the ω-based Lee-Kesler equation. Predictive equations for classes of substances, such as that of Sanjari et al. (2013) for refrigerants, could be used as source correlations.

Although increased complexity in an approach to VLE prediction is not a deterrent to a researcher, it can be to a field practitioner. One of the goals of the work presented here is to develop an overall approach balances ease of implementation with improvement in predictive capability.

3.7 Summary

The R(ω) and A-W(T_b) correlations perform better than their standard counterparts in many cases (Table 3.3). The VLE behavior below and above the normal boiling point of organic acids, and of normal and non-alcohol polar species where $T_{r,b} < 0.7$, can be described accurately on a consistent enough basis by the standard or modified Riedel and Ambrose-Walton correlations such that reasonable Wagner constants can be estimated from $F_{w,j}$ functions whose four points are taken from these predictive correlations. The VLE predictive error of such Wagner constants for the entire two-phase curve approaches or beats the minimum predictive error possible (Table 3.6). For all substance subsets, except the fourteen normal species with $T_{r,b} > 0.7$, the subset best $F_{w,j}$ function results in less average entire-curve error than the subset best correlation. The results clearly support Hypothesis III.

The subset recommended methods have predictive power superior to that of Wagner constants estimated from Antoine analytics, except for some alcohols (Table 3.8). This reinforces the previous conclusions from Chapter 2 that solely using limited VLE data to extrapolate downward to the triple point provides an advantage primarily for species that are problematic for predictive correlations, such as the Riedel and Ambrose-Walton equations.

The approach presented in this chapter has the potential to be modified and improved to provide more avenues for increased predictive power of VLE for species with sparse experimental data. Several modifications could be applied in search of greater error reduction – quantitative fitting constraints, over-determined regression, a three-parameter Wagner form, a different set of source correlations, different anchor points, and species-specific correction factors, to list just a few.

Chapter 4: Final Summary

Several novel elements are used to determine the error segmentation of the Wagner equation, to compare fully- vs. over-determined solutions for predicting VLE outside the parameterization interval, to determine the general level of disagreement for VLE data in the literature, and to reveal an additional beneficial way of using predictive correlations when data is sparse.

An algebraic fully-determined parameterization of the Wagner equation from limited data is used to determine the dependency of predictive error over the entire two-phase curve upon interval width and location. Limited VLE data of good precision from reduced temperature intervals with a width ≥ 0.1 and a lower bound ≤ 0.6 can usually provide reasonable VLE predictions over the entire two-phase curve for pure substances, with average entire-curve error around 1%. Wagner parameterization for a small interval by an over-determined solution has an equal chance of producing more predictive error than that of a fully-determined parameterization, and the difference between the two approaches diminish as the interval width increases, approaching less than a tenth of one percent for an interval width of 0.2. This suggests that the $F_{w,\mathrm{j}}$ function is a viable approach to parameterize limited-data Wagner constants and can be a valuable tool for investigating the extension capability of the Wagner equation outside its parameterization interval.

The deviation between Antoine and entire-curve Wagner analytic data, Δ%Err, exhibited by fifty-five species suggests that the VLE data available in the literature to an engineering practitioner in many cases may deviate significantly from “best” values, and thus, be judged to be well outside what one would consider good precision. The disagreement of VLE data in the literature averages around 2% but varies considerably between species. Data disagreement is not found to be a singularly strong indicator of predictive power of the limited-data Wagner constants; however, it is found to be a discriminator of performance relative to that of Riedel and Ambrose-Walton for some polar species.

Wagner constants estimated from Antoine analytics have an average entire-curve error of 4.8%, with the majority of the error occurring when extending down towards the triple point (9.55%), compared to 1.36% average error when extending up to the critical point. The 4.8%

compares disfavorably to the smaller approximate error of 1% for the $F_{w,j}[RD]$ function for hydrogen, helium, R152a, and water. The difference in the results of $F_{w,j}[RD]$ and $F_{w,j}[AA]$ functions suggests that predictive power lessens when the parameterization data is decoupled from the reference data. The results of the $F_{w,j}[AA]$ function is more representative of the situation in which a practitioner finds himself when attempting to use limited VLE data to extend beyond the parameterization interval, because the reference set, of course, is unknown. Consequently, the poorer results of the $F_{w,j}[AA]$ function relative to those of the $F_{w,j}[RD]$ function suggest that using a limited interval of VLE data to parameterize the Wagner equation to predict VLE over the entire two-phase curve is not generally recommended. The $F_{w,j}[AA]$ function's narrow predictive advantage may lay with alcohols because of the relatively poor predictive power for this substance group by Riedel and Ambrose-Walton.

It is shown that predictions from standard and modified forms of Riedel and Ambrose-Walton can be used as "data" for a fully-determined parameterization of the Wagner equation that has better predictive power than the source correlations themselves, allowing for better predictive accuracy when only the critical and normal boiling points and acentric factor are known. The recommended $F_{w,j}$ functions using predictions as "data" result in less error than the $F_{w,j}[AA]$ function for all substance subsets except for alcohols where $T_{r,b} < 0.7$. Consequently, using predictions to parameterize the Wagner equation is generally recommended over using a limited-data interval. Preliminary recommendations for best predictive methods for substance subsets are given.

The new concept of extrapolation burden is introduced to quantify in a normalized manner the difficulty a species may experience extrapolating vapor pressure down to the triple point. It is found that the $F_{w,j}[AA]$ function, Riedel equation, and the recommended subset $F_{w,j}$ functions using predictions treat all substance types with respect to extrapolation burden in a more consistent manner than does the Ambrose-Walton equation.

The fully-determined approach presented and its application to the Wagner equation, Antoine analytics, and predictive vapor pressure correlations can be modified and expanded in many ways. Any regressed VLE equation and any predictive correlation are potential candidates for study. Any beneficial anchor point is a potential member of the set of four data points. Over-determined regression can replace the fully-determined solution.

Table I.1. Round Off for Parameters as Inputs and Final Outputs.

Parameter	**Significant Digits**
T (K), P (bar)	Chapters 2 & 3: 2 significant digits right of the decimal point
T_r and τ	5 significant digits
$Ln\ P_{v,r}$	4 significant digits in the mantissa, except 5 significant digits for $Ln\ P_{r,b}$
ω	3 significant digits right of the decimal point
Wagner Constants a, b, c, and d	Six digits to the right of the decimal point
η_{ji} in $F_{w,j}$ function	Seven digits to the right of the decimal point

Table 1.1. Summary of Wagner Constant Regressions Using *NIST* Data.

Species	***NIST* Data**			**Regression**								
				# of Points	**T_b (^{o}K)**	**Wagner Constants**				**A%Err in P_r**		
	T_b (^{o}K)	**T_c (^{o}K)**	**P_c (bar)**			**a**	**b**	**c**	**d**	**Ave**	**Max**	**T_r of Max**
H_2	20.369	33.145	12.964	233	20.37	-4.902616	1.065004	0.737305	0.053125	0.005	0.030	0.42411
He	4.230	5.1953	2.2746	203	4.23	-4.265233	1.571259	0.479795	0.751271	0.105	0.612	0.41961
Ar	87.302	150.687	48.63	329	87.30	-5.926538	1.208266	-0.509886	-1.590893	0.009	0.030	0.99756
H_2O	373.1243	647.096	220.64	239	373.13	-7.861942	1.879246	-2.266807	-2.128615	0.019	0.170	0.42213
R152a	249.127	386.411	45.1675	200	249.13	-7.433439	1.755544	-2.169951	-2.774693	0.023	0.080	0.39999

Table 1.2. Entire-Curve Wagner Constants for Set of Seventy-two Species.

Species	***a***	***b***	***c***	***d***
2-Methyl propanoic acid ($C_4H_8O_2$)	-8.53258	1.30605	-5.2242	-2.05813
3-Methyl butanoic acid ($C_5H_{10}O_2$)	-8.67381	1.62939	-6.51756	-2.08757
Acetic Acid ($C_2H_4O_2$)	-8.29430	0.97928	-0.21745	-5.72367
Butanoic acid ($C_4H_8O_2$)	-8.42953	1.34333	-5.37332	-2.74438
Decanoic acid ($C_{10}H_{20}O_2$)	-9.07060	2.77535	-11.1014	-2.43545
Formic acid (CH_2O_2)	-7.24917	0.44255	-0.35558	-0.96906
Octanoic acid ($C_8H_{16}O_2$)	-9.04015	2.16529	-8.66117	-4.69516
Pentanoic acid ($C_5H_{10}O_2$)	-8.76701	1.54990	-6.19961	-4.21927
Propanoic acid ($C_3H_6O_2$)	-8.14882	0.79590	-3.1836	-3.81338
1-butanol ($C_4H_{10}O$)	-8.40615	2.23010	-8.2486	-0.7110
1-Decanol ($C_{10}H_{22}O$)	-9.75478	4.18634	-7.0572	-15.980
1-dodecanol ($C_{12}H_{26}O$)	-9.91901	3.61884	-5.8537	-18.204
1-eicosanol ($C_{20}H_{42}O$)	-11.23154	3.66900	-7.0775	-14.321
1-heptadecanol ($C_{17}H_{36}O$)	-10.73125	3.55515	-6.3591	-15.696
1-Heptanol ($C_7H_{16}O$)	-9.68778	5.35716	-10.1672	-8.0100
1-hexadecanol ($C_{16}H_{34}O$)	-10.54087	3.47260	-6.0770	-15.939
1-Hexanol ($C_6H_{14}O$)	-9.49034	5.13288	-10.5817	-5.1540
1-Nonanol ($C_9H_{20}O$)	-9.91542	5.13670	-8.8075	-12.497
1-octadecanol ($C_{18}H_{38}O$)	-10.91637	3.57835	-6.6199	-15.060
1-Octanol ($C_8H_{18}O$)	-10.01437	5.90629	-10.4026	-9.0480
1-Pentanol ($C_5H_{12}O$)	-8.98005	3.91624	-9.9081	-2.1910
2-butanol ($C_4H_{10}O$)	-8.09820	1.64406	-7.4900	-5.27355
2-ethyl-1-hexanol ($C_8H_{18}O$)	-9.61812	5.17861	-9.1144	-11.004
2-Octanol ($C_8H_{18}O$)	-9.37352	4.73760	-8.3382	-11.646
Benzyl alcohol (C_7H_8O)	-7.29099	1.17084	-4.7167	-5.5300
Cyclohexanol ($C_6H_{12}O$)	-7.12838	1.40189	-5.60756	-9.57158
Ethanol (C_2H_6O)	-8.68587	1.17831	-4.8762	1.5880

Species	***a***	***b***	***c***	***d***
Isopropyl alcohol (C_3H_8O)	-8.73656	2.16240	-8.70785	4.77927
Methanol (CH_4O)	-8.63571	1.17982	-2.4790	-1.0240
Propanol (C_3H_8O)	-8.53706	1.96214	-7.6918	2.9450
Tert-butanol ($C_4H_{10}O$)	-8.47927	2.47845	-9.27918	-2.53992
Acetone (C_3H_6O)	-7.55098	1.60784	-1.9944	-3.2002
Cyclopentanone (C_5H_8O)	-7.36589	1.54092	-2.28143	-3.0514
Methyl isobutyl ketone ($C_6H_{12}O$)	-7.70040	1.69968	-2.80448	-3.81623
Benzene (C_6H_6)	-7.01433	1.55256	-1.8479	-3.7130
Ethylbenzene (C_8H_{10})	-7.53139	1.75439	-2.42012	-3.57146
Naphthalene ($C_{10}H_8$)	-7.61444	1.91553	-2.5075	-3.2300
Toluene (C_7H_8)	-7.31600	1.59425	-1.93165	-3.72220
Pentafluorobenzene (C_6HF_5)	-7.86799	1.71659	-2.53582	-4.59937
Pentafluorotoluene ($C_7H_3F_5$)	-8.08717	1.76131	-2.72838	-4.13797
m-Xylene (C_8H_{10})	-7.67717	1.80240	-2.47745	-3.66068
o-Xylene (C_8H_{10})	-7.60491	1.75383	-2.27531	-3.73771
p-Xylene (C_8H_{10})	-7.71694	1.89119	-2.39695	-3.63026
Acetic Anhydride ($C_4H_6O_3$)	-8.35130	1.89050	-2.8357	-5.1156
Butane (C_4H_{10})	-7.01763	1.67770	-1.9739	-2.1720
Diethyl ether ($C_4H_{10}O$)	-7.43301	1.78847	-2.4793	-3.2811
Decane ($C_{10}H_{22}$)	-8.60643	2.44659	-4.2925	-3.9080
Dodecane ($C_{12}H_{26}$)	-9.08593	2.77846	-5.1985	-4.1730
Eicosane ($C_{20}H_{42}$)	-10.97958	4.25588	-8.9573	-5.0430
Ethane (C_2H_6)	-6.47500	1.41071	-1.1440	-1.8590
Heptadecane ($C_{17}H_{36}$)	-10.23600	3.54177	-7.1898	-5.0000
n-Heptane (C_7H_{16})	-7.77404	1.85614	-2.8298	-3.5070
Hexadecane ($C_{16}H_{34}$)	-10.03664	3.41426	-6.8627	-4.8630
n-Hexane (C_6H_{14})	-7.53998	1.83759	-2.5438	-3.1630
Methane (CH_4)	-6.02242	1.26652	-0.5707	-1.366
Nonadecane ($C_{19}H_{40}$)	-10.68217	3.98054	-8.3030	-4.9950

Species	***a***	***b***	***c***	***d***
Nonane (C_9H_{20})	-8.32886	2.25707	-3.8257	-3.7320
Octadecane ($C_{18}H_{38}$)	-10.47230	3.69655	-7.5779	-5.1090
Octane (C_8H_{18})	-8.04937	2.03865	-3.3120	-3.6480
Pentadecane ($C_{15}H_{32}$)	-9.80239	3.29217	-6.5317	-4.5840
n-Pentane (C_5H_{12})	-7.30698	1.75845	-2.1629	-2.9130
Propane (C_3H_8)	-6.76368	1.55481	-1.5872	-2.024
R152a ($C_2H_4F_2$)	-7.433439	1.755544	-2.169951	-2.774693
n-Tetradecane ($C_{14}H_{30}$)	-9.54470	3.06637	-6.0070	-4.5300
Tridecane ($C_{13}H_{28}$)	-9.32959	2.89925	-5.5550	-4.4700
Undecane ($C_{11}H_{24}$)	-8.85076	2.60205	-4.7305	-4.0810
Argon (Ar)	-5.926538	1.208266	-0.509886	-1.590893
Nitrogen (N_2)	-6.11102	1.2189	-0.69366	-1.89893
Ammonia (NH_3)	-7.28322	1.5716	-1.85672	-2.39312
Water (H_2O)	-7.861942	1.879246	-2.266807	-2.128615
Helium (He normal)	-4.265233	1.571259	0.479795	0.751271
Hydrogen (H_2 normal)	-4.902616	1.065004	0.737305	0.053125

Note: All constants are from Section D of Appendix A of Poling et al. (2001), except for the five *NIST* species (hydrogen, helium, argon, water, and R152a).

Table 1.3. Physical Properties for 72 Species with Entire-Curve Wagner Constants.

Species	T_f (K)	T_b (K)	T_c (K)	P_c (bars)	$T_{r,f}$	$T_{r,b}$	ω	μ (Debye)	$P_{v,r,f}$	$P_{v,r,b}$
2-Methyl propanoic acid ($C_4H_8O_2$)	227.05	427.58	605.00	37.00	0.37529	0.70674	0.618	1.3	3.06E-08	2.74E-02
3-Methyl butanoic acid ($C_5H_{10}O_2$)	243.85	449.68	629.00	34.00	0.38768	0.71491	0.651		3.81E-08	2.98E-02
Acetic Acid ($C_2H_4O_2$)	289.77	391.04	592.71	57.86	0.48889	0.65975	0.459	1.3	2.18E-04	1.75E-02
Butanoic acid ($C_4H_8O_2$)	267.97	436.87	624.00	40.30	0.42944	0.70011	0.600	1.5	1.65E-06	2.51E-02
Decanoic acid ($C_{10}H_{20}O_2$)	305.15	541.92	726.00	22.30	0.42032	0.74644	0.749		5.41E-08	4.54E-02
Formic acid (CH_2O_2)	281.50	374.04	588.00	58.07	0.47874	0.63612	0.316	1.5	4.23E-04	1.75E-02
Octanoic acid ($C_8H_{16}O_2$)	289.45	512.01	695.00	26.40	0.41647	0.7367	0.734		6.68E-08	3.84E-02
Pentanoic acid ($C_5H_{10}O_2$)	239.45	459.31	643.00	35.80	0.3724	0.71432	0.670		5.58E-09	2.83E-02
Propanoic acid ($C_3H_6O_2$)	252.31	414.31	604.00	45.30	0.41773	0.68595	0.539	1.5	2.06E-06	2.24E-02
1-Butanol ($C_4H_{10}O$)	183.35	390.88	563.05	44.24	0.32564	0.69422	0.591	1.8	3.59E-08	4.20E-02
1-Decanol ($C_{10}H_{22}O$)	280.05	504.25	689.00	24.10	0.40646	0.73186	0.629	1.8	4.12E-08	4.87E-02
1-Dodecanol ($C_{12}H_{26}O$)	297.10	537.78	720.00	20.80	0.41264	0.74692	0.684		1.13E-08	7.79E-02
1-Eicosanol ($C_{20}H_{42}O$)	339.00	647.69	809.00	13.00	0.41904	0.80061	0.954		2.55E-08	6.75E-02
1-Peptadecanol ($C_{17}H_{36}O$)	327.00	611.12	780.00	15.00	0.41923	0.78349	0.853		4.83E-09	3.23E-02
1-Heptanol ($C_7H_{16}O$)	239.20	449.70	632.50	31.35	0.37818	0.71099	0.580	1.7	3.33E-08	6.29E-02
1-Hexadecanol ($C_{16}H_{34}O$)	322.45	597.53	770.00	16.10	0.41877	0.77601	0.818		5.35E-09	2.92E-02
1-Hexanol ($C_6H_{14}O$)	229.20	430.44	610.70	34.70	0.37531	0.70483	0.575	1.8	2.41E-08	3.85E-02
1-Nonanol ($C_9H_{20}O$)	268.15	486.52	671.50	26.30	0.39933	0.72453	0.610	1.7	1.86E-08	7.04E-02
1-Octadecanol ($C_{18}H_{38}O$)	331.00	623.56	790.00	14.40	0.41899	0.78932	0.892		2.12E-08	3.54E-02
1-Octanol ($C_8H_{18}O$)	257.65	468.33	652.50	28.60	0.39487	0.71774	0.594	2.0	5.54E-11	2.59E-02
1-Pentanol ($C_5H_{12}O$)	194.25	411.16	588.15	39.09	0.33027	0.69907	0.579	1.7	1.35E-13	2.41E-02
2-Butanol ($C_4H_{10}O$)	158.50	372.67	536.01	41.98	0.2957	0.69526	0.577	1.7	9.32E-13	3.62E-02
2-Ethyl-1-hexanol ($C_8H_{18}O$)	203.20	457.77	640.50	27.99	0.31725	0.71471	0.558	1.8	6.34E-09	3.51E-02
2-Octanol ($C_8H_{18}O$)	241.15	453.03	638.00	28.90	0.37798	0.71008	0.534	1.6	3.43E-08	2.36E-02
Benzyl alcohol (C_7H_8O)	257.80	478.46	715.00	43.00	0.36056	0.66917	0.390	1.7	7.02E-11	2.29E-02
Cyclohexanol ($C_6H_{12}O$)	297.65	433.99	650.00	42.60	0.45792	0.66767	0.370	1.7	1.95E-05	2.38E-02
Ethanol (C_2H_6O)	159.05	351.44	513.92	61.32	0.30948	0.68384	0.643	1.7	1.48E-10	1.65E-02

Species	**T_f (K)**	**T_b (K)**	**T_c (K)**	**P_c (bars)**	**$T_{r,f}$**	**$T_{r,b}$**	**ω**	**μ (Debye)**	**$P_{v,r,f}$**	**$P_{v,r,b}$**
Isopropyl alcohol (C_3H_8O)	183.65	355.39	508.30	47.62	0.3613	0.69917	0.665	1.7	6.57E-09	2.13E-02
Methanol (CH_4O)	175.49	337.69	512.64	80.92	0.34233	0.65872	0.564	1.7	2.14E-08	1.25E-02
Propanol (C_3H_8O)	147.00	370.30	536.78	51.68	0.27386	0.68985	0.620	1.7	3.60E-13	1.96E-02
Tert-butanol ($C_4H_{10}O$)	298.55	355.49	506.20	39.73	0.58979	0.70227	0.613	1.7	1.45E-03	2.55E-02
Acetone (C_3H_6O)	178.50	329.22	508.10	47.02	0.35131	0.64795	0.307	2.9	4.93E-07	2.15E-02
Cyclopentanone (C_5H_8O)	222.50	403.72	624.50	46.00	0.35629	0.64647	0.288	3.0	7.16E-07	2.20E-02
Methyl isobutyl ketone ($C_6H_{12}O$)	189.15	389.15	574.60	32.70	0.32919	0.67726	0.351	2.8	2.34E-08	3.10E-02
Benzene (C_6H_6)	278.68	353.24	562.16	48.98	0.49573	0.62836	0.209	0	9.77E-04	2.07E-02
Ethylbenzene (C_8H_{10})	178.18	409.36	617.20	36.00	0.28869	0.66325	0.302	0.4	9.82E-10	2.81E-02
Naphthalene ($C_{10}H_8$)	351.35	491.16	748.40	40.50	0.46947	0.65628	0.304	0	2.22E-04	2.50E-02
Toluene (C_7H_8)	178.16	383.79	591.80	41.06	0.30105	0.64851	0.264	0.4	8.58E-09	2.47E-02
Pentafluorobenzene (C_6HF_5)	225.85	358.89	530.97	35.37	0.42535	0.67591	0.374		1.60E-05	2.86E-02
Pentafluorotoluene ($C_7H_3F_5$)	243.35	390.66	566.52	31.24	0.42955	0.68958	0.415		1.49E-05	3.24E-02
m-Xylene (C_8H_{10})	225.28	412.34	617.05	35.38	0.36509	0.66825	0.326	0.3	7.77E-07	2.86E-02
o-Xylene (C_8H_{10})	247.97	417.59	630.33	37.35	0.3934	0.6625	0.312	0.5	5.80E-06	2.71E-02
p-Xylene (C_8H_{10})	286.41	411.52	616.23	35.16	0.46478	0.66781	0.322	0.1	1.64E-04	2.88E-02
Acetic Anhydride ($C_4H_6O_3$)	199.00	412.69	606.00	40.00	0.32838	0.68101	0.456	3.0	4.44E-09	2.53E-02
Butane (C_4H_{10})	134.79	272.67	425.25	37.92	0.31697	0.64119	0.199	0	1.76E-07	2.67E-02
Diethyl ether ($C_4H_{10}O$)	156.86	307.58	466.74	36.50	0.33608	0.659	0.282	1.3	1.50E-07	2.78E-02
Decane ($C_{10}H_{22}$)	243.49	447.30	617.65	21.05	0.39422	0.7242	0.490	0	6.69E-07	4.81E-02
Dodecane ($C_{12}H_{26}$)	263.57	489.22	658.00	18.20	0.40056	0.7435	0.573	0	3.76E-07	5.57E-02
Eicosane ($C_{20}H_{42}$)	309.95	616.84	769.00	11.60	0.40306	0.80213	0.891		9.64E-09	8.73E-02
Ethane (C_2H_6)	90.35	184.55	305.33	48.71	0.29591	0.60444	0.099	0	2.30E-07	2.08E-02
Heptadecane ($C_{17}H_{36}$)	295.13	574.56	735.00	13.70	0.40154	0.78171	0.772	0	3.79E-08	7.40E-02
n-Heptane (C_7H_{16})	182.59	371.57	540.15	27.35	0.33804	0.6879	0.350	0	6.37E-08	3.70E-02
Hexadecane ($C_{16}H_{34}$)	291.32	559.98	722.00	14.35	0.40349	0.77560	0.737	0	6.66E-08	7.06E-02
n-Hexane (C_6H_{14})	177.84	341.88	507.90	30.35	0.35015	0.67313	0.299	0	3.87E-07	3.34E-02
Methane (CH_4)	90.69	111.66	190.55	45.99	0.47594	0.58597	0.011	0	2.55E-03	2.20E-02
Nonadecane ($C_{19}H_{40}$)	305.25	602.34	758.00	12.30	0.4027	0.79464	0.844		1.67E-08	8.24E-02

Species	**T_f (K)**	**T_b (K)**	**T_c (K)**	**P_c (bars)**	**$T_{r,f}$**	**$T_{r,b}$**	**ω**	**μ (Debye)**	**$P_{v,r,f}$**	**$P_{v,r,b}$**
Nonane (C_9H_{20})	219.66	423.97	594.90	22.90	0.36924	0.71267	0.443	0	1.95E-07	4.42E-02
Octadecane ($C_{18}H_{38}$)	301.32	588.30	746.00	13.00	0.40391	0.78861	0.812	0	2.94E-08	7.79E-02
Octane (C_8H_{18})	216.39	398.82	568.95	24.90	0.38033	0.70097	0.397	0	8.24E-07	4.07E-02
Pentadecane ($C_{15}H_{32}$)	283.08	543.82	708.00	15.15	0.39983	0.76811	0.696	0	8.03E-08	6.69E-02
n-Pentane (C_5H_{12})	143.43	309.22	469.80	33.75	0.3053	0.65819	0.251	0	2.09E-08	3.00E-02
Propane (C_3H_8)	85.47	231.00	369.83	42.48	0.23111	0.62462	0.152	0	4.26E-11	2.39E-02
R152a ($C_2H_4F_2$)	156.15	249.13	386.41	45.17	0.4041	0.64472	0.275	2.3	1.75E-05	2.24E-02
n-Tetradecane ($C_{14}H_{30}$)	279.01	526.76	693.00	16.10	0.40261	0.76012	0.654	0	1.65E-07	6.29E-02
Tridecane ($C_{13}H_{28}$)	267.76	508.64	676.00	17.10	0.39609	0.75242	0.618	0	1.56E-07	5.93E-02
Undecane ($C_{11}H_{24}$)	247.57	469.08	638.85	19.55	0.38752	0.73425	0.533	0	2.35E-07	5.18E-02
Argon (Ar)	83.80	87.30	150.69	48.63	0.55612	0.57936	-0.002		1.42E-02	2.08E-02
Nitrogen (N_2)	63.15	77.35	126.20	34.00	0.5004	0.61289	0.037	0	3.68E-03	2.98E-02
Ammonia (NH_3)	195.41	239.82	405.50	113.53	0.4819	0.59141	0.256	1.5	5.29E-04	8.93E-03
Water (H_2O)	273.15	373.14	647.10	220.64	0.42211	0.57663	0.344	1.8	2.76E-05	4.59E-03
Helium (He normal)	2.15	4.24	5.20	2.27	0.41346	0.81444	-0.382		2.00E-02	4.46E-01
Hydrogen (H_2 normal)	13.56	20.37	33.15	12.96	0.40905	0.61453	-0.219		4.49E-03	7.82E-02

Table 1.4. Expressions for the Calculation of η_{ji} Coefficients in $F_{w,j}$ Function.

$\eta_{a1} = \left[\varepsilon_{a2} - \varepsilon_{a4}\varepsilon_{c2} - (\varepsilon_{a5} + \varepsilon_{a4}\varepsilon_{c4})\frac{\varepsilon_{d1}}{\varepsilon_d}\right] T_{r1} \mid \eta_{a2} = -\left[\varepsilon_{a3} + \varepsilon_{a4}\varepsilon_{c3} + (\varepsilon_{a5} + \varepsilon_{a4}\varepsilon_{c4})\frac{\varepsilon_{d2}}{\varepsilon_d}\right] T_{r2}$
$\eta_{a3} = -\left[\varepsilon_{a4}\varepsilon_{c1} + (\varepsilon_{a5} + \varepsilon_{a4}\varepsilon_{c4})\frac{\varepsilon_{d3}}{\varepsilon_d}\right] T_{r3} \mid \eta_{a4} = -\left(\frac{\varepsilon_{a5}+\varepsilon_{a4}\varepsilon_{c4}}{\tau_4^5\varepsilon_d}\right) T_{r4}$
$\eta_{b1} = \left[\varepsilon_{b3}\varepsilon_{c2} - \varepsilon_{b1} + (\varepsilon_{b3}\varepsilon_{c4} + \varepsilon_{b4})\frac{\varepsilon_{d1}}{\varepsilon_d}\right] T_{r1} \mid \eta_{b2} = \left[\varepsilon_{b3}\varepsilon_{c3} + \varepsilon_{b2} + (\varepsilon_{b3}\varepsilon_{c4} + \varepsilon_{b4})\frac{\varepsilon_{d2}}{\varepsilon_d}\right] T_{r2}$
$\eta_{b3} = \left[\varepsilon_{b3}\varepsilon_{c1} + (\varepsilon_{b3}\varepsilon_{c4} + \varepsilon_{b4})\frac{\varepsilon_{d3}}{\varepsilon_d}\right] T_{r3} \mid \eta_{b4} = \frac{\varepsilon_{b3}\varepsilon_{c4}+\varepsilon_{b4}}{\tau_4^5\varepsilon_d} T_{r4}$
$\eta_{c1} = \varepsilon_{c2} + \varepsilon_{c4}\frac{\varepsilon_{d1}}{\varepsilon_d} T_{r1} \mid \eta_{c2} = \varepsilon_{c3} + \varepsilon_{c4}\frac{\varepsilon_{d2}}{\varepsilon_d} T_{r2} \mid \eta_{c3} = \varepsilon_{c1} + \varepsilon_{c4}\frac{\varepsilon_{d3}}{\varepsilon_d} T_{r3} \mid \eta_{c4} = \frac{\varepsilon_{c4}}{\tau_4^5\varepsilon_d} T_{r4}$
$\eta_{d1} = \frac{\varepsilon_{d1}}{\varepsilon_d} T_{r1} \mid \eta_{d2} = \frac{\varepsilon_{d2}}{\varepsilon_d} T_{r2} \mid \eta_{d3} = \frac{\varepsilon_{d3}}{\varepsilon_d} T_{r3} \mid \eta_{d4} = \frac{T_{r4}}{\tau_4^5\varepsilon_d}$
$\varepsilon_a = 1 - \left(\frac{\tau_1}{\tau_2}\right)^{0.5} \mid \varepsilon_{a1} = \frac{\tau_1^{0.5}}{\varepsilon_a} \mid \varepsilon_{a2} = \frac{1}{\tau_1}\left(1 + \frac{\varepsilon_{a1}}{\tau_2^{0.5}}\right) \mid \varepsilon_{a3} = \frac{\varepsilon_{a1}}{\tau_2^{1.5}} \mid \varepsilon_{a4} = \tau_1^{1.5} + \varepsilon_{a1}\left(\frac{\tau_1^{1.5}}{\tau_2^{0.5}} - \tau_2\right)$
$\varepsilon_{a5} = \tau_1^4 + \varepsilon_{a1}\left(\frac{\tau_1^4}{\tau_2^{0.5}} - \tau_2^{3.5}\right) \mid \varepsilon_{b1} = \frac{1}{\varepsilon_a\tau_1\tau_2^{0.5}} \mid \varepsilon_{b2} = \frac{1}{\varepsilon_a\tau_2^{1.5}} \mid \varepsilon_{b3} = \frac{\left(\frac{\tau_1^{1.5}}{\tau_2^{0.5}}\right) - \tau_2}{\varepsilon_a} \mid \varepsilon_{b4} = \frac{\left(\frac{\tau_1^4}{\tau_2^{0.5}}\right) - \tau_2^{3.5}}{\varepsilon_a}$
$\varepsilon_c = 1 + \frac{\varepsilon_{b3}}{\tau_3} - \frac{\varepsilon_{a4}}{\tau_3^{1.5}} \mid \varepsilon_{c1} = \frac{1}{\varepsilon_c\tau_3^{2.5}} \mid \varepsilon_{c2} = \frac{\frac{\varepsilon_{b1}}{\tau_3} - \frac{\varepsilon_{a2}}{\tau_3^{1.5}}}{\varepsilon_c} \mid \varepsilon_{c3} = \frac{\frac{\varepsilon_{a3}}{\tau_3^{1.5}} - \frac{\varepsilon_{b2}}{\tau_3}}{\varepsilon_c} \mid \varepsilon_{c4} = \frac{\frac{\varepsilon_{a5}}{\tau_3^{1.5}} - \frac{\varepsilon_{b4}}{\tau_3} - \tau_3^{2.5}}{\varepsilon_c}$
$\varepsilon_d = 1 - \frac{\varepsilon_{a5}+\varepsilon_{a4}\varepsilon_{c4}}{\tau_4^4} + \frac{\varepsilon_{b3}\varepsilon_{c4}+\varepsilon_{b4}}{\tau_4^{3.5}} + \frac{\varepsilon_{c4}}{\tau_4^{2.5}} \mid \varepsilon_{d1} = -\frac{\varepsilon_{a2}-\varepsilon_{a4}\varepsilon_{c2}}{\tau_4^4} - \frac{\varepsilon_{b3}\varepsilon_{c2}-\varepsilon_{b1}}{\tau_4^{3.5}} - \frac{\varepsilon_{c2}}{\tau_4^{2.5}}$
$\varepsilon_{d2} = \frac{\varepsilon_{a3}+\varepsilon_{a4}\varepsilon_{c3}}{\tau_4^4} - \frac{\varepsilon_{b3}\varepsilon_{c3}+\varepsilon_{b2}}{\tau_4^{3.5}} - \frac{\varepsilon_{c3}}{\tau_4^{2.5}} \mid \varepsilon_{d3} = \frac{\varepsilon_{a4}\varepsilon_{c1}}{\tau_4^4} - \frac{\varepsilon_{b3}\varepsilon_{c1}}{\tau_4^{3.5}} - \frac{\varepsilon_{c1}}{\tau_4^{2.5}}$

Table 1.5. Results of t_0* Test. Accepted Alternative Hypothesis is Indicated When Null Hypothesis Is Rejected. Sorted by Descending Interval Width.

T_r Interval	Interval Width	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	All T_rs	
0.5-0.9	0.4	H_1: $\mu_e > \mu_4$ H_1: $\mu_e > \mu_8$	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$	
0.55-0.9	0.35	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	
0.6-0.9	0.3		H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu_4$	
0.50-0.70	0.2	H_1: $\mu_e > \mu_4$	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	**H_2: $\mu_e < \mu_4$**	**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	**H_2: $\mu_e < \mu_4$**	
0.7-0.9	0.2		H_1: $\mu_e > \mu_4$		**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$		
0.55-0.7	0.15		**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu_4$	H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu_4$	
0.50-0.60	0.1		H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$	H_1: $\mu_e > \mu$	H_1: $\mu_e > \mu_4$	H_1: $\mu_e > \mu_4$	
0.55-0.65	0.1		**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$		**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$	H_2: $\mu_e < \mu_8$	
0.6-0.7	0.1		**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$		**H_2: $\mu_e < \mu_4$** H_2: $\mu_e < \mu_8$		
0.55-0.6	0.05		H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$		H_1: $\mu_e > \mu_4$ H_2: $\mu_e < \mu_8$		
0.6-0.65	0.05		H_2: $\mu_e < \mu_8$		H_2: $\mu_e < \mu_8$		
Summary							
H_0: $\mu_e = \mu_4$ Not Rejected		8	2	5	1	5	21
	H_1: $\mu_e > \mu_4$	2	4	4	3	4	17
	H_2: $\mu_e < \mu_4$	1	5	2	7	2	17
H_0: $\mu_e = \mu_8$ Not Rejected		9	1	8	1	8	27
	H_1: $\mu_e > \mu_8$	1	0	0	0	0	1
	H_2: $\mu_e < \mu_8$	1	10	3	10	3	27

Table 1.6. A%Err in $P_{v,r}$ Predictions of $F_{w,j}[WA]$ Function vs. Entire-Curve Analytic Data. Sorted in Ascending Order of Average A%Err at $T_{r,f}$. "Even" Point Distribution.

			Average A%Err					**Maximum A%Err**		
T_r Interval	**4 Points**	**Interval Width**	**$T_{r,f}$**	**$T_{r,b}$**	**$T_r \leq 0.6$**	**$T_r > 0.6$**	**All T_rs**	**$T_{r,f}$**	**$T_{r,b}$**	**Ave $T_r > 0.6$**
0.5-0.9	0.5,0.63333,0.76667,0.9	0.4	0.087	0.005	0.037	0.002	0.017	0.461	0.011	0.010
0.55-0.9	0.55,0.66667,0.78333,0.9	0.35	0.173	0.005	0.077	0.002	0.032	1.064	0.014	0.010
0.50-0.70	0.5,0.56667,0.63333,0.7	0.2	0.187	0.008	0.078	0.021	0.043	1.735	0.035	0.090
0.6-0.9	0.6, 0.7, 0.8, 0.9	0.3	0.462	0.005	0.217	0.003	0.105	3.709	0.013	0.010
0.50-0.60	0.5,0.5333,0.56667,0.6	0.1	0.625	0.088	0.292	0.203	0.222	5.707	0.384	0.833
0.55-0.7	0.55,0.6,0.65,0.7	0.15	0.695	0.010	0.377	0.044	0.168	5.134	0.091	0.180
0.55-0.65	0.55, 0.58333,0.61667,0.65	0.1	1.443	0.041	0.575	0.143	0.308	12.637	0.274	0.763
0.6-0.7	0.6, 0.63333, 0.66667, 0.7	0.1	2.897	0.012	1.282	0.077	0.550	24.058	0.090	0.489
0.7-0.9	0.7, 0.76667, 0.83333, 0.9	0.2	4.512	0.025	1.894	0.009	0.921	47.550	0.344	0.070
0.55-0.6	0.55,0.56667,0.58333,0.6	0.05	8.257	0.472	4.244	1.191	2.098	86.302	2.239	5.802
0.6-0.65	0.6,0.61667,0.63333,0.65	0.05	16.784	0.160	7.681	0.884	3.521	203.861	1.459	4.227

Table 1.7. Predictive Error Due to Data Imprecision: Dependency Upon Interval Location and Width.

Width →	**0.05**	**0.1**	**0.15**	**0.2**	**0.3**	**0.35**	**0.4**
Lower Bound ↓							
				Average A%Err at $T_{r,f}$			
0.5		0.63		0.19			0.09
0.55	8.26	1.44	0.70			0.17	
0.6	16.78	2.90			0.46		
0.7				4.51		▨	▨
				Maximum A%Err at $T_{r,f}$			
0.5		5.71		1.74			0.46
0.55	86.30	12.64	5.13			1.06	
0.6	203.86	24.06			3.71		
0.7				47.55		▨	▨
		At $T_{r,f}$, error ↓ as Lower Bound ↓ and Width ↑					
				Average A%Err for $T_r > 0.6$ Segment			
0.5		0.203		0.021			0.002
0.55	1.191	0.143	0.044			0.002	
0.6	0.884	0.077			0.003		
0.7				0.009		▨	▨
				Maximum A%Err in $T_r > 0.6$ Segment			
0.5		0.83		0.09			0.01
0.55	5.80	0.76	0.18			0.01	
0.6	4.23	0.49			0.01		
0.7				0.07		▨	▨
	For $T_r > 06$ segment, error ↓ as Lower Bound ↑ and Width ↑						

Table 1.8. Error Statistics for $F_{w,j}$ *[WA]* Function Relative to Entire-Curve Wagner Analytics for Four Species.

Generic T_r Interval	4 Points	Actual Width	A%Err in Wagner Constants				Average A%Err in Predicted $P_{v,r}$		
			a	*b*	*c*	*d*	$T_r \leq 0.6$ (5)	$T_r > 0.6$ (7)	All T_rs (13)
Hydrogen									
0.50-0.90	0.50255, 0.63228, 0.76805, 0.89778	0.39523	0.012	0.242	0.666	16.599	0.014	0.003	0.007
0.50-0.70	0.50255, 0.56591, 0.63530, 0.69866	0.19611	0.151	1.901	3.177	39.983	0.004	0.011	0.008
0.6-0.7	0.60211, 0.63228, 0.66849, 0.69866	0.09655	1.958	26.004	49.398	956.463	0.633	0.103	0.299
0.60-0.65	0.60211, 0.61418, 0.63530, 0.64737	0.04526	25.472	327.541	585.696	9,929.779	5.578	1.568	2.990
R152a									
0.50-0.90	0.50198, 0.63099, 0.769, 0.89801	0.39603	0.017	0.212	0.261	0.334	0.010	0.001	0.005
0.50-0.70	0.50198, 0.56499, 0.63399, 0.697	0.19502	0.178	2.073	1.990	1.642	0.030	0.017	0.021
0.6-0.7	0.60099, 0.63099, 0.66698, 0.697	0.09601	0.812	10.333	11.882	15.378	0.712	0.053	0.302
0.60-0.65	0.60099, 0.616, 0.63399, 0.649	0.04801	11.801	139.619	139.928	133.977	4.137	1.106	2.187
Helium									
0.50-0.90	0.50086, 0.63146, 0.76785, 0.89843	0.39757	0.040	0.357	1.745	1.408	0.006	0.001	0.003
0.50-0.70	0.50086, 0.56470, 0.63436, 0.69819	0.19733	0.034	0.232	0.837	0.546	0.000	0.001	0.001
0.6-0.7	0.60243, 0.63146, 0.66918, 0.69819	0.09576	2.228	17.853	80.400	79.393	0.842	0.093	0.381
0.60-0.65	0.60243, 0.61404, 0.63436, 0.64886	0.04643	20.568	157.105	646.220	522.614	4.170	1.072	2.281
Water									
0.50-0.90	0.50014, 0.63306, 0.76885, 0.89888	0.39874	0.030	0.406	0.513	0.785	0.008	0.001	0.005
0.50-0.70	0.50014, 0.56659, 0.63595, 0.69951	0.19937	0.154	1.784	1.767	1.939	0.018	0.014	0.015
0.6-0.7	0.60127, 0.63306, 0.66772, 0.69951	0.09824	1.146	14.003	15.646	24.786	0.646	0.094	0.300
0.60-0.65	0.60127, 0.61572, 0.63595, 0.64751	0.04624	4.099	47.986	49.350	63.955	1.136	0.402	0.654

The number of data points in each temperature segment is given in parenthesis. Points are taken at 0.05 reduced temperature increments, except for the normal fusion point which is included in the $T_r \leq 0.6$ segment and the normal boiling point which is included in the "All T_rs" segment. Cells shaded indicate deviations from the average trend with respect to interval width displayed in Table 1.7.

Table 1.9. A%Err in Wagner Constants Predicted from $F_{w,j}$ *[WA]* Function vs. Entire-Curve Analytic Constants. Sorted in Ascending Order of Average A%Err at $T_{r,f}$ (see Table 1.6).

T_r Interval	Interval Width	Wagner Constants							
		Average A%Err				Maximum A%Err			
		a	*b*	*c*	*d*	*a*	*b*	*c*	*d*
0.5-0.9	0.4	0.016	0.239	0.350	0.824	0.042	2.374	5.129	27.797
0.55-0.9	0.35	0.019	0.264	0.296	1.561	0.058	1.220	1.779	67.639
0.50-0.70	0.2	0.161	2.053	2.108	2.507	0.434	16.393	30.801	75.923
0.6-0.9	0.3	0.022	0.340	0.585	2.742	0.068	1.700	5.912	115.688
0.50-0.60	0.1	1.366	15.536	13.229	22.517	5.309	96.547	125.251	1,053.495
0.55-0.7	0.15	0.334	3.786	3.908	7.216	1.479	12.868	46.192	258.842
0.55-0.65	0.1	1.035	12.136	10.786	8.508	3.420	64.243	94.497	61.086
0.6-0.7	0.1	0.783	9.854	11.461	23.652	2.707	39.508	121.983	940.674
0.7-0.9	0.2	0.055	0.953	1.667	18.010	0.143	3.465	11.102	747.381
0.55-0.6	0.05	8.762	106.008	104.597	166.484	30.539	716.378	1535.513	7,395.573
0.6-0.65	0.05	7.508	101.070	102.439	192.921	21.840	879.916	1,362.777	7,768.563

Table 1.10. A%Err in Wagner Constants Predicted from $F_{w,j}$ *[WA]* Function vs. Entire-Curve Analytic Constants. Sorted in Ascending Order of Average A%Err in *a*.

T_r Interval	Interval Width	Wagner Constants							
		Average A%Err				Maximum A%Err			
		a	*b*	*c*	*d*	*a*	*b*	*c*	*d*
0.5-0.9	0.4	0.016	0.239	0.350	0.824	0.042	2.374	5.129	27.797
0.55-0.9	0.35	0.019	0.264	0.296	1.561	0.058	1.220	1.779	67.639
0.6-0.9	0.3	0.022	0.340	0.585	2.742	0.068	1.700	5.912	115.688
0.7-0.9	0.2	0.055	0.953	1.667	18.010	0.143	3.465	11.102	747.381
0.50-0.70	0.2	0.161	2.053	2.108	2.507	0.434	16.393	30.801	75.923
0.55-0.7	0.15	0.334	3.786	3.908	7.216	1.479	12.868	46.192	258.842
0.6-0.7	0.1	0.783	9.854	11.461	23.652	2.707	39.508	121.983	940.674
0.55-0.65	0.1	1.035	12.136	10.786	8.508	3.420	64.243	94.497	61.086
0.50-0.60	0.1	1.366	15.536	13.229	22.517	5.309	96.547	125.251	1,053.495
0.6-0.65	0.05	7.508	101.070	102.439	192.921	21.840	879.916	1,362.777	7,768.563
0.55-0.6	0.05	8.762	106.008	104.597	166.484	30.539	716.378	1535.513	7,395.573

Table 1.11. A%Err in P_r Predictions of $F_{w,j}$ *[RD]* Functions vs. Entire-Curve Analytic Data. Sorted in Same Ascending Order of Average A%Err at $T_{r,f}$ as Used in Table 1.6.

Generic T_r Interval	**T_r**															
	$T_{r,f}$	**$T_{r,b}$**	**0.45**	**0.50**	**0.55**	**0.60**	**0.65**	**0.70**	**0.75**	**0.80**	**0.85**	**0.90**	**0.95**	**$T_r \leq 0.6^a$**	**$T_r > 0.6^b$**	**All T_rs^c**
								H_2								
0.5-0.9	0.110	0.007	0.040	0	0.010	0.010	0	0	0	0.010	0	0	0	0.034	0.001	0.014
0.5-0.7	0.080	0.010	0.020	0	0	0.010	0	0	0.020	0.040	0.060	0.070	0.060	0.022	0.036	0.028
0.6-0.7	1.921	0.004	0.896	0.290	0.060	0	0	0	0.030	0.100	0.170	0.220	0.200	0.633	0.103	0.299
0.60-0.65	11.521	0.006	5.209	1.489	0.230	0	0	0.180	0.642	1.349	2.071	2.511	2.173	3.690	1.275	2.106
								R152a								
0.5-0.9	0.190	0.003	0.020	0.030	0.040	0.020	0.010	0.020	0.020	0.010	0	0.010	0.020	0.060	0.013	0.030
0.5-0.7	0.090	0.003	0.050	0.030	0.030	0.030	0	0.030	0.060	0.090	0.120	0.130	0.090	0.046	0.074	0.058
0.6-0.7	12.705	0.007	5.243	1.654	0.341	0.020	0.010	0.030	0.230	0.578	0.985	1.262	1.134	3.992	0.604	1.861
0.60-0.65	141.887	0.009	42.918	10.882	1.715	0.030	0.030	1.025	3.719	7.624	11.547	13.869	12.173	39.486	7.141	19.033
								He								
0.5-0.9	1.481	0.053	0.733	0.180	0.060	0.120	0.080	0.040	0.010	0.050	0.060	0.050	0.030	0.515	0.046	0.227
0.5-0.7	0.341	0.239	0.310	0.180	0.020	0.090	0.100	0.060	0.060	0.200	0.331	0.401	0.341	0.188	0.213	0.206
0.6-0.7	3.334	0.059	1.826	0.662	0.120	0.080	0.100	0.060	0	0.050	0.070	0.060	0.030	1.205	0.053	0.496
0.60-0.65	11.979	2.139	5.739	1.528	0.230	0.080	0.090	0.170	0.854	1.837	2.840	3.438	2.963	3.911	1.742	2.607
								H_2O								
0.5-0.9	0.409	0.037	0.230	0.050	0.010	0.030	0.010	0	0.010	0.010	0.010	0	0.010	0.146	0.007	0.063
0.5-0.7	0.648	0.049	0.339	0.050	0.030	0.030	0.000	0.010	0	0.020	0.070	0.100	0.100	0.219	0.043	0.111
0.6-0.7	5.739	0.104	3.355	1.096	0.250	0.040	0.020	0.010	0.130	0.359	0.608	0.787	0.707	2.096	0.375	1.016
0.60-0.65	1.715	0.045	0.975	0.250	0.010	0.040	0	0.030	0.020	0.010	0.090	0.140	0.150	0.598	0.063	0.267
Per Row: ^{a} Excludes $T_{r,b}$. Total of 5 points for each species. ^{b} Excludes $T_{r,b}$. Total of 7 points for each species. ^{c} Includes $T_{r,b}$. Total of 13 points for each species																
								Summary								
Generic T_r Interval	$T_{r,f}$	$T_{r,b}$	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	$T_r \leq 0.6$	$T_r > 0.6$	All T_rs
								# of Predicted Points Pertaining to Each Cell								
	4	4	4	4	4	4	4	4	4	4	4	4	4	20	28	52
0.5-0.9	0.547	0.025	0.256	0.065	0.030	0.045	0.025	0.015	0.010	0.020	0.018	0.015	0.015	0.189	0.017	0.084
0.5-0.7	0.290	0.075	0.180	0.065	0.020	0.040	0.025	0.025	0.035	0.088	0.145	0.175	0.148	0.119	0.092	0.101
0.6-0.7	5.925	0.044	2.830	0.925	0.193	0.035	0.032	0.025	0.097	0.272	0.458	0.582	0.518	1.982	0.284	0.918
0.60-0.65	41.776	0.550	13.710	3.537	0.546	0.037	0.030	0.351	1.309	2.705	4.137	4.989	4.365	11.921	2.555	6.003

Table 1.12. Comparison of Predictive Error Due to Data Imprecision and Wagner Imperfection.

Generic T_r Interval	Average A%Err in Predicted $P_{v,r}$									Ratio of Average A%Err		
	Total: $F_{w,j}[RD]$ (1) (Wagner Imperfection + Data Imprecision)			$F_{w,j}[WA]$ (2) (Data Imprecision)			$F_{w,j}[RD]$ - $F_{w,j}[WA]$ (3) (Wagner Imperfection)			($F_{w,j}[RD]$ - $F_{w,j}[WA]$) / $F_{w,j}[WA]$ (4) (Wagner Imperfection/Data Imprecision)		
	$T_r \le 0.6$	$T_r > 0.6$	All T_rs	$T_r \le 0.6$	$T_r > 0.6$	All T_rs	$T_r \le 0.6$	$T_r > 0.6$	All T_rs	$T_r \le 0.6$	$T_r > 0.6$	All T_rs
H_2												
0.50-0.90	0.034	0.001	0.014	0.014	0.003	0.007	0.020	-0.001	0.007	1.43	-0.50	0.97
0.50-0.70	0.022	0.036	0.028	0.004	0.011	0.008	0.018	0.024	0.021	4.50	2.13	2.66
0.6-0.7	0.633	0.103	0.299	0.633	0.103	0.299	0.000	0.000	0.000	0.00	0.00	0.00
0.60-0.65	3.690	1.275	2.106	5.578	1.568	2.990	-1.889	-0.293	-0.884	-0.34	-0.19	-0.30
R152a												
0.50-0.90	0.060	0.013	0.030	0.010	0.001	0.005	0.050	0.011	0.025	5.00	8.00	5.34
0.50-0.70	0.046	0.074	0.058	0.030	0.017	0.021	0.016	0.057	0.037	0.53	3.33	1.77
0.6-0.7	3.992	0.604	1.861	0.712	0.053	0.302	3.280	0.551	1.559	4.61	10.42	5.15
0.60-0.65	39.486	7.141	19.033	4.137	1.106	2.187	35.350	6.035	16.846	8.55	5.46	7.70
He												
0.50-0.90	0.515	0.046	0.227	0.006	0.001	0.003	0.509	0.044	0.224	84.79	31.00	70.87
0.50-0.70	0.188	0.213	0.206	0.000	0.001	0.001	0.188	0.212	0.204	-	148.20	177.16
0.6-0.7	1.205	0.053	0.496	0.842	0.093	0.381	0.363	-0.040	0.115	0.43	-0.43	0.30
0.60-0.65	3.911	1.742	2.607	4.170	1.072	2.281	-0.259	0.669	0.326	-0.06	0.62	0.14
H_2O												
0.50-0.90	0.146	0.007	0.063	0.008	0.001	0.005	0.138	0.006	0.058	17.22	4.00	11.95
0.50-0.70	0.219	0.043	0.111	0.018	0.014	0.015	0.201	0.029	0.096	11.19	2.00	6.23
0.6-0.7	2.096	0.375	1.016	0.646	0.094	0.300	1.450	0.280	0.716	2.25	2.97	2.38
0.60-0.65	0.598	0.063	0.267	1.136	0.402	0.654	-0.538	-0.339	-0.387	-0.47	-0.84	-0.59

(1) Total error from Table 1.11. Shaded cells indicate inconsistency with error trend for intervals given in Table 1.7.

(2) Data imprecision error from Table 1.8. Shaded cells indicate inconsistency with error trend for intervals given in Table 1.7.

(3) Shaded cells indicate that the error due to Wagner imperfection cancels out to some degree the error due to data imprecision..

(4) Absolute value of shaded cells represents the fraction of the data imprecision error that is cancelled out by Wagner imperfection error.

Note: values in the table are rounded off for display, but the total and data imprecision errors are not rounded off when inputs to the calculations for the Wagner imperfection error and error ratio.

Table 1.13. Comparison of 4 Points vs. the Over-Determined Case to Predict Reduced Vapor Pressure. A%Err Given For Specific Trs and Segments.

Generic T_r Interval	**Data**	**T_r**															
		$T_{r,f}$	**$T_{r,b}$**	**0.45**	**0.50**	**0.55**	**0.60**	**0.65**	**0.70**	**0.75**	**0.80**	**0.85**	**0.90**	**0.95**	**$T_r \leq 0.6^a$**	**$T_r > 0.6^b$**	**All $T_r s^c$**
H_2																	
0.50-0.70	*NIST* $F_{w,j}$ *[RD]*	0.080	0.010	0.020	0	0	0.010	0.000	0	0.020	0.040	0.060	0.070	0.060	0.022	0.036	0.028
0.50-0.70	66 *NIST* Points	0.020	0.009	0.020	**0.010**	0	0.010	0.000	0	0.010	0.020	0.030	0.030	0.030	0.012	0.017	0.015
0.60-0.65	*NIST* $F_{w,j}$ *[RD]*	11.521	0.006	5.209	1.489	0.230	0	0	0.180	0.642	1.349	2.071	2.511	2.173	3.690	1.275	2.106
0.60-0.65	16 *NIST* Points	1.390	**0.009**	0.622	0.180	0.030	**0.010**	0	0.020	0.060	0.110	0.180	0.220	0.180	0.446	0.110	0.232
R152a																	
0.50-0.70	*NIST* $F_{w,j}$ *[RD]*	0.090	0.003	0.050	0.030	0.030	0.030	0	0.030	0.060	0.090	0.120	0.130	0.090	0.046	0.074	0.058
0.50-0.70	66 *NIST* Points	0.090	0.002	0.040	0.020	0.020	0.020	**0.010**	0.030	0.060	0.090	0.120	0.130	0.090	0.038	**0.076**	0.056
0.60-0.65	*NIST* $F_{w,j}$ *[RD]*	141.887	0.009	42.918	10.882	1.715	0.030	0.030	1.025	3.719	7.624	11.547	13.869	12.173	39.486	7.141	19.033
0.60-0.65	17 *NIST* Points	**150.553**	0.009	**44.658**	**11.138**	1.704	0.030	**0.040**	**1.143**	**4.075**	**8.268**	**12.453**	**14.888**	**13.055**	**41.617**	**7.703**	**20.155**
He																	
0.50-0.70	*NIST* $F_{w,j}$ *[RD]*	0.341	0.239	0.310	0.180	0.020	0.090	0.100	0.060	0.060	0.200	0.331	0.401	0.341	0.188	0.213	0.206
0.50-0.70	69 *NIST* Points	**0.451**	0.193	**0.351**	0.180	0.010	0.080	0.100	0.060	0.040	0.160	0.270	0.331	0.280	**0.214**	0.177	0.193
0.60-0.65	*NIST* $F_{w,j}$ *[RD]*	11.979	2.139	5.739	1.528	0.230	0.080	0.090	0.170	0.854	1.837	2.840	3.438	2.963	3.911	1.742	2.607
0.60-0.65	17 *NIST* Points	9.932	1.543	4.810	1.341	**0.240**	**0.090**	**0.100**	0.080	0.582	1.308	2.071	2.532	2.204	3.283	1.268	2.064
H_2O																	
0.50-0.70	*NIST* $F_{w,j}$ *[RD]*	0.648	0.049	0.339	0.050	0.030	0.030	0.000	0.010	0.000	0.020	0.070	0.100	0.100	0.219	0.043	0.111
0.50-0.70	70 *NIST* Points	0.310	0.037	0.200	**0.070**	0.000	**0.040**	**0.020**	0.010	**0.050**	**0.100**	**0.130**	**0.140**	**0.110**	0.124	**0.080**	0.094
0.60-0.65	*NIST* $F_{w,j}$ *[RD]*	1.715	0.045	0.975	0.250	0.010	0.040	0	0.030	0.020	0.010	0.090	0.140	0.150	0.598	0.063	0.267
0.60-0.65	17 *NIST* Points	**3.584**	0.023	**2.098**	**0.628**	**0.090**	0.040	0	**0.040**	0.010	**0.080**	**0.220**	**0.331**	**0.331**	**1.288**	**0.144**	**0.575**

Per Row: [a] Excludes $T_{r,b}$. Total of 5 points for each species. [b] Excludes $T_{r,b}$. Total of 7 points for each species. [c] Includes $T_{r,b}$. Total of 13 points for each species.
Shaded cell indicates over-determined regression results in less error than $F_{w,j}$ *[RD]*, and bold face font indicates regression results in more error.

Table 2.1. Extrapolation Burden.

	Antoine Using T_{min}			Riedel Using T_b			Ambrose-Walton Using T_r=0.7		
Species	$\Delta Log\ P_{v,r}$	ΔT_r	$\Delta Log\ P_{v,r}/\Delta T_r$ *	$\Delta Log\ P_{v,r}$	ΔT_r	$\Delta Log\ P_{v,r}/\Delta T_r$	$\Delta Log\ P_{v,r}$	ΔT_r	$\Delta Log\ P_{v,r}/\Delta T_r$
2-Methyl propanoic acid ($C_4H_8O_2$)	4.2339	0.17678	23.95	5.9511	0.33145	17.95	5.8957	0.32471	18.16
3-Methyl butanoic acid ($C_5H_{10}O_2$)	4.0969	0.16876	24.28	5.8928	0.32723	18.01	5.7678	0.31232	18.47
Acetic Acid ($C_2H_4O_2$)	0.2022	0.01318	15.34	1.9048	0.17086	11.15	2.2022	0.21111	10.43
Butanoic acid ($C_4H_8O_2$)	2.4788	0.11976	20.70	4.1829	0.27067	15.45	4.1820	0.27056	15.46
Pentanoic acid ($C_5H_{10}O_2$)	4.9632	0.18903	26.26	6.7050	0.34192	19.61	6.5834	0.32760	20.10
Propanoic acid ($C_3H_6O_2$)	2.3322	0.11492	20.29	4.0366	0.26822	15.05	4.1483	0.28227	14.70
1-Butanol ($C_4H_{10}O$)	6.8173	0.22525	30.27	8.5136	0.36858	23.10	8.5631	0.37436	22.87
1-Decanol ($C_{10}H_{22}O$)	4.3644	0.16654	26.21	6.0690	0.32540	18.65	5.8165	0.29354	19.81
1-Heptanol ($C_7H_{16}O$)	5.1309	0.18324	28.00	6.8259	0.33281	20.51	6.7364	0.32182	20.93
1-Hexanol ($C_6H_{14}O$)	5.0443	0.18274	27.60	6.7371	0.32952	20.45	6.6972	0.32469	20.63
1-Nonanol ($C_9H_{20}O$)	4.5041	0.16969	26.54	6.2037	0.32520	19.08	6.0079	0.30067	19.98
1-Octanol ($C_8H_{18}O$)	4.5248	0.17034	26.56	6.2230	0.32287	19.27	6.0801	0.30513	19.93
1-Pentanol ($C_5H_{12}O$)	6.9741	0.22403	31.13	8.6703	0.36880	23.51	8.6782	0.36973	23.47
2-Octanol ($C_8H_{18}O$)	5.0115	0.17688	28.33	6.7431	0.33210	20.30	6.6640	0.32202	20.69
Ethanol (C_2H_6O)	6.3449	0.22854	27.76	8.0474	0.37436	21.50	8.1860	0.39052	20.96
Isopropyl alcohol (C_3H_8O)	4.7823	0.19207	24.90	6.5104	0.33787	19.27	6.5177	0.33870	19.24

	Antoine Using T_{min}			**Riedel Using T_b**			**Ambrose-Walton Using T_r=0.7**		
Species	**$\Delta Log\ P_{v,r}$**	**ΔT_r**	**$\Delta Log\ P_{v,r}/\Delta T_r$ ***	**$\Delta Log\ P_{v,r}$**	**ΔT_r**	**$\Delta Log\ P_{v,r}/\Delta T_r$**	**$\Delta Log\ P_{v,r}$**	**ΔT_r**	**$\Delta Log\ P_{v,r}/\Delta T_r$**
Methanol (CH_4O)	4.0660	0.16990	23.93	5.7675	0.31639	18.23	6.1054	0.35767	17.07
Propanol (C_3H_8O)	9.0363	0.27234	33.18	10.7355	0.41599	25.81	10.8234	0.42614	25.40
Tert-butanol ($C_4H_{10}O$)	-0.4642	-0.03072	**0**	1.2465	0.11248	11.08	1.2267	0.11021	11.13
Acetone (C_3H_6O)	2.9407	0.13556	21.69	4.6403	0.29664	15.64	4.9995	0.34869	14.34
Methyl isobutyl ketone ($C_6H_{12}O$)	4.4293	0.18143	24.41	6.1214	0.34807	17.59	6.2788	0.37081	16.93
Benzene (C_6H_6)	0.0226	0.00171	13.21	1.3258	0.13263	10.00	1.8007	0.20427	8.82
Ethylbenzene (C_8H_{10})	5.7544	0.20762	27.72	7.4571	0.37456	19.91	7.7054	0.41131	18.73
Naphthalene ($C_{10}H_8$)	0.3520	0.02283	15.42	2.0517	0.18681	10.98	2.3498	0.23053	10.19
Toluene (C_7H_8)	4.7560	0.18296	26.00	6.4590	0.34746	18.59	6.8029	0.39895	17.05
m-Xylene (C_8H_{10})	2.8493	0.13493	21.12	4.5664	0.30316	15.06	4.7830	0.33491	14.28
o-Xylene (C_8H_{10})	1.9669	0.10277	19.14	3.6702	0.26910	13.64	3.9248	0.30660	12.80
p-Xylene (C_8H_{10})	0.5416	0.03473	15.59	2.2455	0.20303	11.06	2.4635	0.23522	10.47
Butane (C_4H_{10})	3.4808	0.15452	22.53	5.1819	0.32422	15.98	5.5562	0.38303	14.51
Diethyl ether ($C_4H_{10}O$)	3.5648	0.15608	22.84	5.2679	0.32292	16.31	5.5426	0.36392	15.23
Decane ($C_{10}H_{22}$)	3.1565	0.15387	20.51	4.8572	0.32998	14.72	4.6850	0.30578	15.32
Dodecane ($C_{12}H_{26}$)	3.4743	0.16614	20.91	5.1709	0.34294	15.08	4.8522	0.29944	16.20
Eicosane ($C_{20}H_{42}$)	5.2804	0.22256	23.73	6.9574	0.39907	17.43	6.1249	0.29694	20.63
Ethane (C_2H_6)	3.2507	0.14230	22.84	4.9564	0.30853	16.06	5.5392	0.40409	13.71
Heptadecane ($C_{17}H_{36}$)	4.5887	0.20186	22.73	6.2907	0.38017	16.55	5.6502	0.29846	18.93
n-Heptane (C_7H_{16})	4.0627	0.17609	23.07	5.7647	0.34986	16.48	5.8463	0.36196	16.15
Hexadecane ($C_{16}H_{34}$)	4.3250	0.19411	22.28	6.0251	0.37211	16.19	5.4390	0.29651	18.34
n-Hexane (C_6H_{14})	3.2334	0.15042	21.50	4.9357	0.32298	15.28	5.1135	0.34985	14.62
Methane (CH_4)	0.1065	0.01023	10.41	0.9374	0.11003	8.52	1.5830	0.22406	7.06
Nonadecane ($C_{19}H_{40}$)	4.9820	0.21274	23.42	6.6937	0.39194	17.08	5.9340	0.29730	19.96
Nonane (C_9H_{20})	3.6526	0.16794	21.75	5.3551	0.34343	15.59	5.2665	0.33076	15.92
Octadecane ($C_{18}H_{38}$)	4.7183	0.20601	22.90	6.4233	0.38470	16.70	5.7197	0.29609	19.32
Octane (C_8H_{18})	2.9917	0.14594	20.50	4.6935	0.32064	14.64	4.6868	0.31967	14.66
Pentadecane ($C_{15}H_{32}$)	4.2178	0.19028	22.17	5.9203	0.36828	16.08	5.3995	0.30017	17.99

	Antoine Using T_{min}			**Riedel Using T_b**			**Ambrose-Walton Using T_r=0.7**		
Species	**$\Delta Log\ P_{v,r}$**	**ΔT_r**	**$\Delta Log\ P_{v,r}/\Delta T_r$ ***	**$\Delta Log\ P_{v,r}$**	**ΔT_r**	**$\Delta Log\ P_{v,r}/\Delta T_r$**	**$\Delta Log\ P_{v,r}$**	**ΔT_r**	**$\Delta Log\ P_{v,r}/\Delta T_r$**
n-Pentane (C_5H_{12})	4.4556	0.18152	24.55	6.1580	0.35289	17.45	6.4293	0.39470	16.29
Propane (C_3H_8)	7.0493	0.22559	31.25	8.7486	0.39351	22.23	9.2191	0.46889	19.66
R152a ($C_2H_4F_2$)	1.4615	0.08176	17.88	3.1069	0.24062	12.91	3.4809	0.29590	11.76
n-Tetradecane ($C_{14}H_{30}$)	3.8813	0.17992	21.57	5.5814	0.35751	15.61	5.1280	0.29739	17.24
Tridecane ($C_{13}H_{28}$)	3.8798	0.17913	21.66	5.5785	0.35633	15.66	5.1882	0.30391	17.07
Undecane ($C_{11}H_{24}$)	3.6418	0.17012	21.41	5.3426	0.34673	15.41	5.0951	0.31248	16.31
Argon (Ar)	-0.0615	-0.00803	**0**	0.1679	0.02325	7.22	0.8512	0.14389	5.92
Nitrogen (N_2)	-0.1952	-0.01855	**0**	0.9079	0.11249	8.07	1.3965	0.19960	7.00
Ammonia (NH_3)	-0.0844	-0.00587	**0**	1.2269	0.10951	11.20	2.0205	0.21810	9.26
Water (H_2O)	0.0016	0.00008	**0**	2.2204	0.15452	14.37	3.2140	0.27789	11.57
Hydrogen (H_2 normal)	-0.0615	-0.00694	**0**	1.2412	0.20551	6.04	1.5668	0.29095	5.39

* Antoine extrapolation burdens given value of zero for reasons explained in the text are entered in bold font.

Table 2.2. Antoine Constants and Range.

Species	A	B	C	$P_{v,\mathrm{min}}$ (bar)	$P_{v,\mathrm{max}}$ (bar)	T_{min} (K)	T_{max} (K)	$T_{r,\mathrm{min}}$	$T_{r,\mathrm{max}}$	Interval Width
2-Methyl propanoic acid ($C_4H_8O_2$)	3.71153	1097.83	141.74	0.02	2	334.00	453.31	0.55207	0.74927	0.19720
3-Methyl butanoic acid ($C_5H_{10}O_2$)	4.5847	1676.3	189.5	0.02	2	350.00	474.97	0.55644	0.75512	0.19868
Acetic Acid ($C_2H_4O_2$)	4.54456	1555.12	224.65	0.02	2	297.58	414.97	0.50207	0.70012	0.19805
Butanoic acid ($C_4H_8O_2$)	4.8234	1731.708	195.955	0.02	2	342.70	460.12	0.54920	0.73737	0.18817
Pentanoic acid ($C_5H_{10}O_2$)	4.1692	1405.8	151.8	0.02	2	361.00	484.78	0.56143	0.75393	0.19250
Propanoic acid ($C_3H_6O_2$)	4.75466	1662.582	209.046	0.02	2	321.72	437.41	0.53265	0.72419	0.19154
1-Butanol ($C_4H_{10}O$)	4.6493	1395.14	182.739	0.02	2	310.18	411.26	0.55089	0.73041	0.17952
1-Decanol ($C_{10}H_{22}O$)	3.84905	1369	125.078	0.02	2	394.80	533.92	0.57300	0.77492	0.20192
1-Heptanol ($C_7H_{16}O$)	4.01991	1274.89	140.94	0.02	2	355.10	475.03	0.56142	0.75104	0.18962
1-Hexanol ($C_6H_{14}O$)	4.18948	1295.59	152.51	0.02	2	340.80	453.83	0.55805	0.74313	0.18508
1-Nonanol ($C_9H_{20}O$)	3.83303	1297.75	125	0.02	2	382.10	515.58	0.56902	0.76780	0.19878
1-Octanol ($C_8H_{18}O$)	3.90225	1274.8	131.99	0.02	2	368.80	495.15	0.56521	0.75885	0.19364
1-Pentanol ($C_5H_{12}O$)	4.39646	1336.01	166.32	0.02	2	326.01	433.05	0.55430	0.73629	0.18199
2-Octanol ($C_8H_{18}O$)	3.5137	1060.4	122.5	0.02	2	354.00	480.72	0.55486	0.75348	0.19862
Ethanol (C_2H_6O)	5.33675	1648.22	230.918	0.02	2	276.50	369.54	0.53802	0.71906	0.18104
Isopropyl alcohol (C_3H_8O)	5.24268	1580.92	219.61	0.02	2	281.28	373.46	0.55337	0.73472	0.18135
Methanol (CH_4O)	5.20277	1580.08	239.5	0.02	2	262.59	356.00	0.51223	0.69444	0.18221
Propanol (C_3H_8O)	4.99991	1512.94	205.807	0.02	2	293.19	389.32	0.54620	0.72529	0.17909
Tert-butanol ($C_4H_{10}O$)	4.44484	1154.48	177.65	0.02	2	283.00	374.10	0.55907	0.73904	0.17997
Acetone (C_3H_6O)	4.2184	1197.01	228.06	0.02	2	247.38	350.65	0.48687	0.69012	0.20325
Methyl isobutyl ketone ($C_6H_{12}O$)	3.8222	1190.6904	195.45	0.02	2	293.40	415.85	0.51062	0.72372	0.21310
Benzene (C_6H_6)	3.98523	1184.24	217.572	0.05	2	279.64	377.06	0.49744	0.67073	0.17329
Ethylbenzene (C_8H_{10})	4.06861	1415.77	212.3	0.02	2	306.32	436.63	0.49631	0.70744	0.21113
Naphthalene ($C_{10}H_8$)	4.13555	1733.71	201.859	0.02	2	368.44	523.40	0.49230	0.69936	0.20706
Toluene (C_7H_8)	4.05043	1327.62	217.625	0.02	2	286.44	409.61	0.48401	0.69214	0.20813
m-Xylene (C_8H_{10})	4.14051	1468.703	216.12	0.02	2	308.54	439.56	0.50002	0.71236	0.21234

Species	A	B	C	$P_{v,\min}$ (bar)	$P_{v,\max}$ (bar)	$T_{\min}$ (K)	$T_{\max}$ (K)	$T_{r,\min}$	$T_{r,\max}$	Interval Width
o-Xylene (C_8H_{10})	4.09789	1458.706	212.041	0.02	2	312.75	445.30	0.49617	0.70646	0.21029
p-Xylene (C_8H_{10})	4.10494	1446.832	214.627	0.02	2	307.81	438.88	0.49951	0.71220	0.21269
Butane (C_4H_{10})	3.93266	935.773	238.789	0.02	2	200.50	292.03	0.47149	0.68673	0.21524
Diethyl ether ($C_4H_{10}O$)	4.10962	1090.64	231.2	0.02	2	229.71	328.31	0.49216	0.70341	0.21125
Decane ($C_{10}H_{22}$)	4.06853	1495.17	193.858	0.02	2	338.53	476.15	0.54809	0.77091	0.22282
Dodecane ($C_{12}H_{26}$)	4.12285	1639.27	181.84	0.02	2	372.89	520.24	0.56670	0.79064	0.22394
Eicosane ($C_{20}H_{42}$)	4.2771	2032.7	132.1	0.02	2	481.10	652.00	0.62562	0.84785	0.22223
Ethane (C_2H_6)	3.95405	663.72	256.681	0.02	2	133.80	198.16	0.43821	0.64900	0.21079
Heptadecane ($C_{17}H_{36}$)	4.1392	1865.1	149.2	0.02	2	443.50	610.00	0.60340	0.82993	0.22653
n-Heptane (C_7H_{16})	4.02023	1263.909	216.432	0.02	2	277.71	396.53	0.51413	0.73411	0.21998
Hexadecane ($C_{16}H_{34}$)	4.15357	1830.51	154.45	0.02	2	431.47	593.80	0.59760	0.82244	0.22484
n-Hexane (C_6H_{14})	4.00139	1170.875	224.317	0.02	2	254.24	365.25	0.50057	0.71914	0.21857
Methane (CH_4)	3.7687	395.744	266.681	0.15	2	92.64	120.59	0.48617	0.63285	0.14668
Nonadecane ($C_{19}H_{40}$)	4.1402	1932.8	137.6	0.02	2	466.50	639.00	0.61544	0.84301	0.22757
Nonane (C_9H_{20})	4.07356	1438.03	202.694	0.02	2	319.57	451.64	0.53718	0.75919	0.22201
Octadecane ($C_{18}H_{38}$)	4.1271	1894.3	143.3	0.02	2	455.00	625.00	0.60992	0.83780	0.22788
Octane (C_8H_{18})	4.05075	1356.36	209.635	0.02	2	299.42	425.23	0.52627	0.74739	0.22112
Pentadecane ($C_{15}H_{32}$)	4.14849	1789.95	161.38	0.02	2	417.80	576.90	0.59011	0.81483	0.22472
n-Pentane (C_5H_{12})	3.97786	1064.84	232.014	0.02	2	228.71	330.75	0.48682	0.70402	0.21720
Propane (C_3H_8)	3.92828	803.997	247.04	0.02	2	168.90	247.76	0.45670	0.66993	0.21323
R152a ($C_2H_4F_2$)	3.75231	735.16	220.27	0.02	2	187.74	265.89	0.48586	0.68810	0.20224
n-Tetradecane ($C_{14}H_{30}$)	4.1379	1740.88	167.72	0.02	2	403.69	559.15	0.58253	0.80685	0.22432
Tridecane ($C_{13}H_{28}$)	4.13246	1690.67	174.22	0.02	2	388.85	540.19	0.57522	0.79910	0.22388
Undecane ($C_{11}H_{24}$)	4.0971	1569.57	187.7	0.02	2	356.25	499.00	0.55764	0.78109	0.22345
Argon (Ar)	3.74141	304.227	267.32	0.6	2	82.59	94.26	0.54808	0.62552	0.07744
Nitrogen (N_2)	3.61947	255.68	266.55	0.08	2	60.81	83.65	0.48185	0.66284	0.18099
Ammonia (NH_3)	4.4854	926.132	240.17	0.05	2	193.03	254.31	0.47603	0.62715	0.15112
Water (H_2O)	5.11564	1687.537	230.17	0.01	16	273.20	473.20	0.42219	0.73126	0.30907
Hydrogen (H_2 normal)	2.94928	67.5078	275.7	0.05	2	13.33	22.94	0.40211	0.69201	0.28990

Table 2.3. Error at $T_{r,f}$ for Antoine Extrapolated and $F_{w,j}[AA]$.

Species	A%Err at $T_{r,f}$		Incremental % Error
	Antoine Extrapolated	$F_{w,j}[AA]$	
2-Methyl propanoic acid ($C_4H_8O_2$)	98.49	89.56	-8.93
3-Methyl butanoic acid ($C_5H_{10}O_2$)	1.86	41.10	**39.24**
Acetic Acid ($C_2H_4O_2$)	0.44	0.36	-0.08
Butanoic acid ($C_4H_8O_2$)	16.18	12.21	-3.98
Pentanoic acid ($C_5H_{10}O_2$)	90.78	62.47	-28.30
Propanoic acid ($C_3H_6O_2$)	10.53	5.66	-4.87
1-Butanol ($C_4H_{10}O$)	98.60	89.69	-8.91
1-Decanol ($C_{10}H_{22}O$)	65.38	7.39	-57.99
1-Heptanol ($C_7H_{16}O$)	91.60	61.94	-29.66
1-Hexanol ($C_6H_{14}O$)	90.31	66.46	-23.85
1-Nonanol ($C_9H_{20}O$)	83.54	43.73	-39.81
1-Octanol ($C_8H_{18}O$)	85.00	51.29	-33.71
1-Pentanol ($C_5H_{12}O$)	99.40	90.32	-9.08
2-Octanol ($C_8H_{18}O$)	96.58	60.14	-36.44
Ethanol (C_2H_6O)	81.42	70.20	-11.21
Isopropyl alcohol (C_3H_8O)	60.49	51.97	-8.51
Methanol (CH_4O)	33.21	23.70	-9.51
Propanol (C_3H_8O)	99.95	98.51	-1.44
Tert-butanol ($C_4H_{10}O$)	0.02	0.04	**0.02**
Acetone (C_3H_6O)	24.05	9.59	-14.46
Methyl isobutyl ketone ($C_6H_{12}O$)	82.04	53.60	-28.44
Benzene (C_6H_6)	0.63	0.64	0.00
Ethylbenzene (C_8H_{10})	71.59	23.63	-47.96
Naphthalene ($C_{10}H_8$)	2.06	1.77	-0.29
Toluene (C_7H_8)	52.36	13.37	-39.00
m-Xylene (C_8H_{10})	6.27	9.49	**3.23**
o-Xylene (C_8H_{10})	9.64	3.55	-6.10
p-Xylene (C_8H_{10})	0.97	0.48	-0.49
Butane (C_4H_{10})	38.19	18.02	-20.17
Diethyl ether ($C_4H_{10}O$)	24.05	3.92	-20.13
Decane ($C_{10}H_{22}$)	34.83	15.23	-19.60
Dodecane ($C_{12}H_{26}$)	40.87	17.50	-23.37
Eicosane ($C_{20}H_{42}$)	84.37	49.33	-35.05
Ethane (C_2H_6)	16.60	1.00	-15.61
Heptadecane ($C_{17}H_{36}$)	66.22	11.95	-54.27
n-Heptane (C_7H_{16})	45.30	17.00	-28.31
Hexadecane ($C_{16}H_{34}$)	62.96	22.86	-40.10
n-Hexane (C_6H_{14})	28.33	10.23	-18.11
Methane (CH_4)	0.34	0.29	-0.05
Nonadecane ($C_{19}H_{40}$)	72.54	2.08	-70.46
Nonane (C_9H_{20})	39.05	14.02	-25.03
Octadecane ($C_{18}H_{38}$)	68.58	0.26	-68.32
Octane (C_8H_{18})	26.52	10.90	-15.62
Pentadecane ($C_{15}H_{32}$)	58.83	21.61	-37.22
n-Pentane (C_5H_{12})	47.45	10.92	-36.53
Propane (C_3H_8)	86.61	41.38	-45.23
R152a ($C_2H_4F_2$)	45.72	41.45	-4.27

n-Tetradecane ($C_{14}H_{30}$)	51.66	22.65	-29.02
Tridecane ($C_{13}H_{28}$)	50.89	22.83	-28.06
Undecane ($C_{11}H_{24}$)	43.44	17.58	-25.86
Argon (Ar)	0.40	0.41	**0.01**
Nitrogen (N_2)	0.09	0.03	-0.06
Ammonia (NH_3)	1.12	1.13	**0.01**
Water (H_2O)	0.33	0.34	**0.01**
Hydrogen (H_2 normal)	1.29	1.36	**0.07**
Notes: Incremental error is that for extrapolated Antoine subtracted from that for $F_{w,j}[AA]$. Bold font indicates $F_{w,j}[AA]$ error is greater than that for the extrapolated Antoine.			

Table 2.4. Absolute Percent Error (A%Err) of $F_{w,j}[AA]$ Function Relative to Entire-Curve Wagner Analytic Values.

Species	**$F_{w,j}[AA]$ vs. Wagner Analytics**			
	A%Err	**Average A%Err**		
	$T_{r,f}$	**$T_r \leq 0.6$**	**$T_r > 0.6$**	**All T_rs**
2-Methyl propanoic acid ($C_4H_8O_2$)	89.56	35.86	8.60	19.50
3-Methyl butanoic acid ($C_5H_{10}O_2$)	41.10	31.46	2.97	14.37
Acetic Acid ($C_2H_4O_2$)	0.36	0.35	1.88	1.45
Butanoic acid ($C_4H_8O_2$)	12.21	3.33	3.18	3.23
Pentanoic acid ($C_5H_{10}O_2$)	62.47	23.44	4.58	12.56
Propanoic acid ($C_3H_6O_2$)	5.66	1.70	1.64	1.66
1-Butanol ($C_4H_{10}O$)	89.69	31.80	2.84	15.71
1-Decanol ($C_{10}H_{22}O$)	7.39	2.45	0.12	1.00
1-Heptanol ($C_7H_{16}O$)	61.94	21.31	1.77	9.58
1-Hexanol ($C_6H_{14}O$)	66.46	21.83	2.92	10.48
1-Nonanol ($C_9H_{20}O$)	43.73	19.69	1.36	8.70
1-Octanol ($C_8H_{18}O$)	51.29	19.35	1.02	8.35
1-Pentanol ($C_5H_{12}O$)	90.32	33.50	2.92	16.51
2-Octanol ($C_8H_{18}O$)	60.14	19.30	3.82	10.01
Ethanol (C_2H_6O)	70.20	20.77	2.52	10.99
Isopropyl alcohol (C_3H_8O)	51.97	14.83	3.34	8.20
Methanol (CH_4O)	23.70	6.97	0.70	3.49
Propanol (C_3H_8O)	98.51	42.79	2.77	22.78
Tert-butanol ($C_4H_{10}O$)	0.04	0.11	1.90	1.69
Acetone (C_3H_6O)	9.59	2.77	0.22	1.30
Methyl isobutyl ketone ($C_6H_{12}O$)	53.60	16.50	3.73	9.41
Benzene (C_6H_6)	0.64	0.31	0.10	0.16
Ethylbenzene (C_8H_{10})	23.63	6.24	0.30	3.16
Naphthalene ($C_{10}H_8$)	1.77	0.75	0.41	0.52
Toluene (C_7H_8)	13.37	3.16	0.11	1.53
m-Xylene (C_8H_{10})	9.49	4.40	0.21	1.99
o-Xylene (C_8H_{10})	3.55	1.11	0.05	0.48
p-Xylene (C_8H_{10})	0.48	0.18	0.18	0.18
Butane (C_4H_{10})	18.02	5.05	0.32	2.52
Diethyl ether ($C_4H_{10}O$)	3.92	1.11	0.83	0.95
Decane ($C_{10}H_{22}$)	15.23	5.66	0.07	2.30
Dodecane ($C_{12}H_{26}$)	17.50	6.59	0.46	2.76
Eicosane ($C_{20}H_{42}$)	49.33	24.91	1.90	10.53
Ethane (C_2H_6)	1.00	0.60	0.45	0.52
Heptadecane ($C_{17}H_{36}$)	11.95	4.60	1.27	2.52
n-Heptane (C_7H_{16})	17.00	5.01	0.09	2.27
Hexadecane ($C_{16}H_{34}$)	22.86	9.03	0.27	3.55
n-Hexane (C_6H_{14})	10.23	2.64	0.14	1.20
Methane (CH_4)	0.29	0.19	0.62	0.48
Nonadecane ($C_{19}H_{40}$)	2.08	1.41	1.59	1.52
Nonane (C_9H_{20})	14.02	4.63	0.12	2.03
Octadecane ($C_{18}H_{38}$)	0.26	0.61	2.21	1.61
Octane (C_8H_{18})	10.90	3.26	0.12	1.38
Pentadecane ($C_{15}H_{32}$)	21.61	9.17	0.11	3.73
n-Pentane (C_5H_{12})	10.92	2.84	0.03	1.33
Propane (C_3H_8)	41.38	10.43	0.24	5.50
R152a ($C_2H_4F_2$)	41.45	14.57	2.69	7.15

Species		**$F_{w,j}[AA]$ vs. Wagner Analytics**			
		A%Err	**Average A%Err**		
		$T_{r,f}$	**$T_r \leq 0.6$**	**$T_r > 0.6$**	**All T_rs**
n-Tetradecane ($C_{14}H_{30}$)		22.65	8.27	0.08	3.15
Tridecane ($C_{13}H_{28}$)		22.83	9.40	0.13	3.84
Undecane ($C_{11}H_{24}$)		17.58	6.22	0.06	2.52
Argon (Ar)		0.41	0.39	0.11	0.17
Nitrogen (N_2)		0.03	0.03	1.51	1.14
Ammonia (NH_3)		1.13	0.83	0.47	0.61
Water (H_2O)		0.34	0.19	0.76	0.52
Hydrogen (H_2 normal)		1.36	1.18	1.91	1.64
Data Summary					
Acids (6)	Average	35.23	16.02	3.81	8.80
	Maximum	89.56	35.86	8.60	19.50
Alcohols (13)	Average	55.03	19.59	2.15	9.81
	Maximum	98.51	42.79	3.82	22.78
Others (36)	Average	13.68	4.84	0.66	2.39
	Maximum	53.60	24.91	3.73	10.53
All (55)	Average	25.80	9.55	1.36	4.84
	Maximum	98.51	42.79	8.60	22.78

Table 2.5. Number of Species with Lowest & Highest Error Relative to Entire-Curve Wagner Analytic Values for Different Methods at Different T_r Segments, Segregated by Substance Type.

Substance Type	Lowest Average A%Err			Highest Average A%Err		
	$F_{w,j}[AA]$	Riedel	A-W	$F_{w,j}[AA]$	Riedel	A-W
$T_{r,f}$ *						
Organic Acids (6)	2	3	1	2	1	3
Alcohols (13)	9	2	2	0	4	9
Others (36)	12	4	20	6	24	6
All (55)	23	9	23	8	29	18
$T_r \leq 0.6$						
Organic Acids	3	2	1	2	1	3
Alcohols	9	3	1	0	4	9
Others	12	2	22	12	18	6
All	24	7	24	14	23	18
$T_r > 0.6$						
Organic Acids	1	5	0	4	0	2
Alcohols	5	6	2	2	4	7
Others	10	1	25	11	24	1
All	16	12	27	17	28	10
All T_rs						
Organic Acids	2	3	1	2	1	3
Alcohols	9	3	1	0	4	9
Others	10	1	25	13	19	4
All	21	7	27	15	24	16

* The normal fusion point is a singular point; thus, the lowest and highest error pertain to the A%Err at that point.

A-W = Ambrose-Walton equation.

$F_{w,j}[AA]$ = predictions from Wagner constants estimated from four Antoine analytic points using the "even" distribution within the Antoine interval.

Shaded cells indicate best performance, i.e., most number of “Lowest Average A%Err” or least number of “Highest Average A%Err.”

Table 2.6. Incremental Error at $T_{r,f}$.

		Incremental Error Increase		
Species	**Lowest A%Err**	**$F_{w,j}$*[AA]***	**Riedel**	**A-W**
Acetic Acid ($C_2H_4O_2$)	0.36	0.00	19.37	35.02
Propanoic acid ($C_3H_6O_2$)	5.66	0.00	8.87	6.18
Tert-butanol ($C_4H_{10}O$)	0.04	0.00	6.20	29.34
1-Decanol ($C_{10}H_{22}O$)	7.39	0.00	137.88	732.50
Methanol (CH_4O)	23.70	0.00	73.83	64.46
1-Nonanol ($C_9H_{20}O$)	43.73	0.00	90.70	771.40
1-Octanol ($C_8H_{18}O$)	51.29	0.00	59.59	747.52
2-Octanol ($C_8H_{18}O$)	60.14	0.00	78.55	1563.11
1-Heptanol ($C_7H_{16}O$)	61.94	0.00	67.18	1064.13
1-Hexanol ($C_6H_{14}O$)	66.46	0.00	4.32	761.21
Ethanol (C_2H_6O)	70.20	0.00	28.27	23.18
Nitrogen (N_2)	0.03	0.00	0.47	2.95
Octadecane ($C_{18}H_{38}$)	0.26	0.00	34.42	4.64
Methane (CH_4)	0.29	0.00	1.62	0.16
Water (H_2O)	0.34	0.00	16.87	32.39
p-Xylene (C_8H_{10})	0.48	0.00	5.30	4.87
Benzene (C_6H_6)	0.64	0.00	2.74	6.84
Ethane (C_2H_6)	1.00	0.00	13.31	1.65
Ammonia (NH_3)	1.13	0.00	3.97	7.30
Naphthalene ($C_{10}H_8$)	1.77	0.00	1.72	1.45
Nonadecane ($C_{19}H_{40}$)	2.08	0.00	51.88	0.12
Diethyl ether ($C_4H_{10}O$)	3.92	0.00	30.49	12.23
Toluene (C_7H_8)	13.37	0.00	51.67	9.78
Butanoic acid ($C_4H_8O_2$)	10.16	2.05	0.00	11.73
Pentanoic acid ($C_5H_{10}O_2$)	22.85	39.62	0.00	55.99
3-Methyl butanoic acid ($C_5H_{10}O_2$)	27.65	13.45	0.00	7.04
1-Pentanol ($C_5H_{12}O$)	0.39	89.93	0.00	819.15
1-Butanol ($C_4H_{10}O$)	59.47	30.21	0.00	174.80
Argon (Ar)	0.13	0.28	0.00	1.12
o-Xylene (C_8H_{10})	2.72	0.83	0.00	0.43
R152a ($C_2H_4F_2$)	6.75	34.70	0.00	3.91
Acetone (C_3H_6O)	9.00	0.59	0.00	14.84
2-Methyl propanoic acid ($C_4H_8O_2$)	11.29	78.27	33.59	0.00
Isopropyl alcohol (C_3H_8O)	45.35	6.62	34.60	0.00
Propanol (C_3H_8O)	86.50	12.00	12.26	0.00
Pentadecane ($C_{15}H_{32}$)	0.26	21.35	31.38	0.00
n-Heptane (C_7H_{16})	0.27	16.73	22.32	0.00
Octane (C_8H_{18})	0.33	10.57	10.34	0.00

Species		Lowest A%Err	Incremental Error Increase		
			$F_{w,j}[AA]$	Riedel	A-W
Hexadecane ($C_{16}H_{34}$)		0.34	22.52	31.72	0.00
Undecane ($C_{11}H_{24}$)		0.37	17.22	17.84	0.00
Hydrogen (H_2 normal)		0.50	0.86	5.97	0.00
Tridecane ($C_{13}H_{28}$)		0.55	22.28	22.61	0.00
Dodecane ($C_{12}H_{26}$)		0.70	16.80	17.56	0.00
Nonane (C_9H_{20})		0.76	13.26	16.14	0.00
n-Hexane (C_6H_{14})		0.95	9.27	13.35	0.00
n-Pentane (C_5H_{12})		1.08	9.84	26.71	0.00
Decane ($C_{10}H_{22}$)		1.25	13.98	10.67	0.00
n-Tetradecane ($C_{14}H_{30}$)		1.31	21.34	24.19	0.00
m-Xylene (C_8H_{10})		1.45	8.04	8.26	0.00
Heptadecane ($C_{17}H_{36}$)		2.61	9.35	32.54	0.00
Eicosane ($C_{20}H_{42}$)		3.26	46.07	60.10	0.00
Propane (C_3H_8)		4.60	36.78	53.95	0.00
Butane (C_4H_{10})		4.61	13.41	5.17	0.00
Ethylbenzene (C_8H_{10})		20.71	2.92	56.92	0.00
Methyl isobutyl ketone ($C_6H_{12}O$)		21.79	31.81	29.89	0.00
Data Summary					
Acids (6)	Average	13.00	22.23	10.31	19.33
	Maximum	27.65	78.27	33.59	55.99
Alcohols (13)	Average	44.35	10.67	45.64	519.29
	Maximum	86.50	89.93	137.88	1,563.11
Others (36)	Average	3.10	10.58	19.78	2.91
	Maximum	21.79	46.07	60.10	32.39
All (55)	Average	13.93	11.87	24.86	126.75
	Maximum	86.50	89.93	137.88	1,563.11

A-W = Ambrose-Walton equation.
Shaded cells in Summary indicate least incremental error.

Table 2.7. Incremental Error Comparison Between Different Methods - Data Summaries.

Substance Type	Lowest A%Err		Incremental Error Increase		
			$F_{w,j}[AA]$	Riedel	A-W
			$T_{r,f}$		
Acids (6)	Average	13.00	22.23	10.31	19.33
	Maximu	27.65	78.27	33.59	55.99
Alcohols (13)	Average	44.35	10.67	45.64	519.29
	Maximu	86.50	89.93	137.88	1,563.11
Others (36)	Average	3.10	10.58	19.78	2.91
	Maximu	21.79	46.07	60.10	32.39
All (55)	Average	13.93	11.87	24.86	126.75
	Maximu	86.50	89.93	137.88	1,563.11
			$T_r \leq 0.6$		
Acids	Average	5.94	10.08	6.01	12.54
	Maximu	12.93	30.69	15.37	26.37
Alcohols	Average	14.92	4.67	19.04	148.38
	Maximu	26.91	33.10	57.83	351.83
Others	Average	1.20	3.64	5.46	1.40
	Maximu	7.65	23.19	21.00	16.64
All	Average	4.96	4.59	8.73	37.35
	Maximu	26.91	33.10	57.83	351.83
			$T_r > 0.6$		
Acids	Average	0.95	2.86	0.07	1.59
	Maximu	1.88	7.82	0.45	2.47
Alcohols	Average	1.15	1.01	1.08	1.99
	Maximu	2.42	2.63	6.36	4.19
Others	Average	0.13	0.53	0.42	0.05
	Maximu	0.76	3.58	2.79	0.35
All	Average	0.46	0.90	0.54	0.68
	Maximu	2.42	7.82	6.36	4.19
			All T_rs		
Acids	Average	3.32	5.48	1.86	5.22
	Maximu	5.85	16.09	5.27	12.58
Alcohols	Average	7.40	2.41	8.32	60.59
	Maximu	14.93	16.17	29.24	139.89
Others	Average	0.64	1.75	2.41	0.52
	Maximu	3.59	9.81	8.07	7.14
All	Average	2.53	2.31	3.75	15.23
	Maximu	14.93	16.17	29.24	139.89

A-W = Ambrose-Walton equation.
Shaded cells indicate least incremental error.

Table 2.8. Comparison of Antoine Analytic $P_{v,r}$ vs. Entire-Curve Wagner Analytic Values over the Antoine Range, and Predictive Method Lowest & Highest A%Err for “All T^rs.”

Species	Analytic Error: %Err of Antoine Analytic $P_{v,r}$ to entire-curve Wagner Analytic Values										A%Err “All T_rs”	
	$T_{r,f}$	$T_{r,b}$	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	Δ%Err	Lowest	Highest
Organic Acids												
Acetic Acid ($C_2H_4O_2$)		0.015			0.349	0.170	0.220	0.668			0.653	$F_{w,j}[AA]$	A-W
Propanoic acid ($C_3H_6O_2$)		-0.002			0.000	0.000	-0.100	-0.511			0.511	$F_{w,j}[AA]$	R
2-Methyl propanoic acid ($C_4H_8O_2$)		-0.013				-7.670	-6.024	-0.622			7.657	A-W	$F_{w,j}[AA]$
3-Methyl butanoic acid ($C_5H_{10}O_2$)		-0.013				-12.851	-5.781	-0.904	2.088		14.939	R	$F_{w,j}[AA]$
Butanoic acid ($C_4H_8O_2$)		0.010			0.120	0.000	-0.050	-0.682			0.802	R	A-W
Pentanoic acid ($C_5H_{10}O_2$)		0.000				-9.461	-6.258	-2.061	1.921		11.383	R	A-W
Alcohols												
1-Decanol ($C_{10}H_{22}O$)		0.008				-0.100	-0.020	0.040	0.090		0.190	$F_{w,j}[AA]$	A-W
1-Octanol ($C_8H_{18}O$)		0.008				-0.130	-0.230	-0.020	-0.130		0.238	$F_{w,j}[AA]$	A-W
Tert-butanol ($C_4H_{10}O$)	0.020	-0.002				-0.200	-0.070	0.300			0.500	$F_{w,j}[AA]$	A-W
1-Heptanol ($C_7H_{16}O$)		-0.013				0.866	0.548	0.389	-0.230		1.096	$F_{w,j}[AA]$	A-W
1-Nonanol ($C_9H_{20}O$)		-0.011				2.985	2.147	1.911	1.725		2.996	$F_{w,j}[AA]$	A-W
2-Octanol ($C_8H_{18}O$)		0.005				-6.780	-4.258	-0.924	2.293		9.073	$F_{w,j}[AA]$	A-W
Methanol (CH_4O)		0.015			0.170	0.010	-0.020				0.190	$F_{w,j}[AA]$	R
Ethanol (C_2H_6O)		-0.013			0.180	-0.010	0.050	-0.300			0.480	$F_{w,j}[AA]$	R
Isopropyl alcohol (C_3H_8O)		-0.011				-3.118	-0.803	0.110			3.228	$F_{w,j}[AA]$	R
Propanol (C_3H_8O)		0.010			1.025	-0.260	-0.080	-0.150			1.285	A-W	R
1-Butanol ($C_4H_{10}O$)		-0.016				0.090	0.030	-0.170			0.260	R	A-W
1-Pentanol ($C_5H_{12}O$)		-0.004				0.090	-0.030	-0.190			0.280	R	A-W
1-Hexanol ($C_6H_{14}O$)		0.003				0.250	-0.020	-0.341			0.590	R	A-W
Others												
Argon (Ar)	-0.401	-0.022			-0.421	-0.321					0.399	$F_{w,j}[AA]$	A-W
Water (H_2O)		-0.011	-0.220	-0.100	0.220	0.349	0.220	-0.040			0.570	$F_{w,j}[AA]$	A-W
Benzene (C_6H_6)		0.006		0.539	-0.080	-0.240	-0.210				0.779	$F_{w,j}[AA]$	A-W
Acetone (C_3H_6O)		0.015		0.827	0.190	0.060	0.030				0.812	$F_{w,j}[AA]$	A-W
Toluene (C_7H_8)		0.003		0.170	-0.070	-0.080	-0.090				0.260	$F_{w,j}[AA]$	R
p-Xylene (C_8H_{10})		-0.012		0.130	-0.100	-0.090	-0.110	-0.130			0.260	$F_{w,j}[AA]$	R
o-Xylene (C_8H_{10})		0.004		0.220	-0.070	-0.090	-0.040	-0.010			0.310	$F_{w,j}[AA]$	R

Species	Analytic Error: %Err of Antoine Analytic $P_{v,r}$ to entire-curve Wagner Analytic Values											A%Err "All T_rs"	
	$T_{r,f}$	**$T_{r,b}$**	**0.45**	**0.50**	**0.55**	**0.60**	**0.65**	**0.70**	**0.75**	**0.80**	**Δ%Err**	**Lowest**	**Highest**
Diethyl ether ($C_4H_{10}O$)		-0.012		0.379	0.558	0.678	0.489	0.150			0.690	$F_{w,j}[AA]$	R
Naphthalene ($C_{10}H_8$)		0.005		0.936	0.240	0.000	-0.130				1.066	$F_{w,j}[AA]$	R
Ammonia (NH_3)	-1.116	0.003		-1.288	-1.056	-0.341					1.291	$F_{w,j}[AA]$	R
Undecane ($C_{11}H_{24}$)		-0.004				0.160	0.010	-0.010	0.000		0.170	A-W	$F_{w,j}[AA]$
Butane (C_4H_{10})		-0.014		0.210	-0.220	-0.170	0.020				0.430	A-W	$F_{w,j}[AA]$
n-Tetradecane ($C_{14}H_{30}$)		-0.005				0.558	0.020	-0.060	-0.080	-0.030	0.638	A-W	$F_{w,j}[AA]$
Tridecane ($C_{13}H_{28}$)		-0.009				0.737	0.220	0.060	-0.030		0.767	A-W	$F_{w,j}[AA]$
Decane ($C_{10}H_{22}$)		-0.012			0.876	0.070	-0.040	-0.030	0.050		0.916	A-W	$F_{w,j}[AA]$
Propane (C_3H_8)		-0.012		0.906	0.479	0.339	0.329				0.918	A-W	$F_{w,j}[AA]$
Dodecane ($C_{12}H_{26}$)		-0.005				1.153	0.827	0.698	0.558		1.158	A-W	$F_{w,j}[AA]$
Hydrogen (H_2 normal)	1.292	0.120	1.528	1.094	0.846	0.379	0.280				1.408	A-W	$F_{w,j}[AA]$
m-Xylene (C_8H_{10})		-0.011			-1.725	-0.864	-0.381	-0.170			1.714	A-W	$F_{w,j}[AA]$
Methyl isobutyl ketone ($C_6H_{12}O$)		-0.010			0.190	-0.260	0.698	2.264			2.524	A-W	$F_{w,j}[AA]$
Eicosane ($C_{20}H_{42}$)		-0.004					5.029	2.955	1.459	0.250	5.033	A-W	$F_{w,j}[AA]$
R152a ($C_2H_4F_2$)		0.004		9.561	2.566	0.000	-0.040				9.601	A-W	$F_{w,j}[AA]$
n-Hexane (C_6H_{14})		-0.004			0.000	-0.040	-0.060	-0.040			0.060	A-W	R
n-Heptane (C_7H_{16})		0.009			0.120	-0.070	-0.080	-0.050			0.200	A-W	R
Octane (C_8H_{18})		0.000			0.270	0.030	0.020	0.020			0.270	A-W	R
Methane (CH_4)		-0.028		-0.300	-0.140	-0.160					0.272	A-W	R
Nonane (C_9H_{20})		-0.006			0.250	-0.040	-0.040	-0.010	-0.020		0.290	A-W	R
n-Pentane (C_5H_{12})		0.010		0.329	0.020	-0.020	-0.030	0.010			0.359	A-W	R
Ethylbenzene (C_8H_{10})		0.009		0.359	-0.080	-0.120	-0.130	-0.110			0.489	A-W	R
Ethane (C_2H_6)		0.002	0.548	0.399	0.310	0.090					0.546	A-W	R
Pentadecane ($C_{15}H_{32}$)		-0.010				0.558	-0.020	-0.050	0.000	0.100	0.608	A-W	R
Hexadecane ($C_{16}H_{34}$)		-0.011				0.975	0.060	-0.060	0.000	0.180	1.035	A-W	R
Heptadecane ($C_{17}H_{36}$)		-0.005					-0.060	0.359	0.916	1.509	1.569	A-W	R
Octadecane ($C_{18}H_{38}$)		-0.006					-0.060	0.717	1.666	2.635	2.695	A-W	R
Nonadecane ($C_{19}H_{40}$)		0.005					-1.268	-0.381	0.598	1.509	2.776	A-W	R
Nitrogen (N_2)	-0.090	0.022		-0.100	-0.070	0.020	0.220				0.320	R	$F_{w,j}[AA]$

Data Summary														
		Analytic Error: Average A%Err of Antoine Analytic $P_{v,r}$ to entire-curve Wagner Analytic Values										Average Δ%Err		
		$T_{r,f}$	$T_{r,b}$	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	Ave	$F_{w,j}$*[AA]* Lowest A%Err	$F_{w,j}$*[AA]* Not Lowest A%Err
Organic Acids (6)	# of Species	0	6	0	0	3	6	6	6	2	0	6	2	4
	Average		0.009			0.156	5.025	3.072	0.908	2.005		5.99	0.58	8.70
	Max		0.015			0.349	12.851	6.258	2.061	2.088		14.94	0.65	14.94
Alcohols (13)	# of Species	1	13	0	0	3	13	13	12	5	0	13	9	4
	Average	0.020	0.009			0.458	1.145	0.639	0.404	0.894		1.57	2.00	0.60
	Max	0.020	0.016			1.025	6.780	4.258	1.911	2.293		9.07	9.07	1.29
Others (36)	# of Species	4	36	3	18	26	32	32	23	12	7	36	10	26
	Average	0.725	0.012	0.766	0.992	0.429	0.283	0.352	0.365	0.448	0.887	1.20	0.64	1.41
	Max	1.292	0.120	1.528	9.561	2.566	1.153	5.029	2.955	1.666	2.635	9.60	1.29	9.60
All (55)	# of Species	5	55	3	18	32	51	51	41	19	7	55	21	34
	Average	0.584	0.011	0.766	0.992	0.407	1.061	0.745	0.456	0.729	0.887	1.81	1.22	2.18
	Max	1.292	0.120	1.528	9.561	2.566	12.851	6.258	2.955	2.293	2.635	14.94	9.07	14.94

A-W = Ambrose-Walton equation.

R = Riedel equation.

For the substance categories in the Summary, the smallest of the Average Δ%Err values between “$F_{w,j}$*[AA]* Lowest” and “$F_{w,j}$*[AA]* not Lowest” are shaded in gray.

Table 2.9. Incremental Error Comparison For Hypothetical Selection Rules Applied to "All T_rs."

Substance Type	Lowest A%Err		Incremental Error Increase			
			$F_{w,j}$[AA]]	Riedel	A-W	Hypothetical Rules
All T_rs						
Acids	Average	3.32	5.48	1.86	5.22	**0.88**
	Maximum	5.85	16.09	5.27	12.58	5.27
Alcohols	Average	7.40	2.41	8.32	60.59	2.41
	Maximum	14.93	16.17	29.24	139.89	16.17
Others	Average	0.64	1.75	2.42	0.52	**0.27**
	Maximum	3.59	9.81	8.07	7.14	**3.55**
All	Average	2.53	2.31	3.75	15.23	**0.84**
	Maximum	14.93	16.17	29.24	139.89	16.17

A-W = Ambrose-Walton equation.
Values for *$F_{w,j}$[AA]]*, Riedel, and Ambrose-Walton copied from Table 2.7 and included for reference.
Bold font indicates that the hypothetical selection rules result in less incremental error than the method previously determined to have the lowest (cells shaded gray).

Table 3.1. Hypothesized Performance Comparison of Modified Correlations vs. Standard Counterparts.

	$T_r < T_{r,b}$		$T_r > T_{r,b}$	
	R vs. R(ω)	**A-W vs. A-W(T_b)**	**R vs. R(ω)**	**A-W vs. A-W(T_b)**
$T_{b,r} > 0.7$	R(ω)	?	?	A-W(T_b)
$T_{b,r} < 0.7$	?	A-W(T_b)	R(ω)	?

Legend:
R = standard Riedel
R(ω) = Riedel(ω)
A-W = standard Ambrose-Walton
A-W(T_b) = Ambrose-Walton(T_b)

Table 3.2. Comparison of Standard and Modified Riedel and Ambrose-Walton Equations: A%Err @ $T_{r,f}$ Relative to Entire-Curve Wagner Analytics.

Species	**$T_{r,f}$**	**$T_{r,b}$**	**0.7 - $T_{r,b}$**	**A%Err**				**Least A%Err**	
				R	**R(ω)**	**A-W**	**A-W(T_b)**	**R vs. A-W**	**All Four**
Organic Acids with $T_{r,b}$ > 0.7									
Decanoic acid ($C_{10}H_{20}O_2$)	0.42032	0.74644	-0.04644	112.78	29.73	308.16	491.03	R	R(ω)
Octanoic acid ($C_8H_{16}O_2$)	0.41647	0.73670	-0.03670	27.77	10.72	190.58	258.95	R	R(ω)
3-Methyl butanoic acid ($C_5H_{10}O_2$)	0.38768	0.71491	-0.01491	27.65	36.19	34.69	41.91	R	R
Pentanoic acid ($C_5H_{10}O_2$)	0.37240	0.71432	-0.01432	22.85	17.04	78.84	89.34	R	R(ω)
2-Methyl propanoic acid ($C_4H_8O_2$)	0.37529	0.70674	-0.00674	44.88	38.41	11.29	10.04	A-W	A-W(T_b)
Butanoic acid ($C_4H_8O_2$)	0.42944	0.70011	-0.00011	10.16	10.16	21.88	21.88	R	R or R(ω)
Alcohols with $T_{r,b}$ > 0.7									
1-Eicosanol ($C_{20}H_{42}O$)	0.41904	0.80061	-0.10061	995.29	263.97	83.66	64.25	A-W	A-W(T_b)
1-Octadecanol ($C_{18}H_{38}O$)	0.41899	0.78932	-0.08932	483.81	294.28	121.16	104.60	A-W	A-W(T_b)
1-Heptadecanol ($C_{17}H_{36}O$)	0.41923	0.78349	-0.08349	324.57	325.03	153.86	140.20	A-W	A-W(T_b)
1-Hexadecanol ($C_{16}H_{34}O$)	0.41877	0.77601	-0.07601	221.49	331.33	175.41	166.42	A-W	A-W(T_b)
1-Dodecanol ($C_{12}H_{26}O$)	0.41264	0.74692	-0.04692	148.16	534.90	517.99	546.63	R	R
1-Decanol ($C_{10}H_{22}O$)	0.40646	0.73186	-0.03186	145.27	496.20	739.89	800.88	R	R
1-Nonanol ($C_9H_{20}O$)	0.39933	0.72453	-0.02453	134.43	432.12	815.13	884.34	R	R
1-Octanol ($C_8H_{18}O$)	0.39487	0.71774	-0.01774	110.88	267.66	798.81	868.42	R	R
2-Ethyl-1-hexanol ($C_8H_{18}O$)	0.31725	0.71471	-0.01471	850.96	3,524.13	16,749.40	18,499.13	R	R
1-Heptanol ($C_7H_{16}O$)	0.37818	0.71099	-0.01099	129.13	286.28	1,126.07	1,195.01	R	R
2-Octanol ($C_8H_{18}O$)	0.37798	0.71008	-0.01008	138.69	635.07	1,623.25	1,695.38	R	R
1-Hexanol ($C_6H_{14}O$)	0.37531	0.70483	-0.00483	70.78	51.29	827.66	867.17	R	R(ω)
Tert-butanol ($C_4H_{10}O$)	0.58979	0.70227	-0.00227	6.24	0.70	29.38	29.94	R	R(ω)
"Others" with $T_{r,b}$ > 0.7									
Helium (He normal)	0.41346	0.81485	-0.11485	27.83	14.61	31.46	31.46	R	R(ω)
Eicosane ($C_{20}H_{42}$)	0.40306	0.80213	-0.10213	63.36	57.96	3.26	4.53	A-W	A-W
Nonadecane ($C_{19}H_{40}$)	0.40270	0.79464	-0.09464	53.96	50.25	2.20	3.45	A-W	A-W
Octadecane ($C_{18}H_{38}$)	0.40391	0.78861	-0.08861	34.68	46.30	4.90	6.04	A-W	A-W
Heptadecane ($C_{17}H_{36}$)	0.40154	0.78171	-0.08171	35.15	43.02	2.61	2.61	A-W	A-W or A-W(T_b)
Hexadecane ($C_{16}H_{34}$)	0.40349	0.77560	-0.07560	32.06	44.18	0.34	1.53	A-W	A-W
Pentadecane ($C_{15}H_{32}$)	0.39983	0.76811	-0.06811	31.64	35.58	0.26	1.49	A-W	A-W
n-Tetradecane ($C_{14}H_{30}$)	0.40261	0.76012	-0.06012	25.50	39.42	1.31	1.31	A-W	A-W or A-W(T_b)
Tridecane ($C_{13}H_{28}$)	0.39609	0.75242	-0.05242	23.16	32.83	0.55	0.55	A-W	A-W or A-W(T_b)

Species	$T_{r,f}$	$T_{r,b}$	0.7 - $T_{r,b}$	A%Err				Least A%Err	
				R	R(ω)	A-W	A-W(T_b)	R vs. A-W	All Four
Dodecane ($C_{12}H_{26}$)	0.40056	0.74350	-0.04350	18.26	32.46	0.70	0.70	A-W	A-W or A-W(T_b)
Undecane ($C_{11}H_{24}$)	0.38752	0.73425	-0.03425	18.21	34.41	0.37	0.37	A-W	A-W or A-W(T_b)
Decane ($C_{10}H_{22}$)	0.39422	0.72420	-0.02420	11.92	22.86	1.25	1.25	A-W	A-W or A-W(T_b)
Nonane (C_9H_{20})	0.36924	0.71267	-0.01267	16.89	28.27	0.76	0.76	A-W	A-W or A-W(T_b)
Octane (C_8H_{18})	0.38033	0.70097	-0.00097	10.67	146.65	0.33	0.33	A-W	A-W or A-W(T_b)
Organic Acids with $T_{r,b}$ < 0.7									
Propanoic acid ($C_3H_6O_2$)	0.41773	0.68595	0.01405	14.54	1.08	11.84	11.84	A-W	R(ω)
Acetic Acid ($C_2H_4O_2$)	0.48889	0.65975	0.04025	19.73	7.37	35.38	29.49	R	R(ω)
Formic acid (CH_2O_2)	0.47874	0.63612	0.06388	2.58	7.53	34.65	28.41	R	R
Alcohols with $T_{r,b}$ < 0.7									
Isopropyl alcohol (C_3H_8O)	0.36130	0.69917	0.00083	79.95	38.36	45.35	45.35	A-W	R(ω)
1-Pentanol ($C_5H_{12}O$)	0.33027	0.69907	0.00093	0.39	2,306.84	819.54	819.54	R	R
2-Butanol ($C_4H_{10}O$)	0.29570	0.69526	0.00474	144.42	117.49	3,933.02	3,754.01	R	R(ω)
1-Butanol ($C_4H_{10}O$)	0.32564	0.69422	0.00578	59.47	39.66	234.28	221.94	R	R(ω)
Propanol (C_3H_8O)	0.27386	0.68985	0.01015	98.77	96.57	86.50	87.53	A-W	A-W
Ethanol (C_2H_6O)	0.30948	0.68384	0.01616	98.47	87.58	93.38	93.52	A-W	R(ω)
Benzyl alcohol (C_7H_8O)	0.36056	0.66917	0.03083	53.90	36.38	521.77	411.82	R	R(ω)
Cyclohexanol ($C_6H_{12}O$)	0.45792	0.66767	0.03233	15.05	30.72	299.96	236.96	R	R
Methanol (CH_4O)	0.34233	0.65872	0.04128	97.53	36.78	88.16	86.22	A-W	R(ω)
"Others" with $T_{r,b}$ < 0.7 (Normal)									
Pentafluorotoluene ($C_7H_3F_5$)	0.42955	0.68958	0.01042	8.10	5.89	11.05	11.05	R	R(ω)
n-Heptane (C_7H_{16})	0.33804	0.68790	0.01210	22.59	92.63	0.27	0.27	A-W	A-W or A-W(T_b)
Acetic Anhydride ($C_4H_6O_3$)	0.32838	0.68101	0.01899	30.20	141.84	11.89	10.26	A-W	A-W(T_b)
Pentafluorobenzene (C_6HF_5)	0.42535	0.67591	0.02409	3.74	23.23	0.53	1.56	A-W	A-W
n-Hexane (C_6H_{14})	0.35015	0.67313	0.02687	14.30	53.76	0.95	0.95	A-W	A-W or A-W(T_b)
m-Xylene (C_8H_{10})	0.36509	0.66825	0.03175	9.71	35.49	1.45	1.45	A-W	A-W or A-W(T_b)
p-Xylene (C_8H_{10})	0.46478	0.66781	0.03219	5.78	7.42	5.35	4.57	A-W	A-W(T_b)
Ethylbenzene (C_8H_{10})	0.28869	0.66325	0.03675	77.62	142.30	20.71	20.71	A-W	A-W or A-W(T_b)
o-Xylene (C_8H_{10})	0.39340	0.66250	0.03750	2.72	30.32	3.15	1.96	R	A-W(T_b)
n-Pentane (C_5H_{12})	0.30530	0.65819	0.04181	27.79	77.15	1.08	1.08	A-W	A-W or A-W(T_b)
Naphthalene ($C_{10}H_8$)	0.46947	0.65628	0.04372	3.50	8.42	3.23	1.67	A-W	A-W(T_b)
Toluene (C_7H_8)	0.30105	0.64851	0.05149	65.04	145.86	23.15	25.82	A-W	A-W
Cyclopentanone (C_5H_8O)	0.35629	0.64647	0.05353	11.69	26.28	1.18	0.36	A-W	A-W(T_b)
Butane (C_4H_{10})	0.31697	0.64119	0.05881	9.78	42.23	4.61	4.61	A-W	A-W or A-W(T_b)
Benzene (C_6H_6)	0.49573	0.62836	0.07164	3.38	4.11	7.48	5.28	R	R

Species	**$T_{r,f}$**	**$T_{r,b}$**	**0.7 - $T_{r,b}$**	**A%Err**				**Least A%Err**	
				R	**R(ω)**	**A-W**	**A-W(T_b)**	**R vs. A-W**	**All Four**
Propane (C_3H_8)	0.23111	0.62462	0.07538	58.55	159.11	4.60	4.60	A-W	A-W or A-W(T_b)
Hydrogen (H_2 normal)	0.40905	0.61456	0.08544	6.47	0.51	0.50	0.57	A-W	A-W
Nitrogen (N_2)	0.50040	0.61289	0.08711	0.50	1.19	2.98	1.62	R	R
Ethane (C_2H_6)	0.29591	0.60444	0.09556	14.30	46.35	2.64	2.64	A-W	A-W or A-W(T_b)
Methane (CH_4)	0.47594	0.58597	0.11403	1.91	1.12	0.45	0.45	A-W	A-W or A-W(T_b)
Argon (Ar)	0.55611	0.57936	0.12064	0.13	0.13	1.25	0.25	R	R
"Others" with $T_{r,b}$ < 0.7 (Polar)									
Methyl isobutyl ketone ($C_6H_{12}O$)	0.32919	0.67726	0.02274	51.68	50.86	21.79	19.60	A-W	A-W(T_b)
Diethyl ether ($C_4H_{10}O$)	0.33608	0.65900	0.04100	34.41	60.85	16.15	16.15	A-W	A-W or A-W(T_b)
Acetone (C_3H_6O)	0.35131	0.64795	0.05205	9.00	36.32	23.84	20.16	R	R
R152a ($C_2H_4F_2$)	0.40410	0.64472	0.05528	6.75	14.01	10.66	8.58	R	R
Ammonia (NH_3)	0.48190	0.59141	0.10859	5.10	2.06	8.42	4.94	R	R(ω)
Water (H_2O)	0.42211	0.57663	0.12337	17.20	5.00	32.73	21.34	R	R(ω)
Summary									
Acids (9)	$T_{r,b}$ > 0.7 (6)			41.02	23.71	107.57	152.19	R	R(ω)
	$T_{r,b}$ < 0.7 (3)			12.28	5.33	27.29	23.25	R	R(ω)
Alcohols (22)	$T_{r,b}$ > 0.7 (13)			289.21	572.54	1,827.82	1,989.41	R	R
	$T_{r,b}$ < 0.7 (9)			71.99	310.04	680.22	639.65	R	R
"Others" (41)	$T_{r,b}$ > 0.7 (14)			28.81	44.91	3.59	4.03	A-W	A-W
	$T_{r,b}$ < 0.7 (27)			18.59	44.98	8.22	7.17	A-W	A-W(Tb)
	Normal (21)			17.99	49.78	5.17	4.85	A-W	A-W(Tb)
	Polar (6)			20.69	28.18	18.93	15.13	A-W	A-W(Tb)

Legend:
R = Riedel; R(ω) = Riedel(ω); A-W = Ambrose-Walton; and A-W(T_b) = Ambrose-Walton(T_b).
When two correlations are shown in the “All Four” field, both have the same error when rounded off to hundredths of percent.

Table 3.3. Comparison of Standard and Modified Riedel and Ambrose-Walton Equations: A%Err for Below & Above T_b Relative to Entire-Curve Wagner Analytics.

Species	Average A% Error											
	$T_r < T_{r,b}$						$T_r > T_{r,b}$					
	R	R(ω)	A-W	A-W(T_b)	Least		R	R(ω)	A-W	A-W(T_b)	Least	
					R vs. A-W	All Four					R vs. A-W	All Four
Organic Acids with $T_{r,b} > 0.7$												
Decanoic acid ($C_{10}H_{20}O_2$)	40.54	10.12	93.94	148.33	R	R(ω)	2.30	0.52	7.35	4.43	R	R(ω)
Octanoic acid ($C_8H_{16}O_2$)	9.36	4.34	58.16	79.98	R	R(ω)	1.34	0.67	5.52	3.86	R	R(ω)
3-Methyl butanoic acid ($C_5H_{10}O_2$)	8.77	12.37	17.48	20.75	R	R	1.11	0.86	3.63	3.24	R	R(ω)
Pentanoic acid ($C_5H_{10}O_2$)	9.72	7.43	29.59	33.76	R	R(ω)	0.64	0.76	3.47	3.07	R	R
2-Methyl propanoic acid ($C_4H_8O_2$)	14.97	12.27	4.14	4.45	A-W	A-W	0.75	0.95	2.71	2.61	R	R
Butanoic acid ($C_4H_8O_2$)	3.09	3.09	10.59	10.59	R	R or R(ω)	1.29	1.29	2.97	2.97	R	R or R(ω)
Alcohols with $T_{r,b} > 0.7$												
1-Eicosanol ($C_{20}H_{42}O$)	181.31	49.96	15.78	11.96	A-W	A-W(T_b)	0.51	0.39	0.78	0.17	R	A-W(T_b)
1-Octadecanol ($C_{18}H_{38}O$)	96.23	58.17	24.60	20.64	A-W	A-W(T_b)	0.15	0.45	0.79	0.28	R	R
1-Heptadecanol ($C_{17}H_{36}O$)	63.56	63.65	31.37	27.97	A-W	A-W(T_b)	0.54	0.54	0.79	0.43	R	A-W(T_b)
1-Hexadecanol ($C_{16}H_{34}O$)	41.87	64.03	35.45	33.21	A-W	A-W(T_b)	0.96	0.61	0.73	0.51	A-W	A-W(T_b)
1-Dodecanol ($C_{12}H_{26}O$)	27.67	101.45	102.83	109.14	R	R	2.47	1.01	0.43	0.44	A-W	A-W
1-Decanol ($C_{10}H_{22}O$)	24.97	88.09	134.07	145.64	R	R	3.11	1.39	0.80	0.46	A-W	A-W(T_b)
1-Nonanol ($C_9H_{20}O$)	31.19	104.01	196.40	213.40	R	R	3.08	1.55	1.12	0.68	A-W	A-W(T_b)
1-Octanol ($C_8H_{18}O$)	25.06	63.90	186.99	203.36	R	R	3.14	2.02	1.51	1.05	A-W	A-W(T_b)
2-Ethyl-1-hexanol ($C_8H_{18}O$)	131.19	495.70	2,121.92	2,328.96	R	R	3.37	1.85	1.55	1.11	A-W	A-W(T_b)
1-Heptanol ($C_7H_{16}O$)	24.06	56.38	207.53	219.83	R	R	2.56	1.54	2.01	1.63	A-W	R(ω)
2-Octanol ($C_8H_{18}O$)	23.40	109.58	266.58	278.00	R	R	3.59	1.34	1.48	1.22	A-W	A-W(T_b)
1-Hexanol ($C_6H_{14}O$)	14.01	9.66	164.82	172.40	R	R(ω)	1.83	2.09	2.80	2.50	R	R
Tert-butanol ($C_4H_{10}O$)	3.18	0.49	14.03	14.41	R	R(ω)	2.03	1.06	5.94	5.85	R	R(ω)
"Others" with $T_{r,b} > 0.7$												
Helium (He normal)	7.74	3.84	7.11	7.11	A-W	R(ω)	0.26	0.32	0.16	0.16	A-W	A-W W or A-W(T_b)
Eicosane ($C_{20}H_{42}$)	12.26	10.98	0.98	1.46	A-W	A-W	0.40	0.43	0.07	0.01	A-W	A-W(T_b)
Nonadecane ($C_{19}H_{40}$)	10.76	9.82	0.67	1.16	A-W	A-W	0.31	0.33	0.09	0.02	A-W	A-W(T_b)

Species	**Average A% Error**											
	$T_r < T_{r,b}$						**$T_r > T_{r,b}$**					
	R	**R(ω)**	**A-W**	**A-W(T_b)**	**Least**		**R**	**R(ω)**	**A-W**	**A-W(T_b)**	**Least**	
					R vs. A-W	**All Four**					**R vs. A-W**	**All Four**
Octadecane ($C_{18}H_{38}$)	6.17	8.94	1.50	1.98	A-W	A-W	0.32	0.26	0.09	0.02	A-W	A-W(T_b)
Heptadecane ($C_{17}H_{36}$)	6.09	7.92	0.87	0.87	A-W	A-W or A-W(T_b)	0.30	0.25	0.02	0.02	A-W	A-W or A-W(T_b)
Hexadecane ($C_{16}H_{34}$)	5.65	8.61	0.13	0.61	A-W	A-W	0.28	0.19	0.04	0.03	A-W	A-W(T_b)
Pentadecane ($C_{15}H_{32}$)	7.36	8.52	0.14	0.66	A-W	A-W	0.24	0.20	0.06	0.02	A-W	A-W(T_b)
n-Tetradecane ($C_{14}H_{30}$)	4.57	8.17	0.50	0.50	A-W	A-W or A-W(T_b)	0.20	0.08	0.01	0.01	A-W	A-W or A-W(T_b)
Tridecane ($C_{13}H_{28}$)	4.85	7.33	0.29	0.29	A-W	A-W or A-W(T_b)	0.22	0.12	0.03	0.03	A-W	A-W or A-W(T_b)
Dodecane ($C_{12}H_{26}$)	3.27	6.81	0.33	0.33	A-W	A-W or A-W(T_b)	0.20	0.06	0.01	0.01	A-W	A-W or A-W(T_b)
Undecane ($C_{11}H_{24}$)	3.59	7.52	0.11	0.11	A-W	A-W or A-W(T_b)	0.23	0.04	0.01	0.01	A-W	A-W or A-W(T_b)
Decane ($C_{10}H_{22}$)	2.91	5.39	0.52	0.52	A-W	A-W or A-W(T_b)	0.23	0.07	0.02	0.02	A-W	A-W or A-W(T_b)
Nonane (C_9H_{20})	3.78	6.23	0.30	0.30	A-W	A-W or A-W(T_b)	0.25	0.09	0.03	0.03	A-W	A-W or A-W(T_b)
Octane (C_8H_{18})	2.34	37.05	0.06	0.06	A-W	A-W or A-W(T_b)	0.26	1.55	0.03	0.03	A-W	A-W or A-W(T_b)
Organic Acids with $T_{r,b}$ < 0.7												
Propanoic acid ($C_3H_6O_2$)	6.49	1.01	3.49	3.49	A-W	R(ω)	0.77	1.25	1.50	1.50	R	R
Acetic Acid ($C_2H_4O_2$)	10.23	2.35	19.49	14.64	R	R(ω)	2.61	0.38	2.16	3.39	A-W	R(ω)
Formic acid (CH_2O_2)	1.45	3.12	17.95	12.67	R	R	2.15	0.95	0.86	1.90	A-W	A-W
Alcohols with $T_{r,b}$ < 0.7												
Isopropyl alcohol (C_3H_8O)	28.12	11.08	14.49	14.49	A-W	R(ω)	1.52	3.51	4.29	4.29	R	R
1-Pentanol ($C_5H_{12}O$)	0.35	400.17	188.66	188.66	R	R	0.35	4.05	3.72	3.72	R	R
2-Butanol ($C_4H_{10}O$)	33.58	26.97	709.75	680.60	R	R(ω)	1.38	1.25	5.27	5.49	R	R(ω)
1-Butanol ($C_4H_{10}O$)	18.05	9.33	80.50	76.85	R	R(ω)	0.81	1.39	4.60	4.82	R	R
Propanol (C_3H_8O)	46.74	39.26	26.44	26.21	A-W	A-W(T_b)	0.61	1.43	3.85	4.18	R	R
Ethanol (C_2H_6O)	50.65	32.69	35.11	35.49	A-W	R(ω)	1.94	1.23	1.70	1.80	A-W	R(ω)
Benzyl alcohol (C_7H_8O)	26.10	7.94	139.28	109.99	R	R(ω)	2.34	0.56	3.68	4.79	R	R(ω)
Cyclohexanol ($C_6H_{12}O$)	3.77	9.33	102.97	79.00	R	R	0.54	0.30	4.92	6.66	R	R(ω)
Methanol (CH_4O)	56.29	13.34	42.15	38.75	A-W	R(ω)	7.97	0.87	0.87	1.74	A-W	A-W

Species	Average A% Error											
	$T_r < T_{r,b}$						$T_r > T_{r,b}$					
	R	R(ω)	A-W	A-W(T_b)	Least		R	R(ω)	A-W	A-W(T_b)	Least	
					R vs. A-W	All Four					R vs. A-W	All Four
"Others" with $T_{r,b}$ < 0.7 (Normal)												
Pentafluorotoluene ($C_7H_3F_5$)	4.98	1.48	4.57	4.57	A-W	R(ω)	0.63	0.16	0.30	0.30	A-W	R(ω)
n-Heptane (C_7H_{16})	4.68	22.42	0.39	0.39	A-W	A-W or A-W(T_b)	0.30	0.51	0.08	0.08	A-W	A-W or A-W(T_b)
Acetic Anhydride ($C_4H_6O_3$)	6.49	27.00	6.92	6.17	R	A-W(T_b)	1.04	0.12	0.53	0.64	A-W	R(ω)
Pentafluorobenzene (C_6HF_5)	1.70	5.65	0.77	0.50	A-W	A-W(T_b)	0.57	0.21	0.13	0.23	A-W	A-W
n-Hexane (C_6H_{14})	3.07	12.62	0.32	0.32	A-W	A-W or A-W(T_b)	0.41	0.26	0.04	0.04	A-W	A-W or A-W(T_b)
m-Xylene (C_8H_{10})	3.10	8.74	1.34	1.34	A-W	A-W or A-W(T_b)	0.64	0.10	0.21	0.21	A-W	R(ω)
p-Xylene (C_8H_{10})	3.62	2.28	2.89	2.36	A-W	R(ω)	0.96	0.07	0.45	0.54	A-W	R(ω)
Ethylbenzene (C_8H_{10})	14.70	29.12	4.94	4.94	A-W	A-W or A-W(T_b)	0.46	0.09	0.06	0.06	A-W	A-W or A-W(T_b)
o-Xylene (C_8H_{10})	2.30	8.78	2.19	1.50	A-W	A-W(T_b)	0.79	0.14	0.24	0.32	A-W	R(ω)
n-Pentane (C_5H_{12})	5.23	15.73	0.47	0.47	A-W	A-W or A-W(T_b)	0.62	0.07	0.15	0.15	A-W	R(ω)
Naphthalene ($C_{10}H_8$)	2.28	3.06	1.84	0.80	A-W	A-W(T_b)	0.83	0.18	0.24	0.43	A-W	R(ω)
Toluene (C_7H_8)	11.69	29.74	4.77	5.58	A-W	A-W	0.62	0.16	0.10	0.18	A-W	A-W
Cyclopentanone (C_5H_8O)	2.65	6.25	0.74	0.10	A-W	A-W(T_b)	0.27	0.21	0.23	0.30	A-W	R(ω)
Butane (C_4H_{10})	2.78	10.97	1.19	1.19	A-W	A-W or A-W(T_b)	0.47	0.18	0.04	0.04	A-W	A-W or A-W(T_b)
Benzene (C_6H_6)	1.29	1.65	4.04	2.42	R	R	0.15	0.09	0.21	0.48	R	R(ω)
Propane (C_3H_8)	10.17	30.51	0.94	0.94	A-W	A-W or A-W(T_b)	0.52	0.13	0.02	0.02	A-W	A-W or A-W(T_b)
Hydrogen (H_2 normal)	2.92	0.33	1.01	0.47	A-W	R(ω)	0.49	0.04	0.24	0.30	A-W	R(ω)
Nitrogen (N_2)	0.39	0.43	1.72	0.68	R	R	0.28	0.14	0.17	0.34	A-W	R(ω)
Ethane (C_2H_6)	3.52	12.38	0.82	0.82	A-W	A-W or A-W(T_b)	0.66	0.13	0.02	0.02	A-W	A-W or A-W(T_b)
Methane (CH_4)	1.06	0.40	0.23	0.23	A-W	A-W or A-W(T_b)	0.68	0.11	0.05	0.05	A-W	A-W or A-W(T_b)
Argon (Ar)	0.07	0.08	1.09	0.14	R	R	0.33	0.14	0.18	0.36	A-W	R(ω)
"Others" with $T_{r,b}$ < 0.7 (Polar)												
Methyl isobutyl ketone	9.48	9.30	6.22	5.33	A-W	A-W(T_b)	0.15	0.15	0.29	0.39	R	R

Species	Average A% Error											
	$T_r < T_{r,b}$						$T_r > T_{r,b}$					
	R	R(ω)	A-W	A-W(T_b)	Least		R	R(ω)	A-W	A-W(T_b)	Least	
					R vs. A-W	All Four					R vs. A-W	All Four
($C_6H_{12}O$)												
Diethyl ether ($C_4H_{10}O$)	7.15	14.45	4.96	4.96	A-W	A-W or A-W(T_b)	0.31	0.13	0.09	0.09	A-W	A-W or A-W(T_b)
Acetone (C_3H_6O)	6.83	8.39	9.98	7.83	R	R	1.12	0.16	0.42	0.68	A-W	R(ω)
R152a ($C_2H_4F_2$)	4.30	3.82	4.72	3.43	R	A-W(T_b)	0.94	0.10	0.29	0.47	A-W	R(ω)
Ammonia (NH_3)	2.89	0.87	5.50	2.65	R	R(ω)	1.54	0.23	0.46	0.73	A-W	R(ω)
Water (H_2O)	8.84	1.92	19.61	10.34	R	R(ω)	3.41	0.13	1.35	2.57	A-W	R(ω)
Summary												
Organic Acids (9)												
$T_{r,b} > 0.7$ (6)	14.62	8.39	36.18	50.39	R	R(ω)	1.22	0.85	4.20	3.34	R	R(ω)
$T_{r,b} < 0.7$ (3)	6.29	1.95	11.98	9.17	R	R(ω)	1.88	0.85	1.49	2.27	A-W	R(ω)
Alcohols (22)												
$T_{r,b} > 0.7$ (13)	58.83	106.00	298.48	322.45	R	R	2.27	1.30	1.70	1.37	A-W	R(ω)
$T_{r,b} < 0.7$ (9)	30.94	63.82	157.80	148.69	R	R	1.99	1.59	3.64	4.17	R	R(ω)
"Others" (41)												
$T_{r,b} > 0.7$ (14)	9.95	9.63	1.02	1.20	A-W	A-W	0.27	0.29	0.04	0.03	A-W	A-W(T_b)
$T_{r,b} < 0.7$ (27)	5.51	12.55	3.41	2.76	A-W	A-W(T_b)	0.73	0.15	0.25	0.39	A-W	R(ω)
Normal (21)	5.08	13.83	2.17	1.93	A-W	A-W(T_b)	0.55	0.15	0.17	0.24	A-W	R(ω)
Polar (6)	7.07	7.82	8.03	5.84	R	A-W(T_b)	1.35	0.15	0.52	0.88	A-W	R(ω)
R = standard Riedel; R(ω) = Riedel(ω); A-W = standard Ambrose-Walton; and A-W(T_b) = Ambrose-Walton(T_b).												

Table 3.4. Comparison of Average A%Err of $F_{w,j}$ Functions for Entire Two-Phase Curve ("All T_rs").

Species	Average A%Err for Entire Curve						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
Organic Acids with $T_{r,b}$ > 0.7							
Decanoic acid ($C_{10}H_{20}O_2$)	7.68	40.54	25.18	2.75	244.12	92.55	119.53
Octanoic acid ($C_8H_{16}O_2$)	4.62	8.21	6.09	1.23	135.23	49.97	62.98
3-Methyl butanoic acid ($C_5H_{10}O_2$)	9.14	5.27	5.00	5.79	91.91	13.46	14.49
Pentanoic acid ($C_5H_{10}O_2$)	7.63	10.11	5.68	4.29	191.05	21.61	25.28
2-Methyl propanoic acid ($C_4H_8O_2$)	9.08	11.93	8.55	7.18	36.23	3.32	2.88
Butanoic acid ($C_4H_8O_2$)	3.27	3.27	1.92	4.57	20.26	6.85	27,783.21
Alcohols with $T_{r,b}$ > 0.7							
1-Eicosanol ($C_{20}H_{42}O$)	30.06	81.72	131.77	68.39	6.57	9.05	11.19
1-Octadecanol ($C_{18}H_{38}O$)	33.28	52.22	65.54	52.68	11.76	14.40	16.50
1-Heptadecanol ($C_{17}H_{36}O$)	36.64	36.71	43.16	47.02	15.45	19.31	21.75
1-Hexadecanol ($C_{16}H_{34}O$)	36.86	23.30	28.44	40.58	18.02	22.83	25.48
1-Dodecanol ($C_{12}H_{26}O$)	52.09	4.52	16.50	40.40	70.74	65.07	69.81
1-Decanol ($C_{10}H_{22}O$)	44.95	5.10	15.13	35.42	149.27	87.37	93.20
1-Nonanol ($C_9H_{20}O$)	49.06	7.24	18.03	39.70	320.14	123.54	134.90
1-Octanol ($C_8H_{18}O$)	29.48	5.46	14.95	27.54	576.26	119.05	131.88
2-Ethyl-1-hexanol ($C_8H_{18}O$)	190.97	16.49	79.43	136.12	308,214.03	1,448.59	1,671.11
1-Heptanol ($C_7H_{16}O$)	25.13	5.36	14.22	24.57	1,471.85	129.30	140.77
2-Octanol ($C_8H_{18}O$)	50.34	15.02	13.63	35.54	1,128.12	161.67	177.20
1-Hexanol ($C_6H_{14}O$)	2.73	8.78	9.02	8.03	5,286.64	103.57	148.73
Tert-butanol ($C_4H_{10}O$)	0.83	1.73	1.89	0.82	5.50	7.22	6.46
"Others" with $T_{r,b}$ > 0.7							

Species	**Average A%Err for Entire Curve**						
	$\boldsymbol{F_{w,j}[R(\omega)]}$	$\boldsymbol{F_{w,j}^{(1)}}$ $\boldsymbol{[R\mid R(\omega)]}$	$\boldsymbol{F_{w,j}^{(2)}}$ $\boldsymbol{[R\mid R(\omega)]}$	$\boldsymbol{F_{w,j}^{(3)}}$ $\boldsymbol{[R\mid R(\omega)]}$	$\boldsymbol{F_{w,j}^{(1)}}$ $\boldsymbol{[A\text{-}W(T_b)\mid R(\omega)]}$	$\boldsymbol{F_{w,j}^{(2)}}$ $\boldsymbol{[A\text{-}W(T_b)\mid R(\omega)]}$	$\boldsymbol{F_{w,j}^{(3)}}$ $\boldsymbol{[A\text{-}W(T_b)\mid R(\omega)]}$
Helium (He normal)	2.44	4.63	5.73	4.40	3.78	5.28	6.40
Eicosane ($C_{20}H_{42}$)	5.07	5.70	9.19	10.97	2.25	1.61	4.29
Nonadecane ($C_{19}H_{40}$)	3.99	4.45	7.65	9.32	1.96	1.29	3.42
Octadecane ($C_{18}H_{38}$)	3.48	2.03	4.51	7.50	3.06	1.31	0.75
Heptadecane ($C_{17}H_{36}$)	2.91	1.89	4.46	6.86	2.20	0.56	1.26
Hexadecane ($C_{16}H_{34}$)	3.44	1.61	4.13	6.88	1.13	0.36	0.75
Pentadecane ($C_{15}H_{32}$)	2.49	1.73	5.13	7.13	1.17	0.78	2.10
n-Tetradecane ($C_{14}H_{30}$)	2.98	0.54	3.17	5.76	0.76	0.54	1.37
Tridecane ($C_{13}H_{28}$)	1.90	0.59	3.43	5.52	0.13	0.16	0.38
Dodecane ($C_{12}H_{26}$)	1.95	1.30	2.17	4.30	0.23	0.35	0.68
Undecane ($C_{11}H_{24}$)	1.83	2.54	2.41	4.56	0.04	0.09	0.23
Decane ($C_{10}H_{22}$)	0.58	3.15	1.87	3.17	0.90	0.27	0.70
Nonane (C_9H_{20})	0.52	4.14	2.40	3.59	2.84	0.15	1.12
Octane (C_8H_{18})	17.59	15.21	1.39	12.42	12.58	0.60	8.56
Organic Acids with $T_{r,b}$ < 0.7							
Propanoic acid ($C_3H_6O_2$)	2.60	7.48	3.47	1.48	0.83	2.23	3.03
Acetic Acid ($C_2H_4O_2$)	0.83	5.69	3.91	0.34	7.40	5.68	1.53
Formic acid (CH_2O_2)	1.92	0.85	0.79	0.99	4.87	4.20	2.85
Alcohols with $T_{r,b}$ < 0.7							
Isopropyl alcohol (C_3H_8O)	9.38	24.97	16.20	11.22	13.69	9.37	8.99
1-Pentanol ($C_5H_{12}O$)	166.53	29.37	1.89	50.35	57.83	106.33	121.54
2-Butanol ($C_4H_{10}O$)	1.62	11.19	20.27	18.99	67,645,330.60	405.55	131.63
1-Butanol ($C_4H_{10}O$)	9.62	18.19	10.32	7.66	12,791.91	45.74	7.43
Propanol (C_3H_8O)	26.05	32.80	28.29	25.73	6,464.06	16.67	21.13

Species	**Average A%Err for Entire Curve**						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
Ethanol (C_2H_6O)	21.08	33.77	29.30	23.67	18.82	20.75	21.42
Benzyl alcohol (C_7H_8O)	0.79	21.98	12.80	4.81	582.70	51.40	17.36
Cyclohexanol ($C_6H_{12}O$)	3.17	0.84	2.03	3.43	69.90	30.38	9.24
Methanol (CH_4O)	10.16	33.19	29.11	20.08	24.11	19.81	15.98
"Others" with $T_{r,b}$ < 0.7 (Normal)							
Pentafluorotoluene ($C_7H_3F_5$)	0.91	5.32	2.55	0.56	2.99	2.34	1.79
n-Heptane (C_7H_{16})	6.85	12.80	2.72	7.60	7.31	0.42	2.24
Acetic Anhydride ($C_4H_6O_3$)	7.78	15.01	3.81	7.49	11.93	3.51	0.40
Pentafluorobenzene (C_6HF_5)	1.76	3.60	0.98	2.09	0.81	0.30	0.69
n-Hexane (C_6H_{14})	2.93	7.68	1.70	4.14	2.78	0.24	0.86
m-Xylene (C_8H_{10})	1.35	6.48	1.76	2.96	1.65	0.79	0.44
p-Xylene (C_8H_{10})	0.47	3.12	1.53	0.60	1.60	1.06	0.28
Ethylbenzene (C_8H_{10})	5.19	8.34	8.44	11.26	5.88	2.73	2.22
o-Xylene (C_8H_{10})	2.22	5.81	1.19	2.61	2.53	0.70	0.43
n-Pentane (C_5H_{12})	1.73	8.99	2.97	4.96	1.39	0.34	0.24
Naphthalene ($C_{10}H_8$)	0.83	2.27	0.75	0.91	0.60	0.24	0.28
Toluene (C_7H_8)	6.58	6.57	6.40	9.54	2.24	2.96	3.35
Cyclopentanone (C_5H_8O)	0.30	3.44	1.47	2.27	0.54	0.34	0.74
Butane (C_4H_{10})	0.45	6.80	1.36	2.92	0.66	0.72	0.85
Benzene (C_6H_6)	0.36	0.26	0.64	0.72	0.70	0.66	0.42
Propane (C_3H_8)	0.36	8.58	4.40	7.25	0.74	0.49	0.87
Hydrogen (H_2 normal)	0.67	1.20	0.69	0.33	1.39	0.25	0.41
Nitrogen (N_2)	0.12	0.21	0.12	0.16	0.15	0.11	0.11
Ethane (C_2H_6)	0.22	1.19	1.80	3.11	0.55	0.37	0.20
Methane (CH_4)	0.20	0.20	0.06	0.09	0.20	0.06	0.06
Argon (Ar)	0.14	0.14	0.07	0.07	0.14	0.07	0.07

Species	**Average A%Err for Entire Curve**						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
"Others" with $T_{r,b} < 0.7$ (Polar)							
Methyl isobutyl ketone ($C_6H_{12}O$)	0.78	0.88	5.56	5.90	13.13	2.90	1.03
Diethyl ether ($C_4H_{10}O$)	2.56	4.19	4.17	5.97	5.09	2.60	1.76
Acetone (C_3H_6O)	0.81	8.85	2.43	0.90	5.05	3.30	2.07
R152a ($C_2H_4F_2$)	0.31	4.17	1.28	0.62	1.81	1.26	0.75
Ammonia (NH_3)	0.24	0.24	0.22	0.13	0.24	0.49	0.41
Water (H_2O)	0.61	0.61	1.45	0.78	0.61	2.57	1.94
Summary							
Acids (9): Table 3.3 - $F_{w,j}[R(\omega)]$							
$T_{r,b} > 0.7$ (6)	6.97	13.18	8.72	4.33	120.69	31.02	4,384.25
$T_{r,b} < 0.7$ (3)	1.82	4.80	2.76	0.96	4.21	3.95	2.50
Alcohols (22): Table 3.3 - $F_{w,j}[R\|R(\omega)]$							
$T_{r,b} > 0.7$ (13)	47.43	20.46	35.72	44.70	28,204.41	196.96	225.95
$T_{r,b} < 0.7$ (9)	28.03	23.45	17.24	18.95	8,108,568.90	81.53	40.72
"Others" (41)							
$T_{r,b} > 0.7$ (14)	3.565	3.55	4.09	6.58	2.37	0.94	2.28
$T_{r,b} < 0.7$ (27) : Table 3.3 - $F_{w,j}[A\text{-}W(T_b)\|R(\omega)]$	1.85	5.02	2.42	3.49	2.86	1.23	0.97
Normal (21): Table 3.3 - $F_{w,j}[A\text{-}W(T_b)\|R(\omega)]$	2.11	5.52	2.35	3.76	2.36	0.94	0.86
Polar (6); Table 3.3 - $F_{w,j}[A\text{-}W(T_b)\|R(\omega)]$	0.93	3.27	2.66	2.55	4.61	2.26	1.36
Note: The $F_{w,j}$ function with the least average A%Err for a substance subset has its error shaded gray in the Summary section.							

Table 3.5. Comparison of Entire-Curve Average Absolute Percent Error.

	Species-Specific Least Average A%Err				Average A%Err Using Subset Best Method				
	Minimum Possible	R vs. A-W	All Four	$F_{w,j}$	Correlation		$F_{w,j}$		$F_{w,j}$ Success
Acids (9)									
$T_{r,b} > 0.7$ (6)	3.93	7.84	4.09	3.12	5.07	R(ω)	4.33	$F_{w,j}^{(3)}[R \mid R(\omega)]$	S
$T_{r,b} < 0.7$ (3)	0.99	3.18	1.26	0.66	1.26	R(ω)	0.96	$F_{w,j}^{(3)}[R \mid R(\omega)]$	U
Alcohols (22)									
$T_{r,b} > 0.7$ (13)	19.65	21.13	20.12	8.95	35.68	R	20.46	$F_{w,j}^{(1)}[R \mid R(\omega)]$	S
$T_{r,b} < 0.7$ (9)	8.93	13.37	9.22	7.80	17.59	R	17.24	$F_{w,j}^{(2)}[R \mid R(\omega)]$	<S
"Others" (41)									
$T_{r,b} > 0.7$ (14)	0.49	0.66	0.50	0.73	0.66	A-W	0.94	$F_{w,j}^{(2)}[A\text{-}W(T_b) \mid R(\omega)]$	<S
$T_{r,b} < 0.7$ (27)	1.07	1.50	1.13	0.78	1.44	A-W(T_b)	0.87	See breakdown below	U
Normal (21)	0.81	1.02	0.84	0.75	1.00	A-W(T_b)	0.86	$F_{w,j}^{(3)}[A\text{-}W(T_b) \mid R(\omega)]$	S
Polar (6)	1.99	3.18	2.12	0.91	2.98	A-W(T_b)	0.93	$F_{w,j}[R(\omega)]$	U

Legend for Success Levels:

"<S" indicates less than Satisfactory (average error of subset best $F_{w,j}$ function $>$ species-specific subset average error of either standard Riedel or Ambrose-Walton).

"S" indicates Satisfactory (average error of subset best $F_{w,j}$ function $\leq$ species-specific subset average error of both standard Riedel and Ambrose-Walton).

"U" indicates Ultimate (average error of subset best $F_{w,j}$ function $\leq$ species-specific subset average minimum possible error).

Note that achieving Superior success (average error of subset best $F_{w,j}$ function $\leq$ species-specific subset average error for all four correlations) without achieving Ultimate success does not occur.

Table 3.6. Comparison of Entire-Curve Average Absolute Percent Error - Three Alcohol Subsets.

	Species-Specific Least Error				**Best Subset Method**				
	Minimum Possible	**R vs. A-W**	**All Four**	$F_{w,j}$	**Correlation**		$F_{w,j}$		$F_{w,j}$ **Success**
Acids (9)									
$T_{r,b} > 0.7$ (6)	3.93	7.84	4.09	3.12	5.07	R(ω)	4.33	$F_{w,j}^{(3)}[R\|R(\omega)]$	S
$T_{r,b} < 0.7$ (3)	0.99	3.18	1.26	0.66	1.26	R(ω)	0.96	$F_{w,j}^{(3)}[R\|R(\omega)]$	U
Alcohols (22)									
$T_{r,b} > 0.7$ (13)	19.65	21.13	20.12	8.95	35.68	R	20.46	$F_{w,j}^{(1)}[R\|R(\omega)]$	S
$T_{r,b} > 0.76$ (4)	15.85	18.28	15.86	12.95	15.86	A-W(T_b)	12.95	$F_{w,j}^{(1)}[A\text{-}W(T_b)\|R(\omega)]$	U
$0.7 < T_{r,b} < 0.76$ (9)	21.33	22.39	22.00	7.19	22.39	R	8.11	$F_{w,j}^{(1)}[R\|R(\omega)]$	U
$T_{r,b} < 0.7$ (9)	8.93	13.37	9.22	7.80	17.59	R	17.24	$F_{w,j}^{(2)}[R\|R(\omega)]$	<S
"Others" (41)									
$T_{r,b} > 0.7$ (14)	0.49	0.66	0.50	0.73	0.66	A-W	0.94	$F_{w,j}^{(2)}[A\text{-}W(T_b)\|R(\omega)]$	<S
$T_{r,b} < 0.7$ (27)	1.07	1.50	1.13	0.78	1.44	A-W(T_b)	0.87	See breakdown below	U
Normal (21)	0.81	1.02	0.84	0.75	1.00	A-W(T_b)	0.86	$F_{w,j}^{(3)}[A\text{-}W(T_b)\|R(\omega)]$	S
Polar (6)	1.99	3.18	2.12	0.91	2.98	A-W(T_b)	0.93	$F_{w,j}[R(\omega)]$	U

Legend for Success Levels:
"<S" indicates less than Satisfactory
"S" indicates Satisfactory
"U" indicates Ultimate

Table 3.7. Entire-Curve Incremental Error for Recommended Predictive Methods.

$T_{r,b}$ relationship to 0.7	**Minimum Possible Average A%Err**	**Subset Predictive Recommendation**		
		Average A%Err	**Method**	**Incremental Error**
Organic Acids (9)				
$T_{r,b} > 0.7$ (6)	3.93	4.33	$F_{w,j}^{(3)}[R \vert R(\omega)]$	0.40
$T_{r,b} < 0.7$ (3)	0.99	0.96	$F_{w,j}^{(3)}[R \vert R(\omega)]$	-0.03
Alcohols (22)				
$T_{r,b} > 0.7$ (13)	19.65	20.46	$F_{w,j}^{(1)}[R \vert R(\omega)]$	0.81
$T_{r,b} > 0.76$ (4)	15.85	15.86	A-W(T_b)	0.01
$0.7 < T_{r,b} < 0.76$ (9)	21.33	8.11	$F_{w,j}^{(1)}[R \vert R(\omega)]$	-13.22
$T_{r,b} < 0.7$ (9)	8.93	17.59 or 17.24	R or $F_{w,j}^{(2)}[R \vert R(\omega)]$	8.66 or 8.31
"Others" (41)				
$T_{r,b} > 0.7$ (14)	0.49	0.66	A-W	0.17
$T_{r,b} < 0.7$ (27)	1.07	0.87	See breakdown below	-0.20
Normal (21)	0.81	0.86	$F_{w,j}^{(3)}[A\text{-}W(T_b) \vert R(\omega)]$	0.05
Polar (6)	1.99	0.93	$F_{w,j}[R(\omega)]$	-1.06

Table 3.8. Entire-Curve Incremental Errors for Recommended Predictive Methods and *Fw,j[AA]* Functions. All Statistics Are for the Common 55 Species.

$T_{r,b}$ relationship to 0.7	Minimum Possible Average A%Err	Subset Predictive Recommendation			Species-Specific $F_{w,j}[AA]$	
		Average A%Err	Method	Incremental Error	Average A%Err	Incremental Error
Organic Acids (6)						
$T_{r,b} > 0.7$ (4)	3.69	5.46	$F_{w,j}^{(3)}[R \vert R(\omega)]$	1.77	12.60	8.91
$T_{r,b} < 0.7$ (2)	0.98	0.95	$F_{w,j}^{(3)}[R \vert R(\omega)]$	-0.03	1.56	0.58
Alcohols (13)						
$T_{r,b} > 0.7$ (7)	12.15	7.22	$F_{w,j}^{(1)}[R \vert R(\omega)]$	-4.93	7.41	-4.74
$T_{r,b} > 0.76$ (0)	N/A	N/A	A-W(T_b)	N/A	N/A	N/A
$0.7 < T_{r,b} < 0.76$ (7)	12.15	7.22	$F_{w,j}^{(1)}[R \vert R(\omega)]$	-4.93	7.41	-4.74
$T_{r,b} < 0.7$ (6)	9.35	19.77 or 19.43	R or $F_{w,j}^{(2)}[R \vert R(\omega)]$	10.43 or 10.08	13.14	3.79
"Others" (36)						
$T_{r,b} > 0.7$ (13)	0.32	0.33	A-W	0.01	3.17	2.85
$T_{r,b} < 0.7$ (23)	1.04	0.84	See breakdown below	-0.20	2.07	1.03
Normal (17)	0.71	0.85	$F_{w,j}^{(3)}[A\text{-}W(T_b) \vert R(\omega)]$	0.14	1.60	0.89
Polar (6)	1.99	0.80	$F_{w,j}[R(\omega)]$	-1.19	3.43	1.44

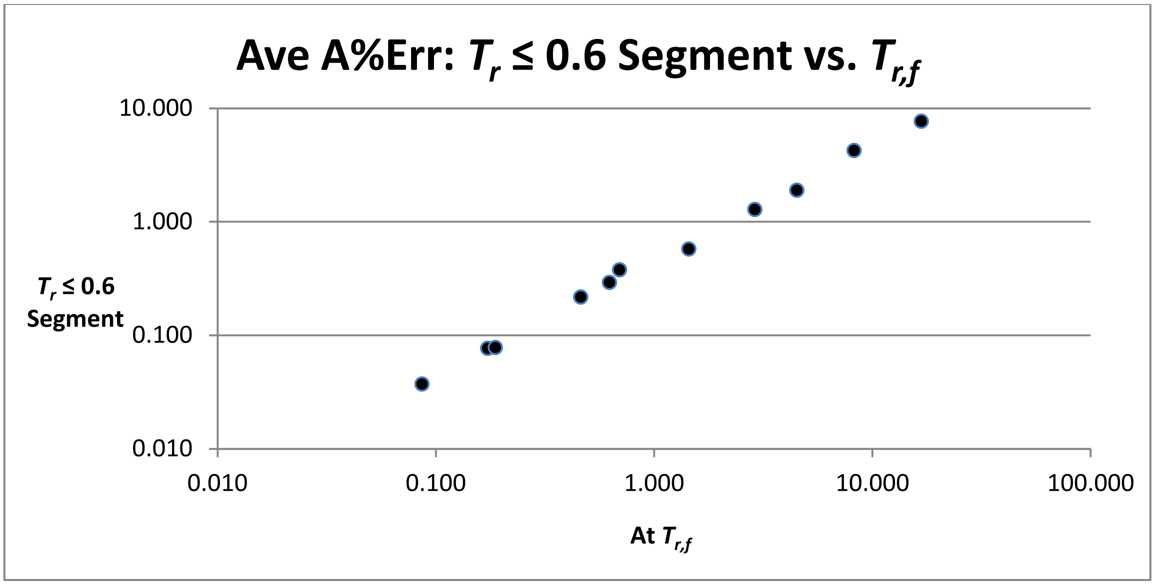

Figure 1.1. Plot of Average Error for Eleven Intervals, the $T_r \leq 0.6$ Segment vs. that at $T_{r,f}$, From Table 1.6.

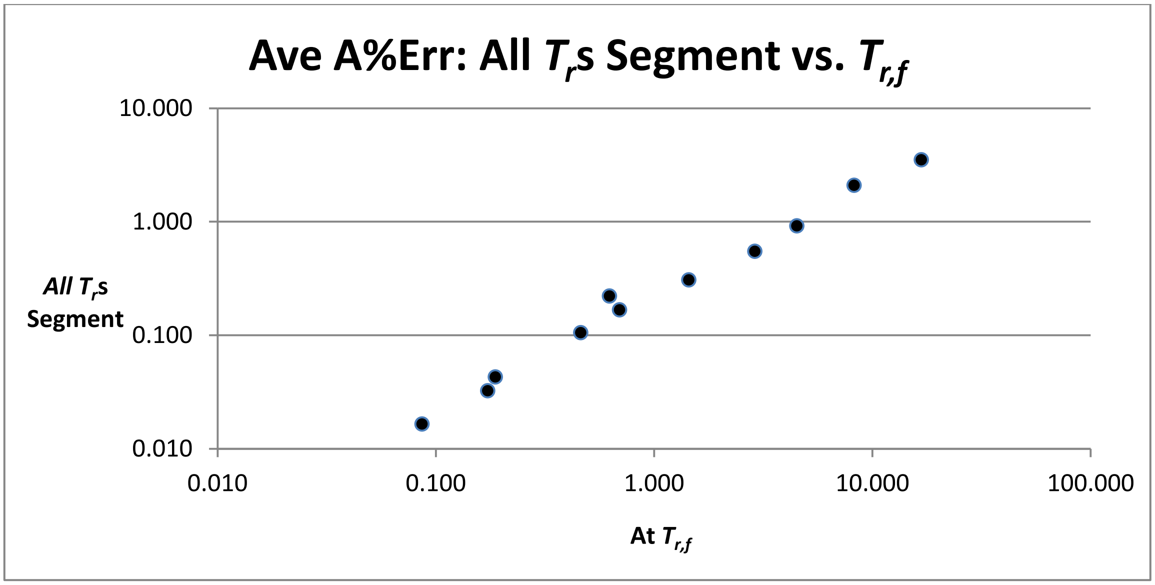

Figure 1.2. Plot of Average Error for Eleven Intervals, All T_rs vs. that at $T_{r,f}$, From Table 1.6.

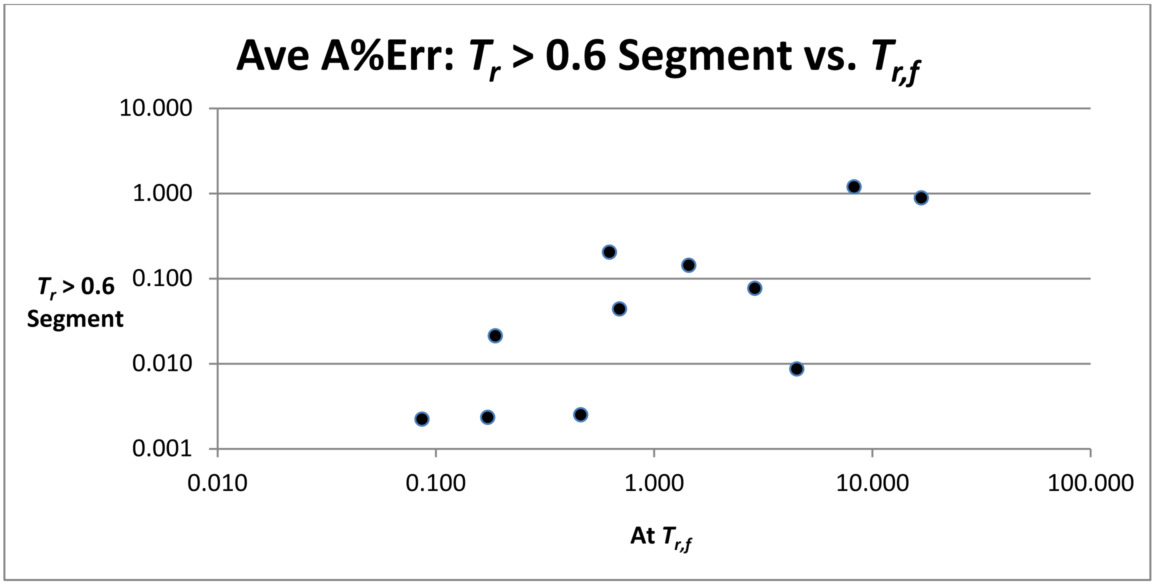

Figure 1.3. Plot of Average Error for Eleven Intervals, the T_r > 0.6 Segment vs. that at $T_{r,f}$, From Table 1.6. Compare with Figure 1.1.

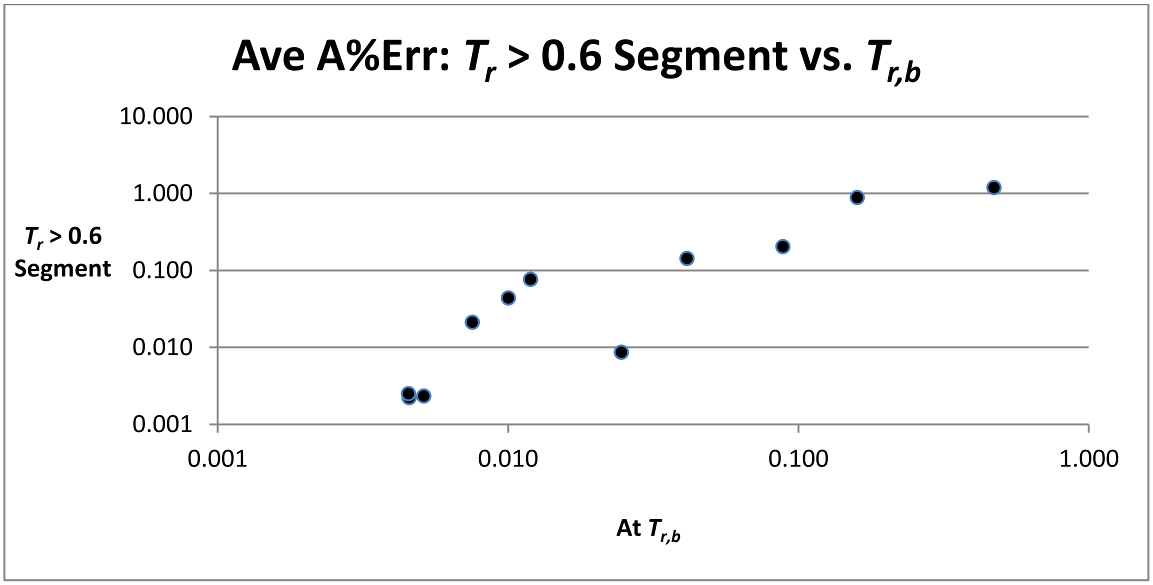

Figure 1.4. Plot of Average Error for Eleven Intervals, the T_r > 0.6 Segment vs. that at $T_{r,b}$, From Table 1.6.

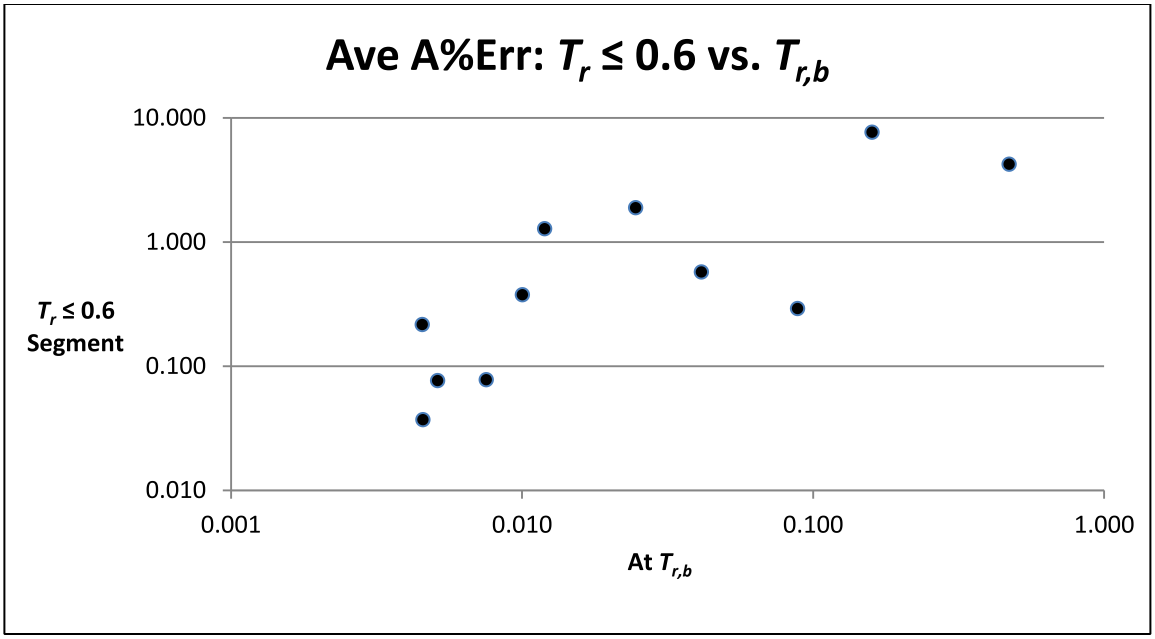

Figure 1.5. Plot of Average Error for Eleven Intervals, the $T_r \leq 0.6$ Segment vs. that at $T_{r,b}$, From Table 1.6.

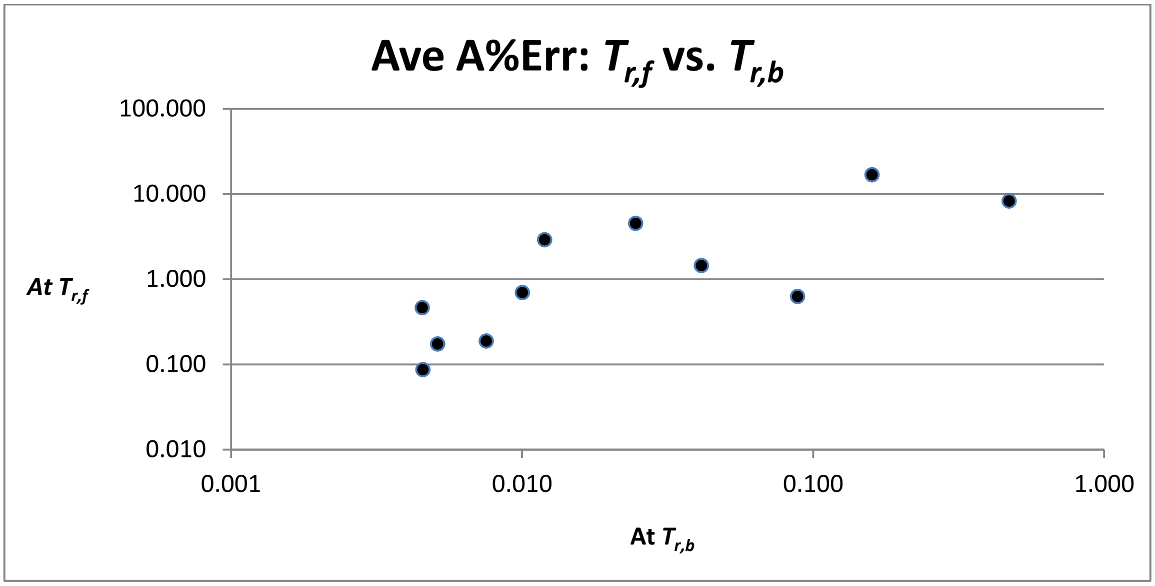

Figure 1.6. Plot of Average Error for Eleven Intervals, at $T_{r,f}$ vs. that at $T_{r,b}$, From Table 1.6.

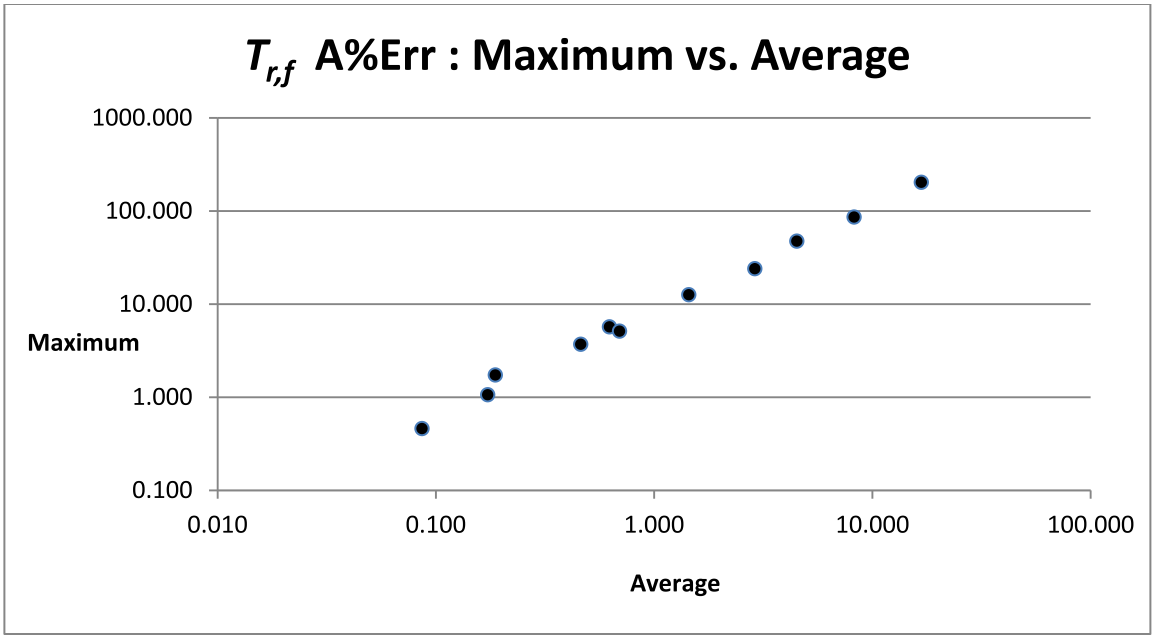

Figure 1.7. Plot of Tr,f Error for Eleven Intervals, Maximum vs. Average. From Table 1.6.

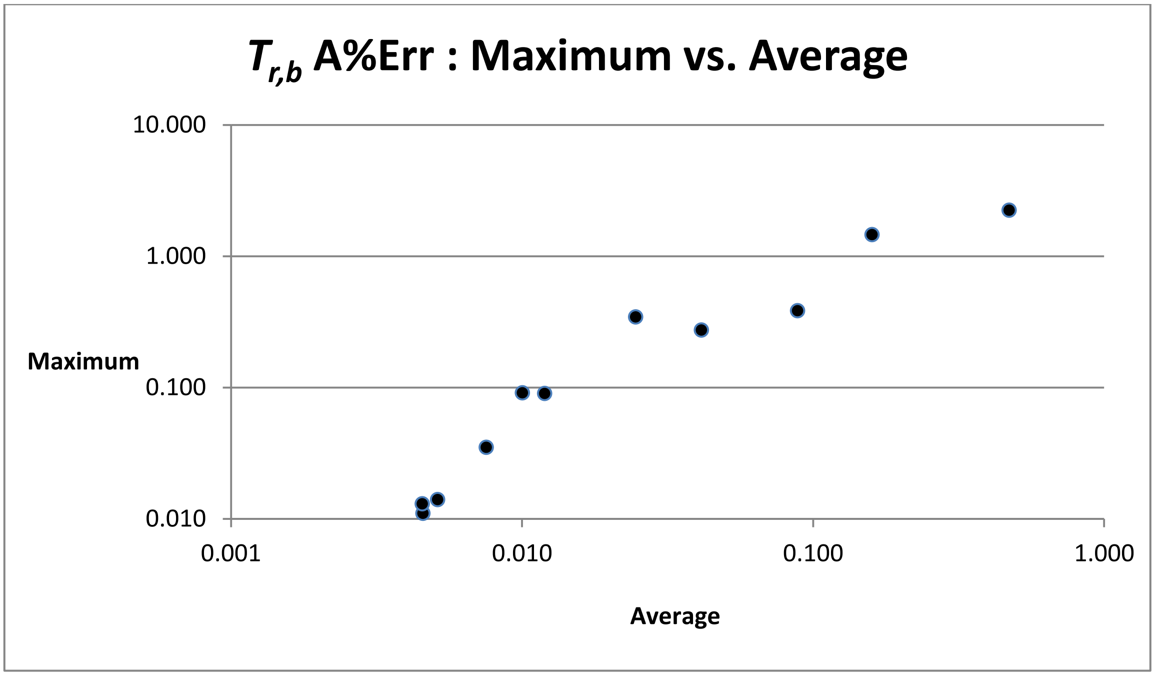

Figure 1.8. Plot of $T_{r,b}$ Error for Eleven Intervals, Maximum vs. Average. From Table 1.6.

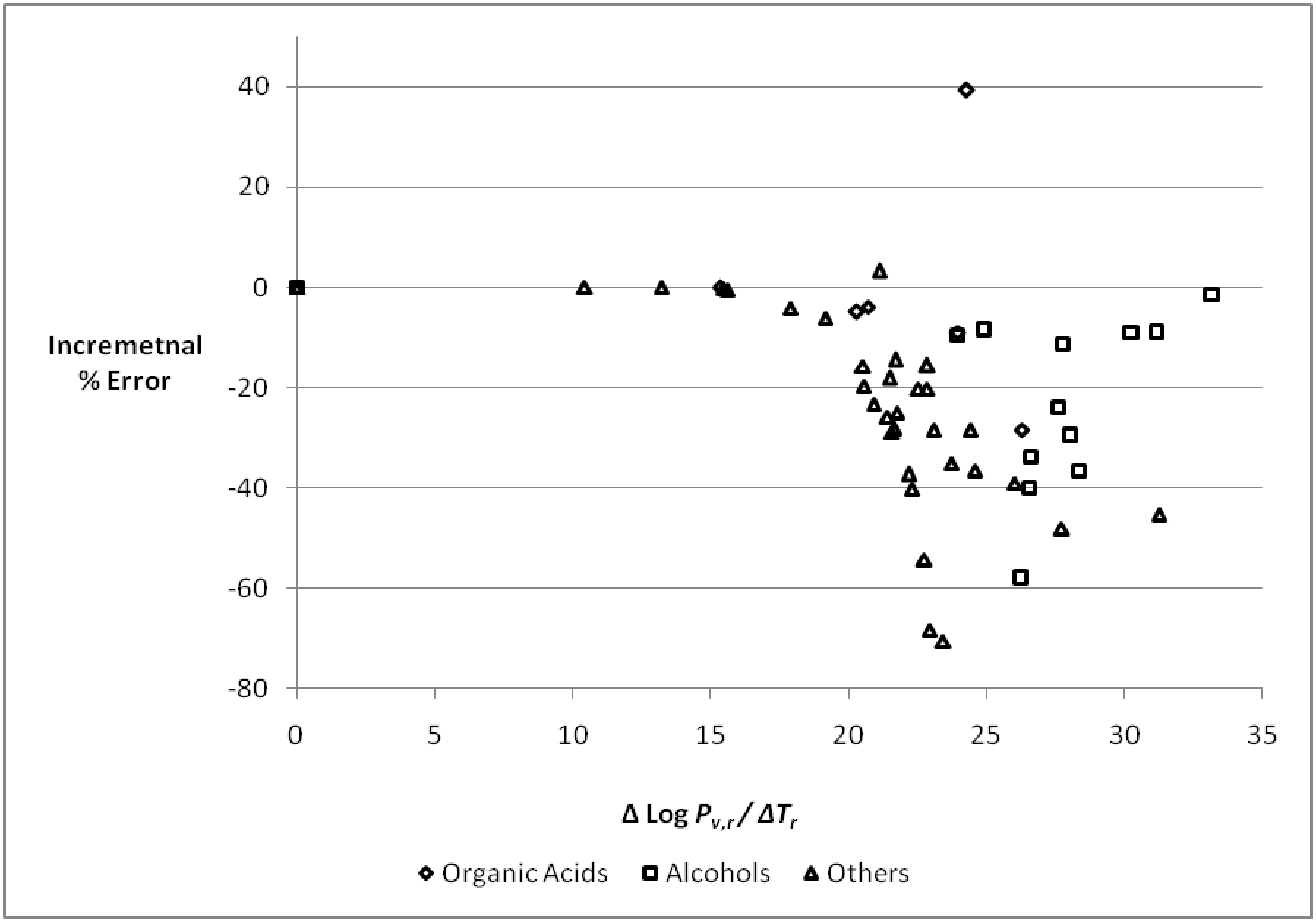

Figure 2.1. Incremental Error of $F_{w,j}[AA]$ relative to Extrapolated Antoine at $T_{r,f}$ vs. Extrapolation Burden.

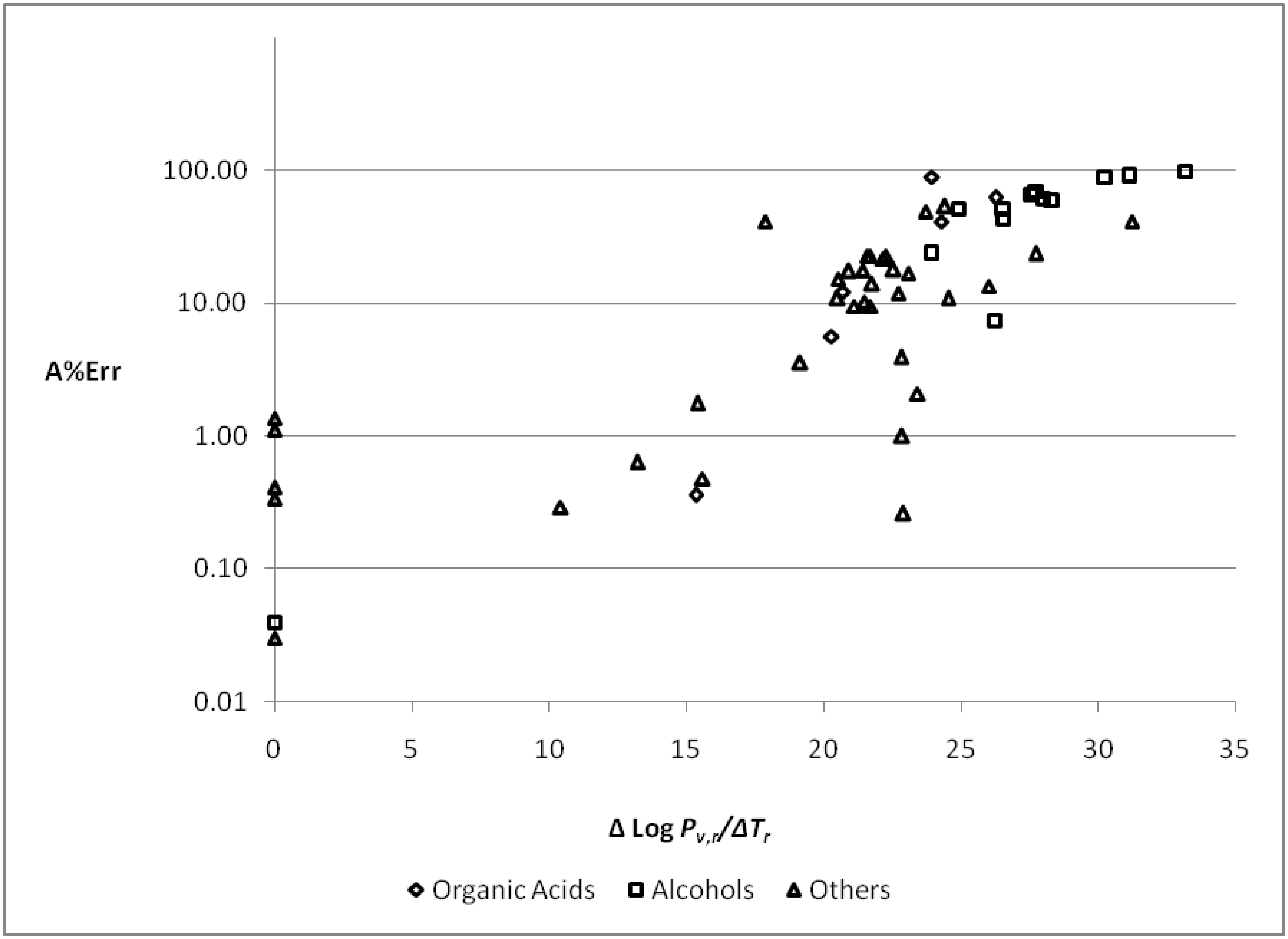

Figure 2.2. Predictive Error of $F_{w,j}[AA]$ Function at the Normal Fusion Point vs. Extrapolation Burden.

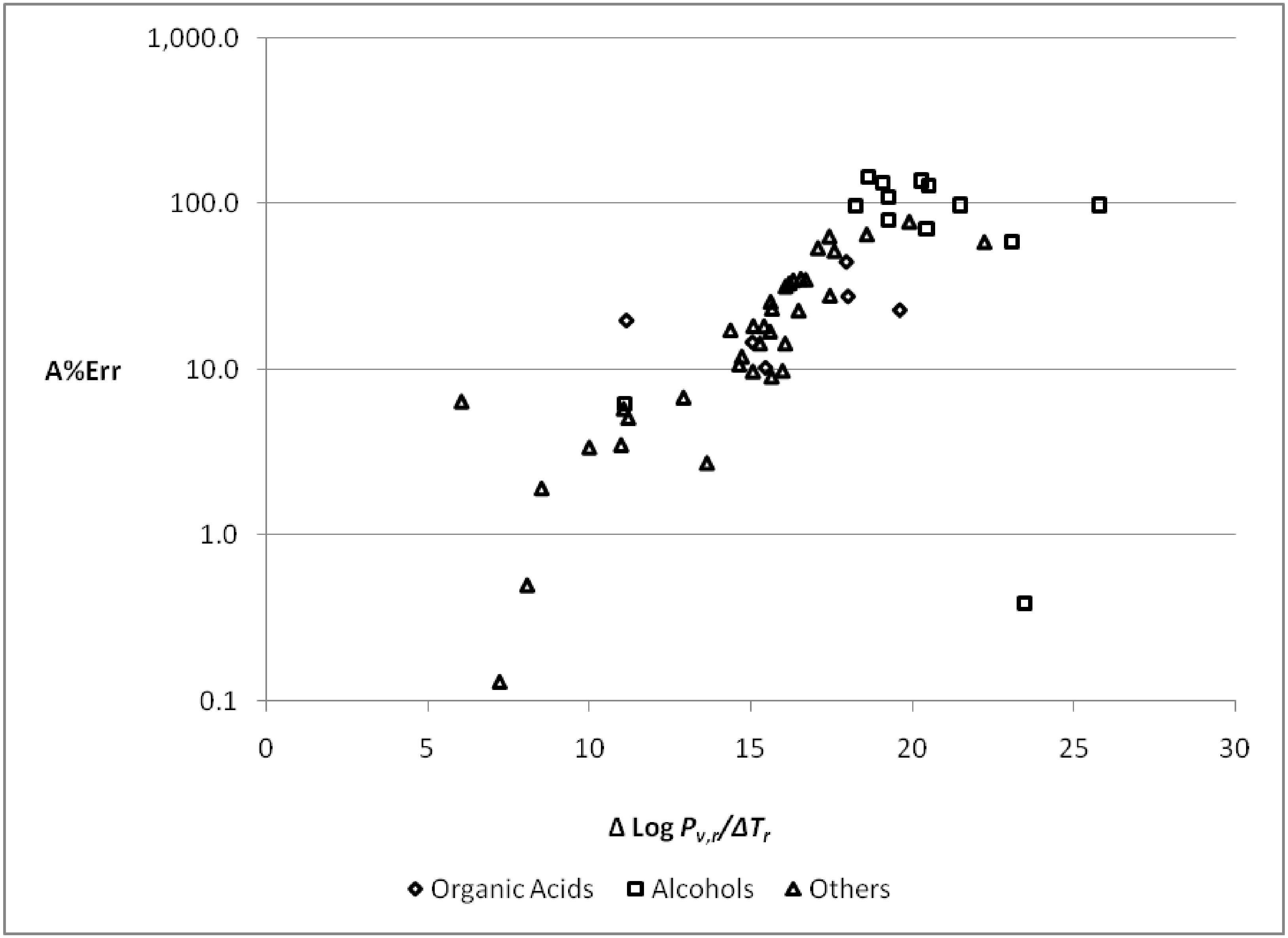

Figure 2.3. Predictive Error of Riedel Equation at the Normal Fusion Point vs. Extrapolation Burden.

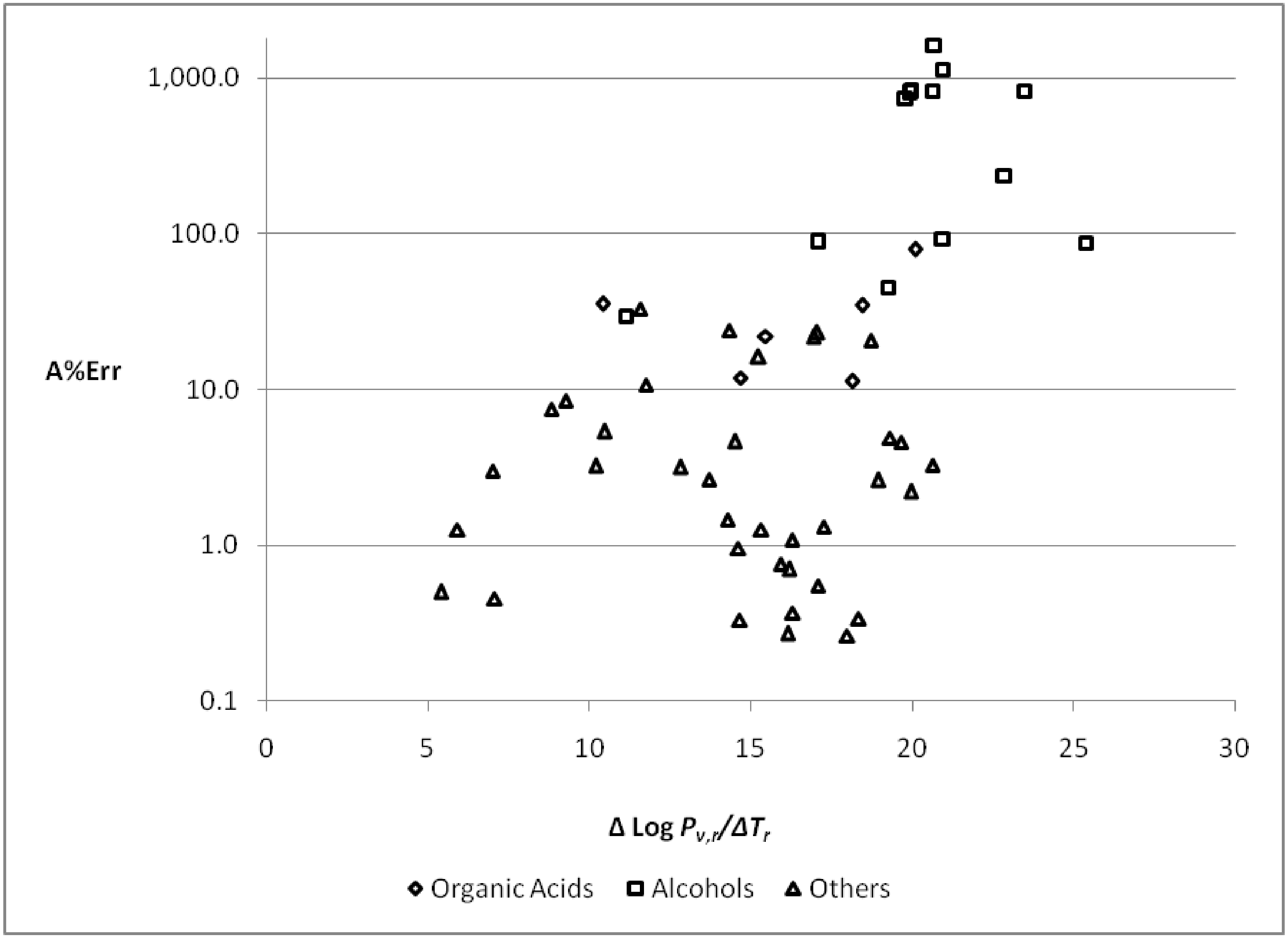

Figure 2.4. Predictive Error of Ambrose-Walton Equation at the Normal Fusion Point vs. Extrapolation Burden.

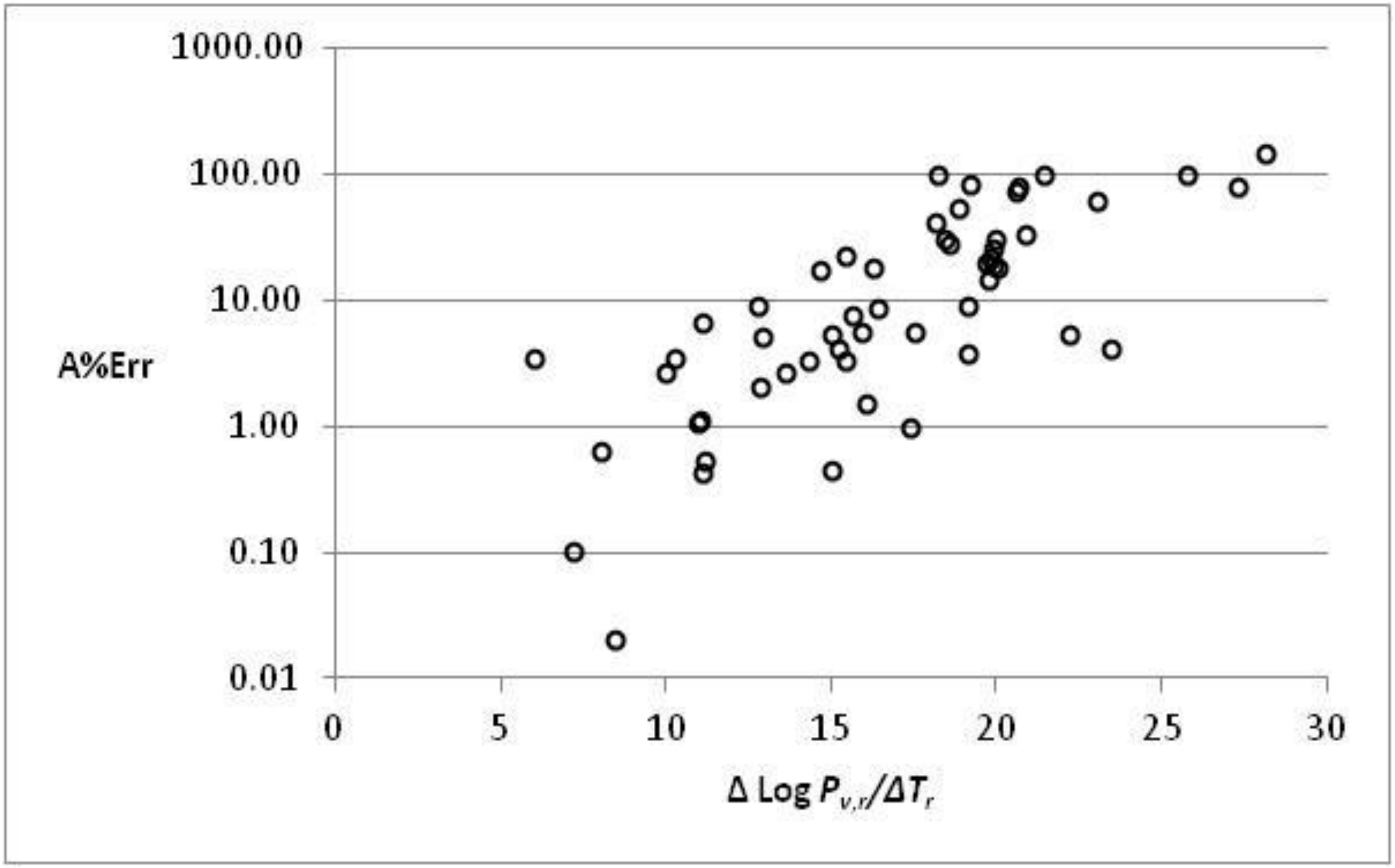

Figure 3.1. A%Err at $T_{r,f}$ for $F_{w,j}$ Functions Recommended in Table 3.7 vs. Extrapolation Burden.

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Appendix A: Results of Entire-Curve Regressions From *NIST* Data

The reduced vapor pressure predicted by this work's regressions of the Wagner constants from the analytic data given in the *NIST* Chemistry WebBook (Lemmon et al., 2011) for hydrogen, helium, argon, water, and R152a, and their absolute percent errors ("A%Err") are presented in this Appendix. The row of the temperature corresponding to the largest absolute percent error is shaded in gray in each table. The temperature interval used between each analytic point for each species is larger at the lower reduced temperatures than at the higher temperatures, except for R152a, which has a consistent interval for its entire co-existence curve. The error statistics and the predominant temperature intervals used are given at the end of each table.

Reduced temperature and τ inputs are rounded to five significant digits, and both input and output values of $Ln\ P_{v,r}$ are rounded off to four digits in the mantissa.

Table A.1. VLE Predictions for Hydrogen Using Wagner Constants Regressed from *NIST*

Analytic (*NIST*)					**Predicted**		
T (^{o}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
13.957	7.3578E-03	0.42109	5.6755E-03	-5.1716	-5.1714	5.6766E-03	0.020
14.057	7.7902E-03	0.42411	6.0090E-03	-5.1145	-5.1142	6.0108E-03	0.030
14.157	8.2419E-03	0.42712	6.3576E-03	-5.0581	-5.0580	6.3583E-03	0.010
14.257	8.7134E-03	0.43014	6.7211E-03	-5.0025	-5.0024	6.7218E-03	0.010
14.357	9.2055E-03	0.43316	7.1011E-03	-4.9475	-4.9474	7.1018E-03	0.010
14.457	9.7186E-03	0.43617	7.4966E-03	-4.8933	-4.8933	7.4966E-03	0.000
14.557	1.0253E-02	0.43919	7.9086E-03	-4.8398	-4.8397	7.9094E-03	0.010
14.657	1.0810E-02	0.44221	8.3383E-03	-4.7869	-4.7868	8.3391E-03	0.010
14.757	1.1390E-02	0.44523	8.7860E-03	-4.7346	-4.7345	8.7868E-03	0.010
14.857	1.1993E-02	0.44824	9.2512E-03	-4.6830	-4.6830	9.2512E-03	0.000
14.957	1.2621E-02	0.45126	9.7353E-03	-4.6320	-4.6320	9.7353E-03	0.000
15.057	1.3273E-02	0.45428	1.0239E-02	-4.5816	-4.5816	1.0239E-02	0.000
15.157	1.3950E-02	0.45729	1.0760E-02	-4.5319	-4.5320	1.0759E-02	0.010
15.257	1.4654E-02	0.46031	1.1304E-02	-4.4826	-4.4827	1.1303E-02	0.010
15.357	1.5383E-02	0.46333	1.1866E-02	-4.4341	-4.4341	1.1866E-02	0.000
15.457	1.6140E-02	0.46634	1.2450E-02	-4.3860	-4.3862	1.2448E-02	0.020
15.557	1.6925E-02	0.46936	1.3055E-02	-4.3386	-4.3386	1.3055E-02	0.000
15.657	1.7739E-02	0.47238	1.3683E-02	-4.2916	-4.2917	1.3682E-02	0.010
15.757	1.8581E-02	0.47540	1.4333E-02	-4.2452	-4.2452	1.4333E-02	0.000
15.857	1.9454E-02	0.47841	1.5006E-02	-4.1993	-4.1994	1.5005E-02	0.010
15.957	2.0357E-02	0.48143	1.5703E-02	-4.1539	-4.1540	1.5701E-02	0.010
16.057	2.1291E-02	0.48445	1.6423E-02	-4.1091	-4.1091	1.6423E-02	0.000
16.157	2.2257E-02	0.48746	1.7168E-02	-4.0647	-4.0649	1.7165E-02	0.020
16.257	2.3255E-02	0.49048	1.7939E-02	-4.0208	-4.0209	1.7937E-02	0.010
16.357	2.4287E-02	0.49350	1.8734E-02	-3.9774	-3.9775	1.8732E-02	0.010
16.457	2.5352E-02	0.49652	1.9555E-02	-3.9345	-3.9345	1.9555E-02	0.000
16.557	2.6452E-02	0.49953	2.0404E-02	-3.8920	-3.8921	2.0402E-02	0.010
16.657	2.7588E-02	0.50255	2.1280E-02	-3.8500	-3.8501	2.1278E-02	0.010
16.757	2.8759E-02	0.50557	2.2184E-02	-3.8084	-3.8084	2.2184E-02	0.000
16.857	2.9967E-02	0.50858	2.3117E-02	-3.7672	-3.7674	2.3112E-02	0.020
16.957	3.1212E-02	0.51160	2.4077E-02	-3.7265	-3.7266	2.4075E-02	0.010
17.057	3.2495E-02	0.51462	2.5065E-02	-3.6863	-3.6863	2.5065E-02	0.000
17.157	3.3817E-02	0.51763	2.6085E-02	-3.6464	-3.6465	2.6082E-02	0.010
17.257	3.5179E-02	0.52065	2.7136E-02	-3.6069	-3.6070	2.7133E-02	0.010
17.357	3.6581E-02	0.52367	2.8218E-02	-3.5678	-3.5679	2.8215E-02	0.010
17.457	3.8023E-02	0.52669	2.9328E-02	-3.5292	-3.5291	2.9331E-02	0.010

Analytic (*NIST*)					**Predicted**		
T (ºK)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
17.557	3.9508E-02	0.52970	3.0476E-02	-3.4908	-3.4909	3.0473E-02	0.010
17.657	4.1034E-02	0.53272	3.1654E-02	-3.4529	-3.4530	3.1651E-02	0.010
17.757	4.2604E-02	0.53574	3.2863E-02	-3.4154	-3.4154	3.2863E-02	0.000
17.857	4.4217E-02	0.53875	3.4109E-02	-3.3782	-3.3783	3.4105E-02	0.010
17.957	4.5875E-02	0.54177	3.5387E-02	-3.3414	-3.3415	3.5384E-02	0.010
18.057	4.7579E-02	0.54479	3.6699E-02	-3.3050	-3.3050	3.6699E-02	0.000
18.157	4.9328E-02	0.54781	3.8048E-02	-3.2689	-3.2688	3.8052E-02	0.010
18.257	5.1124E-02	0.55082	3.9435E-02	-3.2331	-3.2331	3.9435E-02	0.000
18.357	5.2968E-02	0.55384	4.0856E-02	-3.1977	-3.1977	4.0856E-02	0.000
18.457	5.4860E-02	0.55686	4.2316E-02	-3.1626	-3.1625	4.2320E-02	0.010
18.557	5.6800E-02	0.55987	4.3814E-02	-3.1278	-3.1278	4.3814E-02	0.000
18.657	5.8791E-02	0.56289	4.5348E-02	-3.0934	-3.0934	4.5348E-02	0.000
18.757	6.0832E-02	0.56591	4.6925E-02	-3.0592	-3.0592	4.6925E-02	0.000
18.857	6.2924E-02	0.56892	4.8538E-02	-3.0254	-3.0255	4.8534E-02	0.010
18.957	6.5068E-02	0.57194	5.0192E-02	-2.9919	-2.9919	5.0192E-02	0.000
19.057	6.7265E-02	0.57496	5.1886E-02	-2.9587	-2.9587	5.1886E-02	0.000
19.157	6.9515E-02	0.57798	5.3622E-02	-2.9258	-2.9257	5.3627E-02	0.010
19.257	7.1820E-02	0.58099	5.5399E-02	-2.8932	-2.8932	5.5399E-02	0.000
19.357	7.4180E-02	0.58401	5.7217E-02	-2.8609	-2.8608	5.7223E-02	0.010
19.457	7.6595E-02	0.58703	5.9084E-02	-2.8288	-2.8287	5.9090E-02	0.010
19.557	7.9067E-02	0.59004	6.0987E-02	-2.7971	-2.7970	6.0993E-02	0.010
19.657	8.1596E-02	0.59306	6.2938E-02	-2.7656	-2.7655	6.2945E-02	0.010
19.757	8.4184E-02	0.59608	6.4939E-02	-2.7343	-2.7343	6.4939E-02	0.000
19.857	8.6830E-02	0.59909	6.6977E-02	-2.7034	-2.7034	6.6977E-02	0.000
19.957	8.9535E-02	0.60211	6.9065E-02	-2.6727	-2.6727	6.9065E-02	0.000
20.057	9.2301E-02	0.60513	7.1197E-02	-2.6423	-2.6422	7.1204E-02	0.010
20.157	9.5129E-02	0.60815	7.3380E-02	-2.6121	-2.6120	7.3388E-02	0.010
20.257	9.8018E-02	0.61116	7.5607E-02	-2.5822	-2.5822	7.5607E-02	0.000
20.357	1.0097E-01	0.61418	7.7887E-02	-2.5525	-2.5525	7.7887E-02	0.000
20.457	1.0398E-01	0.61720	8.0211E-02	-2.5231	-2.5230	8.0219E-02	0.010
20.557	1.0706E-01	0.62021	8.2579E-02	-2.4940	-2.4939	8.2587E-02	0.010
20.657	1.1021E-01	0.62323	8.5009E-02	-2.4650	-2.4649	8.5017E-02	0.010
20.757	1.1342E-01	0.62625	8.7493E-02	-2.4362	-2.4362	8.7493E-02	0.000
20.857	1.1670E-01	0.62927	9.0022E-02	-2.4077	-2.4077	9.0022E-02	0.000
20.957	1.2004E-01	0.63228	9.2597E-02	-2.3795	-2.3795	9.2597E-02	0.000
21.057	1.2345E-01	0.63530	9.5226E-02	-2.3515	-2.3514	9.5236E-02	0.010
21.157	1.2693E-01	0.63832	9.7911E-02	-2.3237	-2.3236	9.7920E-02	0.010

Analytic (*NIST*)					**Predicted**		
T (ºK)	P (MPa)	T_r	$P_{v,r}$	$Ln\ P_{v,r}$	$Ln\ P_{v,r}$	$P_{v,r}$	**A%Err**
21.257	1.3048E-01	0.64133	1.0065E-01	-2.2961	-2.2961	1.0065E-01	0.000
21.357	1.3410E-01	0.64435	1.0344E-01	-2.2688	-2.2687	1.0345E-01	0.010
21.457	1.3780E-01	0.64737	1.0630E-01	-2.2415	-2.2415	1.0630E-01	0.000
21.557	1.4156E-01	0.65038	1.0920E-01	-2.2146	-2.2146	1.0920E-01	0.000
21.657	1.4540E-01	0.65340	1.1215E-01	-2.1879	-2.1878	1.1216E-01	0.010
21.757	1.4931E-01	0.65642	1.1518E-01	-2.1613	-2.1612	1.1519E-01	0.010
21.857	1.5330E-01	0.65944	1.1826E-01	-2.1349	-2.1349	1.1826E-01	0.000
21.957	1.5736E-01	0.66245	1.2138E-01	-2.1088	-2.1088	1.2138E-01	0.000
22.057	1.6149E-01	0.66547	1.2457E-01	-2.0829	-2.0828	1.2458E-01	0.010
22.157	1.6571E-01	0.66849	1.2782E-01	-2.0571	-2.0571	1.2782E-01	0.000
22.257	1.7000E-01	0.67150	1.3114E-01	-2.0315	-2.0315	1.3114E-01	0.000
22.357	1.7437E-01	0.67452	1.3450E-01	-2.0062	-2.0062	1.3450E-01	0.000
22.457	1.7881E-01	0.67754	1.3793E-01	-1.9810	-1.9809	1.3795E-01	0.010
22.557	1.8334E-01	0.68056	1.4142E-01	-1.9560	-1.9559	1.4144E-01	0.010
22.657	1.8795E-01	0.68357	1.4497E-01	-1.9312	-1.9311	1.4499E-01	0.010
22.757	1.9264E-01	0.68659	1.4860E-01	-1.9065	-1.9065	1.4860E-01	0.000
22.857	1.9742E-01	0.68961	1.5229E-01	-1.8820	-1.8820	1.5229E-01	0.000
22.957	2.0227E-01	0.69262	1.5603E-01	-1.8577	-1.8577	1.5603E-01	0.000
23.057	2.0721E-01	0.69564	1.5984E-01	-1.8336	-1.8336	1.5984E-01	0.000
23.157	2.1224E-01	0.69866	1.6372E-01	-1.8096	-1.8096	1.6372E-01	0.000
23.257	2.1735E-01	0.70167	1.6766E-01	-1.7858	-1.7859	1.6765E-01	0.010
23.357	2.2254E-01	0.70469	1.7167E-01	-1.7622	-1.7622	1.7167E-01	0.000
23.457	2.2783E-01	0.70771	1.7575E-01	-1.7387	-1.7387	1.7575E-01	0.000
23.557	2.3320E-01	0.71073	1.7987E-01	-1.7155	-1.7154	1.7989E-01	0.010
23.657	2.3866E-01	0.71374	1.8410E-01	-1.6923	-1.6923	1.8410E-01	0.000
23.757	2.4421E-01	0.71676	1.8838E-01	-1.6693	-1.6693	1.8838E-01	0.000
23.857	2.4985E-01	0.71978	1.9272E-01	-1.6465	-1.6465	1.9272E-01	0.000
23.957	2.5558E-01	0.72279	1.9715E-01	-1.6238	-1.6238	1.9715E-01	0.000
24.057	2.6140E-01	0.72581	2.0163E-01	-1.6013	-1.6013	2.0163E-01	0.000
24.157	2.6732E-01	0.72883	2.0620E-01	-1.5789	-1.5789	2.0620E-01	0.000
24.257	2.7333E-01	0.73184	2.1083E-01	-1.5567	-1.5567	2.1083E-01	0.000
24.357	2.7943E-01	0.73486	2.1554E-01	-1.5346	-1.5346	2.1554E-01	0.000
24.457	2.8563E-01	0.73788	2.2034E-01	-1.5126	-1.5126	2.2034E-01	0.000
24.557	2.9193E-01	0.74090	2.2519E-01	-1.4908	-1.4908	2.2519E-01	0.000
24.657	2.9832E-01	0.74391	2.3011E-01	-1.4692	-1.4692	2.3011E-01	0.000
24.757	3.0481E-01	0.74693	2.3511E-01	-1.4477	-1.4477	2.3511E-01	0.000
24.857	3.1140E-01	0.74995	2.4020E-01	-1.4263	-1.4263	2.4020E-01	0.000

Analytic (*NIST*)					**Predicted**		
T (^{o}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
24.957	3.1809E-01	0.75296	2.4537E-01	-1.4050	-1.4051	2.4534E-01	0.010
25.057	3.2488E-01	0.75598	2.5060E-01	-1.3839	-1.3839	2.5060E-01	0.000
25.157	3.3177E-01	0.75900	2.5592E-01	-1.3629	-1.3629	2.5592E-01	0.000
25.257	3.3876E-01	0.76202	2.6130E-01	-1.3421	-1.3421	2.6130E-01	0.000
25.357	3.4586E-01	0.76503	2.6679E-01	-1.3213	-1.3214	2.6676E-01	0.010
25.457	3.5305E-01	0.76805	2.7234E-01	-1.3007	-1.3008	2.7231E-01	0.010
25.557	3.6036E-01	0.77107	2.7798E-01	-1.2802	-1.2803	2.7795E-01	0.010
25.657	3.6776E-01	0.77408	2.8368E-01	-1.2599	-1.2600	2.8365E-01	0.010
25.757	3.7528E-01	0.77710	2.8947E-01	-1.2397	-1.2397	2.8947E-01	0.000
25.857	3.8290E-01	0.78012	2.9535E-01	-1.2196	-1.2196	2.9535E-01	0.000
25.957	3.9063E-01	0.78313	3.0131E-01	-1.1996	-1.1997	3.0128E-01	0.010
26.057	3.9847E-01	0.78615	3.0737E-01	-1.1797	-1.1798	3.0734E-01	0.010
26.157	4.0641E-01	0.78917	3.1349E-01	-1.1600	-1.1600	3.1349E-01	0.000
26.257	4.1447E-01	0.79219	3.1972E-01	-1.1403	-1.1404	3.1969E-01	0.010
26.357	4.2264E-01	0.79520	3.2602E-01	-1.1208	-1.1209	3.2599E-01	0.010
26.457	4.3092E-01	0.79822	3.3241E-01	-1.1014	-1.1015	3.3237E-01	0.010
26.557	4.3932E-01	0.80124	3.3888E-01	-1.0821	-1.0822	3.3885E-01	0.010
26.657	4.4782E-01	0.80425	3.4542E-01	-1.0630	-1.0630	3.4542E-01	0.000
26.757	4.5645E-01	0.80727	3.5208E-01	-1.0439	-1.0439	3.5208E-01	0.000
26.857	4.6519E-01	0.81029	3.5883E-01	-1.0249	-1.0249	3.5883E-01	0.000
26.957	4.7404E-01	0.81331	3.6564E-01	-1.0061	-1.0061	3.6564E-01	0.000
27.057	4.8302E-01	0.81632	3.7258E-01	-0.9873	-0.9874	3.7254E-01	0.010
27.157	4.9211E-01	0.81934	3.7961E-01	-0.9686	-0.9687	3.7958E-01	0.010
27.257	5.0132E-01	0.82236	3.8670E-01	-0.9501	-0.9501	3.8670E-01	0.000
27.357	5.1065E-01	0.82537	3.9388E-01	-0.9317	-0.9317	3.9388E-01	0.000
27.457	5.2010E-01	0.82839	4.0120E-01	-0.9133	-0.9134	4.0116E-01	0.010
27.557	5.2968E-01	0.83141	4.0857E-01	-0.8951	-0.8951	4.0857E-01	0.000
27.657	5.3938E-01	0.83442	4.1607E-01	-0.8769	-0.8770	4.1603E-01	0.010
27.757	5.4920E-01	0.83744	4.2363E-01	-0.8589	-0.8589	4.2363E-01	0.000
27.857	5.5915E-01	0.84046	4.3132E-01	-0.8409	-0.8410	4.3128E-01	0.010
27.957	5.6922E-01	0.84348	4.3907E-01	-0.8231	-0.8231	4.3907E-01	0.000
28.057	5.7942E-01	0.84649	4.4695E-01	-0.8053	-0.8054	4.4691E-01	0.010
28.157	5.8975E-01	0.84951	4.5494E-01	-0.7876	-0.7877	4.5489E-01	0.010
28.257	6.0021E-01	0.85253	4.6297E-01	-0.7701	-0.7701	4.6297E-01	0.000
28.357	6.1079E-01	0.85554	4.7114E-01	-0.7526	-0.7526	4.7114E-01	0.000
28.457	6.2151E-01	0.85856	4.7941E-01	-0.7352	-0.7352	4.7941E-01	0.000
28.557	6.3236E-01	0.86158	4.8778E-01	-0.7179	-0.7179	4.8778E-01	0.000

Analytic (*NIST*)					**Predicted**		
T (^{o}K)	P (MPa)	T_r	$P_{v,r}$	$Ln\ P_{v,r}$	$Ln\ P_{v,r}$	$P_{v,r}$	**A%Err**
28.657	6.4335E-01	0.86459	4.9624E-01	-0.7007	-0.7007	4.9624E-01	0.000
28.757	6.5447E-01	0.86761	5.0485E-01	-0.6835	-0.6835	5.0485E-01	0.000
28.857	6.6572E-01	0.87063	5.1350E-01	-0.6665	-0.6665	5.1350E-01	0.000
28.957	6.7711E-01	0.87365	5.2231E-01	-0.6495	-0.6495	5.2231E-01	0.000
29.057	6.8864E-01	0.87666	5.3121E-01	-0.6326	-0.6326	5.3121E-01	0.000
29.157	7.0030E-01	0.87968	5.4021E-01	-0.6158	-0.6158	5.4021E-01	0.000
29.257	7.1211E-01	0.88270	5.4931E-01	-0.5991	-0.5991	5.4931E-01	0.000
29.357	7.2406E-01	0.88571	5.5850E-01	-0.5825	-0.5825	5.5850E-01	0.000
29.457	7.3615E-01	0.88873	5.6785E-01	-0.5659	-0.5659	5.6785E-01	0.000
29.557	7.4838E-01	0.89175	5.7730E-01	-0.5494	-0.5494	5.7730E-01	0.000
29.657	7.6076E-01	0.89477	5.8684E-01	-0.5330	-0.5330	5.8684E-01	0.000
29.757	7.7328E-01	0.89778	5.9649E-01	-0.5167	-0.5167	5.9649E-01	0.000
29.857	7.8595E-01	0.90080	6.0623E-01	-0.5005	-0.5004	6.0629E-01	0.010
29.957	7.9877E-01	0.90382	6.1613E-01	-0.4843	-0.4842	6.1619E-01	0.010
30.057	8.1173E-01	0.90683	6.2613E-01	-0.4682	-0.4682	6.2613E-01	0.000
30.157	8.2485E-01	0.90985	6.3629E-01	-0.4521	-0.4521	6.3629E-01	0.000
30.257	8.3812E-01	0.91287	6.4649E-01	-0.4362	-0.4361	6.4655E-01	0.010
30.357	8.5155E-01	0.91588	6.5685E-01	-0.4203	-0.4203	6.5685E-01	0.000
30.457	8.6513E-01	0.91890	6.6731E-01	-0.4045	-0.4044	6.6738E-01	0.010
30.557	8.7887E-01	0.92192	6.7794E-01	-0.3887	-0.3886	6.7801E-01	0.010
30.657	8.9276E-01	0.92494	6.8867E-01	-0.3730	-0.3729	6.8873E-01	0.010
30.757	9.0682E-01	0.92795	6.9949E-01	-0.3574	-0.3574	6.9949E-01	0.000
30.857	9.2103E-01	0.93097	7.1042E-01	-0.3419	-0.3418	7.1049E-01	0.010
30.957	9.3542E-01	0.93399	7.2152E-01	-0.3264	-0.3263	7.2159E-01	0.010
31.057	9.4996E-01	0.93700	7.3279E-01	-0.3109	-0.3109	7.3279E-01	0.000
31.157	9.6468E-01	0.94002	7.4409E-01	-0.2956	-0.2955	7.4416E-01	0.010
31.257	9.7956E-01	0.94304	7.5563E-01	-0.2802	-0.2802	7.5563E-01	0.000
31.357	9.9461E-01	0.94606	7.6721E-01	-0.2650	-0.2649	7.6728E-01	0.010
31.457	1.0098E+00	0.94907	7.7896E-01	-0.2498	-0.2497	7.7903E-01	0.010
31.557	1.0252E+00	0.95209	7.9081E-01	-0.2347	-0.2346	7.9089E-01	0.010
31.657	1.0408E+00	0.95511	8.0284E-01	-0.2196	-0.2195	8.0292E-01	0.010
31.757	1.0566E+00	0.95812	8.1505E-01	-0.2045	-0.2045	8.1505E-01	0.000
31.857	1.0725E+00	0.96114	8.2729E-01	-0.1896	-0.1895	8.2737E-01	0.010
31.957	1.0887E+00	0.96416	8.3979E-01	-0.1746	-0.1746	8.3979E-01	0.000
32.057	1.1050E+00	0.96717	8.5240E-01	-0.1597	-0.1597	8.5240E-01	0.000
32.157	1.1215E+00	0.97019	8.6511E-01	-0.1449	-0.1449	8.6511E-01	0.000
32.257	1.1382E+00	0.97321	8.7801E-01	-0.1301	-0.1301	8.7801E-01	0.000

Analytic (*NIST*)					**Predicted**		
T (ºK)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
32.357	1.1552E+00	0.97623	8.9110E-01	-0.1153	-0.1153	8.9110E-01	0.000
32.457	1.1723E+00	0.97924	9.0429E-01	-0.1006	-0.1006	9.0429E-01	0.000
32.557	1.1896E+00	0.98226	9.1759E-01	-0.0860	-0.0859	9.1769E-01	0.010
32.657	1.2072E+00	0.98528	9.3118E-01	-0.0713	-0.0713	9.3118E-01	0.000
32.700	1.2148E+00	0.98657	9.3707E-01	-0.0650	-0.0650	9.3707E-01	0.000
32.710	1.2166E+00	0.98688	9.3847E-01	-0.0635	-0.0635	9.3847E-01	0.000
32.720	1.2184E+00	0.98718	9.3979E-01	-0.0621	-0.0621	9.3979E-01	0.000
32.730	1.2202E+00	0.98748	9.4120E-01	-0.0606	-0.0606	9.4120E-01	0.000
32.740	1.2219E+00	0.98778	9.4252E-01	-0.0592	-0.0592	9.4252E-01	0.000
32.750	1.2237E+00	0.98808	9.4393E-01	-0.0577	-0.0577	9.4393E-01	0.000
32.760	1.2255E+00	0.98838	9.4535E-01	-0.0562	-0.0563	9.4526E-01	0.010
32.770	1.2273E+00	0.98869	9.4667E-01	-0.0548	-0.0548	9.4667E-01	0.000
32.780	1.2291E+00	0.98899	9.4810E-01	-0.0533	-0.0533	9.4810E-01	0.000
32.790	1.2309E+00	0.98929	9.4952E-01	-0.0518	-0.0519	9.4942E-01	0.010
32.800	1.2327E+00	0.98959	9.5085E-01	-0.0504	-0.0504	9.5085E-01	0.000
32.810	1.2345E+00	0.98989	9.5228E-01	-0.0489	-0.0490	9.5218E-01	0.010
32.820	1.2363E+00	0.99019	9.5361E-01	-0.0475	-0.0475	9.5361E-01	0.000
32.830	1.2381E+00	0.99050	9.5504E-01	-0.0460	-0.0460	9.5504E-01	0.000
32.840	1.2399E+00	0.99080	9.5638E-01	-0.0446	-0.0446	9.5638E-01	0.000
32.850	1.2417E+00	0.99110	9.5782E-01	-0.0431	-0.0431	9.5782E-01	0.000
32.860	1.2436E+00	0.99140	9.5925E-01	-0.0416	-0.0417	9.5916E-01	0.010
32.870	1.2454E+00	0.99170	9.6069E-01	-0.0401	-0.0402	9.6060E-01	0.010
32.880	1.2472E+00	0.99200	9.6204E-01	-0.0387	-0.0388	9.6194E-01	0.010
32.890	1.2490E+00	0.99231	9.6348E-01	-0.0372	-0.0373	9.6339E-01	0.010
32.900	1.2509E+00	0.99261	9.6493E-01	-0.0357	-0.0358	9.6483E-01	0.010
32.910	1.2527E+00	0.99291	9.6628E-01	-0.0343	-0.0344	9.6618E-01	0.010
32.920	1.2545E+00	0.99321	9.6764E-01	-0.0329	-0.0329	9.6764E-01	0.000
32.930	1.2563E+00	0.99351	9.6909E-01	-0.0314	-0.0315	9.6899E-01	0.010
32.940	1.2582E+00	0.99382	9.7054E-01	-0.0299	-0.0300	9.7045E-01	0.010
32.950	1.2600E+00	0.99412	9.7190E-01	-0.0285	-0.0285	9.7190E-01	0.000
32.960	1.2619E+00	0.99442	9.7336E-01	-0.0270	-0.0271	9.7326E-01	0.010
32.970	1.2637E+00	0.99472	9.7482E-01	-0.0255	-0.0256	9.7472E-01	0.010
32.980	1.2656E+00	0.99502	9.7629E-01	-0.0240	-0.0242	9.7609E-01	0.020
32.990	1.2674E+00	0.99532	9.7765E-01	-0.0226	-0.0227	9.7756E-01	0.010
33.000	1.2693E+00	0.99563	9.7912E-01	-0.0211	-0.0212	9.7902E-01	0.010
33.010	1.2711E+00	0.99593	9.8049E-01	-0.0197	-0.0198	9.8039E-01	0.010
33.020	1.2730E+00	0.99623	9.8196E-01	-0.0182	-0.0183	9.8187E-01	0.010

Analytic (*NIST*)					**Predicted**		
T **(ºK)**	***P*** **(MPa)**	T_r	$P_{v,r}$	$Ln\ P_{v,r}$	$Ln\ P_{v,r}$	$P_{v,r}$	**A%Err**
33.030	1.2748E+00	0.99653	9.8334E-01	-0.0168	-0.0169	9.8324E-01	0.010
33.040	1.2767E+00	0.99683	9.8482E-01	-0.0153	-0.0154	9.8472E-01	0.010
33.050	1.2786E+00	0.99713	9.8629E-01	-0.0138	-0.0139	9.8620E-01	0.010
33.060	1.2804E+00	0.99744	9.8768E-01	-0.0124	-0.0124	9.8768E-01	0.000
33.070	1.2823E+00	0.99774	9.8916E-01	-0.0109	-0.0110	9.8906E-01	0.010
33.080	1.2842E+00	0.99804	9.9054E-01	-0.0095	-0.0095	9.9054E-01	0.000
33.090	1.2861E+00	0.99834	9.9203E-01	-0.0080	-0.0081	9.9193E-01	0.010
33.100	1.2880E+00	0.99864	9.9352E-01	-0.0065	-0.0066	9.9342E-01	0.010
33.110	1.2899E+00	0.99894	9.9501E-01	-0.0050	-0.0052	9.9481E-01	0.020
33.120	1.2917E+00	0.99925	9.9641E-01	-0.0036	-0.0037	9.9631E-01	0.010
33.130	1.2936E+00	0.99955	9.9780E-01	-0.0022	-0.0022	9.9780E-01	0.000
33.140	1.2955E+00	0.99985	9.9930E-01	-0.0007	-0.0007	9.9930E-01	0.000
						Average	0.005
						Maximum	0.030

The temperature interval is 0.1° K up to high reduced temperatures (≈ 0.987), at which point the interval is reduced to 0.01° K.

Table A.2. VLE Predictions for Helium Using Wagner Constants Regressed from *NIST*

Analytic (*NIST*)					**Predicted**		
T (^{0}K)	P (MPa)	T_r	$P_{v,r}$	$Ln\ P_{v,r}$	$Ln\ P_{v,r}$	$P_{v,r}$	A%Err
2.180	4.8960E-03	0.41961	2.1524E-02	-3.8386	-3.8325	2.1655E-02	0.612
2.195	5.0850E-03	0.42252	2.2355E-02	-3.8007	-3.7956	2.2469E-02	0.511
2.210	5.2786E-03	0.42542	2.3207E-02	-3.7633	-3.7592	2.3302E-02	0.411
2.225	5.4769E-03	0.42831	2.4079E-02	-3.7264	-3.7234	2.4152E-02	0.300
2.240	5.6800E-03	0.43122	2.4972E-02	-3.6900	-3.6877	2.5030E-02	0.230
2.255	5.8879E-03	0.43412	2.5885E-02	-3.6541	-3.6524	2.5929E-02	0.170
2.271	6.1007E-03	0.43703	2.6820E-02	-3.6186	-3.6174	2.6852E-02	0.120
2.286	6.3185E-03	0.43992	2.7778E-02	-3.5835	-3.5830	2.7792E-02	0.050
2.301	6.5414E-03	0.44282	2.8759E-02	-3.5488	-3.5488	2.8759E-02	0.000
2.316	6.7694E-03	0.44573	2.9760E-02	-3.5146	-3.5148	2.9754E-02	0.020
2.331	7.0027E-03	0.44864	3.0786E-02	-3.4807	-3.4812	3.0770E-02	0.050
2.346	7.2412E-03	0.45152	3.1835E-02	-3.4472	-3.4483	3.1800E-02	0.110
2.361	7.4851E-03	0.45443	3.2906E-02	-3.4141	-3.4153	3.2867E-02	0.120
2.376	7.7344E-03	0.45734	3.4003E-02	-3.3813	-3.3826	3.3959E-02	0.130
2.391	7.9892E-03	0.46024	3.5123E-02	-3.3489	-3.3504	3.5070E-02	0.150
2.406	8.2496E-03	0.46313	3.6269E-02	-3.3168	-3.3186	3.6203E-02	0.180
2.421	8.5157E-03	0.46604	3.7437E-02	-3.2851	-3.2869	3.7370E-02	0.180
2.436	8.7875E-03	0.46894	3.8635E-02	-3.2536	-3.2556	3.8558E-02	0.200
2.451	9.0651E-03	0.47185	3.9855E-02	-3.2225	-3.2244	3.9780E-02	0.190
2.467	9.3485E-03	0.47476	4.1098E-02	-3.1918	-3.1936	4.1024E-02	0.180
2.482	9.6380E-03	0.47764	4.2371E-02	-3.1613	-3.1634	4.2282E-02	0.210
2.497	9.9334E-03	0.48055	4.3670E-02	-3.1311	-3.1331	4.3582E-02	0.200
2.512	1.0235E-02	0.48346	4.4995E-02	-3.1012	-3.1031	4.4910E-02	0.190
2.527	1.0543E-02	0.48636	4.6352E-02	-3.0715	-3.0735	4.6259E-02	0.200
2.542	1.0857E-02	0.48925	4.7730E-02	-3.0422	-3.0442	4.7634E-02	0.200
2.557	1.1177E-02	0.49216	4.9139E-02	-3.0131	-3.0150	4.9046E-02	0.190
2.572	1.1503E-02	0.49506	5.0570E-02	-2.9844	-2.9861	5.0484E-02	0.170
2.587	1.1836E-02	0.49797	5.2037E-02	-2.9558	-2.9575	5.1949E-02	0.170
2.602	1.2176E-02	0.50086	5.3531E-02	-2.9275	-2.9292	5.3440E-02	0.170
2.617	1.2522E-02	0.50376	5.5051E-02	-2.8995	-2.9011	5.4963E-02	0.160
2.632	1.2875E-02	0.50667	5.6603E-02	-2.8717	-2.8732	5.6518E-02	0.150
2.647	1.3235E-02	0.50958	5.8187E-02	-2.8441	-2.8455	5.8105E-02	0.140
2.662	1.3601E-02	0.51246	5.9797E-02	-2.8168	-2.8183	5.9707E-02	0.150
2.678	1.3974E-02	0.51537	6.1433E-02	-2.7898	-2.7910	6.1360E-02	0.120
2.693	1.4355E-02	0.51828	6.3108E-02	-2.7629	-2.7640	6.3039E-02	0.110
2.708	1.4742E-02	0.52118	6.4810E-02	-2.7363	-2.7373	6.4745E-02	0.100

Analytic (*NIST)*					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
2.723	1.5136E-02	0.52409	6.6543E-02	-2.7099	-2.7108	6.6484E-02	0.090
2.738	1.5537E-02	0.52698	6.8303E-02	-2.6838	-2.6846	6.8248E-02	0.080
2.753	1.5946E-02	0.52988	7.0102E-02	-2.6578	-2.6586	7.0046E-02	0.080
2.768	1.6362E-02	0.53279	7.1934E-02	-2.6320	-2.6327	7.1884E-02	0.070
2.783	1.6785E-02	0.53570	7.3792E-02	-2.6065	-2.6070	7.3755E-02	0.050
2.798	1.7216E-02	0.53858	7.5691E-02	-2.5811	-2.5817	7.5645E-02	0.060
2.813	1.7654E-02	0.54149	7.7615E-02	-2.5560	-2.5565	7.7576E-02	0.050
2.828	1.8100E-02	0.54440	7.9571E-02	-2.5311	-2.5314	7.9548E-02	0.030
2.843	1.8553E-02	0.54730	8.1569E-02	-2.5063	-2.5066	8.1545E-02	0.030
2.858	1.9014E-02	0.55019	8.3593E-02	-2.4818	-2.4820	8.3576E-02	0.020
2.874	1.9483E-02	0.55310	8.5657E-02	-2.4574	-2.4575	8.5649E-02	0.010
2.889	1.9960E-02	0.55600	8.7756E-02	-2.4332	-2.4333	8.7747E-02	0.010
2.904	2.0444E-02	0.55891	8.9878E-02	-2.4093	-2.4092	8.9887E-02	0.010
2.919	2.0937E-02	0.56180	9.2043E-02	-2.3855	-2.3854	9.2052E-02	0.010
2.934	2.1437E-02	0.56470	9.4241E-02	-2.3619	-2.3617	9.4260E-02	0.020
2.949	2.1945E-02	0.56761	9.6482E-02	-2.3384	-2.3382	9.6501E-02	0.020
2.964	2.2462E-02	0.57052	9.8756E-02	-2.3151	-2.3148	9.8786E-02	0.030
2.979	2.2987E-02	0.57342	1.0106E-01	-2.2920	-2.2916	1.0110E-01	0.040
2.994	2.3520E-02	0.57631	1.0341E-01	-2.2691	-2.2687	1.0345E-01	0.040
3.009	2.4062E-02	0.57922	1.0579E-01	-2.2463	-2.2458	1.0584E-01	0.050
3.024	2.4611E-02	0.58212	1.0820E-01	-2.2238	-2.2232	1.0826E-01	0.060
3.039	2.5170E-02	0.58503	1.1066E-01	-2.2013	-2.2007	1.1073E-01	0.060
3.054	2.5737E-02	0.58792	1.1315E-01	-2.1790	-2.1784	1.1322E-01	0.060
3.070	2.6312E-02	0.59082	1.1568E-01	-2.1569	-2.1563	1.1575E-01	0.060
3.085	2.6896E-02	0.59373	1.1824E-01	-2.1350	-2.1342	1.1834E-01	0.080
3.100	2.7489E-02	0.59664	1.2085E-01	-2.1132	-2.1123	1.2096E-01	0.090
3.115	2.8091E-02	0.59952	1.2350E-01	-2.0915	-2.0908	1.2359E-01	0.070
3.130	2.8701E-02	0.60243	1.2619E-01	-2.0700	-2.0692	1.2629E-01	0.080
3.145	2.9320E-02	0.60534	1.2890E-01	-2.0487	-2.0478	1.2902E-01	0.090
3.160	2.9949E-02	0.60824	1.3166E-01	-2.0275	-2.0266	1.3178E-01	0.090
3.175	3.0586E-02	0.61113	1.3447E-01	-2.0064	-2.0056	1.3458E-01	0.080
3.190	3.1232E-02	0.61404	1.3731E-01	-1.9855	-1.9846	1.3744E-01	0.090
3.205	3.1888E-02	0.61694	1.4020E-01	-1.9647	-1.9638	1.4032E-01	0.090
3.220	3.2553E-02	0.61985	1.4312E-01	-1.9441	-1.9431	1.4326E-01	0.100
3.235	3.3227E-02	0.62276	1.4608E-01	-1.9236	-1.9225	1.4624E-01	0.110
3.250	3.3910E-02	0.62564	1.4908E-01	-1.9033	-1.9023	1.4923E-01	0.100
3.266	3.4603E-02	0.62855	1.5213E-01	-1.8830	-1.8820	1.5229E-01	0.100

Analytic (*NIST*)					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**Ln $P_{v,r}$**	**Ln $P_{v,r}$**	**$P_{v,r}$**	**A%Err**
3.281	3.5305E-02	0.63146	1.5522E-01	-1.8629	-1.8619	1.5538E-01	0.100
3.296	3.6017E-02	0.63436	1.5834E-01	-1.8430	-1.8419	1.5852E-01	0.110
3.311	3.6738E-02	0.63725	1.6151E-01	-1.8232	-1.8222	1.6167E-01	0.100
3.326	3.7469E-02	0.64016	1.6472E-01	-1.8035	-1.8024	1.6490E-01	0.110
3.341	3.8210E-02	0.64306	1.6798E-01	-1.7839	-1.7829	1.6815E-01	0.100
3.356	3.8961E-02	0.64597	1.7129E-01	-1.7644	-1.7634	1.7146E-01	0.100
3.371	3.9721E-02	0.64886	1.7463E-01	-1.7451	-1.7441	1.7480E-01	0.100
3.386	4.0491E-02	0.65176	1.7801E-01	-1.7259	-1.7249	1.7819E-01	0.100
3.401	4.1271E-02	0.65467	1.8145E-01	-1.7068	-1.7058	1.8163E-01	0.100
3.416	4.2062E-02	0.65758	1.8493E-01	-1.6878	-1.6868	1.8511E-01	0.100
3.431	4.2862E-02	0.66046	1.8844E-01	-1.6690	-1.6681	1.8861E-01	0.090
3.446	4.3672E-02	0.66337	1.9199E-01	-1.6503	-1.6493	1.9218E-01	0.100
3.462	4.4493E-02	0.66628	1.9562E-01	-1.6316	-1.6307	1.9579E-01	0.090
3.477	4.5324E-02	0.66918	1.9927E-01	-1.6131	-1.6122	1.9945E-01	0.090
3.492	4.6165E-02	0.67209	2.0295E-01	-1.5948	-1.5938	2.0315E-01	0.100
3.507	4.7016E-02	0.67498	2.0670E-01	-1.5765	-1.5756	2.0688E-01	0.090
3.522	4.7878E-02	0.67788	2.1049E-01	-1.5583	-1.5575	2.1066E-01	0.080
3.537	4.8751E-02	0.68079	2.1434E-01	-1.5402	-1.5394	2.1451E-01	0.080
3.552	4.9634E-02	0.68369	2.1821E-01	-1.5223	-1.5215	2.1838E-01	0.080
3.567	5.0527E-02	0.68658	2.2213E-01	-1.5045	-1.5038	2.2228E-01	0.070
3.582	5.1432E-02	0.68949	2.2612E-01	-1.4867	-1.4860	2.2628E-01	0.070
3.597	5.2347E-02	0.69240	2.3013E-01	-1.4691	-1.4683	2.3032E-01	0.080
3.612	5.3273E-02	0.69530	2.3422E-01	-1.4515	-1.4509	2.3436E-01	0.060
3.627	5.4210E-02	0.69819	2.3833E-01	-1.4341	-1.4335	2.3847E-01	0.060
3.642	5.5157E-02	0.70110	2.4249E-01	-1.4168	-1.4162	2.4263E-01	0.060
3.658	5.6116E-02	0.70400	2.4670E-01	-1.3996	-1.3990	2.4684E-01	0.060
3.673	5.7086E-02	0.70691	2.5098E-01	-1.3824	-1.3819	2.5110E-01	0.050
3.688	5.8067E-02	0.70981	2.5528E-01	-1.3654	-1.3649	2.5541E-01	0.050
3.703	5.9059E-02	0.71270	2.5966E-01	-1.3484	-1.3480	2.5976E-01	0.040
3.718	6.0062E-02	0.71561	2.6405E-01	-1.3316	-1.3312	2.6416E-01	0.040
3.733	6.1077E-02	0.71851	2.6853E-01	-1.3148	-1.3145	2.6861E-01	0.030
3.748	6.2103E-02	0.72142	2.7302E-01	-1.2982	-1.2978	2.7313E-01	0.040
3.763	6.3140E-02	0.72431	2.7759E-01	-1.2816	-1.2813	2.7768E-01	0.030
3.778	6.4189E-02	0.72721	2.8221E-01	-1.2651	-1.2649	2.8227E-01	0.020
3.793	6.5250E-02	0.73012	2.8688E-01	-1.2487	-1.2485	2.8693E-01	0.020
3.808	6.6322E-02	0.73303	2.9156E-01	-1.2325	-1.2322	2.9165E-01	0.030
3.823	6.7406E-02	0.73592	2.9635E-01	-1.2162	-1.2161	2.9638E-01	0.010

Analytic (*NIST)*					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
3.838	6.8501E-02	0.73882	3.0116E-01	-1.2001	-1.2001	3.0116E-01	0.000
3.854	6.9608E-02	0.74173	3.0602E-01	-1.1841	-1.1840	3.0605E-01	0.010
3.869	7.0728E-02	0.74463	3.1096E-01	-1.1681	-1.1681	3.1096E-01	0.000
3.884	7.1859E-02	0.74752	3.1591E-01	-1.1523	-1.1524	3.1588E-01	0.010
3.899	7.3002E-02	0.75043	3.2094E-01	-1.1365	-1.1366	3.2091E-01	0.010
3.914	7.4157E-02	0.75333	3.2602E-01	-1.1208	-1.1209	3.2599E-01	0.010
3.929	7.5325E-02	0.75624	3.3114E-01	-1.1052	-1.1053	3.3111E-01	0.010
3.944	7.6504E-02	0.75915	3.3635E-01	-1.0896	-1.0898	3.3628E-01	0.020
3.959	7.7696E-02	0.76203	3.4157E-01	-1.0742	-1.0745	3.4147E-01	0.030
3.974	7.8901E-02	0.76494	3.4687E-01	-1.0588	-1.0591	3.4677E-01	0.030
3.989	8.0117E-02	0.76785	3.5222E-01	-1.0435	-1.0438	3.5211E-01	0.030
4.004	8.1346E-02	0.77075	3.5761E-01	-1.0283	-1.0286	3.5751E-01	0.030
4.019	8.2588E-02	0.77364	3.6309E-01	-1.0131	-1.0135	3.6295E-01	0.040
4.034	8.3842E-02	0.77655	3.6862E-01	-0.9980	-0.9985	3.6843E-01	0.050
4.050	8.5109E-02	0.77945	3.7419E-01	-0.9830	-0.9835	3.7400E-01	0.050
4.065	8.6389E-02	0.78236	3.7980E-01	-0.9681	-0.9686	3.7961E-01	0.050
4.080	8.7682E-02	0.78525	3.8547E-01	-0.9533	-0.9538	3.8527E-01	0.050
4.095	8.8987E-02	0.78815	3.9121E-01	-0.9385	-0.9391	3.9098E-01	0.060
4.110	9.0306E-02	0.79106	3.9701E-01	-0.9238	-0.9244	3.9677E-01	0.060
4.125	9.1637E-02	0.79397	4.0289E-01	-0.9091	-0.9097	4.0264E-01	0.060
4.140	9.2982E-02	0.79685	4.0877E-01	-0.8946	-0.8953	4.0849E-01	0.070
4.155	9.4340E-02	0.79976	4.1474E-01	-0.8801	-0.8808	4.1445E-01	0.070
4.170	9.5711E-02	0.80267	4.2080E-01	-0.8656	-0.8664	4.2046E-01	0.080
4.185	9.7095E-02	0.80557	4.2686E-01	-0.8513	-0.8520	4.2656E-01	0.070
4.200	9.8493E-02	0.80848	4.3301E-01	-0.8370	-0.8377	4.3270E-01	0.070
4.215	9.9904E-02	0.81137	4.3920E-01	-0.8228	-0.8236	4.3885E-01	0.080
4.230	1.0133E-01	0.81427	4.4548E-01	-0.8086	-0.8095	4.4508E-01	0.090
4.246	1.0277E-01	0.81718	4.5181E-01	-0.7945	-0.7953	4.5145E-01	0.080
4.261	1.0422E-01	0.82009	4.5818E-01	-0.7805	-0.7813	4.5781E-01	0.080
4.276	1.0569E-01	0.82297	4.6464E-01	-0.7665	-0.7674	4.6422E-01	0.090
4.291	1.0717E-01	0.82588	4.7114E-01	-0.7526	-0.7535	4.7072E-01	0.090
4.306	1.0866E-01	0.82879	4.7769E-01	-0.7388	-0.7396	4.7730E-01	0.080
4.321	1.1017E-01	0.83169	4.8437E-01	-0.7249	-0.7259	4.8389E-01	0.100
4.336	1.1169E-01	0.83458	4.9105E-01	-0.7112	-0.7122	4.9056E-01	0.100
4.351	1.1323E-01	0.83749	4.9778E-01	-0.6976	-0.6985	4.9733E-01	0.090
4.366	1.1478E-01	0.84039	5.0459E-01	-0.6840	-0.6849	5.0414E-01	0.090
4.381	1.1634E-01	0.84330	5.1145E-01	-0.6705	-0.6714	5.1099E-01	0.090

Analytic (*NIST*)					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
4.396	1.1792E-01	0.84619	5.1840E-01	-0.6570	-0.6579	5.1794E-01	0.090
4.411	1.1952E-01	0.84909	5.2545E-01	-0.6435	-0.6445	5.2492E-01	0.100
4.426	1.2113E-01	0.85200	5.3254E-01	-0.6301	-0.6311	5.3201E-01	0.100
4.442	1.2275E-01	0.85491	5.3967E-01	-0.6168	-0.6177	5.3918E-01	0.090
4.457	1.2439E-01	0.85781	5.4684E-01	-0.6036	-0.6045	5.4635E-01	0.090
4.472	1.2604E-01	0.86070	5.5411E-01	-0.5904	-0.5913	5.5361E-01	0.090
4.487	1.2771E-01	0.86361	5.6147E-01	-0.5772	-0.5781	5.6096E-01	0.090
4.502	1.2940E-01	0.86651	5.6887E-01	-0.5641	-0.5650	5.6836E-01	0.090
4.517	1.3110E-01	0.86942	5.7637E-01	-0.5510	-0.5519	5.7585E-01	0.090
4.532	1.3281E-01	0.87231	5.8386E-01	-0.5381	-0.5389	5.8339E-01	0.080
4.547	1.3454E-01	0.87521	5.9150E-01	-0.5251	-0.5260	5.9096E-01	0.090
4.562	1.3629E-01	0.87812	5.9918E-01	-0.5122	-0.5130	5.9870E-01	0.080
4.577	1.3805E-01	0.88103	6.0689E-01	-0.4994	-0.5001	6.0647E-01	0.070
4.592	1.3983E-01	0.88391	6.1477E-01	-0.4865	-0.4874	6.1422E-01	0.090
4.607	1.4162E-01	0.88682	6.2263E-01	-0.4738	-0.4745	6.2220E-01	0.070
4.622	1.4343E-01	0.88973	6.3059E-01	-0.4611	-0.4618	6.3015E-01	0.070
4.638	1.4526E-01	0.89263	6.3865E-01	-0.4484	-0.4491	6.3820E-01	0.070
4.653	1.4710E-01	0.89552	6.4668E-01	-0.4359	-0.4365	6.4629E-01	0.060
4.668	1.4896E-01	0.89843	6.5488E-01	-0.4233	-0.4238	6.5455E-01	0.050
4.683	1.5083E-01	0.90133	6.6312E-01	-0.4108	-0.4113	6.6279E-01	0.050
4.698	1.5273E-01	0.90424	6.7146E-01	-0.3983	-0.3987	6.7119E-01	0.040
4.713	1.5464E-01	0.90715	6.7984E-01	-0.3859	-0.3862	6.7963E-01	0.030
4.728	1.5656E-01	0.91003	6.8832E-01	-0.3735	-0.3738	6.8811E-01	0.030
4.743	1.5851E-01	0.91294	6.9684E-01	-0.3612	-0.3614	6.9670E-01	0.020
4.758	1.6047E-01	0.91585	7.0546E-01	-0.3489	-0.3489	7.0546E-01	0.000
4.773	1.6245E-01	0.91875	7.1419E-01	-0.3366	-0.3366	7.1419E-01	0.000
4.788	1.6445E-01	0.92164	7.2296E-01	-0.3244	-0.3243	7.2303E-01	0.010
4.803	1.6646E-01	0.92455	7.3184E-01	-0.3122	-0.3120	7.3198E-01	0.020
4.818	1.6850E-01	0.92745	7.4082E-01	-0.3000	-0.2998	7.4097E-01	0.020
4.834	1.7055E-01	0.93036	7.4984E-01	-0.2879	-0.2876	7.5006E-01	0.030
4.849	1.7262E-01	0.93325	7.5889E-01	-0.2759	-0.2754	7.5927E-01	0.050
4.864	1.7471E-01	0.93615	7.6813E-01	-0.2638	-0.2633	7.6851E-01	0.050
4.879	1.7682E-01	0.93906	7.7740E-01	-0.2518	-0.2512	7.7787E-01	0.060
4.894	1.7895E-01	0.94197	7.8671E-01	-0.2399	-0.2390	7.8741E-01	0.090
4.909	1.8110E-01	0.94485	7.9620E-01	-0.2279	-0.2271	7.9684E-01	0.080
4.924	1.8327E-01	0.94776	8.0574E-01	-0.2160	-0.2150	8.0654E-01	0.100
4.939	1.8546E-01	0.95067	8.1538E-01	-0.2041	-0.2029	8.1636E-01	0.120

Analytic (*NIST)*					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
4.954	1.8767E-01	0.95357	8.2506E-01	-0.1923	-0.1910	8.2613E-01	0.130
4.969	1.8990E-01	0.95648	8.3485E-01	-0.1805	-0.1790	8.3611E-01	0.150
4.984	1.9215E-01	0.95937	8.4476E-01	-0.1687	-0.1671	8.4611E-01	0.160
4.999	1.9443E-01	0.96227	8.5479E-01	-0.1569	-0.1551	8.5633E-01	0.180
5.014	1.9672E-01	0.96518	8.6485E-01	-0.1452	-0.1432	8.6658E-01	0.200
5.030	1.9905E-01	0.96809	8.7511E-01	-0.1334	-0.1312	8.7704E-01	0.220
5.045	2.0139E-01	0.97097	8.8541E-01	-0.1217	-0.1194	8.8745E-01	0.230
5.060	2.0376E-01	0.97388	8.9583E-01	-0.1100	-0.1075	8.9808E-01	0.250
5.075	2.0615E-01	0.97679	9.0629E-01	-0.0984	-0.0956	9.0883E-01	0.280
5.090	2.0857E-01	0.97969	9.1695E-01	-0.0867	-0.0838	9.1962E-01	0.290
5.105	2.1102E-01	0.98258	9.2774E-01	-0.0750	-0.0719	9.3062E-01	0.310
5.120	2.1350E-01	0.98549	9.3866E-01	-0.0633	-0.0600	9.4176E-01	0.331
5.135	2.1600E-01	0.98839	9.4961E-01	-0.0517	-0.0481	9.5304E-01	0.361
5.145	2.1768E-01	0.99032	9.5705E-01	-0.0439	-0.0402	9.6060E-01	0.371
5.155	2.1938E-01	0.99224	9.6445E-01	-0.0362	-0.0323	9.6822E-01	0.391
5.165	2.2109E-01	0.99417	9.7200E-01	-0.0284	-0.0243	9.7599E-01	0.411
5.175	2.2281E-01	0.99609	9.7951E-01	-0.0207	-0.0164	9.8373E-01	0.431
5.185	2.2456E-01	0.99802	9.8728E-01	-0.0128	-0.0083	9.9173E-01	0.451
5.195	2.2632E-01	0.99994	9.9501E-01	-0.0050	-0.0003	9.9970E-01	0.471
						Average	0.105
						Maximum	0.612

The temperature interval is 0.015° K up to high reduced temperatures (≈ 0.988), at which point the interval is reduced to 0.01° K.

Table A.3. VLE Predictions for Argon Using Wagner Constants Regressed from *NIST*

Analytic (*NIST*)					**Predicted**		
T **(^{0}K)**	***P*** **(MPa)**	T_r	$P_{v,r}$	***Ln*** $P_{v,r}$	***Ln*** $P_{v,r}$	$P_{v,r}$	**A%Err**
83.806	6.8891E-02	0.55616	1.4166E-02	-4.2569	-4.2568	1.4168E-02	0.010
84.306	7.2952E-02	0.55948	1.5002E-02	-4.1996	-4.1995	1.5003E-02	0.010
84.806	7.7197E-02	0.56280	1.5874E-02	-4.1431	-4.1429	1.5877E-02	0.020
85.306	8.1631E-02	0.56611	1.6786E-02	-4.0872	-4.0872	1.6786E-02	0.000
85.806	8.6259E-02	0.56943	1.7737E-02	-4.0321	-4.0321	1.7737E-02	0.000
86.306	9.1086E-02	0.57275	1.8731E-02	-3.9776	-3.9776	1.8731E-02	0.000
86.806	9.6120E-02	0.57607	1.9766E-02	-3.9238	-3.9238	1.9766E-02	0.000
87.306	1.0136E-01	0.57939	2.0844E-02	-3.8707	-3.8706	2.0846E-02	0.010
87.806	1.0683E-01	0.58270	2.1967E-02	-3.8182	-3.8183	2.1965E-02	0.010
88.306	1.1251E-01	0.58602	2.3135E-02	-3.7664	-3.7664	2.3135E-02	0.000
88.806	1.1842E-01	0.58934	2.4351E-02	-3.7152	-3.7152	2.4351E-02	0.000
89.306	1.2457E-01	0.59266	2.5617E-02	-3.6645	-3.6645	2.5617E-02	0.000
89.806	1.3096E-01	0.59598	2.6930E-02	-3.6145	-3.6145	2.6930E-02	0.000
90.306	1.3759E-01	0.59930	2.8294E-02	-3.5651	-3.5651	2.8294E-02	0.000
90.806	1.4448E-01	0.60261	2.9709E-02	-3.5163	-3.5164	2.9706E-02	0.010
91.306	1.5163E-01	0.60593	3.1179E-02	-3.4680	-3.4681	3.1176E-02	0.010
91.806	1.5904E-01	0.60925	3.2703E-02	-3.4203	-3.4203	3.2703E-02	0.000
92.306	1.6672E-01	0.61257	3.4283E-02	-3.3731	-3.3731	3.4283E-02	0.000
92.806	1.7468E-01	0.61589	3.5919E-02	-3.3265	-3.3265	3.5919E-02	0.000
93.306	1.8292E-01	0.61920	3.7613E-02	-3.2804	-3.2805	3.7609E-02	0.010
93.806	1.9146E-01	0.62252	3.9372E-02	-3.2347	-3.2348	3.9368E-02	0.010
94.306	2.0029E-01	0.62584	4.1188E-02	-3.1896	-3.1897	4.1184E-02	0.010
94.806	2.0942E-01	0.62916	4.3063E-02	-3.1451	-3.1451	4.3063E-02	0.000
95.306	2.1886E-01	0.63248	4.5004E-02	-3.1010	-3.1010	4.5004E-02	0.000
95.806	2.2861E-01	0.63579	4.7010E-02	-3.0574	-3.0575	4.7005E-02	0.010
96.306	2.3869E-01	0.63911	4.9085E-02	-3.0142	-3.0144	4.9075E-02	0.020
96.806	2.4910E-01	0.64243	5.1221E-02	-2.9716	-2.9717	5.1216E-02	0.010
97.306	2.5984E-01	0.64575	5.3434E-02	-2.9293	-2.9294	5.3429E-02	0.010
97.806	2.7092E-01	0.64907	5.5710E-02	-2.8876	-2.8876	5.5710E-02	0.000
98.306	2.8236E-01	0.65239	5.8065E-02	-2.8462	-2.8463	5.8059E-02	0.010
98.806	2.9414E-01	0.65570	6.0483E-02	-2.8054	-2.8055	6.0477E-02	0.010
99.306	3.0629E-01	0.65902	6.2982E-02	-2.7649	-2.7650	6.2976E-02	0.010
99.806	3.1881E-01	0.66234	6.5559E-02	-2.7248	-2.7250	6.5546E-02	0.020
100.310	3.3170E-01	0.66568	6.8208E-02	-2.6852	-2.6851	6.8214E-02	0.010
100.810	3.4497E-01	0.66900	7.0934E-02	-2.6460	-2.6458	7.0949E-02	0.020

101.310	3.5863E-01	0.67232	7.3748E-02	-2.6071	-2.6070	7.3755E-02	0.010
101.810	3.7268E-01	0.67564	7.6635E-02	-2.5687	-2.5685	7.6650E-02	0.020
102.310	3.8714E-01	0.67896	7.9611E-02	-2.5306	-2.5304	7.9627E-02	0.020
102.810	4.0200E-01	0.68228	8.2662E-02	-2.4930	-2.4928	8.2678E-02	0.020
103.310	4.1728E-01	0.68559	8.5803E-02	-2.4557	-2.4555	8.5820E-02	0.020
103.810	4.3299E-01	0.68891	8.9037E-02	-2.4187	-2.4186	8.9046E-02	0.010
104.310	4.4912E-01	0.69223	9.2356E-02	-2.3821	-2.3820	9.2366E-02	0.010
104.810	4.6568E-01	0.69555	9.5761E-02	-2.3459	-2.3458	9.5771E-02	0.010
105.310	4.8269E-01	0.69887	9.9261E-02	-2.3100	-2.3099	9.9271E-02	0.010
105.810	5.0015E-01	0.70218	1.0285E-01	-2.2745	-2.2744	1.0286E-01	0.010
106.310	5.1807E-01	0.70550	1.0653E-01	-2.2393	-2.2392	1.0654E-01	0.010
106.810	5.3645E-01	0.70882	1.1032E-01	-2.2044	-2.2044	1.1032E-01	0.000
107.310	5.5530E-01	0.71214	1.1419E-01	-2.1699	-2.1698	1.1420E-01	0.010
107.810	5.7463E-01	0.71546	1.1816E-01	-2.1357	-2.1356	1.1817E-01	0.010
108.310	5.9444E-01	0.71877	1.2224E-01	-2.1018	-2.1018	1.2224E-01	0.000
108.810	6.1474E-01	0.72209	1.2641E-01	-2.0682	-2.0682	1.2641E-01	0.000
109.310	6.3554E-01	0.72541	1.3069E-01	-2.0349	-2.0349	1.3069E-01	0.000
109.810	6.5685E-01	0.72873	1.3506E-01	-2.0020	-2.0019	1.3508E-01	0.010
110.310	6.7867E-01	0.73205	1.3955E-01	-1.9693	-1.9692	1.3957E-01	0.010
110.810	7.0100E-01	0.73537	1.4415E-01	-1.9369	-1.9368	1.4416E-01	0.010
111.310	7.2387E-01	0.73868	1.4885E-01	-1.9048	-1.9048	1.4885E-01	0.000
111.810	7.4727E-01	0.74200	1.5366E-01	-1.8730	-1.8730	1.5366E-01	0.000
112.310	7.7121E-01	0.74532	1.5858E-01	-1.8415	-1.8415	1.5858E-01	0.000
112.810	7.9569E-01	0.74864	1.6362E-01	-1.8102	-1.8102	1.6362E-01	0.000
113.310	8.2074E-01	0.75196	1.6877E-01	-1.7792	-1.7792	1.6877E-01	0.000
113.810	8.4634E-01	0.75527	1.7403E-01	-1.7485	-1.7485	1.7403E-01	0.000
114.310	8.7251E-01	0.75859	1.7942E-01	-1.7180	-1.7181	1.7941E-01	0.010
114.810	8.9926E-01	0.76191	1.8493E-01	-1.6878	-1.6879	1.8491E-01	0.010
115.310	9.2660E-01	0.76523	1.9054E-01	-1.6579	-1.6579	1.9054E-01	0.000
115.810	9.5452E-01	0.76855	1.9628E-01	-1.6282	-1.6282	1.9628E-01	0.000
116.310	9.8305E-01	0.77186	2.0214E-01	-1.5988	-1.5988	2.0214E-01	0.000
116.810	1.0122E+00	0.77518	2.0815E-01	-1.5695	-1.5696	2.0813E-01	0.010
117.310	1.0419E+00	0.77850	2.1425E-01	-1.5406	-1.5406	2.1425E-01	0.000
117.810	1.0723E+00	0.78182	2.2051E-01	-1.5118	-1.5119	2.2049E-01	0.010
118.310	1.1033E+00	0.78514	2.2689E-01	-1.4833	-1.4834	2.2687E-01	0.010
118.810	1.1349E+00	0.78846	2.3338E-01	-1.4551	-1.4551	2.3338E-01	0.000
119.310	1.1672E+00	0.79177	2.4003E-01	-1.4270	-1.4272	2.3998E-01	0.020
119.810	1.2001E+00	0.79509	2.4677E-01	-1.3993	-1.3993	2.4677E-01	0.000
120.310	1.2337E+00	0.79841	2.5370E-01	-1.3716	-1.3717	2.5368E-01	0.010

120.810	1.2679E+00	0.80173	2.6072E-01	-1.3443	-1.3443	2.6072E-01	0.000
121.310	1.3028E+00	0.80505	2.6791E-01	-1.3171	-1.3172	2.6788E-01	0.010
121.810	1.3384E+00	0.80836	2.7522E-01	-1.2902	-1.2903	2.7519E-01	0.010
122.310	1.3747E+00	0.81168	2.8269E-01	-1.2634	-1.2635	2.8266E-01	0.010
122.810	1.4116E+00	0.81500	2.9028E-01	-1.2369	-1.2370	2.9025E-01	0.010
123.310	1.4493E+00	0.81832	2.9802E-01	-1.2106	-1.2106	2.9802E-01	0.000
123.810	1.4877E+00	0.82164	3.0593E-01	-1.1844	-1.1844	3.0593E-01	0.000
124.310	1.5268E+00	0.82496	3.1396E-01	-1.1585	-1.1585	3.1396E-01	0.000
124.810	1.5667E+00	0.82827	3.2216E-01	-1.1327	-1.1328	3.2213E-01	0.010
125.310	1.6072E+00	0.83159	3.3048E-01	-1.1072	-1.1072	3.3048E-01	0.000
125.810	1.6485E+00	0.83491	3.3898E-01	-1.0818	-1.0818	3.3898E-01	0.000
126.310	1.6906E+00	0.83823	3.4764E-01	-1.0566	-1.0566	3.4764E-01	0.000
126.810	1.7334E+00	0.84155	3.5644E-01	-1.0316	-1.0316	3.5644E-01	0.000
127.310	1.7770E+00	0.84486	3.6542E-01	-1.0067	-1.0068	3.6539E-01	0.010
127.810	1.8214E+00	0.84818	3.7452E-01	-0.9821	-0.9821	3.7452E-01	0.000
128.310	1.8665E+00	0.85150	3.8381E-01	-0.9576	-0.9576	3.8381E-01	0.000
128.810	1.9125E+00	0.85482	3.9329E-01	-0.9332	-0.9333	3.9325E-01	0.010
129.310	1.9592E+00	0.85814	4.0289E-01	-0.9091	-0.9091	4.0289E-01	0.000
129.810	2.0068E+00	0.86145	4.1267E-01	-0.8851	-0.8852	4.1263E-01	0.010
130.310	2.0551E+00	0.86477	4.2261E-01	-0.8613	-0.8613	4.2261E-01	0.000
130.810	2.1043E+00	0.86809	4.3270E-01	-0.8377	-0.8377	4.3270E-01	0.000
131.310	2.1544E+00	0.87141	4.4304E-01	-0.8141	-0.8141	4.4304E-01	0.000
131.810	2.2053E+00	0.87473	4.5348E-01	-0.7908	-0.7908	4.5348E-01	0.000
132.310	2.2570E+00	0.87805	4.6413E-01	-0.7676	-0.7676	4.6413E-01	0.000
132.810	2.3096E+00	0.88136	4.7492E-01	-0.7446	-0.7446	4.7492E-01	0.000
133.310	2.3631E+00	0.88468	4.8593E-01	-0.7217	-0.7217	4.8593E-01	0.000
133.810	2.4174E+00	0.88800	4.9708E-01	-0.6990	-0.6989	4.9713E-01	0.010
134.310	2.4727E+00	0.89132	5.0849E-01	-0.6763	-0.6763	5.0849E-01	0.000
134.810	2.5288E+00	0.89464	5.2001E-01	-0.6539	-0.6538	5.2007E-01	0.010
135.310	2.5859E+00	0.89795	5.3174E-01	-0.6316	-0.6316	5.3174E-01	0.000
135.810	2.6439E+00	0.90127	5.4368E-01	-0.6094	-0.6094	5.4368E-01	0.000
136.310	2.7028E+00	0.90459	5.5577E-01	-0.5874	-0.5873	5.5583E-01	0.010
136.810	2.7627E+00	0.90791	5.6813E-01	-0.5654	-0.5654	5.6813E-01	0.000
137.310	2.8235E+00	0.91123	5.8060E-01	-0.5437	-0.5436	5.8065E-01	0.010
137.810	2.8853E+00	0.91454	5.9333E-01	-0.5220	-0.5220	5.9333E-01	0.000
138.310	2.9481E+00	0.91786	6.0623E-01	-0.5005	-0.5005	6.0623E-01	0.000
138.810	3.0118E+00	0.92118	6.1934E-01	-0.4791	-0.4790	6.1940E-01	0.010
139.310	3.0766E+00	0.92450	6.3267E-01	-0.4578	-0.4578	6.3267E-01	0.000
139.810	3.1424E+00	0.92782	6.4617E-01	-0.4367	-0.4366	6.4623E-01	0.010

140.310	3.2092E+00	0.93114	6.5994E-01	-0.4156	-0.4155	6.6001E-01	0.010
140.810	3.2771E+00	0.93445	6.7388E-01	-0.3947	-0.3946	6.7395E-01	0.010
141.310	3.3460E+00	0.93777	6.8805E-01	-0.3739	-0.3738	6.8811E-01	0.010
141.810	3.4160E+00	0.94109	7.0244E-01	-0.3532	-0.3531	7.0251E-01	0.010
142.310	3.4871E+00	0.94441	7.1706E-01	-0.3326	-0.3325	7.1713E-01	0.010
142.810	3.5593E+00	0.94773	7.3191E-01	-0.3121	-0.3120	7.3198E-01	0.010
143.310	3.6326E+00	0.95104	7.4699E-01	-0.2917	-0.2916	7.4707E-01	0.010
143.810	3.7071E+00	0.95436	7.6231E-01	-0.2714	-0.2713	7.6239E-01	0.010
144.310	3.7827E+00	0.95768	7.7787E-01	-0.2512	-0.2511	7.7794E-01	0.010
144.810	3.8595E+00	0.96100	7.9366E-01	-0.2311	-0.2310	7.9374E-01	0.010
145.310	3.9375E+00	0.96432	8.0969E-01	-0.2111	-0.2110	8.0977E-01	0.010
145.810	4.0167E+00	0.96763	8.2597E-01	-0.1912	-0.1911	8.2605E-01	0.010
146.310	4.0972E+00	0.97095	8.4248E-01	-0.1714	-0.1712	8.4265E-01	0.020
146.810	4.1790E+00	0.97427	8.5933E-01	-0.1516	-0.1515	8.5942E-01	0.010
147.310	4.2621E+00	0.97759	8.7643E-01	-0.1319	-0.1318	8.7652E-01	0.010
147.810	4.3466E+00	0.98091	8.9378E-01	-0.1123	-0.1121	8.9395E-01	0.020
148.000	4.3797E+00	0.98217	9.0059E-01	-0.1047	-0.1047	9.0059E-01	0.000
148.010	4.3820E+00	0.98223	9.0105E-01	-0.1042	-0.1043	9.0095E-01	0.010
148.030	4.3843E+00	0.98237	9.0159E-01	-0.1036	-0.1035	9.0168E-01	0.010
148.040	4.3867E+00	0.98243	9.0204E-01	-0.1031	-0.1031	9.0204E-01	0.000
148.050	4.3890E+00	0.98250	9.0249E-01	-0.1026	-0.1027	9.0240E-01	0.010
148.070	4.3913E+00	0.98263	9.0303E-01	-0.1020	-0.1020	9.0303E-01	0.000
148.080	4.3936E+00	0.98270	9.0348E-01	-0.1015	-0.1016	9.0339E-01	0.010
148.090	4.3959E+00	0.98277	9.0393E-01	-0.1010	-0.1011	9.0384E-01	0.010
148.110	4.3982E+00	0.98290	9.0439E-01	-0.1005	-0.1004	9.0448E-01	0.010
148.120	4.4005E+00	0.98296	9.0493E-01	-0.0999	-0.1000	9.0484E-01	0.010
148.130	4.4028E+00	0.98303	9.0538E-01	-0.0994	-0.0996	9.0520E-01	0.020
148.150	4.4051E+00	0.98316	9.0583E-01	-0.0989	-0.0988	9.0592E-01	0.010
148.160	4.4074E+00	0.98323	9.0629E-01	-0.0984	-0.0984	9.0629E-01	0.000
148.170	4.4098E+00	0.98330	9.0683E-01	-0.0978	-0.0980	9.0665E-01	0.020
148.190	4.4121E+00	0.98343	9.0728E-01	-0.0973	-0.0973	9.0728E-01	0.000
148.200	4.4144E+00	0.98350	9.0774E-01	-0.0968	-0.0968	9.0774E-01	0.000
148.210	4.4167E+00	0.98356	9.0819E-01	-0.0963	-0.0965	9.0801E-01	0.020
148.230	4.4190E+00	0.98369	9.0874E-01	-0.0957	-0.0957	9.0874E-01	0.000
148.240	4.4214E+00	0.98376	9.0919E-01	-0.0952	-0.0953	9.0910E-01	0.010
148.260	4.4237E+00	0.98389	9.0965E-01	-0.0947	-0.0945	9.0983E-01	0.020
148.270	4.4260E+00	0.98396	9.1010E-01	-0.0942	-0.0941	9.1019E-01	0.010
148.280	4.4283E+00	0.98403	9.1065E-01	-0.0936	-0.0937	9.1056E-01	0.010
148.300	4.4307E+00	0.98416	9.1110E-01	-0.0931	-0.0930	9.1119E-01	0.010

148.310	4.4330E+00	0.98423	9.1156E-01	-0.0926	-0.0925	9.1165E-01	0.010
148.320	4.4353E+00	0.98429	9.1201E-01	-0.0921	-0.0922	9.1192E-01	0.010
148.340	4.4376E+00	0.98442	9.1256E-01	-0.0915	-0.0914	9.1265E-01	0.010
148.350	4.4400E+00	0.98449	9.1302E-01	-0.0910	-0.0910	9.1302E-01	0.000
148.360	4.4423E+00	0.98456	9.1347E-01	-0.0905	-0.0906	9.1338E-01	0.010
148.380	4.4446E+00	0.98469	9.1393E-01	-0.0900	-0.0898	9.1411E-01	0.020
148.390	4.4470E+00	0.98476	9.1448E-01	-0.0894	-0.0894	9.1448E-01	0.000
148.400	4.4493E+00	0.98482	9.1494E-01	-0.0889	-0.0891	9.1475E-01	0.020
148.420	4.4516E+00	0.98496	9.1539E-01	-0.0884	-0.0882	9.1558E-01	0.020
148.430	4.4540E+00	0.98502	9.1585E-01	-0.0879	-0.0879	9.1585E-01	0.000
148.440	4.4563E+00	0.98509	9.1640E-01	-0.0873	-0.0875	9.1622E-01	0.020
148.460	4.4586E+00	0.98522	9.1686E-01	-0.0868	-0.0867	9.1695E-01	0.010
148.470	4.4610E+00	0.98529	9.1732E-01	-0.0863	-0.0863	9.1732E-01	0.000
148.480	4.4633E+00	0.98535	9.1778E-01	-0.0858	-0.0860	9.1759E-01	0.020
148.500	4.4657E+00	0.98549	9.1833E-01	-0.0852	-0.0851	9.1842E-01	0.010
148.510	4.4680E+00	0.98555	9.1879E-01	-0.0847	-0.0848	9.1870E-01	0.010
148.520	4.4703E+00	0.98562	9.1925E-01	-0.0842	-0.0844	9.1906E-01	0.020
148.540	4.4727E+00	0.98575	9.1971E-01	-0.0837	-0.0836	9.1980E-01	0.010
148.550	4.4750E+00	0.98582	9.2026E-01	-0.0831	-0.0832	9.2017E-01	0.010
148.560	4.4774E+00	0.98588	9.2072E-01	-0.0826	-0.0828	9.2054E-01	0.020
148.580	4.4797E+00	0.98602	9.2118E-01	-0.0821	-0.0820	9.2127E-01	0.010
148.590	4.4821E+00	0.98608	9.2164E-01	-0.0816	-0.0817	9.2155E-01	0.010
148.600	4.4844E+00	0.98615	9.2210E-01	-0.0811	-0.0812	9.2201E-01	0.010
148.620	4.4868E+00	0.98628	9.2265E-01	-0.0805	-0.0805	9.2265E-01	0.000
148.630	4.4891E+00	0.98635	9.2312E-01	-0.0800	-0.0801	9.2302E-01	0.010
148.640	4.4915E+00	0.98642	9.2358E-01	-0.0795	-0.0797	9.2339E-01	0.020
148.660	4.4938E+00	0.98655	9.2404E-01	-0.0790	-0.0789	9.2413E-01	0.010
148.670	4.4962E+00	0.98661	9.2459E-01	-0.0784	-0.0785	9.2450E-01	0.010
148.690	4.4985E+00	0.98675	9.2506E-01	-0.0779	-0.0777	9.2524E-01	0.020
148.700	4.5009E+00	0.98681	9.2552E-01	-0.0774	-0.0774	9.2552E-01	0.000
148.710	4.5033E+00	0.98688	9.2608E-01	-0.0768	-0.0770	9.2589E-01	0.020
148.730	4.5056E+00	0.98701	9.2654E-01	-0.0763	-0.0762	9.2663E-01	0.010
148.740	4.5080E+00	0.98708	9.2700E-01	-0.0758	-0.0758	9.2700E-01	0.000
148.750	4.5103E+00	0.98715	9.2747E-01	-0.0753	-0.0754	9.2737E-01	0.010
148.770	4.5127E+00	0.98728	9.2793E-01	-0.0748	-0.0746	9.2811E-01	0.020
148.780	4.5151E+00	0.98734	9.2849E-01	-0.0742	-0.0743	9.2839E-01	0.010
148.790	4.5174E+00	0.98741	9.2895E-01	-0.0737	-0.0738	9.2886E-01	0.010
148.810	4.5198E+00	0.98754	9.2941E-01	-0.0732	-0.0731	9.2951E-01	0.010
148.820	4.5222E+00	0.98761	9.2988E-01	-0.0727	-0.0727	9.2988E-01	0.000

148.830	4.5245E+00	0.98768	9.3044E-01	-0.0721	-0.0723	9.3025E-01	0.020
148.850	4.5269E+00	0.98781	9.3090E-01	-0.0716	-0.0715	9.3100E-01	0.010
148.860	4.5293E+00	0.98788	9.3137E-01	-0.0711	-0.0711	9.3137E-01	0.000
148.870	4.5316E+00	0.98794	9.3183E-01	-0.0706	-0.0707	9.3174E-01	0.010
148.890	4.5340E+00	0.98807	9.3230E-01	-0.0701	-0.0700	9.3239E-01	0.010
148.900	4.5364E+00	0.98814	9.3286E-01	-0.0695	-0.0696	9.3277E-01	0.010
148.910	4.5388E+00	0.98821	9.3333E-01	-0.0690	-0.0692	9.3314E-01	0.020
148.930	4.5411E+00	0.98834	9.3379E-01	-0.0685	-0.0684	9.3389E-01	0.010
148.940	4.5435E+00	0.98841	9.3426E-01	-0.0680	-0.0680	9.3426E-01	0.000
148.950	4.5459E+00	0.98847	9.3482E-01	-0.0674	-0.0676	9.3463E-01	0.020
148.970	4.5483E+00	0.98861	9.3529E-01	-0.0669	-0.0668	9.3538E-01	0.010
148.980	4.5506E+00	0.98867	9.3576E-01	-0.0664	-0.0665	9.3566E-01	0.010
148.990	4.5530E+00	0.98874	9.3622E-01	-0.0659	-0.0660	9.3613E-01	0.010
149.010	4.5554E+00	0.98887	9.3679E-01	-0.0653	-0.0653	9.3679E-01	0.000
149.020	4.5578E+00	0.98894	9.3725E-01	-0.0648	-0.0649	9.3716E-01	0.010
149.030	4.5602E+00	0.98900	9.3772E-01	-0.0643	-0.0645	9.3754E-01	0.020
149.050	4.5626E+00	0.98914	9.3819E-01	-0.0638	-0.0637	9.3829E-01	0.010
149.060	4.5650E+00	0.98920	9.3876E-01	-0.0632	-0.0633	9.3866E-01	0.010
149.070	4.5673E+00	0.98927	9.3923E-01	-0.0627	-0.0629	9.3904E-01	0.020
149.090	4.5697E+00	0.98940	9.3969E-01	-0.0622	-0.0622	9.3969E-01	0.000
149.100	4.5721E+00	0.98947	9.4016E-01	-0.0617	-0.0618	9.4007E-01	0.010
149.120	4.5745E+00	0.98960	9.4064E-01	-0.0612	-0.0610	9.4082E-01	0.020
149.130	4.5769E+00	0.98967	9.4120E-01	-0.0606	-0.0606	9.4120E-01	0.000
149.140	4.5793E+00	0.98973	9.4167E-01	-0.0601	-0.0602	9.4158E-01	0.010
149.160	4.5817E+00	0.98987	9.4214E-01	-0.0596	-0.0594	9.4233E-01	0.020
149.170	4.5841E+00	0.98993	9.4261E-01	-0.0591	-0.0591	9.4261E-01	0.000
149.180	4.5865E+00	0.99000	9.4318E-01	-0.0585	-0.0586	9.4308E-01	0.010
149.200	4.5889E+00	0.99013	9.4365E-01	-0.0580	-0.0579	9.4374E-01	0.010
149.210	4.5913E+00	0.99020	9.4412E-01	-0.0575	-0.0575	9.4412E-01	0.000
149.220	4.5937E+00	0.99026	9.4459E-01	-0.0570	-0.0571	9.4450E-01	0.010
149.240	4.5961E+00	0.99040	9.4516E-01	-0.0564	-0.0563	9.4526E-01	0.010
149.250	4.5985E+00	0.99046	9.4563E-01	-0.0559	-0.0560	9.4554E-01	0.010
149.260	4.6009E+00	0.99053	9.4611E-01	-0.0554	-0.0555	9.4601E-01	0.010
149.280	4.6033E+00	0.99066	9.4658E-01	-0.0549	-0.0548	9.4667E-01	0.010
149.290	4.6057E+00	0.99073	9.4705E-01	-0.0544	-0.0544	9.4705E-01	0.000
149.300	4.6081E+00	0.99080	9.4762E-01	-0.0538	-0.0540	9.4743E-01	0.020
149.320	4.6105E+00	0.99093	9.4810E-01	-0.0533	-0.0532	9.4819E-01	0.010
149.330	4.6129E+00	0.99099	9.4857E-01	-0.0528	-0.0528	9.4857E-01	0.000
149.340	4.6153E+00	0.99106	9.4904E-01	-0.0523	-0.0524	9.4895E-01	0.010

149.360	4.6178E+00	0.99119	9.4961E-01	-0.0517	-0.0517	9.4961E-01	0.000
149.370	4.6202E+00	0.99126	9.5009E-01	-0.0512	-0.0513	9.4999E-01	0.010
149.380	4.6226E+00	0.99133	9.5056E-01	-0.0507	-0.0509	9.5037E-01	0.020
149.400	4.6250E+00	0.99146	9.5104E-01	-0.0502	-0.0501	9.5113E-01	0.010
149.410	4.6274E+00	0.99153	9.5151E-01	-0.0497	-0.0497	9.5151E-01	0.000
149.420	4.6298E+00	0.99159	9.5209E-01	-0.0491	-0.0493	9.5190E-01	0.020
149.440	4.6323E+00	0.99172	9.5256E-01	-0.0486	-0.0486	9.5256E-01	0.000
149.450	4.6347E+00	0.99179	9.5304E-01	-0.0481	-0.0482	9.5294E-01	0.010
149.460	4.6371E+00	0.99186	9.5352E-01	-0.0476	-0.0477	9.5342E-01	0.010
149.480	4.6395E+00	0.99199	9.5409E-01	-0.0470	-0.0470	9.5409E-01	0.000
149.490	4.6419E+00	0.99206	9.5456E-01	-0.0465	-0.0466	9.5447E-01	0.010
149.500	4.6444E+00	0.99212	9.5504E-01	-0.0460	-0.0462	9.5485E-01	0.020
149.520	4.6468E+00	0.99226	9.5552E-01	-0.0455	-0.0454	9.5562E-01	0.010
149.530	4.6492E+00	0.99232	9.5600E-01	-0.0450	-0.0451	9.5590E-01	0.010
149.550	4.6517E+00	0.99245	9.5657E-01	-0.0444	-0.0443	9.5667E-01	0.010
149.560	4.6541E+00	0.99252	9.5705E-01	-0.0439	-0.0439	9.5705E-01	0.000
149.570	4.6565E+00	0.99259	9.5753E-01	-0.0434	-0.0435	9.5743E-01	0.010
149.590	4.6589E+00	0.99272	9.5801E-01	-0.0429	-0.0427	9.5820E-01	0.020
149.600	4.6614E+00	0.99279	9.5858E-01	-0.0423	-0.0423	9.5858E-01	0.000
149.610	4.6638E+00	0.99285	9.5906E-01	-0.0418	-0.0419	9.5897E-01	0.010
149.630	4.6663E+00	0.99299	9.5954E-01	-0.0413	-0.0411	9.5973E-01	0.020
149.640	4.6687E+00	0.99305	9.6002E-01	-0.0408	-0.0408	9.6002E-01	0.000
149.650	4.6711E+00	0.99312	9.6050E-01	-0.0403	-0.0404	9.6041E-01	0.010
149.670	4.6736E+00	0.99325	9.6108E-01	-0.0397	-0.0396	9.6117E-01	0.010
149.680	4.6760E+00	0.99332	9.6156E-01	-0.0392	-0.0392	9.6156E-01	0.000
149.690	4.6785E+00	0.99338	9.6204E-01	-0.0387	-0.0388	9.6194E-01	0.010
149.710	4.6809E+00	0.99352	9.6252E-01	-0.0382	-0.0380	9.6271E-01	0.020
149.720	4.6833E+00	0.99358	9.6300E-01	-0.0377	-0.0377	9.6300E-01	0.000
149.730	4.6858E+00	0.99365	9.6358E-01	-0.0371	-0.0373	9.6339E-01	0.020
149.750	4.6882E+00	0.99378	9.6406E-01	-0.0366	-0.0365	9.6416E-01	0.010
149.760	4.6907E+00	0.99385	9.6454E-01	-0.0361	-0.0361	9.6454E-01	0.000
149.770	4.6931E+00	0.99391	9.6503E-01	-0.0356	-0.0357	9.6493E-01	0.010
149.790	4.6956E+00	0.99405	9.6561E-01	-0.0350	-0.0349	9.6570E-01	0.010
149.800	4.6980E+00	0.99411	9.6609E-01	-0.0345	-0.0346	9.6599E-01	0.010
149.810	4.7005E+00	0.99418	9.6657E-01	-0.0340	-0.0342	9.6638E-01	0.020
149.830	4.7029E+00	0.99431	9.6705E-01	-0.0335	-0.0334	9.6715E-01	0.010
149.840	4.7054E+00	0.99438	9.6764E-01	-0.0329	-0.0330	9.6754E-01	0.010
149.850	4.7079E+00	0.99445	9.6812E-01	-0.0324	-0.0326	9.6793E-01	0.020
149.870	4.7103E+00	0.99458	9.6860E-01	-0.0319	-0.0318	9.6870E-01	0.010

149.880	4.7128E+00	0.99464	9.6909E-01	-0.0314	-0.0315	9.6899E-01	0.010
149.890	4.7152E+00	0.99471	9.6957E-01	-0.0309	-0.0311	9.6938E-01	0.020
149.910	4.7177E+00	0.99484	9.7015E-01	-0.0303	-0.0303	9.7015E-01	0.000
149.920	4.7202E+00	0.99491	9.7064E-01	-0.0298	-0.0299	9.7054E-01	0.010
149.930	4.7226E+00	0.99498	9.7113E-01	-0.0293	-0.0295	9.7093E-01	0.020
149.950	4.7251E+00	0.99511	9.7161E-01	-0.0288	-0.0287	9.7171E-01	0.010
149.960	4.7276E+00	0.99518	9.7219E-01	-0.0282	-0.0283	9.7210E-01	0.010
149.970	4.7300E+00	0.99524	9.7268E-01	-0.0277	-0.0279	9.7249E-01	0.020
149.990	4.7325E+00	0.99537	9.7317E-01	-0.0272	-0.0272	9.7317E-01	0.000
150.000	4.7350E+00	0.99544	9.7365E-01	-0.0267	-0.0268	9.7356E-01	0.010
150.020	4.7375E+00	0.99557	9.7424E-01	-0.0261	-0.0260	9.7434E-01	0.010
150.030	4.7399E+00	0.99564	9.7472E-01	-0.0256	-0.0256	9.7472E-01	0.000
150.040	4.7424E+00	0.99571	9.7521E-01	-0.0251	-0.0252	9.7511E-01	0.010
150.060	4.7449E+00	0.99584	9.7570E-01	-0.0246	-0.0244	9.7590E-01	0.020
150.070	4.7474E+00	0.99591	9.7619E-01	-0.0241	-0.0240	9.7629E-01	0.010
150.080	4.7498E+00	0.99597	9.7668E-01	-0.0236	-0.0237	9.7658E-01	0.010
150.100	4.7523E+00	0.99610	9.7726E-01	-0.0230	-0.0229	9.7736E-01	0.010
150.110	4.7548E+00	0.99617	9.7775E-01	-0.0225	-0.0225	9.7775E-01	0.000
150.120	4.7573E+00	0.99624	9.7824E-01	-0.0220	-0.0221	9.7814E-01	0.010
150.140	4.7598E+00	0.99637	9.7883E-01	-0.0214	-0.0213	9.7893E-01	0.010
150.150	4.7623E+00	0.99644	9.7932E-01	-0.0209	-0.0209	9.7932E-01	0.000
150.160	4.7647E+00	0.99650	9.7981E-01	-0.0204	-0.0206	9.7961E-01	0.020
150.180	4.7672E+00	0.99664	9.8030E-01	-0.0199	-0.0197	9.8049E-01	0.020
150.190	4.7697E+00	0.99670	9.8079E-01	-0.0194	-0.0194	9.8079E-01	0.000
150.200	4.7722E+00	0.99677	9.8138E-01	-0.0188	-0.0190	9.8118E-01	0.020
150.220	4.7747E+00	0.99690	9.8187E-01	-0.0183	-0.0182	9.8196E-01	0.010
150.230	4.7772E+00	0.99697	9.8236E-01	-0.0178	-0.0178	9.8236E-01	0.000
150.240	4.7797E+00	0.99703	9.8285E-01	-0.0173	-0.0175	9.8265E-01	0.020
150.260	4.7822E+00	0.99717	9.8334E-01	-0.0168	-0.0166	9.8354E-01	0.020
150.270	4.7847E+00	0.99723	9.8393E-01	-0.0162	-0.0163	9.8383E-01	0.010
150.280	4.7872E+00	0.99730	9.8442E-01	-0.0157	-0.0159	9.8423E-01	0.020
150.300	4.7897E+00	0.99743	9.8491E-01	-0.0152	-0.0151	9.8501E-01	0.010
150.310	4.7922E+00	0.99750	9.8541E-01	-0.0147	-0.0147	9.8541E-01	0.000
150.320	4.7947E+00	0.99756	9.8600E-01	-0.0141	-0.0144	9.8570E-01	0.030
150.340	4.7972E+00	0.99770	9.8649E-01	-0.0136	-0.0135	9.8659E-01	0.010
150.350	4.7997E+00	0.99776	9.8699E-01	-0.0131	-0.0132	9.8689E-01	0.010
150.360	4.8022E+00	0.99783	9.8748E-01	-0.0126	-0.0128	9.8728E-01	0.020
150.380	4.8048E+00	0.99796	9.8807E-01	-0.0120	-0.0120	9.8807E-01	0.000
150.390	4.8073E+00	0.99803	9.8857E-01	-0.0115	-0.0116	9.8847E-01	0.010

150.400	4.8098E+00	0.99810	9.8906E-01	-0.0110	-0.0112	9.8886E-01	0.020
150.420	4.8123E+00	0.99823	9.8955E-01	-0.0105	-0.0104	9.8965E-01	0.010
150.430	4.8148E+00	0.99829	9.9005E-01	-0.0100	-0.0101	9.8995E-01	0.010
150.450	4.8173E+00	0.99843	9.9064E-01	-0.0094	-0.0092	9.9084E-01	0.020
150.460	4.8199E+00	0.99849	9.9114E-01	-0.0089	-0.0089	9.9114E-01	0.000
150.470	4.8224E+00	0.99856	9.9164E-01	-0.0084	-0.0085	9.9154E-01	0.010
150.490	4.8249E+00	0.99869	9.9213E-01	-0.0079	-0.0077	9.9233E-01	0.020
150.500	4.8274E+00	0.99876	9.9273E-01	-0.0073	-0.0073	9.9273E-01	0.000
150.510	4.8300E+00	0.99883	9.9322E-01	-0.0068	-0.0069	9.9312E-01	0.010
150.530	4.8325E+00	0.99896	9.9372E-01	-0.0063	-0.0061	9.9392E-01	0.020
150.540	4.8350E+00	0.99902	9.9422E-01	-0.0058	-0.0058	9.9422E-01	0.000
150.550	4.8376E+00	0.99909	9.9481E-01	-0.0052	-0.0054	9.9461E-01	0.020
150.570	4.8401E+00	0.99922	9.9531E-01	-0.0047	-0.0046	9.9541E-01	0.010
150.580	4.8426E+00	0.99929	9.9581E-01	-0.0042	-0.0042	9.9581E-01	0.000
150.590	4.8452E+00	0.99936	9.9631E-01	-0.0037	-0.0038	9.9621E-01	0.010
150.610	4.8477E+00	0.99949	9.9681E-01	-0.0032	-0.0030	9.9700E-01	0.020
150.620	4.8502E+00	0.99956	9.9740E-01	-0.0026	-0.0026	9.9740E-01	0.000
150.630	4.8528E+00	0.99962	9.9790E-01	-0.0021	-0.0022	9.9780E-01	0.010
150.650	4.8553E+00	0.99975	9.9840E-01	-0.0016	-0.0015	9.9850E-01	0.010
150.660	4.8579E+00	0.99982	9.9900E-01	-0.0010	-0.0011	9.9890E-01	0.010
150.670	4.8604E+00	0.99989	9.9950E-01	-0.0005	-0.0007	9.9930E-01	0.020
						Average	0.009
						Maximum	0.030

The temperature interval is 0.5° K up to high reduced temperatures (≈ 0.98), at which point the interval is reduced to 0.01-0.02° K.

Table A.4. VLE Predictions for Water Using Wagner Constants Regressed from *NIST*

Analytic (*NIST*)					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
273.160	6.1165E-04	0.42213	2.7722E-05	-10.4933	-10.4950	2.7674E-05	0.16986
275.030	6.9994E-04	0.42502	3.1722E-05	-10.3585	-10.3599	3.1678E-05	0.13990
276.900	7.9932E-04	0.42791	3.6227E-05	-10.2257	-10.2268	3.6187E-05	0.10994
278.770	9.1098E-04	0.43080	4.1290E-05	-10.0949	-10.0958	4.1252E-05	0.08996
280.640	1.0362E-03	0.43369	4.6965E-05	-9.9661	-9.9668	4.6933E-05	0.06998
282.510	1.1764E-03	0.43658	5.3320E-05	-9.8392	-9.8397	5.3293E-05	0.04999
284.380	1.3330E-03	0.43947	6.0413E-05	-9.7143	-9.7145	6.0401E-05	0.02000
286.250	1.5077E-03	0.44236	6.8334E-05	-9.5911	-9.5911	6.8334E-05	0.00000
288.120	1.7022E-03	0.44525	7.7147E-05	-9.4698	-9.4696	7.7162E-05	0.02000
289.990	1.9184E-03	0.44814	8.6948E-05	-9.3502	-9.3499	8.6974E-05	0.03000
291.860	2.1584E-03	0.45103	9.7828E-05	-9.2323	-9.2319	9.7867E-05	0.04001
293.730	2.4242E-03	0.45392	1.0987E-04	-9.1162	-9.1157	1.0993E-04	0.05001
295.600	2.7182E-03	0.45681	1.2320E-04	-9.0017	-9.0011	1.2327E-04	0.06002
297.470	3.0429E-03	0.45970	1.3791E-04	-8.8889	-8.8882	1.3801E-04	0.07002
299.340	3.4010E-03	0.46259	1.5415E-04	-8.7776	-8.7768	1.5427E-04	0.08003
301.210	3.7952E-03	0.46548	1.7200E-04	-8.6680	-8.6671	1.7216E-04	0.09004
303.070	4.2287E-03	0.46835	1.9166E-04	-8.5598	-8.5596	1.9170E-04	0.02000
304.940	4.7046E-03	0.47124	2.1322E-04	-8.4532	-8.4529	2.1328E-04	0.03000
306.810	5.2262E-03	0.47413	2.3687E-04	-8.3480	-8.3477	2.3694E-04	0.03000
308.680	5.7974E-03	0.47702	2.6275E-04	-8.2443	-8.2440	2.6283E-04	0.03000
310.550	6.4218E-03	0.47991	2.9105E-04	-8.1420	-8.1416	2.9117E-04	0.04001
312.420	7.1036E-03	0.48280	3.2195E-04	-8.0411	-8.0407	3.2208E-04	0.04001
314.290	7.8470E-03	0.48569	3.5564E-04	-7.9416	-7.9412	3.5578E-04	0.04001
316.160	8.6565E-03	0.48858	3.9233E-04	-7.8434	-7.8430	3.9249E-04	0.04001
318.030	9.5371E-03	0.49147	4.3225E-04	-7.7465	-7.7461	4.3243E-04	0.04001
319.900	1.0494E-02	0.49436	4.7562E-04	-7.6509	-7.6505	4.7581E-04	0.04001
321.770	1.1532E-02	0.49725	5.2265E-04	-7.5566	-7.5562	5.2286E-04	0.04001
323.640	1.2656E-02	0.50014	5.7359E-04	-7.4636	-7.4631	5.7387E-04	0.05001
325.510	1.3874E-02	0.50303	6.2880E-04	-7.3717	-7.3713	6.2905E-04	0.04001
327.380	1.5190E-02	0.50592	6.8843E-04	-7.2811	-7.2806	6.8877E-04	0.05001
329.250	1.6612E-02	0.50881	7.5288E-04	-7.1916	-7.1912	7.5318E-04	0.04001
331.120	1.8146E-02	0.51170	8.2239E-04	-7.1033	-7.1029	8.2272E-04	0.04001
332.990	1.9799E-02	0.51459	8.9732E-04	-7.0161	-7.0157	8.9768E-04	0.04001
334.860	2.1579E-02	0.51748	9.7800E-04	-6.9300	-6.9296	9.7839E-04	0.04001
336.730	2.3492E-02	0.52037	1.0648E-03	-6.8450	-6.8447	1.0651E-03	0.03000

Analytic (*NIST*)					**Predicted**		
T **(^{0}K)**	***P*** **(MPa)**	T_r	$P_{v,r}$	$Ln\ P_{v,r}$	$Ln\ P_{v,r}$	$P_{v,r}$	**A%Err**
338.600	2.5549E-02	0.52326	1.1580E-03	-6.7611	-6.7608	1.1583E-03	0.03000
340.470	2.7755E-02	0.52615	1.2579E-03	-6.6783	-6.6780	1.2583E-03	0.03000
342.340	3.0122E-02	0.52904	1.3653E-03	-6.5964	-6.5962	1.3655E-03	0.02000
344.210	3.2656E-02	0.53193	1.4800E-03	-6.5157	-6.5154	1.4805E-03	0.03000
346.080	3.5369E-02	0.53482	1.6030E-03	-6.4359	-6.4356	1.6034E-03	0.03000
347.950	3.8269E-02	0.53771	1.7344E-03	-6.3571	-6.3568	1.7349E-03	0.03000
349.820	4.1367E-02	0.54060	1.8749E-03	-6.2792	-6.2790	1.8753E-03	0.02000
351.690	4.4674E-02	0.54349	2.0248E-03	-6.2023	-6.2021	2.0252E-03	0.02000
353.560	4.8200E-02	0.54638	2.1846E-03	-6.1263	-6.1262	2.1849E-03	0.01000
355.430	5.1956E-02	0.54927	2.3548E-03	-6.0513	-6.0512	2.3550E-03	0.01000
357.300	5.5956E-02	0.55216	2.5362E-03	-5.9771	-5.9770	2.5364E-03	0.01000
359.170	6.0209E-02	0.55505	2.7288E-03	-5.9039	-5.9038	2.7291E-03	0.01000
361.030	6.4730E-02	0.55792	2.9337E-03	-5.8315	-5.8319	2.9325E-03	0.03999
362.900	6.9530E-02	0.56081	3.1514E-03	-5.7599	-5.7604	3.1499E-03	0.04999
364.770	7.4624E-02	0.56370	3.3823E-03	-5.6892	-5.6897	3.3806E-03	0.04999
366.640	8.0025E-02	0.56659	3.6268E-03	-5.6194	-5.6198	3.6254E-03	0.03999
368.510	8.5747E-02	0.56948	3.8863E-03	-5.5503	-5.5507	3.8847E-03	0.03999
370.380	9.1805E-02	0.57237	4.1610E-03	-5.4820	-5.4825	4.1589E-03	0.04999
372.250	9.8214E-02	0.57526	4.4511E-03	-5.4146	-5.4150	4.4493E-03	0.03999
374.120	1.0499E-01	0.57815	4.7586E-03	-5.3478	-5.3483	4.7562E-03	0.04999
375.990	1.1215E-01	0.58104	5.0828E-03	-5.2819	-5.2823	5.0807E-03	0.03999
377.860	1.1970E-01	0.58393	5.4252E-03	-5.2167	-5.2171	5.4230E-03	0.03999
379.730	1.2767E-01	0.58682	5.7861E-03	-5.1523	-5.1526	5.7843E-03	0.03000
381.600	1.3608E-01	0.58971	6.1673E-03	-5.0885	-5.0889	6.1648E-03	0.03999
383.470	1.4493E-01	0.59260	6.5683E-03	-5.0255	-5.0258	6.5663E-03	0.03000
385.340	1.5425E-01	0.59549	6.9912E-03	-4.9631	-4.9635	6.9884E-03	0.03999
387.210	1.6406E-01	0.59838	7.4354E-03	-4.9015	-4.9018	7.4332E-03	0.03000
389.080	1.7438E-01	0.60127	7.9031E-03	-4.8405	-4.8409	7.8999E-03	0.03999
390.950	1.8522E-01	0.60416	8.3943E-03	-4.7802	-4.7805	8.3918E-03	0.03000
392.820	1.9660E-01	0.60705	8.9107E-03	-4.7205	-4.7209	8.9072E-03	0.03999
394.690	2.0855E-01	0.60994	9.4523E-03	-4.6615	-4.6618	9.4494E-03	0.03000
396.560	2.2109E-01	0.61283	1.0021E-02	-4.6031	-4.6034	1.0018E-02	0.03000
398.430	2.3424E-01	0.61572	1.0616E-02	-4.5454	-4.5457	1.0613E-02	0.03000
400.300	2.4801E-01	0.61861	1.1241E-02	-4.4882	-4.4885	1.1237E-02	0.03000
402.170	2.6243E-01	0.62150	1.1894E-02	-4.4317	-4.4320	1.1891E-02	0.03000
404.040	2.7753E-01	0.62439	1.2578E-02	-4.3758	-4.3760	1.2576E-02	0.02000
405.910	2.9333E-01	0.62728	1.3295E-02	-4.3204	-4.3206	1.3292E-02	0.02000

Analytic (*NIST*)					**Predicted**		
T **(^{0}K)**	***P*** **(MPa)**	T_r	$P_{v,r}$	***Ln*** $P_{v,r}$	***Ln*** $P_{v,r}$	$P_{v,r}$	**A%Err**
407.780	3.0985E-01	0.63017	1.4043E-02	-4.2656	-4.2658	1.4041E-02	0.02000
409.650	3.2711E-01	0.63306	1.4826E-02	-4.2114	-4.2116	1.4823E-02	0.02000
411.520	3.4514E-01	0.63595	1.5642E-02	-4.1578	-4.1579	1.5640E-02	0.01000
413.390	3.6396E-01	0.63884	1.6495E-02	-4.1047	-4.1048	1.6493E-02	0.01000
415.260	3.8360E-01	0.64173	1.7386E-02	-4.0521	-4.0522	1.7384E-02	0.01000
417.130	4.0409E-01	0.64462	1.8314E-02	-4.0001	-4.0002	1.8312E-02	0.01000
419.000	4.2545E-01	0.64751	1.9282E-02	-3.9486	-3.9486	1.9282E-02	0.00000
420.860	4.4770E-01	0.65038	2.0291E-02	-3.8976	-3.8980	2.0282E-02	0.03999
422.730	4.7088E-01	0.65327	2.1342E-02	-3.8471	-3.8475	2.1333E-02	0.03999
424.600	4.9502E-01	0.65616	2.2436E-02	-3.7971	-3.7974	2.2429E-02	0.03000
426.470	5.2013E-01	0.65905	2.3574E-02	-3.7476	-3.7479	2.3567E-02	0.03000
428.340	5.4625E-01	0.66194	2.4758E-02	-3.6986	-3.6989	2.4751E-02	0.03000
430.210	5.7341E-01	0.66483	2.5989E-02	-3.6501	-3.6504	2.5981E-02	0.03000
432.080	6.0163E-01	0.66772	2.7266E-02	-3.6021	-3.6023	2.7261E-02	0.02000
433.950	6.3096E-01	0.67061	2.8596E-02	-3.5545	-3.5547	2.8590E-02	0.02000
435.820	6.6140E-01	0.67350	2.9978E-02	-3.5073	-3.5075	2.9972E-02	0.02000
437.690	6.9301E-01	0.67639	3.1408E-02	-3.4607	-3.4608	3.1405E-02	0.01000
439.560	7.2580E-01	0.67928	3.2896E-02	-3.4144	-3.4145	3.2893E-02	0.01000
441.430	7.5982E-01	0.68217	3.4438E-02	-3.3686	-3.3687	3.4434E-02	0.01000
443.300	7.9508E-01	0.68506	3.6034E-02	-3.3233	-3.3233	3.6034E-02	0.00000
445.170	8.3163E-01	0.68795	3.7692E-02	-3.2783	-3.2783	3.7692E-02	0.00000
447.040	8.6949E-01	0.69084	3.9407E-02	-3.2338	-3.2338	3.9407E-02	0.00000
448.910	9.0871E-01	0.69373	4.1184E-02	-3.1897	-3.1897	4.1184E-02	0.00000
450.780	9.4930E-01	0.69662	4.3024E-02	-3.1460	-3.1459	4.3028E-02	0.01000
452.650	9.9131E-01	0.69951	4.4928E-02	-3.1027	-3.1026	4.4932E-02	0.01000
454.520	1.0348E+00	0.70240	4.6902E-02	-3.0597	-3.0597	4.6902E-02	0.00000
456.390	1.0797E+00	0.70529	4.8933E-02	-3.0173	-3.0171	4.8943E-02	0.02000
458.260	1.1262E+00	0.70818	5.1042E-02	-2.9751	-2.9750	5.1047E-02	0.01000
460.130	1.1742E+00	0.71107	5.3216E-02	-2.9334	-2.9332	5.3226E-02	0.02000
462.000	1.2238E+00	0.71396	5.5465E-02	-2.8920	-2.8918	5.5476E-02	0.02000
463.870	1.2751E+00	0.71685	5.7792E-02	-2.8509	-2.8507	5.7804E-02	0.02000
465.740	1.3280E+00	0.71974	6.0187E-02	-2.8103	-2.8100	6.0205E-02	0.03000
467.610	1.3826E+00	0.72263	6.2662E-02	-2.7700	-2.7697	6.2681E-02	0.03000
469.480	1.4390E+00	0.72552	6.5219E-02	-2.7300	-2.7298	6.5232E-02	0.02000
471.350	1.4971E+00	0.72841	6.7854E-02	-2.6904	-2.6901	6.7874E-02	0.03000
473.220	1.5571E+00	0.73130	7.0574E-02	-2.6511	-2.6509	7.0588E-02	0.02000
475.090	1.6189E+00	0.73419	7.3373E-02	-2.6122	-2.6119	7.3395E-02	0.03000

Analytic (*NIST*)					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
476.960	1.6826E+00	0.73708	7.6261E-02	-2.5736	-2.5733	7.6283E-02	0.03000
478.820	1.7482E+00	0.73995	7.9230E-02	-2.5354	-2.5353	7.9238E-02	0.01000
480.690	1.8158E+00	0.74284	8.2299E-02	-2.4974	-2.4973	8.2307E-02	0.01000
482.560	1.8854E+00	0.74573	8.5452E-02	-2.4598	-2.4597	8.5461E-02	0.01000
484.430	1.9571E+00	0.74862	8.8700E-02	-2.4225	-2.4224	8.8708E-02	0.01000
486.300	2.0309E+00	0.75151	9.2043E-02	-2.3855	-2.3854	9.2052E-02	0.01000
488.170	2.1068E+00	0.75440	9.5484E-02	-2.3488	-2.3487	9.5493E-02	0.01000
490.040	2.1849E+00	0.75729	9.9023E-02	-2.3124	-2.3123	9.9033E-02	0.01000
491.910	2.2652E+00	0.76018	1.0266E-01	-2.2763	-2.2761	1.0268E-01	0.02000
493.780	2.3478E+00	0.76307	1.0641E-01	-2.2405	-2.2403	1.0643E-01	0.02000
495.650	2.4326E+00	0.76596	1.1025E-01	-2.2050	-2.2048	1.1027E-01	0.02000
497.520	2.5199E+00	0.76885	1.1421E-01	-2.1697	-2.1696	1.1422E-01	0.01000
499.390	2.6095E+00	0.77174	1.1827E-01	-2.1348	-2.1346	1.1829E-01	0.02000
501.260	2.7016E+00	0.77463	1.2244E-01	-2.1001	-2.0999	1.2247E-01	0.02000
503.130	2.7961E+00	0.77752	1.2673E-01	-2.0657	-2.0655	1.2675E-01	0.02000
505.000	2.8932E+00	0.78041	1.3113E-01	-2.0316	-2.0314	1.3115E-01	0.02000
506.870	2.9928E+00	0.78330	1.3565E-01	-1.9977	-1.9976	1.3566E-01	0.01000
508.740	3.0951E+00	0.78619	1.4028E-01	-1.9641	-1.9640	1.4030E-01	0.01000
510.610	3.2000E+00	0.78908	1.4503E-01	-1.9308	-1.9306	1.4506E-01	0.02000
512.480	3.3076E+00	0.79197	1.4991E-01	-1.8977	-1.8975	1.4994E-01	0.02000
514.350	3.4180E+00	0.79486	1.5491E-01	-1.8649	-1.8647	1.5494E-01	0.02000
516.220	3.5312E+00	0.79775	1.6005E-01	-1.8323	-1.8321	1.6008E-01	0.02000
518.090	3.6473E+00	0.80064	1.6530E-01	-1.8000	-1.7998	1.6533E-01	0.02000
519.960	3.7662E+00	0.80353	1.7069E-01	-1.7679	-1.7677	1.7073E-01	0.02000
521.830	3.8881E+00	0.80642	1.7622E-01	-1.7360	-1.7358	1.7626E-01	0.02000
523.700	4.0130E+00	0.80931	1.8188E-01	-1.7044	-1.7042	1.8192E-01	0.02000
525.570	4.1410E+00	0.81220	1.8768E-01	-1.6730	-1.6728	1.8772E-01	0.02000
527.440	4.2720E+00	0.81509	1.9361E-01	-1.6419	-1.6417	1.9365E-01	0.02000
529.310	4.4062E+00	0.81798	1.9971E-01	-1.6109	-1.6108	1.9973E-01	0.01000
531.180	4.5436E+00	0.82087	2.0593E-01	-1.5802	-1.5800	2.0598E-01	0.02000
533.050	4.6843E+00	0.82376	2.1231E-01	-1.5497	-1.5496	2.1233E-01	0.01000
534.920	4.8283E+00	0.82665	2.1882E-01	-1.5195	-1.5193	2.1887E-01	0.02000
536.780	4.9756E+00	0.82952	2.2551E-01	-1.4894	-1.4895	2.2549E-01	0.01000
538.650	5.1263E+00	0.83241	2.3233E-01	-1.4596	-1.4596	2.3233E-01	0.00000
540.520	5.2805E+00	0.83530	2.3933E-01	-1.4299	-1.4300	2.3931E-01	0.01000
542.390	5.4382E+00	0.83819	2.4647E-01	-1.4005	-1.4006	2.4645E-01	0.01000
544.260	5.5995E+00	0.84108	2.5378E-01	-1.3713	-1.3713	2.5378E-01	0.00000

Analytic (*NIST*)					**Predicted**		
***T* (^{0}K)**	***P* (MPa)**	**T_r**	**$P_{v,r}$**	***Ln* $P_{v,r}$**	***Ln* $P_{v,r}$**	**$P_{v,r}$**	**A%Err**
546.130	5.7644E+00	0.84397	2.6127E-01	-1.3422	-1.3423	2.6124E-01	0.01000
548.000	5.9330E+00	0.84686	2.6890E-01	-1.3134	-1.3135	2.6888E-01	0.01000
549.870	6.1053E+00	0.84975	2.7671E-01	-1.2848	-1.2849	2.7668E-01	0.01000
551.740	6.2814E+00	0.85264	2.8468E-01	-1.2564	-1.2564	2.8468E-01	0.00000
553.610	6.4614E+00	0.85553	2.9285E-01	-1.2281	-1.2282	2.9282E-01	0.01000
555.480	6.6453E+00	0.85842	3.0119E-01	-1.2000	-1.2001	3.0116E-01	0.01000
557.350	6.8332E+00	0.86131	3.0968E-01	-1.1722	-1.1722	3.0968E-01	0.00000
559.220	7.0251E+00	0.86420	3.1838E-01	-1.1445	-1.1445	3.1838E-01	0.00000
561.090	7.2211E+00	0.86709	3.2729E-01	-1.1169	-1.1170	3.2726E-01	0.01000
562.960	7.4212E+00	0.86998	3.3635E-01	-1.0896	-1.0897	3.3632E-01	0.01000
564.830	7.6256E+00	0.87287	3.4563E-01	-1.0624	-1.0625	3.4559E-01	0.01000
566.700	7.8343E+00	0.87576	3.5508E-01	-1.0354	-1.0355	3.5505E-01	0.01000
568.570	8.0473E+00	0.87865	3.6473E-01	-1.0086	-1.0087	3.6469E-01	0.01000
570.440	8.2647E+00	0.88154	3.7456E-01	-0.9820	-0.9820	3.7456E-01	0.00000
572.310	8.4866E+00	0.88443	3.8462E-01	-0.9555	-0.9555	3.8462E-01	0.00000
574.180	8.7130E+00	0.88732	3.9491E-01	-0.9291	-0.9292	3.9487E-01	0.01000
576.050	8.9441E+00	0.89021	4.0535E-01	-0.9030	-0.9030	4.0535E-01	0.00000
577.920	9.1798E+00	0.89310	4.1607E-01	-0.8769	-0.8770	4.1603E-01	0.01000
579.790	9.4203E+00	0.89599	4.2695E-01	-0.8511	-0.8511	4.2695E-01	0.00000
581.660	9.6657E+00	0.89888	4.3806E-01	-0.8254	-0.8254	4.3806E-01	0.00000
583.530	9.9159E+00	0.90177	4.4942E-01	-0.7998	-0.7999	4.4937E-01	0.01000
585.400	1.0171E+01	0.90466	4.6098E-01	-0.7744	-0.7745	4.6093E-01	0.01000
587.270	1.0431E+01	0.90755	4.7274E-01	-0.7492	-0.7492	4.7274E-01	0.00000
589.140	1.0697E+01	0.91044	4.8481E-01	-0.7240	-0.7240	4.8481E-01	0.00000
591.010	1.0967E+01	0.91333	4.9703E-01	-0.6991	-0.6991	4.9703E-01	0.00000
592.880	1.1243E+01	0.91622	5.0956E-01	-0.6742	-0.6742	5.0956E-01	0.00000
594.740	1.1525E+01	0.91909	5.2236E-01	-0.6494	-0.6497	5.2220E-01	0.03000
596.610	1.1811E+01	0.92198	5.3531E-01	-0.6249	-0.6251	5.3521E-01	0.02000
598.480	1.2104E+01	0.92487	5.4859E-01	-0.6004	-0.6006	5.4848E-01	0.02000
600.350	1.2402E+01	0.92776	5.6209E-01	-0.5761	-0.5763	5.6197E-01	0.02000
602.220	1.2705E+01	0.93065	5.7580E-01	-0.5520	-0.5521	5.7574E-01	0.01000
604.090	1.3015E+01	0.93354	5.8990E-01	-0.5278	-0.5280	5.8978E-01	0.02000
605.960	1.3331E+01	0.93643	6.0417E-01	-0.5039	-0.5040	6.0411E-01	0.01000
607.830	1.3652E+01	0.93932	6.1872E-01	-0.4801	-0.4802	6.1866E-01	0.01000
609.700	1.3980E+01	0.94221	6.3362E-01	-0.4563	-0.4564	6.3356E-01	0.01000
611.570	1.4314E+01	0.94510	6.4876E-01	-0.4327	-0.4328	6.4869E-01	0.01000
613.440	1.4654E+01	0.94799	6.6418E-01	-0.4092	-0.4093	6.6411E-01	0.01000

Analytic (*NIST*)					**Predicted**		
T (^{0}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
615.310	1.5001E+01	0.95088	6.7991E-01	-0.3858	-0.3859	6.7984E-01	0.01000
617.180	1.5355E+01	0.95377	6.9593E-01	-0.3625	-0.3626	6.9586E-01	0.01000
619.050	1.5715E+01	0.95666	7.1227E-01	-0.3393	-0.3394	7.1220E-01	0.01000
620.920	1.6082E+01	0.95955	7.2891E-01	-0.3162	-0.3163	7.2884E-01	0.01000
622.790	1.6457E+01	0.96244	7.4587E-01	-0.2932	-0.2932	7.4587E-01	0.00000
624.660	1.6838E+01	0.96533	7.6315E-01	-0.2703	-0.2703	7.6315E-01	0.00000
626.530	1.7227E+01	0.96822	7.8075E-01	-0.2475	-0.2475	7.8075E-01	0.00000
628.400	1.7623E+01	0.97111	7.9876E-01	-0.2247	-0.2247	7.9876E-01	0.00000
630.270	1.8028E+01	0.97400	8.1709E-01	-0.2020	-0.2020	8.1709E-01	0.00000
632.140	1.8440E+01	0.97689	8.3577E-01	-0.1794	-0.1794	8.3577E-01	0.00000
634.010	1.8860E+01	0.97978	8.5479E-01	-0.1569	-0.1569	8.5479E-01	0.00000
635.880	1.9289E+01	0.98267	8.7424E-01	-0.1344	-0.1344	8.7424E-01	0.00000
637.750	1.9726E+01	0.98556	8.9404E-01	-0.1120	-0.1119	8.9413E-01	0.01000
639.620	2.0173E+01	0.98845	9.1430E-01	-0.0896	-0.0895	9.1439E-01	0.01000
641.490	2.0629E+01	0.99134	9.3501E-01	-0.0672	-0.0672	9.3501E-01	0.00000
643.000	2.1006E+01	0.99367	9.5209E-01	-0.0491	-0.0491	9.5209E-01	0.00000
643.100	2.1031E+01	0.99382	9.5323E-01	-0.0479	-0.0480	9.5313E-01	0.01000
643.200	2.1056E+01	0.99398	9.5428E-01	-0.0468	-0.0467	9.5437E-01	0.01000
643.300	2.1081E+01	0.99413	9.5542E-01	-0.0456	-0.0456	9.5542E-01	0.00000
643.400	2.1107E+01	0.99429	9.5667E-01	-0.0443	-0.0443	9.5667E-01	0.00000
643.500	2.1132E+01	0.99444	9.5772E-01	-0.0432	-0.0432	9.5772E-01	0.00000
643.600	2.1157E+01	0.99460	9.5887E-01	-0.0420	-0.0419	9.5897E-01	0.01000
643.700	2.1183E+01	0.99475	9.6012E-01	-0.0407	-0.0408	9.6002E-01	0.01000
643.800	2.1208E+01	0.99491	9.6117E-01	-0.0396	-0.0395	9.6127E-01	0.01000
643.900	2.1233E+01	0.99506	9.6233E-01	-0.0384	-0.0384	9.6233E-01	0.00000
644.000	2.1259E+01	0.99522	9.6348E-01	-0.0372	-0.0371	9.6358E-01	0.01000
644.100	2.1284E+01	0.99537	9.6464E-01	-0.0360	-0.0360	9.6464E-01	0.00000
644.200	2.1310E+01	0.99552	9.6580E-01	-0.0348	-0.0348	9.6580E-01	0.00000
644.300	2.1335E+01	0.99568	9.6696E-01	-0.0336	-0.0336	9.6696E-01	0.00000
644.400	2.1361E+01	0.99583	9.6812E-01	-0.0324	-0.0324	9.6812E-01	0.00000
644.500	2.1387E+01	0.99599	9.6928E-01	-0.0312	-0.0312	9.6928E-01	0.00000
644.600	2.1412E+01	0.99614	9.7045E-01	-0.0300	-0.0300	9.7045E-01	0.00000
644.700	2.1438E+01	0.99630	9.7161E-01	-0.0288	-0.0288	9.7161E-01	0.00000
644.800	2.1464E+01	0.99645	9.7278E-01	-0.0276	-0.0276	9.7278E-01	0.00000
644.900	2.1489E+01	0.99661	9.7395E-01	-0.0264	-0.0264	9.7395E-01	0.00000
645.000	2.1515E+01	0.99676	9.7511E-01	-0.0252	-0.0252	9.7511E-01	0.00000
645.100	2.1541E+01	0.99692	9.7629E-01	-0.0240	-0.0240	9.7629E-01	0.00000

Analytic (*NIST*)					**Predicted**		
T (°K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
645.200	2.1567E+01	0.99707	9.7746E-01	-0.0228	-0.0228	9.7746E-01	0.00000
645.300	2.1593E+01	0.99722	9.7863E-01	-0.0216	-0.0216	9.7863E-01	0.00000
645.400	2.1619E+01	0.99738	9.7981E-01	-0.0204	-0.0204	9.7981E-01	0.00000
645.500	2.1645E+01	0.99753	9.8098E-01	-0.0192	-0.0192	9.8098E-01	0.00000
645.600	2.1671E+01	0.99769	9.8216E-01	-0.0180	-0.0180	9.8216E-01	0.00000
645.700	2.1697E+01	0.99784	9.8334E-01	-0.0168	-0.0168	9.8334E-01	0.00000
645.800	2.1723E+01	0.99800	9.8452E-01	-0.0156	-0.0156	9.8452E-01	0.00000
645.900	2.1749E+01	0.99815	9.8570E-01	-0.0144	-0.0144	9.8570E-01	0.00000
646.000	2.1775E+01	0.99831	9.8689E-01	-0.0132	-0.0132	9.8689E-01	0.00000
646.100	2.1801E+01	0.99846	9.8807E-01	-0.0120	-0.0120	9.8807E-01	0.00000
646.200	2.1827E+01	0.99862	9.8926E-01	-0.0108	-0.0108	9.8926E-01	0.00000
646.300	2.1854E+01	0.99877	9.9045E-01	-0.0096	-0.0096	9.9045E-01	0.00000
646.400	2.1880E+01	0.99892	9.9164E-01	-0.0084	-0.0084	9.9164E-01	0.00000
646.500	2.1906E+01	0.99908	9.9283E-01	-0.0072	-0.0072	9.9283E-01	0.00000
646.600	2.1932E+01	0.99923	9.9402E-01	-0.0060	-0.0060	9.9402E-01	0.00000
646.700	2.1959E+01	0.99939	9.9521E-01	-0.0048	-0.0048	9.9521E-01	0.00000
646.800	2.1985E+01	0.99954	9.9641E-01	-0.0036	-0.0036	9.9641E-01	0.00000
646.900	2.2012E+01	0.99970	9.9760E-01	-0.0024	-0.0023	9.9770E-01	0.01000
647.000	2.2038E+01	0.99985	9.9880E-01	-0.0012	-0.0012	9.9880E-01	0.00000
						Average	0.019
						Maximum	0.170

The temperature interval is 1.87° K up to high reduced temperatures (≈ 0.99), at which point the interval is reduced to 0.1° K.

Table A.5. VLE Predictions for R152a Using Wagner Constants Regressed from *NIST*

Analytic (*NIST*)					**Predicted**		
T **(^{0}K)**	***P*** **(MPa)**	T_r	$P_{v,r}$	***Ln*** $P_{v,r}$	***Ln*** $P_{v,r}$	$P_{v,r}$	**A%Err**
154.560	6.4139E-05	0.39999	1.4200E-05	-11.1623	-11.1631	1.4188E-05	0.080
155.720	7.4894E-05	0.40299	1.6582E-05	-11.0072	-11.0079	1.6570E-05	0.070
156.880	8.7223E-05	0.40599	1.9312E-05	-10.8548	-10.8553	1.9302E-05	0.050
158.040	1.0132E-04	0.40899	2.2432E-05	-10.7050	-10.7053	2.2426E-05	0.030
159.200	1.1740E-04	0.41200	2.5993E-05	-10.5577	-10.5574	2.6000E-05	0.030
160.360	1.3570E-04	0.41500	3.0042E-05	-10.4129	-10.4124	3.0057E-05	0.050
161.520	1.5648E-04	0.41800	3.4644E-05	-10.2704	-10.2699	3.4661E-05	0.050
162.670	1.8001E-04	0.42098	3.9854E-05	-10.1303	-10.1306	3.9842E-05	0.030
163.830	2.0661E-04	0.42398	4.5742E-05	-9.9925	-9.9927	4.5733E-05	0.020
164.990	2.3661E-04	0.42698	5.2384E-05	-9.8569	-9.8571	5.2374E-05	0.020
166.150	2.7038E-04	0.42998	5.9860E-05	-9.7235	-9.7237	5.9848E-05	0.020
167.310	3.0829E-04	0.43298	6.8252E-05	-9.5923	-9.5924	6.8245E-05	0.010
168.470	3.5079E-04	0.43599	7.7665E-05	-9.4631	-9.4628	7.7689E-05	0.030
169.630	3.9833E-04	0.43899	8.8191E-05	-9.3360	-9.3357	8.8218E-05	0.030
170.790	4.5140E-04	0.44199	9.9944E-05	-9.2109	-9.2106	9.9974E-05	0.030
171.950	5.1054E-04	0.44499	1.1304E-04	-9.0878	-9.0875	1.1307E-04	0.030
173.110	5.7632E-04	0.44799	1.2760E-04	-8.9666	-8.9663	1.2764E-04	0.030
174.270	6.4936E-04	0.45100	1.4377E-04	-8.8473	-8.8466	1.4387E-04	0.070
175.430	7.3030E-04	0.45400	1.6169E-04	-8.7298	-8.7291	1.6181E-04	0.070
176.590	8.1986E-04	0.45700	1.8151E-04	-8.6142	-8.6135	1.8164E-04	0.070
177.750	9.1878E-04	0.46000	2.0341E-04	-8.5003	-8.4996	2.0355E-04	0.070
178.900	1.0279E-03	0.46298	2.2758E-04	-8.3880	-8.3882	2.2754E-04	0.020
180.060	1.1480E-03	0.46598	2.5417E-04	-8.2775	-8.2777	2.5412E-04	0.020
181.220	1.2800E-03	0.46898	2.8339E-04	-8.1687	-8.1688	2.8336E-04	0.010
182.380	1.4248E-03	0.47198	3.1545E-04	-8.0615	-8.0616	3.1542E-04	0.010
183.540	1.5836E-03	0.47499	3.5062E-04	-7.9558	-7.9557	3.5066E-04	0.010
184.700	1.7573E-03	0.47799	3.8905E-04	-7.8518	-7.8516	3.8913E-04	0.020
185.860	1.9471E-03	0.48099	4.3109E-04	-7.7492	-7.7491	4.3113E-04	0.010
187.020	2.1542E-03	0.48399	4.7695E-04	-7.6481	-7.6480	4.7700E-04	0.010
188.180	2.3798E-03	0.48699	5.2690E-04	-7.5485	-7.5484	5.2695E-04	0.010
189.340	2.6253E-03	0.49000	5.8121E-04	-7.4504	-7.4499	5.8150E-04	0.050
190.500	2.8921E-03	0.49300	6.4028E-04	-7.3536	-7.3532	6.4054E-04	0.040
191.660	3.1817E-03	0.49600	7.0445E-04	-7.2581	-7.2578	7.0466E-04	0.030

Analytic (*NIST*)					**Predicted**		
T (^{o}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
192.820	3.4955E-03	0.49900	7.7388E-04	-7.1641	-7.1637	7.7418E-04	0.040
193.970	3.8352E-03	0.50198	8.4913E-04	-7.0713	-7.0716	8.4887E-04	0.030
195.130	4.2024E-03	0.50498	9.3040E-04	-6.9799	-6.9802	9.3012E-04	0.030
196.290	4.5990E-03	0.50798	1.0182E-03	-6.8897	-6.8900	1.0179E-03	0.030
197.450	5.0268E-03	0.51098	1.1129E-03	-6.8008	-6.8011	1.1126E-03	0.030
198.610	5.4876E-03	0.51399	1.2149E-03	-6.7131	-6.7131	1.2149E-03	0.000
199.770	5.9836E-03	0.51699	1.3248E-03	-6.6265	-6.6266	1.3247E-03	0.010
200.930	6.5167E-03	0.51999	1.4428E-03	-6.5412	-6.5413	1.4426E-03	0.010
202.090	7.0892E-03	0.52299	1.5695E-03	-6.4570	-6.4571	1.5693E-03	0.010
203.250	7.7033E-03	0.52599	1.7055E-03	-6.3739	-6.3740	1.7053E-03	0.010
204.410	8.3613E-03	0.52900	1.8512E-03	-6.2919	-6.2918	1.8514E-03	0.010
205.570	9.0657E-03	0.53200	2.0072E-03	-6.2110	-6.2109	2.0074E-03	0.010
206.730	9.8189E-03	0.53500	2.1740E-03	-6.1312	-6.1311	2.1742E-03	0.010
207.890	1.0624E-02	0.53800	2.3522E-03	-6.0524	-6.0524	2.3522E-03	0.000
209.040	1.1483E-02	0.54098	2.5423E-03	-5.9747	-5.9752	2.5410E-03	0.050
210.200	1.2398E-02	0.54398	2.7449E-03	-5.8980	-5.8984	2.7438E-03	0.040
211.360	1.3374E-02	0.54698	2.9611E-03	-5.8222	-5.8227	2.9596E-03	0.050
212.520	1.4413E-02	0.54998	3.1911E-03	-5.7474	-5.7479	3.1895E-03	0.050
213.680	1.5517E-02	0.55299	3.4355E-03	-5.6736	-5.6738	3.4348E-03	0.020
214.840	1.6690E-02	0.55599	3.6953E-03	-5.6007	-5.6009	3.6945E-03	0.020
216.000	1.7936E-02	0.55899	3.9711E-03	-5.5287	-5.5290	3.9700E-03	0.030
217.160	1.9257E-02	0.56199	4.2634E-03	-5.4577	-5.4579	4.2625E-03	0.020
218.320	2.0658E-02	0.56499	4.5738E-03	-5.3874	-5.3877	4.5725E-03	0.030
219.480	2.2141E-02	0.56800	4.9021E-03	-5.3181	-5.3181	4.9021E-03	0.000
220.640	2.3710E-02	0.57100	5.2491E-03	-5.2497	-5.2497	5.2491E-03	0.000
221.800	2.5369E-02	0.57400	5.6168E-03	-5.1820	-5.1820	5.6168E-03	0.000
222.960	2.7122E-02	0.57700	6.0048E-03	-5.1152	-5.1152	6.0048E-03	0.000
224.120	2.8973E-02	0.58000	6.4145E-03	-5.0492	-5.0492	6.4145E-03	0.000
225.270	3.0925E-02	0.58298	6.8466E-03	-4.9840	-4.9844	6.8439E-03	0.040
226.430	3.2983E-02	0.58598	7.3021E-03	-4.9196	-4.9200	7.2991E-03	0.040
227.590	3.5151E-02	0.58898	7.7823E-03	-4.8559	-4.8563	7.7792E-03	0.040
228.750	3.7434E-02	0.59199	8.2876E-03	-4.7930	-4.7932	8.2859E-03	0.020
229.910	3.9835E-02	0.59499	8.8194E-03	-4.7308	-4.7310	8.8176E-03	0.020
231.070	4.2360E-02	0.59799	9.3788E-03	-4.6693	-4.6695	9.3770E-03	0.020
232.230	4.5012E-02	0.60099	9.9658E-03	-4.6086	-4.6088	9.9638E-03	0.020

Analytic (*NIST*)					**Predicted**		
T (^{o}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
233.390	4.7797E-02	0.60399	1.0582E-02	-4.5486	-4.5487	1.0581E-02	0.010
234.550	5.0720E-02	0.60700	1.1230E-02	-4.4892	-4.4892	1.1230E-02	0.000
235.710	5.3784E-02	0.61000	1.1907E-02	-4.4306	-4.4305	1.1909E-02	0.010
236.870	5.6996E-02	0.61300	1.2618E-02	-4.3726	-4.3725	1.2620E-02	0.010
238.030	6.0359E-02	0.61600	1.3364E-02	-4.3152	-4.3152	1.3364E-02	0.000
239.190	6.3881E-02	0.61900	1.4144E-02	-4.2585	-4.2585	1.4144E-02	0.000
240.340	6.7564E-02	0.62198	1.4958E-02	-4.2025	-4.2028	1.4954E-02	0.030
241.500	7.1416E-02	0.62498	1.5812E-02	-4.1470	-4.1473	1.5807E-02	0.030
242.660	7.5441E-02	0.62798	1.6702E-02	-4.0922	-4.0925	1.6697E-02	0.030
243.820	7.9645E-02	0.63099	1.7633E-02	-4.0380	-4.0380	1.7633E-02	0.000
244.980	8.4033E-02	0.63399	1.8605E-02	-3.9843	-3.9844	1.8604E-02	0.010
246.140	8.8612E-02	0.63699	1.9618E-02	-3.9313	-3.9313	1.9618E-02	0.000
247.300	9.3386E-02	0.63999	2.0676E-02	-3.8788	-3.8789	2.0674E-02	0.010
248.460	9.8362E-02	0.64299	2.1777E-02	-3.8269	-3.8269	2.1777E-02	0.000
249.620	1.0355E-01	0.64600	2.2926E-02	-3.7755	-3.7754	2.2928E-02	0.010
250.780	1.0894E-01	0.64900	2.4118E-02	-3.7248	-3.7246	2.4123E-02	0.020
251.940	1.1456E-01	0.65200	2.5365E-02	-3.6744	-3.6743	2.5367E-02	0.010
253.100	1.2041E-01	0.65500	2.6660E-02	-3.6246	-3.6245	2.6662E-02	0.010
254.260	1.2648E-01	0.65800	2.8001E-02	-3.5755	-3.5753	2.8007E-02	0.020
255.420	1.3280E-01	0.66101	2.9402E-02	-3.5267	-3.5264	2.9411E-02	0.030
256.570	1.3936E-01	0.66398	3.0854E-02	-3.4785	-3.4786	3.0851E-02	0.010
257.730	1.4617E-01	0.66698	3.2361E-02	-3.4308	-3.4309	3.2358E-02	0.010
258.890	1.5324E-01	0.66999	3.3928E-02	-3.3835	-3.3835	3.3928E-02	0.000
260.050	1.6057E-01	0.67299	3.5551E-02	-3.3368	-3.3367	3.5554E-02	0.010
261.210	1.6818E-01	0.67599	3.7235E-02	-3.2905	-3.2904	3.7239E-02	0.010
262.370	1.7606E-01	0.67899	3.8980E-02	-3.2447	-3.2446	3.8984E-02	0.010
263.530	1.8423E-01	0.68199	4.0787E-02	-3.1994	-3.1993	4.0791E-02	0.010
264.690	1.9270E-01	0.68500	4.2664E-02	-3.1544	-3.1542	4.2673E-02	0.020
265.850	2.0146E-01	0.68800	4.4601E-02	-3.1100	-3.1097	4.4614E-02	0.030
267.010	2.1053E-01	0.69100	4.6612E-02	-3.0659	-3.0657	4.6621E-02	0.020
268.170	2.1991E-01	0.69400	4.8689E-02	-3.0223	-3.0221	4.8699E-02	0.020
269.330	2.2962E-01	0.69700	5.0839E-02	-2.9791	-2.9789	5.0849E-02	0.020
270.490	2.3965E-01	0.70001	5.3056E-02	-2.9364	-2.9360	5.3078E-02	0.040
271.640	2.5002E-01	0.70298	5.5354E-02	-2.8940	-2.8940	5.5354E-02	0.000
272.800	2.6073E-01	0.70598	5.7723E-02	-2.8521	-2.8521	5.7723E-02	0.000

Analytic (*NIST*)					**Predicted**		
T (^{o}K)	**P (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
273.960	2.7179E-01	0.70899	6.0175E-02	-2.8105	-2.8104	6.0181E-02	0.010
275.120	2.8321E-01	0.71199	6.2700E-02	-2.7694	-2.7692	6.2712E-02	0.020
276.280	2.9500E-01	0.71499	6.5311E-02	-2.7286	-2.7284	6.5324E-02	0.020
277.440	3.0716E-01	0.71799	6.8003E-02	-2.6882	-2.6880	6.8017E-02	0.020
278.600	3.1970E-01	0.72099	7.0778E-02	-2.6482	-2.6480	7.0793E-02	0.020
279.760	3.3263E-01	0.72400	7.3645E-02	-2.6085	-2.6082	7.3667E-02	0.030
280.920	3.4596E-01	0.72700	7.6597E-02	-2.5692	-2.5689	7.6620E-02	0.030
282.080	3.5970E-01	0.73000	7.9635E-02	-2.5303	-2.5300	7.9659E-02	0.030
283.240	3.7385E-01	0.73300	8.2769E-02	-2.4917	-2.4914	8.2794E-02	0.030
284.400	3.8842E-01	0.73600	8.5992E-02	-2.4535	-2.4532	8.6018E-02	0.030
285.560	4.0342E-01	0.73901	8.9314E-02	-2.4156	-2.4152	8.9349E-02	0.040
286.720	4.1886E-01	0.74201	9.2736E-02	-2.3780	-2.3776	9.2773E-02	0.040
287.870	4.3474E-01	0.74498	9.6251E-02	-2.3408	-2.3408	9.6251E-02	0.000
289.030	4.5108E-01	0.74799	9.9869E-02	-2.3039	-2.3038	9.9879E-02	0.010
290.190	4.6788E-01	0.75099	1.0359E-01	-2.2673	-2.2672	1.0360E-01	0.010
291.350	4.8516E-01	0.75399	1.0741E-01	-2.2311	-2.2310	1.0742E-01	0.010
292.510	5.0292E-01	0.75699	1.1135E-01	-2.1951	-2.1950	1.1136E-01	0.010
293.670	5.2116E-01	0.75999	1.1538E-01	-2.1595	-2.1594	1.1539E-01	0.010
294.830	5.3990E-01	0.76300	1.1953E-01	-2.1242	-2.1240	1.1955E-01	0.020
295.990	5.5915E-01	0.76600	1.2380E-01	-2.0891	-2.0889	1.2382E-01	0.020
297.150	5.7892E-01	0.76900	1.2817E-01	-2.0544	-2.0542	1.2820E-01	0.020
298.310	5.9920E-01	0.77200	1.3266E-01	-2.0200	-2.0198	1.3268E-01	0.020
299.470	6.2003E-01	0.77500	1.3727E-01	-1.9858	-1.9856	1.3730E-01	0.020
300.630	6.4139E-01	0.77801	1.4200E-01	-1.9519	-1.9517	1.4203E-01	0.020
301.790	6.6330E-01	0.78101	1.4686E-01	-1.9183	-1.9181	1.4689E-01	0.020
302.940	6.8578E-01	0.78398	1.5183E-01	-1.8850	-1.8851	1.5181E-01	0.010
304.100	7.0882E-01	0.78699	1.5694E-01	-1.8519	-1.8520	1.5692E-01	0.010
305.260	7.3245E-01	0.78999	1.6216E-01	-1.8192	-1.8192	1.6216E-01	0.000
306.420	7.5666E-01	0.79299	1.6753E-01	-1.7866	-1.7867	1.6751E-01	0.010
307.580	7.8147E-01	0.79599	1.7301E-01	-1.7544	-1.7544	1.7301E-01	0.000
308.740	8.0689E-01	0.79899	1.7864E-01	-1.7224	-1.7224	1.7864E-01	0.000
309.900	8.3292E-01	0.80200	1.8441E-01	-1.6906	-1.6906	1.8441E-01	0.000
311.060	8.5958E-01	0.80500	1.9031E-01	-1.6591	-1.6591	1.9031E-01	0.000
312.220	8.8687E-01	0.80800	1.9636E-01	-1.6278	-1.6278	1.9636E-01	0.000
313.380	9.1481E-01	0.81100	2.0254E-01	-1.5968	-1.5968	2.0254E-01	0.000

Analytic (*NIST*)					**Predicted**		
***T* (ºK)**	***P* (MPa)**	**T_r**	**$P_{v,r}$**	**$Ln\ P_{v,r}$**	**$Ln\ P_{v,r}$**	**$P_{v,r}$**	**A%Err**
314.540	9.4341E-01	0.81400	2.0888E-01	-1.5660	-1.5661	2.0886E-01	0.010
315.700	9.7267E-01	0.81701	2.1535E-01	-1.5355	-1.5354	2.1537E-01	0.010
316.860	1.0026E+00	0.82001	2.2197E-01	-1.5052	-1.5051	2.2200E-01	0.010
318.010	1.0332E+00	0.82298	2.2876E-01	-1.4751	-1.4754	2.2869E-01	0.030
319.170	1.0645E+00	0.82599	2.3568E-01	-1.4453	-1.4454	2.3565E-01	0.010
320.330	1.0966E+00	0.82899	2.4278E-01	-1.4156	-1.4158	2.4273E-01	0.020
321.490	1.1293E+00	0.83199	2.5002E-01	-1.3862	-1.3864	2.4997E-01	0.020
322.650	1.1628E+00	0.83499	2.5743E-01	-1.3570	-1.3572	2.5738E-01	0.020
323.810	1.1970E+00	0.83799	2.6501E-01	-1.3280	-1.3282	2.6495E-01	0.020
324.970	1.2319E+00	0.84100	2.7275E-01	-1.2992	-1.2994	2.7270E-01	0.020
326.130	1.2676E+00	0.84400	2.8064E-01	-1.2707	-1.2708	2.8061E-01	0.010
327.290	1.3041E+00	0.84700	2.8872E-01	-1.2423	-1.2424	2.8869E-01	0.010
328.450	1.3414E+00	0.85000	2.9698E-01	-1.2141	-1.2143	2.9692E-01	0.020
329.610	1.3794E+00	0.85300	3.0541E-01	-1.1861	-1.1863	3.0535E-01	0.020
330.770	1.4183E+00	0.85601	3.1402E-01	-1.1583	-1.1585	3.1396E-01	0.020
331.930	1.4579E+00	0.85901	3.2277E-01	-1.1308	-1.1309	3.2274E-01	0.010
333.090	1.4984E+00	0.86201	3.3174E-01	-1.1034	-1.1035	3.3171E-01	0.010
334.240	1.5398E+00	0.86499	3.4092E-01	-1.0761	-1.0765	3.4079E-01	0.040
335.400	1.5819E+00	0.86799	3.5022E-01	-1.0492	-1.0495	3.5011E-01	0.030
336.560	1.6250E+00	0.87099	3.5977E-01	-1.0223	-1.0226	3.5966E-01	0.030
337.720	1.6689E+00	0.87399	3.6950E-01	-0.9956	-0.9960	3.6935E-01	0.040
338.880	1.7137E+00	0.87699	3.7942E-01	-0.9691	-0.9695	3.7927E-01	0.040
340.040	1.7594E+00	0.88000	3.8954E-01	-0.9428	-0.9431	3.8942E-01	0.030
341.200	1.8060E+00	0.88300	3.9984E-01	-0.9167	-0.9170	3.9972E-01	0.030
342.360	1.8535E+00	0.88600	4.1037E-01	-0.8907	-0.8910	4.1025E-01	0.030
343.520	1.9019E+00	0.88900	4.2109E-01	-0.8649	-0.8652	4.2097E-01	0.030
344.680	1.9513E+00	0.89200	4.3201E-01	-0.8393	-0.8395	4.3193E-01	0.020
345.840	2.0017E+00	0.89501	4.4317E-01	-0.8138	-0.8140	4.4308E-01	0.020
347.000	2.0530E+00	0.89801	4.5453E-01	-0.7885	-0.7886	4.5448E-01	0.010
348.160	2.1053E+00	0.90101	4.6613E-01	-0.7633	-0.7635	4.6603E-01	0.020
349.310	2.1587E+00	0.90399	4.7793E-01	-0.7383	-0.7386	4.7778E-01	0.030
350.470	2.2130E+00	0.90699	4.8998E-01	-0.7134	-0.7137	4.8983E-01	0.030
351.630	2.2684E+00	0.90999	5.0223E-01	-0.6887	-0.6890	5.0208E-01	0.030
352.790	2.3248E+00	0.91299	5.1469E-01	-0.6642	-0.6644	5.1458E-01	0.020
353.950	2.3823E+00	0.91599	5.2745E-01	-0.6397	-0.6399	5.2735E-01	0.020

Analytic (*NIST*)					**Predicted**		
T **(ºK)**	***P*** **(MPa)**	T_r	$P_{v,r}$	$Ln\ P_{v,r}$	$Ln\ P_{v,r}$	$P_{v,r}$	**A%Err**
355.110	2.4408E+00	0.91900	5.4037E-01	-0.6155	-0.6156	5.4032E-01	0.010
356.270	2.5005E+00	0.92200	5.5361E-01	-0.5913	-0.5914	5.5355E-01	0.010
357.430	2.5613E+00	0.92500	5.6705E-01	-0.5673	-0.5674	5.6700E-01	0.010
358.590	2.6232E+00	0.92800	5.8077E-01	-0.5434	-0.5434	5.8077E-01	0.000
359.750	2.6862E+00	0.93100	5.9470E-01	-0.5197	-0.5197	5.9470E-01	0.000
360.910	2.7504E+00	0.93401	6.0896E-01	-0.4960	-0.4959	6.0902E-01	0.010
362.070	2.8158E+00	0.93701	6.2344E-01	-0.4725	-0.4724	6.2350E-01	0.010
363.230	2.8824E+00	0.94001	6.3814E-01	-0.4492	-0.4490	6.3827E-01	0.020
364.390	2.9502E+00	0.94301	6.5318E-01	-0.4259	-0.4257	6.5331E-01	0.020
365.540	3.0192E+00	0.94599	6.6845E-01	-0.4028	-0.4027	6.6851E-01	0.010
366.700	3.0896E+00	0.94899	6.8400E-01	-0.3798	-0.3796	6.8414E-01	0.020
367.860	3.1612E+00	0.95199	6.9991E-01	-0.3568	-0.3566	7.0005E-01	0.020
369.020	3.2341E+00	0.95499	7.1605E-01	-0.3340	-0.3338	7.1620E-01	0.020
370.180	3.3084E+00	0.95800	7.3249E-01	-0.3113	-0.3109	7.3279E-01	0.040
371.340	3.3841E+00	0.96100	7.4924E-01	-0.2887	-0.2883	7.4954E-01	0.040
372.500	3.4612E+00	0.96400	7.6629E-01	-0.2662	-0.2657	7.6667E-01	0.050
373.660	3.5397E+00	0.96700	7.8364E-01	-0.2438	-0.2432	7.8411E-01	0.060
374.820	3.6197E+00	0.97000	8.0140E-01	-0.2214	-0.2208	8.0188E-01	0.060
375.980	3.7012E+00	0.97301	8.1947E-01	-0.1991	-0.1985	8.1996E-01	0.060
377.140	3.7843E+00	0.97601	8.3786E-01	-0.1769	-0.1762	8.3845E-01	0.070
378.300	3.8690E+00	0.97901	8.5659E-01	-0.1548	-0.1541	8.5719E-01	0.070
379.460	3.9554E+00	0.98201	8.7573E-01	-0.1327	-0.1320	8.7634E-01	0.070
380.610	4.0436E+00	0.98499	8.9521E-01	-0.1107	-0.1101	8.9574E-01	0.060
381.770	4.1337E+00	0.98799	9.1521E-01	-0.0886	-0.0881	9.1567E-01	0.050
382.930	4.2257E+00	0.99099	9.3557E-01	-0.0666	-0.0661	9.3604E-01	0.050
384.090	4.3200E+00	0.99399	9.5648E-01	-0.0445	-0.0441	9.5686E-01	0.040
385.250	4.4167E+00	0.99700	9.7785E-01	-0.0224	-0.0221	9.7814E-01	0.030
						Average	0.023
						Maximum	0.080

The temperature interval is 1.15-1.16° K for the entire range.

Appendix B: Ancillary Data For Chapter 1

This appendix contains more detailed information pertaining to Chapter 1.

Table B.1. Physical Properties of Seventy-Two Species With Entire-Curve Wagner Constants. From Section A of Appendix A of Poling et al. (2001).

Species	CAS #	No. (1)	T_f (K)	T_b (K)	T_c (K)	P_c (bars)	ω
2-Methyl propanoic acid ($C_4H_8O_2$)	79-31-2	120	227.05	427.57	605.00	37.00	0.618
3-Methyl butanoic acid ($C_5H_{10}O_2$)	503-74-2	159	243.85	449.68	629.00	34.00	0.651
Acetic Acid ($C_2H_4O_2$)	64-19-7	60	289.77	391.04	594.45	57.90	0.445
Butanoic acid ($C_4H_8O_2$)	107-92-6	119	267.97	436.87	624.00	40.30	0.600
Decanoic acid ($C_{10}H_{20}O_2$)	334-48-5	359	305.15	541.92	726.00	22.30	0.749
Formic acid (CH_2O_2)	64-18-6	22	281.50	374.04	588.00	58.07	0.316
Octanoic acid ($C_8H_{16}O_2$)	124-07-2	289	289.45	512.01	695.00	26.40	0.734
Pentanoic acid ($C_5H_{10}O_2$)	109-52-4	158	239.45	459.31	643.00	35.80	0.670
Propanoic acid ($C_3H_6O_2$)	79-09-4	90	252.31	414.31	604.00	45.30	0.539
1-Decanol ($C_{10}H_{22}O$)	112-30-1	365	280.05	504.25	684.40	23.70	0.661
1-Dodecanol ($C_{12}H_{26}O$)	112-53-8	378	297.10	537.79	720.00	20.80	0.684
1-Eicosanol ($C_{20}H_{42}O$)	629-96-9	402	339.00	647.69	809.00	13.00	0.954
1-Heptadecanol ($C_{17}H_{36}O$)	1454-85-9	393	327.00	611.12	780.00	15.00	0.853
1-Heptanol ($C_7H_{16}O$)	111-70-6	268	239.20	449.81	631.90	31.50	0.588
1-Hexadecanol ($C_{16}H_{34}O$)	4485-13-6	391	322.45	597.53	770.00	16.10	0.818
1-Hexanol ($C_6H_{14}O$)	111-27-3	221	229.20	430.44	611.40	35.10	0.573
1-Nonanol ($C_9H_{20}O$)	143-08-8	342	268.15	486.52	668.90	26.30	0.633
1-Octadecanol ($C_{18}H_{38}O$)	112-92-5	398	331.00	623.57	790.00	14.40	0.892
1-Octanol ($C_8H_{18}O$)	111-87-5	314	257.65	468.33	652.50	28.60	0.594
1-Pentanol ($C_5H_{12}O$)	71-41-0	169	194.25	411.16	588.15	39.09	0.579
2-Butanol ($C_4H_{10}O$)	78-92-2	133	158.50	372.66	536.05	41.79	0.574
2-Ethyl-1-hexanol ($C_8H_{18}O$)	104-76-7	318	203.20	457.77	640.50	27.99	0.558
2-Octanol ($C_8H_{18}O$)	123-96-6	315	241.15	453.03	637.00	28.10	0.531
Benzyl alcohol (C_7H_8O)	100-51-6	235	257.80	478.46	715.00	43.00	0.390
Butanol-1 ($C_4H_{10}O$)	71-36-3	130	183.35	390.88	563.05	44.23	0.590
Cyclohexanol ($C_6H_{12}O$)	108-93-0	201	297.65	433.94	648.00	40.75	0.366
Ethanol (C_2H_6O)	64-17-5	66	159.05	351.80	513.92	61.48	0.649
Isopropyl alcohol (C_3H_8O)	67-63-0	97	183.65	355.39	508.30	47.62	0.665
Methanol (CH_4O)	67-56-1	27	175.49	337.69	512.64	80.97	0.565
Propanol (C_3H_8O)	71-23-8	96	147.00	370.93	536.78	51.75	0.629
Tert-butanol ($C_4H_{10}O$)	75-65-0	132	298.55	355.49	506.21	39.73	0.613
Acetone (C_3H_6O)	67-64-1	89	178.50	329.22	508.10	47.00	0.307
Cyclopentanone (C_5H_8O)	120-92-3	147	222.50	403.72	624.50	46.00	0.288
Methyl isobutyl ketone ($C_6H_{12}O$)	108-10-1	204	189.15	389.15	574.60	32.70	0.351
Benzene (C_6H_6)	71-43-2	187	278.68	353.24	562.05	48.95	0.210
Ethylbenzene (C_8H_{10})	100-41-4	273	178.18	409.36	617.15	36.09	0.304
Naphthalene ($C_{10}H_8$)	91-20-3	345	351.35	491.16	748.40	40.50	0.304

Species	**CAS #**	**No.** (1)	***T_f* (K)**	***T_b* (K)**	***T_c* (K)**	***P_c* (bars)**	**ω**
Toluene (C_7H_8)	108-88-3	234	178.16	383.79	591.75	41.08	0.264
Pentafluorobenzene (C_6HF_5)	363-72-4	184	225.85	358.89	530.97	35.37	0.374
Pentafluorotoluene ($C_7H_3F_5$)	771-56-2	233	243.35	390.65	566.52	31.24	0.415
m-Xylene (C_8H_{10})	108-38-3	275	225.28	412.34	617.00	35.41	0.327
o-Xylene (C_8H_{10})	95-47-6	274	247.97	417.59	630.30	37.32	0.312
p-Xylene (C_8H_{10})	106-42-3	276	286.41	411.53	616.20	35.11	0.322
Acetic Anhydride ($C_4H_6O_3$)	108-24-7	111	199.00	412.69	606.00	40.00	0.456
Butane (C_4H_{10})	106-97-8	127	134.79	272.66	425.12	37.96	0.200
Diethyl ether ($C_4H_{10}O$)	60-29-7	134	156.86	307.59	466.70	36.40	0.281
Decane ($C_{10}H_{22}$)	124-18-5	360	243.49	447.30	617.70	21.10	0.490
Dodecane ($C_{12}H_{26}$)	112-40-3	377	263.57	489.48	658.00	18.20	0.576
Eicosane ($C_{20}H_{42}$)	112-95-8	401	309.95	616.84	768.00	10.70	0.865
Ethane (C_2H_6)	74-84-0	65	90.35	184.55	305.32	48.72	0.099
Heptadecane ($C_{17}H_{36}$)	629-78-7	392	295.13	574.56	736.00	13.40	0.753
n-Heptane (C_7H_{16})	142-82-5	259	182.59	371.57	540.20	27.40	0.350
Hexadecane ($C_{16}H_{34}$)	544-76-3	389	291.32	559.98	723.00	14.00	0.718
n-Hexane (C_6H_{14})	110-54-3	216	177.84	341.88	507.60	30.25	0.300
Methane (CH_4)	74-82-8	26	90.69	111.66	190.56	45.99	0.011
Nonadecane ($C_{19}H_{40}$)	629-92-5	399	305.25	602.34	755.00	11.60	0.845
Nonane (C_9H_{20})	111-84-2	334	219.66	423.97	594.60	22.90	0.445
Octadecane ($C_{18}H_{38}$)	593-45-3	397	301.32	588.30	747.00	12.90	0.800
Octane (C_8H_{18})	111-65-9	296	216.39	398.82	568.70	24.90	0.399
Pentadecane ($C_{15}H_{32}$)	629-62-9	387	283.08	543.83	708.00	14.80	0.685
n-Pentane (C_5H_{12})	109-66-0	166	143.43	309.22	469.70	33.70	0.252
Propane (C_3H_8)	74-98-6	95	85.47	231.02	369.83	42.48	0.152
R152a ($C_2H_4F_2$)	75-37-6	59	156.15	249.10	386.41	45.16	0.276
n-Tetradecane ($C_{14}H_{30}$)	629-59-4	385	279.01	526.76	693.00	15.70	0.644
Tridecane ($C_{13}H_{28}$)	629-50-5	380	267.76	508.63	675.00	16.80	0.618
Undecane ($C_{11}H_{24}$)	1120-21-4	369	247.57	469.08	639.00	19.80	0.537
Argon (Ar)	7440-37-1	1	83.80	87.27	150.86	48.98	-0.002
Nitrogen (N_2)	7727-37-9	455	63.15	77.35	126.20	33.98	0.037
Ammonia (NH_3)	7664-41-7	447	195.41	239.82	405.40	113.53	0.257
Water (H_2O)	7732-18-5	440	273.15	373.15	647.14	220.64	0.344
Helium (He normal)	7440-59-7	450	2.15	4.30	5.19	2.27	-0.390
Hydrogen (H_2 normal)	800000-51-5	439	13.56	20.38	33.25	12.97	-0.216

(1) Unique number given to each species in Appendix A of Poling et al. (2001).

Table B.2. Calculated T_b and ω from Wagner Constants, Critical Constants Corresponding to Wagner Constants if Different From Those in Table B.1, and Absolute Difference from Values in Table B.1.

Species	T_c (K)	P_c (bars)	ω	T_b (K)	$\lvert\Delta\rvert\ T_c$	$\lvert\Delta\rvert\ P_c$	$\lvert\Delta\rvert\ \omega$	$\lvert\Delta\rvert\ T_b$
2-Methyl propanoic acid ($C_4H_8O_2$)			0.618	427.58				0.01
3-Methyl butanoic acid ($C_5H_{10}O_2$)			0.651	449.68				
Acetic Acid ($C_2H_4O_2$)	592.71	57.86	0.459	391.04	1.74	0.04	0.014	
Butanoic acid ($C_4H_8O_2$)			0.600	436.87				
Decanoic acid ($C_{10}H_{20}O_2$)			0.749	541.92				
Formic acid (CH_2O_2)			0.316	374.04				
Octanoic acid ($C_8H_{16}O_2$)			0.734	512.01				
Pentanoic acid ($C_5H_{10}O_2$)			0.670	459.31				
Propanoic acid ($C_3H_6O_2$)			0.539	414.31				
1-Decanol ($C_{10}H_{22}O$)	689.00	24.10	0.629	504.25	4.60	0.40	0.032	
1-Dodecanol ($C_{12}H_{26}O$)			0.684	537.78				0.01
1-Eicosanol ($C_{20}H_{42}O$)			0.954	647.69				
1-Heptadecanol ($C_{17}H_{36}O$)			0.853	611.12				
1-Heptanol ($C_7H_{16}O$)	632.50	31.35	0.580	449.70	0.60	0.15	0.008	0.11
1-hexadecanol ($C_{16}H_{34}O$)			0.818	597.53				
1-Hexanol ($C_6H_{14}O$)	610.70	34.70	0.575	430.44	0.70	0.40	0.002	
1-Nonanol ($C_9H_{20}O$)	671.50		0.610	486.52	2.60		0.023	
1-Octadecanol ($C_{18}H_{38}O$)			0.892	623.56				0.01
1-Octanol ($C_8H_{18}O$)			0.594	468.33				
1-Pentanol ($C_5H_{12}O$)			0.579	411.16				
2-Butanol ($C_4H_{10}O$)	536.01	41.98	0.577	372.67	0.04	0.19	0.003	0.01
2-Ethyl-1-hexanol ($C_8H_{18}O$)			0.558	457.77				
2-Octanol ($C_8H_{18}O$)	638.00	28.90	0.534	453.03	1.00	0.80	0.003	
Benzyl alcohol (C_7H_8O)			0.390	478.46				
Butanol-1 ($C_4H_{10}O$)		44.24	0.591	390.88		0.01	0.001	
Cyclohexanol ($C_6H_{12}O$)	650.00	42.60	0.370	433.99	2.00	1.85	0.004	0.05
Ethanol (C_2H_6O)		61.32	0.643	351.44		0.16	0.006	0.36
Isopropyl alcohol (C_3H_8O)			0.665	355.39				
Methanol (CH_4O)		80.92	0.564	337.69		0.05	0.001	
Propanol (C_3H_8O)		51.68	0.620	370.30		0.07	0.009	0.63
Tert-butanol ($C_4H_{10}O$)	506.20		0.613	355.49	0.01			
Acetone (C_3H_6O)		47.02	0.307	329.22		0.02		
Cyclopentanone (C_5H_8O)			0.288	403.72				
Methyl isobutyl ketone ($C_6H_{12}O$)			0.351	389.15				
Benzene (C_6H_6)	562.16	48.98	0.209	353.24	0.11	0.03	0.001	
Ethylbenzene (C_8H_{10})	617.20	36.00	0.302	409.36	0.05	0.09	0.002	
Naphthalene ($C_{10}H_8$)			0.304	491.16				
Toluene (C_7H_8)	591.80	41.06	0.264	383.79	0.05	0.02		

Species	***T_c (K)***	***P_c (bars)***	**ω**	***T_b (K)***	**|Δ| T_c**	**|Δ| P_c**	**|Δ| ω**	**|Δ| T_b**
Pentafluorobenzene (C_6HF_5)			0.374	358.89				
Pentafluorotoluene ($C_7H_3F_5$)			0.415	390.66				0.01
m-Xylene (C_8H_{10})	617.05	35.38	0.326	412.34	0.05	0.03	0.001	
o-Xylene (C_8H_{10})	630.33	37.35	0.312	417.59	0.03	0.03		
p-Xylene (C_8H_{10})	616.23	35.16	0.322	411.52	0.03	0.05		0.01
Acetic Anhydride ($C_4H_6O_3$)			0.456	412.69				
Butane (C_4H_{10})	425.25	37.92	0.199	272.67	0.13	0.04	0.001	0.01
Diethyl ether ($C_4H_{10}O$)	466.74	36.50	0.282	307.58	0.04	0.10	0.001	0.01
Decane ($C_{10}H_{22}$)	617.65	21.05	0.490	447.30	0.05	0.05		
Dodecane ($C_{12}H_{26}$)			0.573	489.22			0.003	0.26
Eicosane ($C_{20}H_{42}$)	769.00	11.60	0.891	616.84	1.00	0.90	0.026	
Ethane (C_2H_6)	305.33	48.71	0.099	184.55	0.01	0.01		
Heptadecane ($C_{17}H_{36}$)	735.00	13.70	0.772	574.56	1.00	0.30	0.019	
n-Heptane (C_7H_{16})	540.15	27.35	0.350	371.57	0.05	0.05		
Hexadecane ($C_{16}H_{34}$)	722.00	14.35	0.737	559.98	1.00	0.35	0.019	
n-Hexane (C_6H_{14})	507.90	30.35	0.299	341.88	0.30	0.10	0.001	
Methane (CH_4)	190.55		0.011	111.66	0.01			
Nonadecane ($C_{19}H_{40}$)	758.00	12.30	0.844	602.34	3.00	0.70	0.001	
Nonane (C_9H_{20})	594.90		0.443	423.97	0.30		0.002	
Octadecane ($C_{18}H_{38}$)	746.00	13.00	0.812	588.30	1.00	0.10	0.012	
Octane (C_8H_{18})	568.95		0.397	398.82	0.25		0.002	
Pentadecane ($C_{15}H_{32}$)		15.15	0.696	543.82		0.35	0.011	0.01
n-Pentane (C_5H_{12})	469.80	33.75	0.251	309.22	0.10	0.05	0.001	
Propane (C_3H_8)			0.152	231.00				0.02
R152a ($C_2H_4F_2$)		45.17	0.275	249.13		0.01	0.001	0.03
n-Tetradecane ($C_{14}H_{30}$)		16.10	0.654	526.76		0.40	0.010	
Tridecane ($C_{13}H_{28}$)	676.00	17.10	0.618	508.64	1.00	0.30		0.01
Undecane ($C_{11}H_{24}$)	638.85	19.55	0.533	469.08	0.15	0.25	0.004	
Argon (Ar)	150.69	48.63	-0.002	87.30	0.17	0.35		0.03
Nitrogen (N_2)		34.00	0.037	77.35		0.02		
Ammonia (NH_3)	405.50		0.256	239.82	0.10		0.001	
Water (H_2O)	647.10		0.344	373.13	0.04			0.01
Helium (He normal)	5.20		-0.382	4.23	0.01		0.008	0.06
Hydrogen (H_2 normal)	33.15	12.96	-0.219	20.37	0.10	0.01	0.003	0.01

Table B.3. Reduced Temperatures For Each Interval and Point Distribution Combination.

T_r Interval		Point Distributions		
Bounds	**Width**	**Eighth**	**Quarter**	**Even**
0.5-0.9	0.4	0.5,0.55,0.85,0.9	0.5,0.6,0.8,0.9	0.5,0.63333,0.76667,0.9
0.55-0.9	0.35	0.55,0.59375,0.85625,0.9	0.55,0.6375,0.8125,0.9	0.55,0.66667,0.78333,0.9
0.6-0.9	0.3	0.6, 0.6375, 0.8625, 0.9	0.6, 0.675, 0.825, 0.9	0.6, 0.7, 0.8, 0.9
0.50-0.70	0.2	0.5, 0.525, 0.675, 0.7	0.5, 0.55, 0.65, 0.7	0.5,0.56667,0.63333,0.7
0.7-0.9	0.2	0.7, 0.725, 0.875, 0.9	0.7, 0.75, 0.85, 0.9	0.7, 0.76667, 0.83333, 0.9
0.55-0.7	0.15	0.55,0.56875,0.68125,0.7	0.55,0.5875,0.6625,0.7	0.55,0.6,0.65,0.7
0.50-0.60	0.1	0.5,0.5125,0.5875,0.6	0.5,0.525,0.575,0.6	0.5,0.5333,0.56667,0.6
0.55-0.65	0.1	0.55,0.5625,0.6375,0.65	0.55, 0.575, 0.625, 0.65	0.55, 0.58333,0.61667,0.65
0.6-0.7	0.1	0.6, 0.6125, 0.6875, 0.7	0.6, 0.625, 0.675, 0.7	0.6, 0.63333, 0.66667, 0.7
0.55-0.6	0.05	0.55,0.55625,0.59375,0.6	0.55,0.5625,0.5875,0.6	0.55,0.56667,0.58333,0.6
0.6-0.65	0.05	0.6,0.60625,0.64375,0.65	0.6,0.6125,0.6375,0.65	0.6,0.61667,0.63333,0.65

Table B.4. η Values for Three Distributions. Intervals: 0.5-0.9, 0.55-0.9, and 0.6-0.9.

Interval	**0.5-0.9**			**0.55-0.9**			**0.6-0.9**		
Dist'n	**Even**	**Quarter**	**Eighth**	**Even**	**Quarter**	**Eighth**	**Even**	**Quarter**	**Eighth**
η_{a1}	-1.2527554	-1.4129707	-2.1370735	-1.9105592	-2.1654787	-3.3203808	-3.0648585	-3.4926088	-5.4352515
η_{a2}	9.9705508	5.8526808	4.0957105	14.1258539	8.4759213	6.1784668	21.0364707	12.9213950	9.8258144
η_{a3}	-29.4781293	-30.4698805	-53.3527652	-38.9065851	-39.5423295	-67.2692216	-53.6598599	-53.5269091	-88.2027067
η_{a4}	49.0651727	55.1578821	82.8110837	56.3577392	63.6954003	97.0440850	66.9831631	76.1506766	117.8781688
η_{b1}	5.1785201	5.9409679	9.3961917	8.0261779	9.2437401	14.7710866	13.1164427	15.1682227	24.4998958
η_{b2}	-40.5699180	-24.3781898	-17.9515145	-58.3589341	-35.8171968	-27.3898073	-88.4498187	-55.5083188	-44.1178005
η_{b3}	113.6738071	116.5675397	202.1502788	152.3792779	153.6171521	258.7507652	214.0719880	211.7908155	345.4598562
η_{b4}	-146.5746040	-169.4765370	-273.4395073	-175.8251796	-203.8187770	-331.0645449	-219.1970428	-254.8012084	-416.8798364
η_{c1}	-12.3186676	-14.9037679	-26.6815685	-20.1398146	-24.3078771	-43.3055045	-34.8740634	-41.9798100	-74.3884861
η_{c2}	91.0850608	59.1865857	50.4651298	138.1776272	91.0603729	79.4263269	221.8890227	148.3688744	132.3618243
η_{c3}	-205.6613258	-203.1382406	-335.8145571	-295.4540008	-287.5292484	-462.8447553	-447.7420970	-428.7014193	-670.2352401
η_{c4}	199.5827894	236.0754381	401.8797830	262.0185950	310.1556500	529.1218036	360.8064394	427.3770531	730.5916821
η_{d1}	47.1407272	55.7015939	94.8211471	93.3576437	110.3395309	187.9336418	198.8988093	235.1378002	400.7469026
η_{d2}	-215.7874989	-152.6450493	-147.9070499	-406.9881397	-291.1101374	-287.3021894	-829.2917811	-599.5913230	-601.8927563
η_{d3}	348.9738959	317.8303432	466.2289211	631.0236629	567.9385136	814.8147393	1,232.0169271	1,095.0183534	1,534.0743645
η_{d4}	-255.7511714	-300.5623216	-504.7378201	-426.9095742	-502.2658486	-845.8417970	-766.7340723	-903.0873184	-1,525.2699404

Table B.5. η Values for Three Distributions. Intervals: 0.5-0.7 and 0.7-0.9.

Interval	**0.5-0.7**			**0.7-0.9**		
Dist'n	**Even**	**Quarter**	**Eighth**	**Even**	**Quarter**	**Eighth**
η_{a1}	-53.4948579	-62.9974339	-106.4265140	-10.2674466	-11.8500429	-19.0645187
η_{a2}	246.8027629	173.8408042	166.6125121	59.8206316	38.7723578	32.4020036
η_{a3}	-385.0215692	-339.2018638	-456.1817116	-126.8429885	-120.8476519	-184.4209443
η_{a4}	206.9114116	243.6261474	411.4247820	113.0724079	130.3247411	209.0334781
η_{b1}	153.3724856	181.1662193	308.1926435	46.0655860	53.7505178	88.8017617
η_{b2}	-695.4278764	-493.8566662	-479.8132148	-263.1848603	-173.6580294	-150.1822393
η_{b3}	1,056.0997651	925.2589189	1,234.8841196	531.9809075	502.7276301	759.2916190
η_{b4}	-543.7060369	-642.4087022	-1,093.5161082	-414.3859331	-484.7991029	-806.0620695
η_{c1}	-198.4706878	-235.6462631	-405.5565636	-140.0221564	-167.5669407	-293.3265443
η_{c2}	863.7799007	623.8835718	622.9261307	755.7094489	521.9786487	489.0922646
η_{c3}	-1,236.7042293	-1,069.6726100	-1,402.1310033	-1,329.7498676	-1,223.9328396	-1,785.1694004
η_{c4}	592.5243792	702.7384636	1,206.4659686	863.7444870	1,024.2870158	1,756.9603861
η_{d1}	259.4258867	307.3137116	526.1968648	1,281.1861021	1,515.6868113	2,587.3572202
η_{d2}	-967.2529320	-723.3209400	-761.1356767	-4,919.0222742	-3,632.8125774	-3,766.6497750
η_{d3}	1,207.7957950	1,010.1021747	1,259.4391508	6,662.3759056	5,753.7131085	7,638.6495874
η_{d4}	-511.0750277	-605.2826286	-1,035.8761659	-3,460.6897117	-4,086.0330567	-6,942.3642942

Table B.6. η Values for Three Distributions. Intervals: 0.55-0.7 and 0.5-0.6.

Interval	0.55-0.7			0.5-0.6		
Dist'n	**Even**	**Quarter**	**Eighth**	**Even**	**Quarter**	**Eighth**
η_{a1}	-136.6250998	-161.2645048	-273.8962731	-727.4575657	-861.0426632	-1,471.8796624
η_{a2}	572.9181326	414.2693895	413.6632482	2,682.2204661	2,010.1686085	2,120.1106442
η_{a3}	-810.4193486	-697.4110263	-905.5464471	-3,305.1323566	-2,749.8170099	-3,393.5815145
η_{a4}	390.1762668	460.5032865	781.9845744	1,363.3546069	1,613.6881892	2,758.3747439
η_{b1}	398.9723046	471.8544968	805.0161599	1,898.6584959	2,248.7181439	3,849.4168954
η_{b2}	-1,647.5815867	-1,198.9389224	-1,209.6478046	-6,930.2994427	-5,211.2317784	-5,525.1172252
η_{b3}	2,280.3726904	1,953.2339606	2,519.6499583	8,435.6054681	6,998.5416565	8,601.9964029
η_{b4}	-1,063.8533459	-1,258.3627147	-2,147.5134216	-3,427.8522373	-4,059.9439370	-6,950.2757784
η_{c1}	-537.4356375	-637.6321812	-1,095.6599610	-2,050.7734063	-2,431.1159568	-4,170.2894681
η_{c2}	2,143.0399417	1,579.7260599	1,626.8459090	7,324.7479144	5,544.5403296	5,939.2815559
η_{c3}	-2,832.2942375	-2,401.0410303	-3,052.1364851	-8,695.6752625	-7,172.0772361	-8,740.2594088
η_{c4}	1,250.9193319	1,483.3035974	2,545.5976386	3,436.6153531	4,073.5914795	6,986.2602698
η_{d1}	791.1920078	937.3841723	1,605.6871582	1,775.3785475	2,103.8096656	3,605.6136515
η_{d2}	-2,794.8058666	-2,118.3920892	-2,275.2987121	-5,943.1711190	-4,568.9970004	-5,009.8547063
η_{d3}	3,308.7925393	2,729.8797728	3,332.6578261	6,634.3039888	5,389.0075302	6,419.1979990
η_{d4}	-1,320.1825597	-1,563.9457773	-2,678.2805164	-2,472.3848837	-2,929.7020732	-5,020.8578535

Table B.7. η Values for Three Distributions. Intervals: 0.55-0.65 and 0.6-0.7.

Interval	0.55-0.65			0.6-0.7		
Dist'n	**Even**	**Quarter**	**Eighth**	**Even**	**Quarter**	**Eighth**
η_{a1}	-614.3660881	-726.9403478	-1,241.7008896	-494.4312092	-584.7430890	-997.7038595
η_{a2}	2,290.8757193	1,711.1491487	1,795.6923947	1,874.8838684	1,393.5554390	1,451.5403282
η_{a3}	-2,861.1949547	-2,388.6306641	-2,963.2274709	-2,387.8676411	-2,003.2941462	-2,503.7612066
η_{a4}	1,199.4477670	1,419.2013822	2,424.0541642	1,024.4781288	1,211.5704905	2,067.0714165
η_{b1}	1,705.9216235	2,020.0983174	3,456.7136456	1,473.6279245	1,744.5821458	2,983.5513474
η_{b2}	-6,291.1520819	-4,716.9701561	-4,979.7230552	-5,520.1196208	-4,120.9930479	-4,322.4798821
η_{b3}	7,749.7828166	6,449.5762069	7,965.2174998	6,920.8429486	5,785.8069224	7,195.0369806
η_{b4}	-3,193.1287148	-3,781.3234384	-6,470.9239161	-2,909.3950267	-3,444.5082553	-5,891.3760662
η_{c1}	-2,084.6502362	-2,471.4819057	-4,240.3248767	-2,073.4365889	-2,458.4971162	-4,219.2356609
η_{c2}	7,505.3684468	5,670.0303919	6,056.5949406	7,561.1235990	5,694.3404812	6,055.0866868
η_{c3}	-8,988.4061886	-7,431.3722089	-9,090.6157074	-9,177.7115880	-7,615.4124972	-9,368.6226235
η_{c4}	3,587.7785900	4,252.9553035	7,294.5700305	3,718.2193433	4,407.8390534	7,561.2121070
η_{d1}	2,451.1616415	2,904.5238481	4,977.5945188	3,455.8458065	4,094.8632970	7,016.8702558
η_{d2}	-8,200.7499241	-6,304.3263270	-6,913.3838498	-11,581.3850072	-8,897.5563992	-9,749.7360711
η_{d3}	9,164.5877493	7,448.2701812	8,880.9344197	12,989.8444519	10,570.0178072	12,629.4979429
η_{d4}	-3,425.6162632	-4,059.1037549	-6,955.8247707	-4,885.0979091	-5,788.1666691	-9,917.5860361

Table B.8. η Values for Three Distributions. Intervals: 0.55-0.6 and 0.6-0.65.

Interval	**0.55-0.6**			**0.6-0.65**		
Dist'n	**Even**	**Quarter**	**Eighth**	**Even**	**Quarter**	**Eighth**
η_{a1}	-6,353.3071338	-7,527.9338624	-12,894.7570311	-5,310.7685105	-6,292.0133254	-10,775.2811738
η_{a2}	21,209.8877160	16,305.9465163	17,891.5020226	17,862.9708572	13,704.9591261	14,991.7682243
η_{a3}	-23,614.1456056	-19,157.2275787	-22,785.2226296	-20,050.3070137	-16,299.3083392	-19,445.7557316
η_{a4}	8,771.2992555	10,392.9526987	17,802.2233872	7,513.8126368	8,902.0756664	15,244.9934287
η_{b1}	16,882.9931310	20,007.9468830	34,285.7377961	15,046.7146863	17,830.8819167	30,551.6301230
η_{b2}	-56,031.6611433	-43,150.1986821	-47,470.1967131	-50,278.6903281	-38,650.3318415	-42,406.1348746
η_{b3}	61,977.6052018	50,201.5715164	59,572.2501242	56,019.9348039	45,459.7877492	54,096.2368171
η_{b4}	-22,854.7858716	-27,085.1769495	-46,413.6676918	-20,819.1698036	-24,671.5617277	-42,272.9858434
η_{c1}	-18,924.0860383	-22,432.4324889	-38,461.9307584	-19,170.1598302	-22,724.6278738	-38,964.8515423
η_{c2}	62,042.1987151	47,941.2086685	53,014.0524685	63,183.3342836	48,758.4082471	53,812.9993576
η_{c3}	-67,732.1246807	-54,688.7323363	-64,593.7165595	-69,358.8867708	-56,082.7044774	-66,385.8913672
η_{c4}	24,631.0581051	29,197.0099474	50,058.6659549	25,369.0450629	30,072.2703710	51,561.1202783
η_{d1}	18,086.7926683	21,437.6398989	36,747.5329859	25,218.7508637	29,890.6273845	51,236.2521478
η_{d2}	-57,340.8740499	-44,673.3478649	-50,012.7268875	-80,007.6068646	-62,318.4745949	-69,746.3002478
η_{d3}	60,589.4185099	48,525.0968286	56,620.5012471	84,638.8279834	67,810.1863828	79,169.5778183
η_{d4}	-21,343.0890998	-25,297.1439429	-43,363.0694264	-29,864.4796542	-35,396.8543185	-60,674.0617029

Table B.9. Average A%Err at $T_{r,f}$ Based on Interval and Point Distribution.

Interval →	0.5-0.9	0.55-0.9	0.6-0.9	0.5-0.7	0.7-0.9	0.55-0.7	0.5-0.6	0.55-0.65	0.6-0.7	0.55-0.6	0.6-0.65
Distribution ↓											
Even	0.0865	**0.1730**	0.4617	0.1875	4.5115	0.6952	0.6250	1.4434	2.8971	8.2574	16.7836
Quarter	*0.0604*	0.2082	0.4181	*0.1678*	2.5622	0.5564	0.4722	1.6173	3.5297	6.8585	18.7755
Eighth	0.0758	0.2071	0.5494	0.1936	4.3275	0.8937	0.5598	1.7881	3.6794	10.0678	24.1425

Table B.10. Average A%Err at $T_{r,b}$ Based on Interval and Point Distribution.

Interval →	0.5-0.9	0.55-0.9	0.6-0.9	0.5-0.7	0.7-0.9	0.55-0.7	0.5-0.6	0.55-0.65	0.6-0.7	0.55-0.6	0.6-0.65
Distribution ↓											
Even	**0.0046**	0.0051	0.0045	**0.0075**	0.0246	**0.0100**	0.0885	**0.0413**	**0.0120**	0.4720	0.1595
Quarter	0.0048	*0.0048*	0.0045	0.0085	*0.0231*	0.0101	*0.0732*	0.0432	0.0153	*0.3358*	0.1643
Eighth	0.0076	0.0072	0.0065	0.0089	0.0194	0.0130	0.1064	0.0479	0.0216	0.6315	0.2167

Table B.11. Average A%Err in the $T_r \leq 0.6$ Segment Based on Interval and Point Distribution.

Interval →	0.5-0.9	0.55-0.9	0.6-0.9	0.5-0.7	0.7-0.9	0.55-0.7	0.5-0.6	0.55-0.65	0.6-0.7	0.55-0.6	0.6-0.65
Distribution ↓											
Even	0.0371	**0.0766**	0.2167	**0.0779**	1.8939	0.3768	0.2916	0.5746	1.2822	4.2442	7.6815
Quarter	*0.0319*	0.0923	*0.1947*	0.0845	1.0840	*0.2463*	*0.2329*	0.6812	1.6414	3.4382	8.3869
Eighth	0.0394	0.0919	0.2574	0.0769	1.7643	0.3625	0.2640	0.7376	1.6774	4.7446	9.7575

Table B.12. Average A%Err in the Tr > 0.6 Segment Based on Interval and Point Distribution.

Interval →	0.5-0.9	0.55-0.9	0.6-0.9	0.5-0.7	0.7-0.9	0.55-0.7	0.5-0.6	0.55-0.65	0.6-0.7	0.55-0.6	0.6-0.65
Distribution ↓											
Even	**0.0022**	**0.0023**	**0.0025**	**0.0212**	**0.0086**	0.0438	0.2035	**0.1427**	**0.0766**	1.1908	0.8842
Quarter	0.0028	0.0029	0.0028	0.0232	0.0096	*0.0334*	*0.1542*	0.1502	0.0833	*0.8648*	0.8385
Eighth	0.0057	0.0054	0.0053	0.0229	0.0091	0.0515	0.2053	0.1785	0.1054	1.4480	1.0588

Table B.13. Average A%Err in the "All T_rs" Segment Based on Interval and Point Distribution.

Interval →	0.5-0.9	0.55-0.9	0.6-0.9	0.5-0.7	0.7-0.9	0.55-0.7	0.5-0.6	0.55-0.65	0.6-0.7	0.55-0.6	0.6-0.65
Distribution ↓											
Even	0.0165	**0.0325**	0.1055	**0.0430**	0.9211	0.1676	0.2219	0.3079	0.5498	2.0976	3.5212
Quarter	*0.0142*	0.0390	*0.0792*	0.0453	0.6382	*0.1171*	*0.1725*	0.3548	0.6962	1.6356	3.7781
Eighth	0.0189	0.0404	0.1055	0.0435	0.8582	0.1733	0.2156	0.3924	0.7225	2.4236	4.4408

Table B.14. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.5-0.9.

Distribution	**Parameter**	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	**All T_rs**
Even	# of Points	69	69	328	414	811
	Average A%Err $(\overline{X})$	0.0865	0.0046	0.0371	0.0022	0.0165
	Maximum A%Err	0.4611	0.0110	0.4611	0.0100	0.4611
	S^2	0.012	0.000	0.005	0.000	0.002
Quarter	# of Points	69	69	259	345	673
	Average A%Err $(\overline{X})$	0.0604	0.0048	0.0319	0.0028	0.0142
	Maximum A%Err	0.4191	0.0130	0.4191	0.0100	0.4191
	S^2	7.496E-03	1.126E-05	3.713E-03	2.027E-05	1.633E-03
	$\nu_{e,4}$	117	132	583	682	1,440
	t_0*	15.619	-114.718	14.279	-433.467	22.114
	$t_{0.05,\nu}$	1.659	1.658	1.658	1.658	1.658
	S-S Test Result	H_1	**H_2**	H_1	**H_2**	H_1
Eighth	# of Points	69	69	259	345	673
	Average A%Err $(\overline{X})$	0.0758	0.0076	0.0394	0.0057	0.0189
	Maximum A%Err	0.3394	0.0250	0.3394	0.0200	0.3394
	S^2	7.892E-03	3.580E-05	4.077E-03	4.026E-05	1.854E-03
	$\nu_{e,8}$	121	77	587	450	1,480
	t_0*	6.304	-674.671	-6.070	-1502.829	-21.942
	$t_{0.05,\nu}$	1.658	1.667	1.658	1.658	1.658
	S-S Test Result	H_1	H_2	H_2	H_2	H_2

Table B.15. *t for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.55-0.9.**

Distribution	**Parameter**	$T_{r,f}$	$T_{r,b}$	$\mathbf{T_r \leq 0.6}$	$\mathbf{T_r > 0.6}$	**All T_rs**
Even	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	0.1730	0.0051	0.0766	0.0023	0.0325
	Maximum A%Err	1.0643	0.0140	1.0643	0.0100	1.0643
	S^2	0.047	0.000	0.021	0.000	0.010
Quarter	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	0.2082	0.0048	0.0923	0.0029	0.0390
	Maximum A%Err	1.2027	0.0120	1.2027	0.0100	1.2027
	S^2	6.947E-02	1.071E-05	3.019E-02	2.046E-05	1.405E-02
	$\nu_{e,4}$	123	140	584	826	1,452
	t_0*	-3.501	164.918	-7.791	-452.015	-10.922
	$t_{0.05,\ \nu}$	1.658	1.658	1.658	1.658	1.658
	S-S Test Result	$\mathbf{H_2}$	H_1	$\mathbf{H_2}$	$\mathbf{H_2}$	$\mathbf{H_2}$
Eighth	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	0.2071	0.0072	0.0919	0.0054	0.0404
	Maximum A%Err	1.1434	0.0200	1.1434	0.0200	1.1434
	S^2	4.859E-02	2.976E-05	2.387E-02	3.591E-05	1.140E-02
	$\nu_{e,8}$	140	87	647	617	1,596
	t_0*	-4.201	-554.984	-8.798	-1582.826	-15.151
	$t_{0.05,\ \nu}$	1.658	1.665	1.658	1.658	1.658
	S-S Test Result	H_2	H_2	H_2	H_2	H_2

Table B.16. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.6-0.9.

Distribution	**Parameter**	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	**All T_rs**
Even	# of Points	72	72	332	288	692
	Average A%Err $(\overline{X})$	0.4617	0.0045	0.2167	0.0025	0.1055
	Maximum A%Err	3.7094	0.0130	3.7094	0.0100	3.7094
	S^2	0.341	0.000	0.134	0.000	0.076
Quarter	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	0.4181	0.0045	0.1947	0.0028	0.0792
	Maximum A%Err	2.1173	0.0110	2.1173	0.0100	2.1173
	S^2	2.051E-01	8.027E-06	9.372E-02	2.021E-05	4.597E-02
	$\nu_{e,4}$	118	143	594	647	1,095
	t_0*	0.930	0.000	2.451	-203.428	8.005
	$t_{0.05,\ \nu}$	1.658	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	Fail to Reject	H_1	$\mathbf{H_2}$	H_1
Eighth	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	0.5494	0.0065	0.2574	0.0053	0.1055
	Maximum A%Err	2.9943	0.0170	2.9943	0.0200	2.9943
	S^2	3.354E-01	1.884E-05	1.686E-01	3.332E-05	8.205E-02
	$\nu_{e,8}$	144	101	632	703	1,510
	t_0*	-1.557	-815.742	-3.444	-1436.528	0.000
	$t_{0.05,\ \nu}$	1.658	1.662	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	$\mathrm{H_2}$	$\mathrm{H_2}$	$\mathrm{H_2}$	Fail to Reject

Table B.17. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.5-0.7.

Distribution	Parameter	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	All T_rs
Even	# of Points	69	69	328	414	811
	Average A%Err $(\overline{X})$	0.1875	0.0075	0.0779	0.0212	0.0430
	Maximum A%Err	1.7349	0.0350	1.7349	0.0900	1.7349
	S^2	0.081	0.000	0.033	0.000	0.014
Quarter	# of Points	69	69	259	345	673
	Average A%Err $(\overline{X})$	0.1678	0.0085	0.0845	0.0232	0.0453
	Maximum A%Err	0.9242	0.0460	0.9242	0.0900	0.9242
	S^2	5.178E-02	5.954E-05	2.572E-02	4.113E-04	1.107E-02
	$\nu_{e,4}$	117	137	587	725	1,475
	t_0*	1.703	-93.588	-2.712	-67.767	-3.466
	$t_{0.05/2,\ \nu}$	1.981	1.980	1.980	1.980	1.980
	2-S Test Result	Fail to Reject	Reject	Reject	Reject	Reject
	$t_{0.05,\ \nu}$	1.659	1.658	1.658	1.658	1.658
	S-S Test Result	H_1	$\mathbf{H_2}$	$\mathbf{H_2}$	$\mathbf{H_2}$	$\mathbf{H_2}$
Eighth	# of Points	69	69	328	414	811
	Average A%Err $(\overline{X})$	0.1936	0.0089	0.0769	0.0229	0.0435
	Maximum A%Err	3.0234	0.0350	3.0234	0.1199	3.0234
	S^2	1.692E-01	6.326E-05	5.222E-02	5.769E-04	2.215E-02
	$\nu_{e,8}$	98	138	556	734	1,396
	t_0*	-0.270	-127.380	0.293	-49.395	-0.538
	$t_{0.05/2,\ \nu}$	1.987	1.980	1.980	1.980	1.980
	2-S Test Result	Fail to Reject	Reject	Fail to Reject	Reject	Fail to Reject
	$t_{0.05,\ \nu}$	1.663	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	$\mathrm{H_2}$	Fail to Reject	$\mathrm{H_2}$	Fail to Reject

Table B.18. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.7-0.9.

Distribution	**Parameter**	$T_{r,f}$	$T_{r,b}$	$T_r \le 0.6$	$T_r > 0.6$	**All T_rs**
Even	# of Points	72	72	404	360	836
	Average A%Err $(\overline{X})$	4.5115	0.0246	1.8939	0.0086	0.9211
	Maximum A%Err	47.5505	0.3444	47.5505	0.0700	47.5505
	S^2	43.172	0.003	13.931	0.000	7.610
Quarter	# of Points	72	72	404	216	692
	Average A%Err $(\overline{X})$	2.5622	0.0231	1.0840	0.0096	0.6382
	Maximum A%Err	12.6821	0.5183	12.6821	0.0800	12.6821
	S^2	6.703E+00	4.271E-03	2.935E+00	1.617E-04	1.991E+00
	$\nu_{e,4}$	75	122	439	536	971
	t_0*	0.379	2.517	1.143	-64.737	1.033
	$t_{0.05,\ \nu}$	1.668	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_1	Fail to Reject	$\mathbf{H_2}$	Fail to Reject
Eighth	# of Points	72	72	404	360	836
	Average A%Err $(\overline{X})$	4.3275	0.0194	1.7643	0.0091	0.8582
	Maximum A%Err	32.3659	0.2684	32.3659	0.0800	32.3659
	S^2	3.732E+01	1.476E-03	1.192E+01	1.724E-04	6.523E+00
	$\nu_{e,8}$	141	111	789	699	1,634
	t_0*	0.027	0.883	0.142	-35.352	0.181
	$t_{0.05,\ \nu}$	1.658	1.660	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	Fail to Reject	Fail to Reject	H_2	Fail to Reject

Table B.19. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.55-0.7.

Distribution	**Parameter**	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	**All T_rs**
Even	# of Points	70	70	260	350	680
	Average A%Err $(\overline{X})$	0.6952	0.0100	0.3768	0.0438	0.1676
	Maximum A%Err	5.1335	0.0910	5.1335	0.1802	5.1335
	S^2	1.153	0.000	0.566	0.002	0.244
Quarter	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	0.5564	0.0101	0.2463	0.0334	0.1171
	Maximum A%Err	4.8200	0.0500	4.8200	0.1501	4.8200
	S^2	7.891E-01	1.207E-04	3.243E-01	1.074E-03	1.421E-01
	$\nu_{e,4}$	124	116	391	591	1,048
	t_0^*	0.831	-3.642	3.315	103.453	4.770
	$t_{0.05,\,\nu}$	1.658	1.659	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	**H_2**	H_1	H_1	H_1
Eighth	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	0.8937	0.0130	0.3625	0.0515	0.1733
	Maximum A%Err	13.6447	0.0730	13.6447	0.2202	13.6447
	S^2	2.974E+00	2.297E-04	9.043E-01	2.247E-03	3.886E-01
	$\nu_{e,8}$	90	136	563	753	1,402
	t_0^*	-0.521	-83.219	0.235	-55.309	-0.346
	$t_{0.05,\,\nu}$	1.665	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_2	Fail to Reject	H_2	Fail to Reject

Table B.20. *t for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.5-0.6.**

Distribution	Parameter	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	All T_rs
Even	# of Points	69	69	259	483	811
	Average A%Err $(\overline{X})$	0.6250	0.0885	0.2916	0.2035	0.2219
	Maximum A%Err	5.7069	0.3843	5.7069	0.8335	5.7069
	S^2	0.922	0.008	0.387	0.033	0.147
Quarter	# of Points	69	69	259	483	811
	Average A%Err $(\overline{X})$	0.4722	0.0732	0.2329	0.1542	0.1725
	Maximum A%Err	5.1335	0.5063	5.1335	0.7830	5.1335
	S^2	6.034E-01	7.505E-03	3.120E-01	1.939E-02	1.138E-01
	$\nu_{e,4}$	119	137	496	781	1,527
	t_0*	1.152	11.572	1.901	28.327	7.577
	$t_{0.05,\ \nu}$	1.658	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_1	H_1	H_1	H_1
Eighth	# of Points	69	69	259	483	811
	Average A%Err $(\overline{X})$	0.5598	0.1064	0.2640	0.2053	0.2156
	Maximum A%Err	4.3416	0.7599	4.3416	1.0346	4.3416
	S^2	7.585E-01	1.944E-02	3.285E-01	4.502E-02	1.349E-01
	$\nu_{e,8}$	133	91	505	885	1,611
	t_0*	0.454	-7.070	0.875	-0.709	0.900
	$t_{0.05,\ \nu}$	1.658	1.664	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_2	Fail to Reject	Fail to Reject	Fail to Reject

Table B.21. ***t**** **for** $F_{w,j}$ ***[WA]*** **Function Comparing Point Distributions.** T_r **Interval = 0.55-0.65.**

Distribution	**Parameter**	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	All T_rs
Even	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	1.4434	0.0413	0.5746	0.1427	0.3079
	Maximum A%Err	12.6370	0.2736	12.6370	0.7629	12.6370
	S^2	4.025	0.004	1.424	0.016	0.629
Quarter	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	1.6173	0.0432	0.6812	0.1502	0.3548
	Maximum A%Err	9.9769	0.3085	9.9769	0.5214	9.9769
	S^2	5.022E+00	4.550E-03	2.175E+00	1.609E-02	9.550E-01
	$\nu_{e,4}$	134	132	569	840	1,419
	t_0*	-0.226	-2.753	-0.745	-6.778	-1.174
	$t_{0.05,\,\nu}$	1.658	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	$\mathbf{H_2}$	Fail to Reject	$\mathbf{H_2}$	Fail to Reject
Eighth	# of Points	70	70	330	420	820
	Average A%Err $(\overline{X})$	1.7881	0.0479	0.7376	0.1785	0.3924
	Maximum A%Err	12.6483	0.3005	12.6483	0.8435	12.6483
	S^2	6.962E+00	4.256E-03	2.853E+00	2.741E-02	1.242E+00
	$\nu_{e,8}$	112	136	484	676	1,214
	t_0*	-0.359	-9.959	-0.929	-23.125	-1.738
	$t_{0.05,\,\nu}$	1.660	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_2	Fail to Reject	H_2	H_2

Table B.22. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.6-0.7.

Distribution	**Parameter**	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	**All T_rs**
Even	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	2.8971	0.0120	1.2822	0.0766	0.5498
	Maximum A%Err	24.0580	0.0900	24.0580	0.4888	24.0580
	S^2	15.621	0.000	5.981	0.008	2.729
Quarter	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	3.5297	0.0153	1.6414	0.0833	0.6962
	Maximum A%Err	38.9941	0.1191	38.9941	0.3807	38.9941
	S^2	3.574E+01	4.933E-04	1.364E+01	8.682E-03	6.002E+00
	$\nu_{e,4}$	98	124	454	862	1,167
	t_0*	-0.138	-47.412	-0.439	-11.593	-0.642
	$t_{0.05,\,\nu}$	1.663	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	$\mathbf{H_2}$	Fail to Reject	$\mathbf{H_2}$	Fail to Reject
Eighth	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	3.6794	0.0216	1.6774	0.1054	0.7225
	Maximum A%Err	30.8001	0.1982	30.8001	0.6119	30.8001
	S^2	2.609E+01	1.299E-03	1.172E+01	1.292E-02	5.256E+00
	$\nu_{e,8}$	117	80	493	736	1,256
	t_0*	-0.218	-60.847	-0.547	-38.968	-0.843
	$t_{0.05,\,\nu}$	1.659	1.667	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_2	Fail to Reject	H_2	Fail to Reject

Table B.23. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.55-0.6.

Distribution	Parameter	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	All T_rs
Even	# of Points	70	70	260	490	820
	Average A%Err $(\overline{X})$	8.2574	0.4720	4.2442	1.1908	2.0976
	Maximum A%Err	86.3022	2.2386	86.3022	5.8021	86.3022
	S^2	174.384	0.322	76.674	1.390	27.285
Quarter	# of Points	70	70	260	490	820
	Average A%Err $(\overline{X})$	6.8585	0.3358	3.4382	0.8648	1.6356
	Maximum A%Err	86.2463	2.0037	86.2463	4.6103	86.2463
	S^2	1.657E+02	1.706E-01	6.467E+01	8.090E-01	2.248E+01
	$\nu_{e,4}$	140	106	506	787	1,582
	t_0^*	0.049	3.126	0.130	4.486	0.374
	$t_{0.05,\ \nu}$	1.658	1.661	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_1	Fail to Reject	H_1	Fail to Reject
Eighth	# of Points	70	70	260	490	820
	Average A%Err $(\overline{X})$	10.0678	0.6315	4.7446	1.4480	2.4236
	Maximum A%Err	171.2308	3.6131	171.2308	6.8334	171.2308
	S^2	4.560E+02	6.826E-01	1.522E+02	1.962E+00	5.191E+01
	$\nu_{e,8}$	89	99	384	883	1,241
	t_0^*	-0.031	-1.768	-0.047	-2.368	-0.159
	$t_{0.05,\ \nu}$	1.665	1.663	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_2	Fail to Reject	H_2	Fail to Reject

Table B.24. t^* for $F_{w,j}$ *[WA]* Function Comparing Point Distributions. T_r Interval = 0.6-0.65.

Distribution	Parameter	$T_{r,f}$	$T_{r,b}$	$T_r \leq 0.6$	$T_r > 0.6$	All T_rs
Even	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	16.7836	0.1595	7.6815	0.8842	3.5212
	Maximum A%Err	203.8609	1.4585	203.8609	4.2269	203.8609
	S^2	772.515	0.082	342.749	0.904	147.796
Quarter	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	18.7755	0.1643	8.3869	0.8385	3.7781
	Maximum A%Err	140.9213	1.2748	140.9213	4.0082	140.9213
	S^2	8.305E+02	6.994E-02	3.442E+02	7.202E-01	1.509E+02
	$\nu_{e,4}$	143	141	664	823	1,671
	t_0*	-0.015	-0.378	-0.026	0.822	-0.035
	$t_{0.05,\nu}$	1.658	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	Fail to Reject	Fail to Reject	Fail to Reject	Fail to Reject
Eighth	# of Points	72	72	332	432	836
	Average A%Err $(\overline{X})$	24.1425	0.2167	9.7575	1.0588	4.4408
	Maximum A%Err	442.5445	1.9801	442.5445	5.3609	442.5445
	S^2	3.118E+03	1.279E-01	8.480E+02	1.123E+00	3.554E+02
	$\nu_{e,8}$	80	122	437	826	1,116
	t_0*	-0.019	-3.197	-0.041	-2.516	-0.069
	$t_{0.05,\nu}$	1.667	1.658	1.658	1.658	1.658
	S-S Test Result	Fail to Reject	H_2	Fail to Reject	H_2	Fail to Reject

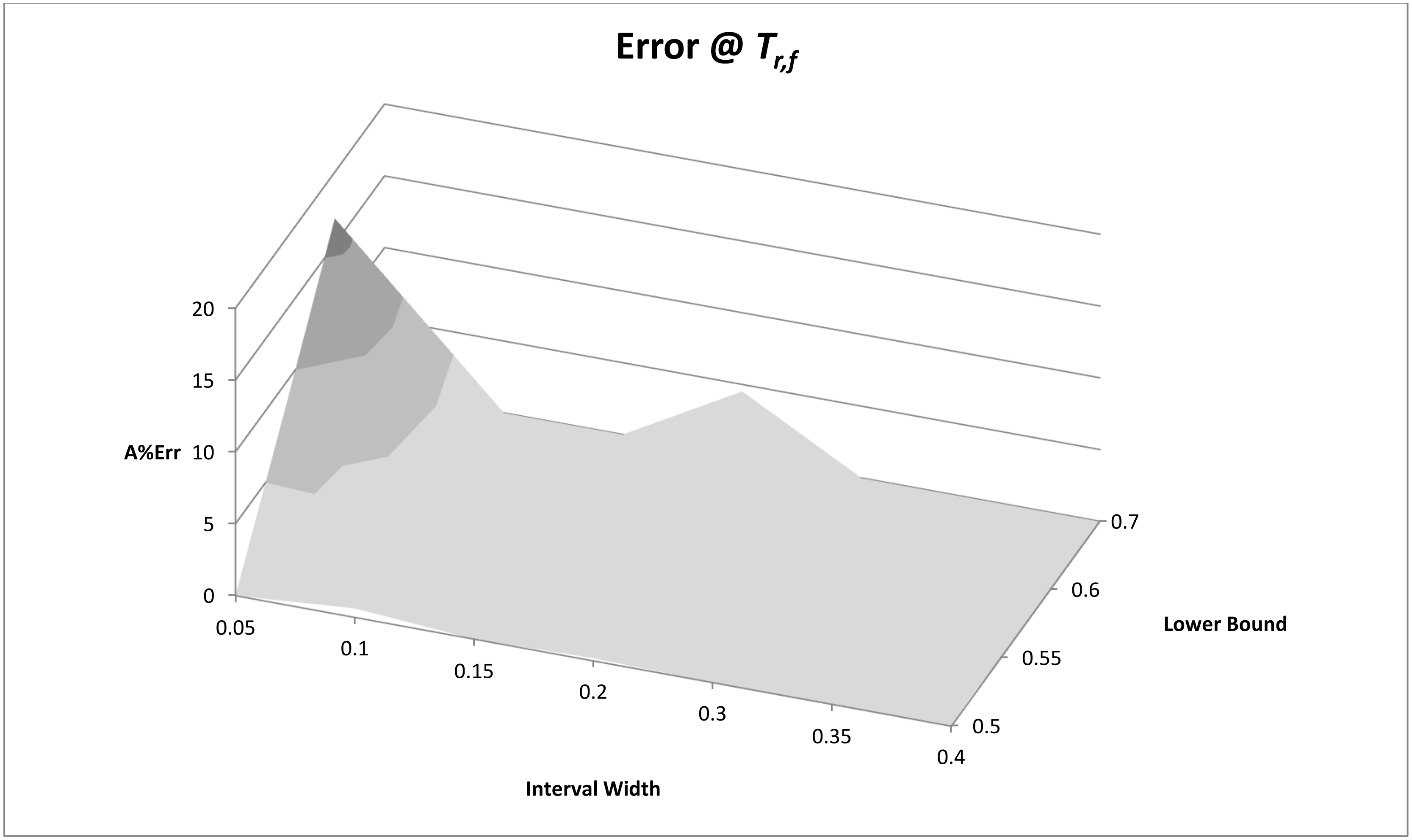

Figure B.1. A%Err at $T_{r,f}$ vs. Interval Width and Lower Bound.

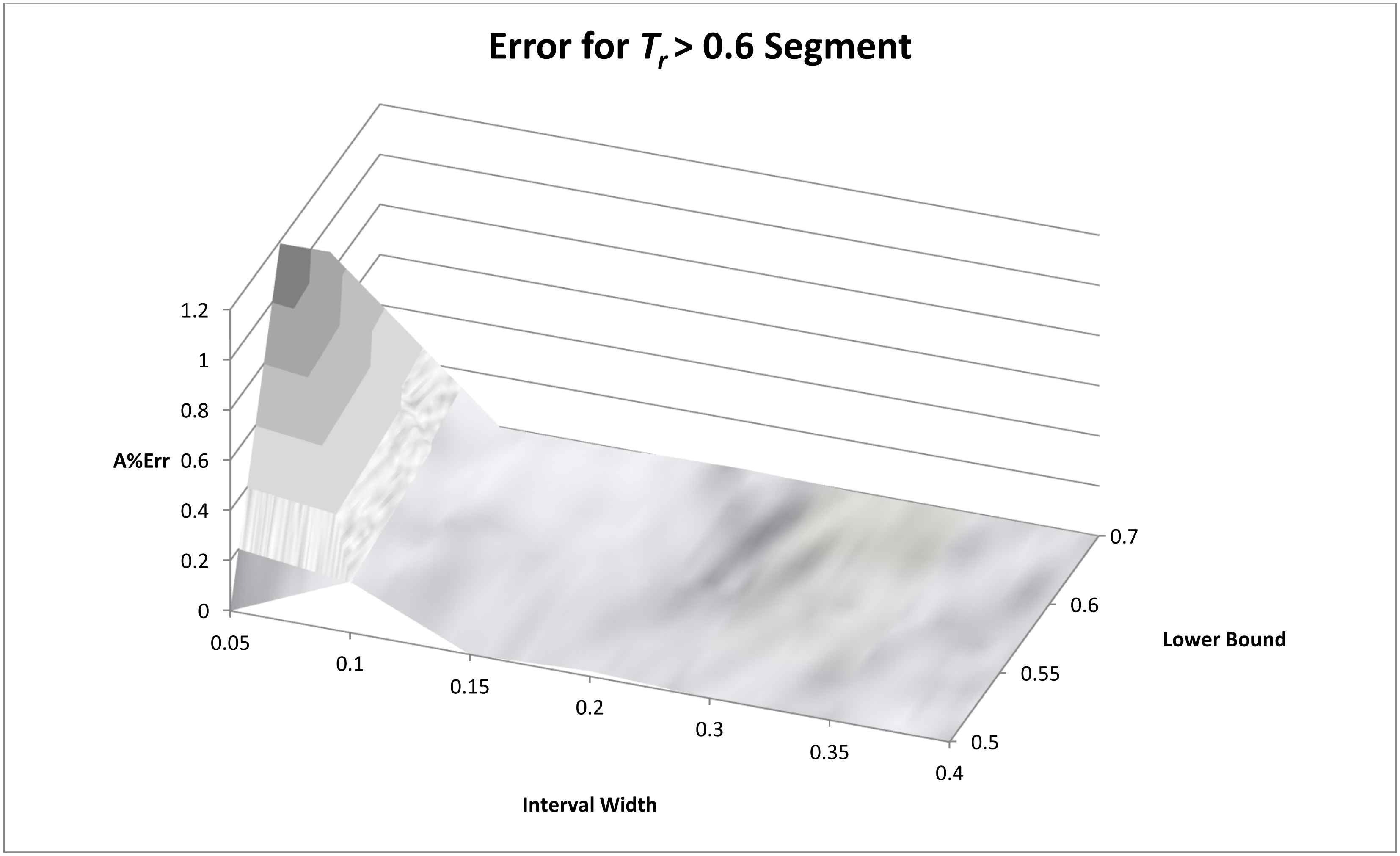

Figure B.2. A%Err for T_r > 0.6 Segment vs. Interval Width and Lower Bound.

Appendix C: Ancillary Data for Chapter 2

Table C.1. Reduced Temperatures and Pressures Used for $F_{w,j}$ *[AA]*.

Species	$T_{r,1}$	$T_{r,2}$	$T_{r,3}$	$T_{r,4}$	$Ln\ P_{v,r,T_{r1}}$	$Ln\ P_{v,r,T_{r2}}$	$Ln\ P_{v,r,T_{r3}}$	$Ln\ P_{v,r,T_{r4}}$
2-Methyl propanoic acid ($C_4H_8O_2$)	0.55207	0.61780	0.68354	0.74927	-7.5425	-5.4949	-4.0247	-2.9177
3-Methyl butanoic acid ($C_5H_{10}O_2$)	0.55644	0.62267	0.68889	0.75512	-7.4612	-5.5012	-4.0085	-2.8333
Acetic Acid ($C_2H_4O_2$)	0.50207	0.56809	0.63410	0.70012	-7.9699	-6.0181	-4.5329	-3.3648
Butanoic acid ($C_4H_8O_2$)	0.54920	0.61192	0.67465	0.73737	-7.6083	-5.6788	-4.1886	-3.0031
Pentanoic acid ($C_5H_{10}O_2$)	0.56143	0.62560	0.68976	0.75393	-7.4851	-5.5012	-4.0254	-2.8847
Propanoic acid ($C_3H_6O_2$)	0.53265	0.59650	0.66034	0.72419	-7.7255	-5.7904	-4.3015	-3.1203
1-Butanol ($C_4H_{10}O$)	0.55089	0.61073	0.67057	0.73041	-7.7015	-5.7586	-4.2715	-3.0965
1-Decanol ($C_{10}H_{22}O$)	0.57300	0.64031	0.70761	0.77492	-7.0956	-5.0743	-3.6053	-2.4891
1-Heptanol ($C_7H_{16}O$)	0.56142	0.62463	0.68783	0.75104	-7.3594	-5.3563	-3.8824	-2.7520
1-Hexanol ($C_6H_{14}O$)	0.55805	0.61974	0.68144	0.74313	-7.4503	-5.4701	-3.9949	-2.8536
1-Nonanol ($C_9H_{20}O$)	0.56902	0.63528	0.70154	0.76780	-7.2164	-5.1756	-3.6970	-2.5763
1-Octanol ($C_8H_{18}O$)	0.56521	0.62976	0.69430	0.75885	-7.2628	-5.2494	-3.7802	-2.6603
1-Pentanol ($C_5H_{12}O$)	0.55430	0.61496	0.67563	0.73629	-7.5780	-5.6131	-4.1308	-2.9727
2-Octanol ($C_8H_{18}O$)	0.55486	0.62107	0.68727	0.75348	-7.2804	-5.2153	-3.7562	-2.6707
Ethanol (C_2H_6O)	0.53802	0.59837	0.65871	0.71906	-8.0279	-6.1342	-4.6368	-3.4229
Isopropyl alcohol (C_3H_8O)	0.55337	0.61382	0.67427	0.73472	-7.7756	-5.8757	-4.3791	-3.1700
Methanol (CH_4O)	0.51223	0.57297	0.63370	0.69444	-8.3054	-6.4027	-4.9073	-3.7003
Propanol (C_3H_8O)	0.54620	0.60590	0.66559	0.72529	-7.8573	-5.9404	-4.4476	-3.2520
Tert-butanol ($C_4H_{10}O$)	0.55907	0.61906	0.67905	0.73904	-7.6250	-5.6487	-4.1560	-2.9891
Acetone (C_3H_6O)	0.48687	0.55462	0.62237	0.69012	-7.7624	-5.7812	-4.3026	-3.1576
Methyl isobutyl ketone ($C_6H_{12}O$)	0.51062	0.58165	0.65269	0.72372	-7.3970	-5.3744	-3.9071	-2.7943
Benzene (C_6H_6)	0.49744	0.55520	0.61297	0.67073	-6.8850	-5.3446	-4.1500	-3.1971
Ethylbenzene (C_8H_{10})	0.49631	0.56669	0.63706	0.70744	-7.4956	-5.4987	-4.0242	-2.8903
Naphthalene ($C_{10}H_8$)	0.49230	0.56132	0.63034	0.69936	-7.6132	-5.6239	-4.1474	-3.0086
Toluene (C_7H_8)	0.48401	0.55339	0.62276	0.69214	-7.6270	-5.6284	-4.1544	-3.0220
m-Xylene (C_8H_{10})	0.50002	0.57080	0.64158	0.71236	-7.4783	-5.4891	-4.0122	-2.8729
o-Xylene (C_8H_{10})	0.49617	0.56627	0.63636	0.70646	-7.5322	-5.5384	-4.0631	-2.9271
p-Xylene (C_8H_{10})	0.49951	0.57041	0.64130	0.71220	-7.4719	-5.4790	-4.0033	-2.8667
Butane (C_4H_{10})	0.47149	0.54324	0.61498	0.68673	-7.5494	-5.5373	-4.0656	-2.9425
Diethyl ether ($C_4H_{10}O$)	0.49216	0.56258	0.63299	0.70341	-7.5096	-5.5169	-4.0414	-2.9043
Decane ($C_{10}H_{22}$)	0.54809	0.62236	0.69664	0.77091	-6.9591	-4.9625	-3.4875	-2.3538
Dodecane ($C_{12}H_{26}$)	0.56670	0.64135	0.71599	0.79064	-6.8131	-4.8221	-3.3462	-2.2081

Species	$T_{r,1}$	$T_{r,2}$	$T_{r,3}$	$T_{r,4}$	$Ln\ P_{v,r,T_{r1}}$	$Ln\ P_{v,r,T_{r2}}$	$Ln\ P_{v,r,T_{r3}}$	$Ln\ P_{v,r,T_{r4}}$
Eicosane ($C_{20}H_{42}$)	0.62562	0.69970	0.77377	0.84785	-6.3667	-4.3916	-2.9125	-1.7629
Ethane (C_2H_6)	0.43821	0.50847	0.57874	0.64900	-7.8067	-5.7935	-4.3187	-3.1927
Heptadecane ($C_{17}H_{36}$)	0.60340	0.67891	0.75442	0.82993	-6.5259	-4.5371	-3.0611	-1.9222
n-Heptane (C_7H_{16})	0.51413	0.58746	0.66078	0.73411	-7.2209	-5.2192	-3.7461	-2.6161
Hexadecane ($C_{16}H_{34}$)	0.59760	0.67255	0.74749	0.82244	-6.5759	-4.5883	-3.1117	-1.9714
n-Hexane (C_6H_{14})	0.50057	0.57343	0.64628	0.71914	-7.3246	-5.3208	-3.8481	-2.7198
Methane (CH_4)	0.48617	0.53506	0.58396	0.63285	-5.7254	-4.6933	-3.8456	-3.1355
Nonadecane ($C_{19}H_{40}$)	0.61544	0.69130	0.76715	0.84301	-6.4239	-4.4331	-2.9561	-1.8163
Nonane (C_9H_{20})	0.53718	0.61118	0.68519	0.75919	-7.0433	-5.0472	-3.5721	-2.4380
Octadecane ($C_{18}H_{38}$)	0.60992	0.68588	0.76184	0.83780	-6.4766	-4.4856	-3.0095	-1.8710
Octane (C_8H_{18})	0.52627	0.59998	0.67368	0.74739	-7.1266	-5.1282	-3.6543	-2.5219
Pentadecane ($C_{15}H_{32}$)	0.59011	0.66502	0.73992	0.81483	-6.6334	-4.6444	-3.1672	-2.0267
n-Pentane (C_5H_{12})	0.48682	0.55922	0.63162	0.70402	-7.4312	-5.4249	-3.9521	-2.8257
Propane (C_3H_8)	0.45670	0.52778	0.59885	0.66993	-7.6688	-5.6529	-4.1800	-3.0561
R152a ($C_2H_4F_2$)	0.48586	0.55327	0.62069	0.68810	-7.7225	-5.6904	-4.2246	-3.1173
n-Tetradecane ($C_{14}H_{30}$)	0.58253	0.65730	0.73208	0.80685	-6.6907	-4.7013	-3.2249	-2.0857
Tridecane ($C_{13}H_{28}$)	0.57522	0.64985	0.72447	0.79910	-6.7513	-4.7610	-3.2849	-2.1460
Undecane ($C_{11}H_{24}$)	0.55764	0.63212	0.70661	0.78109	-6.8849	-4.8905	-3.4144	-2.2782
Argon (Ar)	0.54808	0.57389	0.59971	0.62552	-4.3953	-3.9551	-3.5554	-3.1909
Nitrogen (N_2)	0.48185	0.54218	0.60251	0.66284	-6.0523	-4.7154	-3.6704	-2.8330
Ammonia (NH_3)	0.47603	0.52640	0.57678	0.62715	-7.7280	-6.2198	-5.0188	-4.0390
Water (H_2O)	0.42219	0.52521	0.62824	0.73126	-10.4955	-6.7058	-4.3055	-2.6492
Hydrogen (H_2 normal)	0.40211	0.49874	0.59538	0.69201	-5.5595	-3.9178	-2.7445	-1.8691

Table C.2. η_{ai} Used for $F_{w,j}$ [AA].

Species	η_{a1}	η_{a2}	η_{a3}	η_{a4}
2-Methyl propanoic acid ($C_4H_8O_2$)	-43.7551361	206.6100610	-333.1570168	188.0425857
3-Methyl butanoic acid ($C_5H_{10}O_2$)	-41.2779066	196.3292783	-319.2306861	182.2401171
Acetic Acid ($C_2H_4O_2$)	-55.2288971	253.8836907	-394.6306672	211.2095908
Butanoic acid ($C_4H_8O_2$)	-54.4361062	250.6960182	-392.9856383	213.9661672
Pentanoic acid ($C_5H_{10}O_2$)	-46.0452398	216.2896487	-347.0205029	194.8931914
Propanoic acid ($C_3H_6O_2$)	-55.0407775	253.1167318	-395.1851559	213.5868928
1-Butanol ($C_4H_{10}O$)	-65.8096820	296.8901603	-454.8993375	240.8477618
1-Decanol ($C_{10}H_{22}O$)	-34.6387618	168.3878975	-281.2988456	166.8305738
1-Heptanol ($C_7H_{16}O$)	-49.1699316	229.2376755	-364.7062933	202.6403638
1-Hexanol ($C_6H_{14}O$)	-55.6390848	255.7076467	-400.3514322	217.9111426
1-Nonanol ($C_9H_{20}O$)	-38.1418880	183.2163971	-301.8315679	175.6238792
1-Octanol ($C_8H_{18}O$)	-43.8668703	207.2576455	-334.8727581	189.8807876
1-Pentanol ($C_5H_{12}O$)	-61.0133374	277.5235174	-429.3586999	230.1509560
2-Octanol ($C_8H_{18}O$)	-41.7180732	198.1621145	-321.6658670	183.1843236
Ethanol (C_2H_6O)	-67.8609643	305.0512090	-464.8035132	244.0231311
Isopropyl alcohol (C_3H_8O)	-62.2374197	282.5044062	-435.9291242	232.8902275
Methanol (CH_4O)	-74.5043377	331.5197420	-498.0915023	256.3157225
Propanol (C_3H_8O)	-68.1132204	306.1377454	-466.8075921	245.5483973
Tert-butanol ($C_4H_{10}O$)	-62.3080671	282.8629533	-436.8295614	233.7724511
Acetone (C_3H_6O)	-52.8800081	244.3480389	-381.1956243	204.4582933
Methyl isobutyl ketone ($C_6H_{12}O$)	-38.8561607	185.9500901	-302.5096897	171.4933880
Benzene (C_6H_6)	-96.8433868	419.4501467	-611.4554937	303.2519138
Ethylbenzene (C_8H_{10})	-43.2452649	204.4615513	-327.3964901	181.5306899
Naphthalene ($C_{10}H_8$)	-47.8092497	223.4261977	-353.1169337	192.5605464
Toluene (C_7H_8)	-48.4493575	226.1676319	-356.5181802	193.5411799
m-Xylene (C_8H_{10})	-41.4947692	197.0979073	-317.4448206	177.3950665
o-Xylene (C_8H_{10})	-44.0151324	207.6736925	-331.7883071	183.4498450
p-Xylene (C_8H_{10})	-41.2977115	196.2967721	-316.3126483	176.8540497
Butane (C_4H_{10})	-44.2498945	208.8794685	-332.5870960	182.3778918
Diethyl ether ($C_4H_{10}O$)	-43.9417813	207.3936818	-331.2515804	182.9707966
Decane ($C_{10}H_{22}$)	-25.8344700	130.0558113	-225.3052376	139.6400275
Dodecane ($C_{12}H_{26}$)	-22.3040115	114.5426942	-203.5971806	131.2718808

Species	η_{a1}	η_{a2}	η_{a3}	η_{a4}
Eicosane ($C_{20}H_{42}$)	-14.1663281	77.7489333	-151.0746987	113.0040012
Ethane (C_2H_6)	-54.3550146	251.1898867	-389.0645219	205.3487638
Heptadecane ($C_{17}H_{36}$)	-15.7840024	85.1156270	-161.3048481	115.2994812
n-Heptane (C_7H_{16})	-33.2031993	161.9733356	-269.2078923	156.9181716
Hexadecane ($C_{16}H_{34}$)	-17.2428328	91.8330547	-171.2667713	119.2937946
n-Hexane (C_6H_{14})	-36.5164411	176.1316868	-288.4597597	164.6121317
Methane (CH_4)	-191.3521089	778.2261146	-1060.5612891	487.0997662
Nonadecane ($C_{19}H_{40}$)	-13.7915718	75.8732198	-147.5794557	110.2466254
Nonane (C_9H_{20})	-28.0699964	139.7969961	-238.7996495	144.9107761
Octadecane ($C_{18}H_{38}$)	-14.4254910	78.8101263	-151.8860363	111.6399482
Octane (C_8H_{18})	-30.4163609	149.9860370	-252.8070973	150.4085381
Pentadecane ($C_{15}H_{32}$)	-18.3916023	97.0415673	-178.7571363	122.0078251
n-Pentane (C_5H_{12})	-39.9442495	190.6742176	-308.1096817	172.4863085
Propane (C_3H_8)	-48.6753475	227.4730155	-357.4669433	192.4807084
R152a ($C_2H_4F_2$)	-54.2135464	249.7886650	-388.4862644	207.5743782
n-Tetradecane ($C_{14}H_{30}$)	-19.6968022	102.8994759	-187.1658266	125.1681196
Tridecane ($C_{13}H_{28}$)	-21.0093835	108.7959610	-195.5474255	128.3337329
Undecane ($C_{11}H_{24}$)	-23.9731138	121.8891673	-213.9169329	135.2317548
Argon (Ar)	-1500.4616761	5315.2083609	-6293.8103946	2493.2638988
Nitrogen (N_2)	-86.4365400	378.9073018	-558.3908882	279.9125279
Ammonia (NH_3)	-176.7925675	724.1660375	-993.4510482	459.2409718
Water (H_2O)	-10.5467093	60.5997678	-118.0202957	82.9663512
Hydrogen (H_2 normal)	-15.4816555	84.4695459	-154.5693731	99.2399808

Table C.3. η_{bi} Used for $F_{w,j}$ [AA].

Species	η_{b1}	η_{b2}	η_{b3}	η_{b4}
2-Methyl propanoic acid ($C_4H_8O_2$)	135.5677399	-628.5214202	983.4403390	-527.3476332
3-Methyl butanoic acid ($C_5H_{10}O_2$)	129.0992911	-602.7812415	950.4856718	-514.6021115
Acetic Acid ($C_2H_4O_2$)	158.4794110	-716.0348985	1083.6392688	-555.8464141
Butanoic acid ($C_4H_8O_2$)	165.9502973	-750.7780572	1144.0901428	-594.6878267
Pentanoic acid ($C_5H_{10}O_2$)	144.0668661	-664.4587552	1034.5856035	-552.1733462
Propanoic acid ($C_3H_6O_2$)	164.1048438	-741.5023811	1126.0924991	-581.9303352
1-Butanol ($C_4H_{10}O$)	199.0531420	-882.5623240	1316.4092178	-667.7314627
1-Decanol ($C_{10}H_{22}O$)	112.0904584	-534.6558789	864.4205060	-483.2946794
1-Heptanol ($C_7H_{16}O$)	153.2595229	-701.6673199	1083.9155254	-573.1538306
1-Hexanol ($C_6H_{14}O$)	171.4384690	-773.9814453	1177.8788517	-611.8953911
1-Nonanol ($C_9H_{20}O$)	121.9842880	-575.0665448	917.7383800	-504.8544922
1-Octanol ($C_8H_{18}O$)	138.3650311	-641.7890146	1005.8120867	-541.2003856
1-Pentanol ($C_5H_{12}O$)	186.1224239	-831.8528937	1251.9821512	-641.8688749
2-Octanol ($C_8H_{18}O$)	130.1120720	-606.7339615	955.2322491	-516.1193521
Ethanol (C_2H_6O)	201.5247944	-890.5198122	1321.7038239	-665.7698032
Isopropyl alcohol (C_3H_8O)	189.4210973	-844.8896033	1268.5312049	-648.4657566
Methanol (CH_4O)	213.2542105	-933.2870668	1367.8128153	-677.5799947
Propanol (C_3H_8O)	204.3919427	-902.9810341	1340.9102393	-676.3969538
Tert-butanol ($C_4H_{10}O$)	191.0800265	-852.3563795	1280.5461492	-655.4589150
Acetone (C_3H_6O)	149.3421369	-678.2853597	1030.3881825	-529.8364853
Methyl isobutyl ketone ($C_6H_{12}O$)	114.8584819	-539.7433674	852.3681550	-459.5546380
Benzene (C_6H_6)	269.1248390	-1147.4720898	1635.2754394	-784.4759357
Ethylbenzene (C_8H_{10})	124.8432888	-579.8180257	902.4345896	-477.5228144
Naphthalene ($C_{10}H_8$)	136.6116127	-627.3176533	964.5416832	-503.1138445
Toluene (C_7H_8)	136.9877069	-628.4229075	964.0652767	-501.0437060
m-Xylene (C_8H_{10})	120.6083577	-562.6804542	880.4770289	-469.0231775
o-Xylene (C_8H_{10})	126.9214536	-588.2839597	913.6704599	-482.2890134
p-Xylene (C_8H_{10})	119.9924453	-560.1877555	876.9987619	-467.3855586
Butane (C_4H_{10})	123.8870994	-574.6367584	890.1702635	-466.9663089
Diethyl ether ($C_4H_{10}O$)	126.1097902	-584.7285636	908.0045172	-478.9586495
Decane ($C_{10}H_{22}$)	82.3026569	-406.4034250	680.2681454	-395.3664004
Dodecane ($C_{12}H_{26}$)	73.7089604	-371.1740489	636.2512487	-382.0783049

Species	η_{b1}	η_{b2}	η_{b3}	η_{b4}
Eicosane ($C_{20}H_{42}$)	53.2955791	-286.6843612	533.9178880	-361.9651804
Ethane (C_2H_6)	145.0943374	-659.4510025	996.2216175	-506.0220128
Heptadecane ($C_{17}H_{36}$)	56.6884840	-299.6253279	545.2026761	-356.3697398
n-Heptane (C_7H_{16})	99.5049880	-476.4675875	767.6713355	-423.8983327
Hexadecane ($C_{16}H_{34}$)	60.9080550	-317.9655606	569.9400777	-364.6892766
n-Hexane (C_6H_{14})	106.9857933	-506.6879684	805.4004043	-436.8976569
Methane (CH_4)	511.2278557	-2051.0350293	2744.5945168	-1229.7502388
Nonadecane ($C_{19}H_{40}$)	51.1190785	-275.6343386	513.9324749	-348.2300303
Nonane (C_9H_{20})	87.6183368	-428.1117610	707.3669734	-403.9587727
Octadecane ($C_{18}H_{38}$)	52.7700261	-282.5640609	522.3307764	-349.3101088
Octane (C_8H_{18})	93.0960832	-450.4854702	735.2367089	-413.0018153
Pentadecane ($C_{15}H_{32}$)	63.8768797	-330.3889096	585.4275062	-368.4206559
n-Pentane (C_5H_{12})	114.5046670	-536.8732768	842.9566657	-449.9766265
Propane (C_3H_8)	133.3359645	-612.5245202	937.5686397	-484.3225180
R152a ($C_2H_4F_2$)	152.7324867	-691.7386181	1047.8191646	-537.0244836
n-Tetradecane ($C_{14}H_{30}$)	67.2601672	-344.4749060	603.2437910	-373.3314018
Tridecane ($C_{13}H_{28}$)	70.6140831	-358.5209586	620.9268045	-378.3474007
Undecane ($C_{11}H_{24}$)	77.8009714	-387.9393852	657.2035590	-388.2833154
Argon (Ar)	4071.9072605	-14298.0543652	16755.8633202	-6556.7905446
Nitrogen (N_2)	237.0934074	-1022.9861838	1473.3051793	-713.8627244
Ammonia (NH_3)	468.3694846	-1892.3453543	2548.5371571	-1148.8786223
Water (H_2O)	30.5601862	-172.1478089	322.8457263	-210.1930026
Hydrogen (H_2 normal)	42.6560354	-228.3139125	403.9480730	-243.7390005

Table C.4. η_{ci} Used for $F_{w,j}$ *[AA]*.

Species	η_{c1}	η_{c2}	η_{c3}	η_{c4}
2-Methyl propanoic acid ($C_4H_8O_2$)	-204.3006995	906.1448033	-1325.1664436	653.5348868
3-Methyl butanoic acid ($C_5H_{10}O_2$)	-198.1200042	884.4303256	-1301.1947369	646.3574144
Acetic Acid ($C_2H_4O_2$)	-205.4584549	891.1917030	-1272.1316007	607.6525934
Butanoic acid ($C_4H_8O_2$)	-242.5188683	1051.5918988	-1505.2773435	724.5580678
Pentanoic acid ($C_5H_{10}O_2$)	-221.4249621	977.0968581	-1422.3813237	698.4708091
Propanoic acid ($C_3H_6O_2$)	-229.5096833	994.5628259	-1421.0727210	681.5336675
1-Butanol ($C_4H_{10}O$)	-286.6902731	1220.1204186	-1715.8533640	810.0411710
1-Decanol ($C_{10}H_{22}O$)	-183.7455272	836.3715096	-1254.2262643	638.1595537
1-Heptanol ($C_7H_{16}O$)	-233.8862006	1025.0477117	-1482.6032281	722.7648571
1-Hexanol ($C_6H_{14}O$)	-255.9231635	1107.2633656	-1582.3937580	760.9316267
1-Nonanol ($C_9H_{20}O$)	-195.5271009	880.3946699	-1306.8304929	656.7738108
1-Octanol ($C_8H_{18}O$)	-216.0170796	958.1650130	-1401.8834968	692.6390619
1-Pentanol ($C_5H_{12}O$)	-272.5181035	1168.2641702	-1654.8086105	787.7009588
2-Octanol ($C_8H_{18}O$)	-198.5900181	885.5153807	-1301.2813266	645.4353470
Ethanol (C_2H_6O)	-279.9216856	1188.1102602	-1665.2338364	782.3833326
Isopropyl alcohol (C_3H_8O)	-276.1180133	1181.5351863	-1670.3704272	793.3121558
Methanol (CH_4O)	-275.4645869	1159.8090612	-1611.0132684	748.0165534
Propanol (C_3H_8O)	-289.8332328	1229.6015855	-1723.3376249	810.2095398
Tert-butanol ($C_4H_{10}O$)	-282.7553518	1209.8162533	-1710.6704287	813.0189996
Acetone (C_3H_6O)	-187.5623608	817.9448833	-1172.3741719	561.6424291
Methyl isobutyl ketone ($C_6H_{12}O$)	-157.6119679	708.8321229	-1047.3586603	520.1101094
Benzene (C_6H_6)	-328.1446287	1349.5550629	-1832.6737974	830.0349306
Ethylbenzene (C_8H_{10})	-163.5881083	728.0834590	-1064.0655007	521.1336618
Naphthalene ($C_{10}H_8$)	-175.5098678	773.0646622	-1118.7971487	541.9015174
Toluene (C_7H_8)	-172.3676116	758.7591432	-1096.6483115	529.9184914
m-Xylene (C_8H_{10})	-160.1436727	715.6502965	-1050.2657552	516.9764771
o-Xylene (C_8H_{10})	-165.9539750	737.2361629	-1075.5687472	525.7565478
p-Xylene (C_8H_{10})	-159.2083336	711.9370776	-1045.2654894	514.7097245
Butane (C_4H_{10})	-152.8032844	679.8837466	-991.4516482	483.0345016
Diethyl ether ($C_4H_{10}O$)	-163.3500556	726.0097199	-1059.3396540	517.6683318
Decane ($C_{10}H_{22}$)	-130.4949908	614.0264417	-948.4865201	498.1744566
Dodecane ($C_{12}H_{26}$)	-125.4175388	600.8493500	-944.4982398	508.1029902

Species	η_{c1}	η_{c2}	η_{c3}	η_{c4}
Eicosane ($C_{20}H_{42}$)	-116.0998396	591.5731222	-986.7716296	580.0275134
Ethane (C_2H_6)	-162.9933369	712.5957882	-1019.9374418	485.3779493
Heptadecane ($C_{17}H_{36}$)	-113.0167624	566.4745924	-930.1039838	532.5875487
n-Heptane (C_7H_{16})	-140.1497623	641.3830294	-963.0907157	487.1819866
Hexadecane ($C_{16}H_{34}$)	-117.7066587	583.1129556	-946.8475939	533.6365564
n-Hexane (C_6H_{14})	-144.1944176	653.4535375	-971.3842276	485.0142071
Methane (CH_4)	-577.4149601	2247.2124421	-2894.9883780	1241.1817434
Nonadecane ($C_{19}H_{40}$)	-108.1316320	552.3379321	-922.9704548	542.7049694
Nonane (C_9H_{20})	-133.5516628	622.4071891	-952.2545073	493.7513482
Octadecane ($C_{18}H_{38}$)	-108.8854122	552.5393084	-917.7231788	534.4826390
Octane (C_8H_{18})	-136.6038409	631.0828706	-956.7586821	490.0977962
Pentadecane ($C_{15}H_{32}$)	-119.5347155	587.0602081	-945.3632242	526.3411684
n-Pentane (C_5H_{12})	-147.9007040	664.3197481	-978.5650202	482.8996708
Propane (C_3H_8)	-157.5794928	695.2785992	-1004.8793950	484.0940233
R152a ($C_2H_4F_2$)	-190.9112990	830.4129164	-1187.4940784	567.4412521
n-Tetradecane ($C_{14}H_{30}$)	-121.8631294	593.0123185	-946.8040582	520.7198950
Tridecane ($C_{13}H_{28}$)	-124.1206929	599.1462408	-948.8701939	515.9051680
Undecane ($C_{11}H_{24}$)	-127.8425605	606.9372719	-945.8661056	502.8172997
Argon (Ar)	-4756.9650803	16394.1564323	-18812.9119496	7194.1120416
Nitrogen (N_2)	-281.5914378	1171.4566411	-1606.3482575	734.0188033
Ammonia (NH_3)	-520.1260564	2037.9435947	-2641.0128279	1138.5003484
Water (H_2O)	-39.8814624	213.4874884	-365.2870868	211.5552754
Hydrogen (H_2 normal)	-50.6325450	258.3940871	-422.7697585	231.1996735

Table C.5. η_{di} Used for $F_{w,j}$ *[AA]*.

Species	η_{d1}	η_{d2}	η_{d3}	η_{d4}
2-Methyl propanoic acid ($C_4H_8O_2$)	385.0881862	-1431.0055043	1794.3288608	-770.6493594
3-Methyl butanoic acid ($C_5H_{10}O_2$)	389.5488673	-1450.4913088	1823.7023097	-786.7850573
Acetic Acid ($C_2H_4O_2$)	270.0028672	-1004.5144252	1251.7372885	-528.4755852
Butanoic acid ($C_4H_8O_2$)	427.0580858	-1571.5141759	1947.6151408	-822.9877249
Pentanoic acid ($C_5H_{10}O_2$)	438.6573472	-1622.9738162	2026.9292207	-867.2075401
Propanoic acid ($C_3H_6O_2$)	363.0726385	-1340.7407688	1663.9449471	-702.3940014
1-Butanol ($C_4H_{10}O$)	489.7855678	-1786.0056445	2190.7599238	-913.5171588
1-Decanol ($C_{10}H_{22}O$)	421.2611415	-1575.7375698	1997.3806015	-874.8217311
1-Heptanol ($C_7H_{16}O$)	456.3814597	-1683.3291462	2094.7105308	-891.7713629
1-Hexanol ($C_6H_{14}O$)	475.0284304	-1742.8638317	2155.2219337	-909.3890597
1-Nonanol ($C_9H_{20}O$)	426.1347834	-1587.9213421	2002.6268881	-869.9953100
1-Octanol ($C_8H_{18}O$)	443.8468618	-1644.5561936	2058.5528997	-884.1416932
1-Pentanol ($C_5H_{12}O$)	483.7343616	-1768.6311813	2177.2930891	-912.7175312
2-Octanol ($C_8H_{18}O$)	385.4747234	-1435.1201243	1803.6335601	-777.4398755
Ethanol (C_2H_6O)	437.9186754	-1599.1899693	1961.4022472	-816.1626038
Isopropyl alcohol (C_3H_8O)	485.0902204	-1772.5200871	2179.9721696	-912.4910996
Methanol (CH_4O)	361.3891683	-1321.5799831	1618.4477460	-669.7279774
Propanol (C_3H_8O)	477.0483895	-1738.7301897	2130.0575894	-886.0751741
Tert-butanol ($C_4H_{10}O$)	515.4012200	-1880.9343090	2311.6917415	-967.5906609
Acetone (C_3H_6O)	227.7992946	-852.8135189	1067.7814889	-452.3910973
Methyl isobutyl ketone ($C_6H_{12}O$)	235.5054807	-889.8152934	1129.6305019	-489.3579997
Benzene (C_6H_6)	375.5369002	-1360.7059036	1647.8385343	-671.6388652
Ethylbenzene (C_8H_{10})	219.1623363	-826.9865797	1045.6648099	-449.2988974
Naphthalene ($C_{10}H_8$)	224.7140142	-844.3828620	1062.2885805	-453.1972116
Toluene (C_7H_8)	209.8207198	-789.8347882	994.2234850	-423.8110103
m-Xylene (C_8H_{10})	221.3075445	-835.9114629	1058.8691571	-456.3938172
o-Xylene (C_8H_{10})	221.2835301	-834.2539948	1053.8131078	-452.2122216
p-Xylene (C_8H_{10})	219.5879869	-829.8307987	1051.5140253	-453.3497133
Butane (C_4H_{10})	176.7180511	-670.9826212	850.7986509	-365.1690033
Diethyl ether ($C_4H_{10}O$)	212.8608131	-803.4977486	1015.7067992	-435.9428435
Decane ($C_{10}H_{22}$)	272.4594108	-1040.3834008	1346.1503101	-604.2141717
Dodecane ($C_{12}H_{26}$)	308.2133676	-1179.8949487	1536.8417794	-700.4035932

Species	η_{d1}	η_{d2}	η_{d3}	η_{d4}
Eicosane ($C_{20}H_{42}$)	500.0115732	-1926.6243858	2567.0059879	-1241.8950202
Ethane (C_2H_6)	150.7468053	-571.9518483	721.2412211	-305.7281540
Heptadecane ($C_{17}H_{36}$)	397.4294800	-1532.2052456	2031.5999701	-965.7136953
n-Heptane (C_7H_{16})	221.9122847	-844.6871025	1081.6629047	-474.3985211
Hexadecane ($C_{16}H_{34}$)	386.6134354	-1486.5943509	1961.0981402	-921.8366433
n-Hexane (C_6H_{14})	205.8129089	-782.5902184	998.6172881	-434.6225076
Methane (CH_4)	552.5342398	-1946.7876934	2287.7748480	-900.1523944
Nonadecane ($C_{19}H_{40}$)	433.3901432	-1676.4294875	2239.6527647	-1084.6462357
Nonane (C_9H_{20})	254.4161177	-970.3070076	1250.9965325	-557.0053872
Octadecane ($C_{18}H_{38}$)	412.8359714	-1595.7012793	2126.7673877	-1023.1507359
Octane (C_8H_{18})	238.1043292	-907.3078475	1165.8617497	-515.2113732
Pentadecane ($C_{15}H_{32}$)	365.0438639	-1402.0330163	1843.4444055	-859.4123765
n-Pentane (C_5H_{12})	190.8666776	-725.2067070	922.6264450	-398.8777257
Propane (C_3H_8)	164.5831931	-624.5915081	789.7547499	-336.8879879
R152a ($C_2H_4F_2$)	229.3309707	-857.5916041	1072.4811135	-453.6593982
n-Tetradecane ($C_{14}H_{30}$)	345.8523170	-1326.2696643	1737.8382326	-803.5874769
Tridecane ($C_{13}H_{28}$)	328.7574048	-1259.4067970	1644.8583581	-754.7820976
Undecane ($C_{11}H_{24}$)	289.9143862	-1108.3301944	1438.8850134	-650.7951167
Argon (Ar)	5023.0946391	-16397.2574601	17863.6896998	-6498.4951277
Nitrogen (N_2)	301.4352864	-1102.4020900	1345.6988009	-552.5463600
Ammonia (NH_3)	476.8373032	-1689.2659176	1994.7721281	-788.4131266
Water (H_2O)	49.9165693	-210.9232238	296.5283900	-144.5198822
Hydrogen (H_2 normal)	51.4842004	-214.3213380	294.8141228	-138.1868047

Table C.6. Wagner Constants Estimated by $F_{w,j}$ *[AA]*, and Error Relative to Entire-Curve Constants.

	$F_{w,j}$ *[AA]*				A%Err			
Species	***a***	***b***	***c***	***d***	***a***	***b***	***c***	***d***
2-Methyl propanoic acid ($C_4H_8O_2$)	-13.073317	11.732531	-11.658407	-14.407229	53.22	798.32	123.16	600.02
3-Methyl butanoic acid ($C_5H_{10}O_2$)	-8.768628	0.784882	-2.700491	-8.171826	1.09	51.83	58.57	291.45
Acetic Acid ($C_2H_4O_2$)	-9.585332	4.388138	-3.981562	-2.412895	15.57	348.10	1731.02	57.84
Butanoic acid ($C_4H_8O_2$)	-5.988473	-5.310175	2.460578	-11.137674	28.96	495.30	145.79	305.84
Pentanoic acid ($C_5H_{10}O_2$)	-10.511448	5.199168	-7.042215	-12.657846	19.90	235.45	13.59	200.00
Propanoic acid ($C_3H_6O_2$)	-6.995831	-2.286243	0.315278	-7.271508	14.15	387.25	109.90	90.68
1-Butanol ($C_4H_{10}O$)	-5.520985	-6.095874	2.734854	-16.316578	34.32	373.35	133.16	2194.88
1-Decanol ($C_{10}H_{22}O$)	-9.759163	4.128806	-6.796183	-16.972917	0.04	1.37	3.70	6.21
1-Heptanol ($C_7H_{16}O$)	-7.735135	-0.431761	-2.191067	-20.627183	20.16	108.06	78.45	157.52
1-Hexanol ($C_6H_{14}O$)	-6.685825	-2.915658	-0.026657	-20.328351	29.55	156.80	99.75	294.42
1-Nonanol ($C_9H_{20}O$)	-9.596158	3.804831	-6.262919	-19.056041	3.22	25.93	28.89	52.48
1-Octanol ($C_8H_{18}O$)	-8.635838	1.674241	-4.130275	-20.297230	13.77	71.65	60.30	124.33
1-Pentanol ($C_5H_{12}O$)	-5.983014	-4.766516	1.643343	-18.962196	33.37	221.71	116.59	765.46
2-Octanol ($C_8H_{18}O$)	-10.739659	7.388280	-8.304859	-20.327895	14.57	55.95	0.40	74.55
Ethanol (C_2H_6O)	-6.529936	-4.807096	2.413685	-6.803188	24.82	507.97	149.50	528.41
Isopropyl alcohol (C_3H_8O)	-5.262652	-7.933393	4.556534	-10.790584	39.76	466.88	152.33	325.78
Methanol (CH_4O)	-7.993764	-0.622991	-0.226137	-3.815630	7.43	152.80	90.88	272.62
Propanol (C_3H_8O)	-5.744598	-6.089763	2.896399	-11.687160	32.71	410.36	137.66	496.85
Tert-butanol ($C_4H_{10}O$)	-6.014529	-4.997274	1.471697	-20.266304	29.07	301.63	115.86	697.91
Acetone (C_3H_6O)	-7.614321	1.713410	-1.953912	-3.750234	0.84	6.57	2.03	17.19
Methyl isobutyl ketone ($C_6H_{12}O$)	-9.219509	5.034470	-4.900292	-5.977003	19.73	196.20	74.73	56.62
Benzene (C_6H_6)	-7.012931	1.509755	-1.664638	-4.376087	0.02	2.76	9.92	17.86
Ethylbenzene (C_8H_{10})	-7.292722	1.076937	-1.541726	-4.757827	3.17	38.61	36.30	33.22
Naphthalene ($C_{10}H_8$)	-7.365703	1.248356	-1.712239	-4.314483	3.27	34.83	31.72	33.58
Toluene (C_7H_8)	-7.200968	1.251546	-1.450124	-4.441681	1.57	21.50	24.93	19.33
m-Xylene (C_8H_{10})	-7.565968	1.470551	-2.019073	-3.823634	1.45	18.41	18.50	4.45
o-Xylene (C_8H_{10})	-7.536169	1.527835	-1.908848	-4.397125	0.90	12.89	16.11	17.64
p-Xylene (C_8H_{10})	-7.630723	1.662198	-2.121534	-4.005008	1.12	12.11	11.49	10.32
Butane (C_4H_{10})	-7.048977	1.634995	-1.630355	-3.180389	0.45	2.55	17.40	46.43
Diethyl ether ($C_4H_{10}O$)	-6.866950	0.285082	-0.878305	-4.451491	7.62	84.06	64.57	35.67
Decane ($C_{10}H_{22}$)	-8.549984	2.202853	-3.734824	-5.669548	0.66	9.96	12.99	45.08

	$F_{w,j}$ *[AA]*				**A%Err**			
Species	***a***	***b***	***c***	***d***	***a***	***b***	***c***	***d***
Dodecane ($C_{12}H_{26}$)	-8.961419	2.295040	-4.335620	-6.335851	1.37	17.40	16.60	51.83
Eicosane ($C_{20}H_{42}$)	-10.459148	2.758645	-7.337807	-9.528239	4.74	35.18	18.08	88.94
Ethane (C_2H_6)	-6.299364	1.015600	-0.845965	-1.958236	2.71	28.01	26.05	5.34
Heptadecane ($C_{17}H_{36}$)	-11.031682	5.580700	-9.214265	-4.452427	7.77	57.57	28.16	10.95
n-Heptane (C_7H_{16})	-7.648195	1.450903	-2.181554	-4.758927	1.62	21.83	22.91	35.70
Hexadecane ($C_{16}H_{34}$)	-10.215435	3.862003	-7.175407	-6.430754	1.78	13.11	4.56	32.24
n-Hexane (C_6H_{14})	-7.383229	1.370152	-1.887145	-4.184089	2.08	25.44	25.81	32.28
Methane (CH_4)	-5.688083	0.407938	0.331408	-2.059978	5.55	67.79	158.07	50.80
Nonadecane ($C_{19}H_{40}$)	-11.739209	6.785153	-11.264570	-2.869960	9.90	70.46	35.67	42.54
Nonane (C_9H_{20})	-8.154237	1.709371	-2.986600	-5.301093	2.10	24.27	21.93	42.04
Octadecane ($C_{18}H_{38}$)	-11.859884	7.303743	-11.392172	-2.287220	13.25	97.58	50.33	55.23
Octane (C_8H_{18})	-7.875474	1.494814	-2.492625	-5.115239	2.16	26.68	24.74	40.22
Pentadecane ($C_{15}H_{32}$)	-9.814658	3.249504	-6.202091	-6.665884	0.13	1.30	5.05	45.42
n-Pentane (C_5H_{12})	-7.269145	1.626673	-1.931273	-3.397774	0.52	7.49	10.71	16.64
Propane (C_3H_8)	-6.629174	1.114149	-0.938653	-3.013730	1.99	28.34	40.86	48.90
R152a ($C_2H_4F_2$)	-8.605844	4.242384	-3.266285	-7.580427	15.77	141.66	50.52	173.20
n-Tetradecane ($C_{14}H_{30}$)	-9.447984	2.718678	-5.296251	-7.114640	1.01	11.34	11.83	57.06
Tridecane ($C_{13}H_{28}$)	-9.187372	2.432486	-4.748009	-6.936946	1.52	16.10	14.53	55.19
Undecane ($C_{11}H_{24}$)	-8.733490	2.196873	-3.996625	-6.030297	1.32	15.57	15.51	47.77
Argon (Ar)	-5.943681	1.247338	-0.504456	-1.729142	0.29	3.23	1.06	8.69
Nitrogen (N_2)	-7.033895	3.582390	-3.145412	0.000990	15.10	193.90	353.45	100.05
Ammonia (NH_3)	-6.857123	0.172729	0.244867	-5.064263	5.85	89.01	113.19	111.62
Water (H_2O)	-7.335010	0.475371	-0.737194	-3.331310	6.70	74.70	67.48	56.50
Hydrogen (H_2 normal)	-6.138327	4.279097	-2.688428	2.609323	25.21	301.79	464.63	4811.67
Summary								
Organic Acids (6)				Average	22.15	386.04	363.67	257.64
				Maximum	53.22	798.32	1,731.02	600.02
Alcohols (13)				Average	21.75	219.57	89.80	460.88
				Maximum	39.76	507.97	152.33	2,194.88
Others (36)				Average	4.76	50.28	52.85	176.62
				Maximum	25.21	301.79	464.63	4,811.67
All (55)				Average	10.67	126.93	95.49	252.64
				Maximum	53.22	798.32	1,731.02	4,811.67

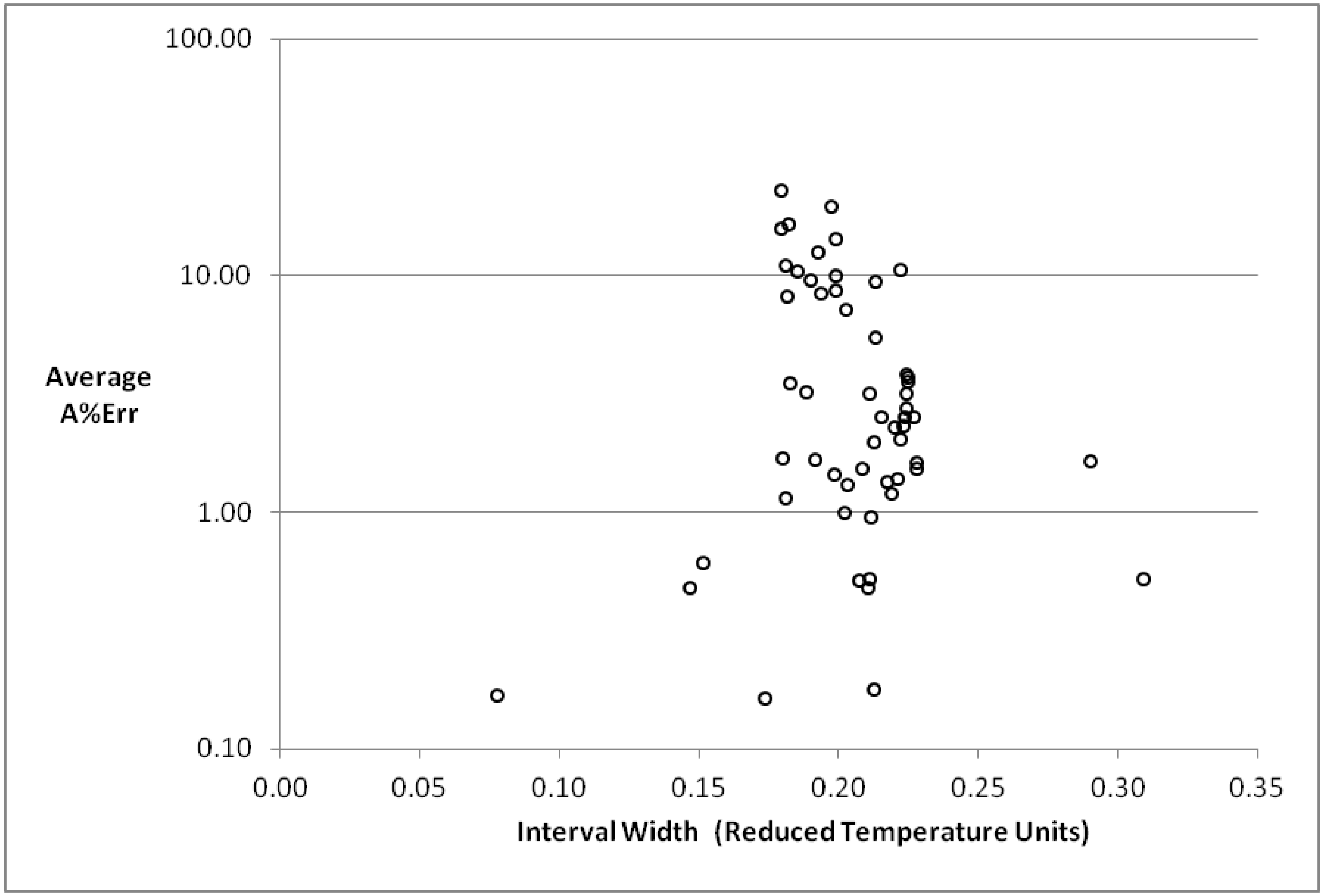

Figure C.1. Average A%Err of "All T_rs" for $F_{w,j}$*[AA]* vs. Interval Width.

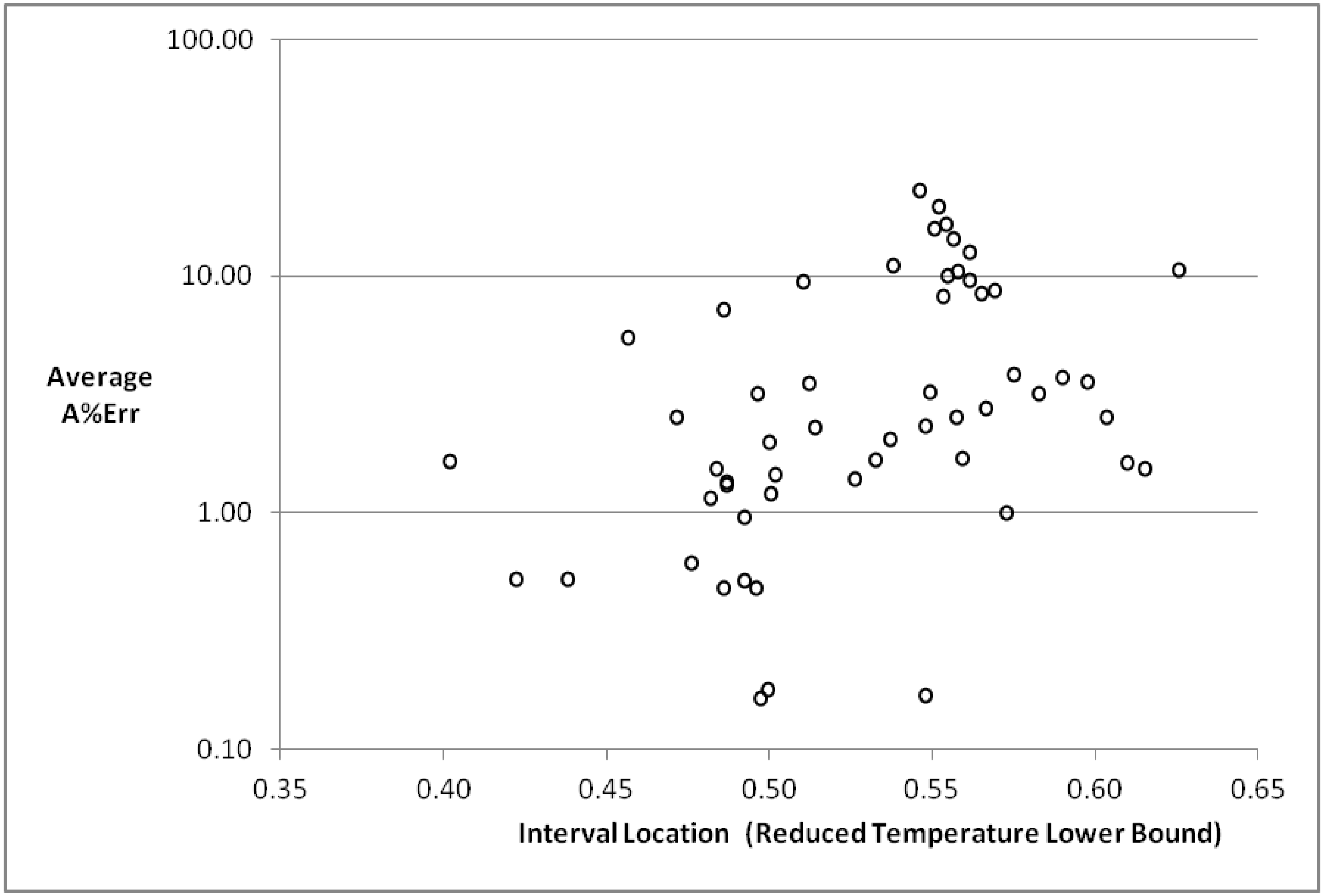

Figure C.2. Average A%Err of "All T_rs" for $F_{w,j}[AA]$ vs. Interval Location.

Appendix D: Ancillary Data for Chapter 3

Table D.1. Point Distributions and η_{ji} Values for the Three Fully-Determined Cases Used.

(a) T_r = 0.6, 0.7, 0.8, 0.9			**(b) T_r = 0.3, 0.6, 0.7, 0.95**		
$F_{w,j}$ Function	**$P_{v,r}$ Correlation**		**$F_{w,j}$ Function**	**$P_{v,r}$ Correlation**	
	$T_r < T_{r,b}$	**$T_r > T_{r,b}$**		**$T_r < T_{r,b}$**	**$T_r > T_{r,b}$**
$F_{w,j}[R(\omega)]$	R(ω)	R(ω)			
$F_{w,j}^{(1)}[R \mid R(\omega)]$	R	R(ω)	$F_{w,j}^{(2)}[R \mid R(\omega)]$	R	R(ω)
$F_{w,j}^{(1)}[A\text{-}W(T_b) \mid R(\omega)]$	A-W(T_b)	R(ω)	$F_{w,j}^{(2)}[A\text{-}W(T_b) \mid R(\omega)]$	A-W(T_b)	R(ω)
η_{ji} Values			η_{ji} Values		
η_{a1}	-3.0648585		η_{a1}	-0.0773462	
η_{a2}	21.0364707		η_{a2}	4.4993457	
η_{a3}	-53.6598599		η_{a3}	-9.6419666	
η_{a4}	66.9831631		η_{a4}	43.9504566	
η_{b1}	13.1164427		η_{b1}	0.3961452	
η_{b2}	-88.4498187		η_{b2}	-22.6938397	
η_{b3}	214.071988		η_{b3}	47.6499234	
η_{b4}	-219.1970428		η_{b4}	-118.1136539	
η_{c1}	-34.8740634		η_{c1}	-1.0066326	
η_{c2}	221.8890227		η_{c2}	51.4795436	
η_{c3}	-447.742097		η_{c3}	-90.6479963	
η_{c4}	360.8064394		η_{c4}	130.6868447	
η_{d1}	198.8988093		η_{d1}	3.1821126	
η_{d2}	-829.2917811		η_{d2}	-65.2308649	
η_{d3}	1232.016927		η_{d3}	95.2281085	
η_{d4}	-766.7340723		η_{d4}	-90.2449189	
(c) T_r = 0.2, $T_{r,b}$, 0.7, 0.95					
$F_{w,j}$ Function	**$P_{v,r}$ Correlation**				
	0.2	**$T_{r,b}$**	**0.7**	**0.95**	
$F_{w,j}^{(3)}[R \mid R(\omega)]$	R	1.01325/P_c	R(ω)	R(ω)	
$F_{w,j}^{(3)}[A\text{-}W(T_b) \mid R(\omega)]$	A-W(T_b)		A-W(T_b) for 0.7 < $T_{r,b}$ R(ω) for 0.7 > $T_{r,b}$	R(ω)	
η_{ji} Values are species-specific					

Notes:
The η_{ji} values are shown for cases (a) and (b) because they apply to every species. The η_{ji} values for case (c), however, are species-dependent because the normal boiling point is one of the four points. The algebraic equations for the η_{ji} parameters, which are dependent only upon the chosen four reduced temperatures, can be found in Table 1.4.

Table D.2. Comparison of Average A%Err of $F_{w,j}$ Functions for T_r < $\mathrm{T}_{r,b}$ Segment.

Species	Average A%Err for $T_r < T_{r,b}$ Segment						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
Organic Acids with $T_{r,b}$ > 0.7							
Decanoic acid ($C_{10}H_{20}O_2$)	12.80	69.00	42.49	4.59	417.76	157.30	203.23
Octanoic acid ($C_8H_{16}O_2$)	7.46	13.60	10.01	1.83	231.18	84.41	106.40
3-Methyl butanoic acid ($C_5H_{10}O_2$)	15.69	8.77	8.42	9.87	163.44	22.63	24.45
Pentanoic acid ($C_5H_{10}O_2$)	12.71	17.00	9.53	7.05	330.57	36.25	42.51
2-Methyl propanoic acid ($C_4H_8O_2$)	15.52	20.60	14.83	12.27	63.97	4.70	3.99
Butanoic acid ($C_4H_8O_2$)	5.18	5.18	2.84	8.21	37.69	11.38	53,229.99
Alcohols with $T_{r,b}$ > 0.7							
1-Eicosanol ($C_{20}H_{42}O$)	42.30	115.21	185.78	96.33	9.15	12.44	15.56
1-Octadecanol ($C_{18}H_{38}O$)	49.73	78.14	97.95	78.75	17.45	21.19	24.44
1-Heptadecanol ($C_{17}H_{36}O$)	54.74	54.84	64.33	70.22	22.93	28.53	32.28
1-Hexadecanol ($C_{16}H_{34}O$)	55.04	34.68	42.16	60.53	26.77	33.78	37.86
1-Dodecanol ($C_{12}H_{26}O$)	88.66	7.01	27.01	68.55	120.59	110.88	119.12
1-Decanol ($C_{10}H_{22}O$)	76.18	7.82	24.28	59.76	254.95	149.15	159.18
1-Nonanol ($C_9H_{20}O$)	86.52	11.77	30.31	69.71	570.48	219.82	240.12
1-Octanol ($C_8H_{18}O$)	51.23	8.29	24.60	47.64	1027.53	211.61	234.49
2-Ethyl-1-hexanol ($C_8H_{18}O$)	313.47	26.07	129.07	223.04	507645.51	2385.16	2,751.63
1-Heptanol ($C_7H_{16}O$)	43.79	8.48	23.67	42.67	2627.19	229.90	250.34
2-Octanol ($C_8H_{18}O$)	88.96	25.82	22.28	62.44	2013.54	287.85	315.52
1-Hexanol ($C_6H_{14}O$)	3.41	14.21	14.50	12.67	9438.99	183.75	263.98
Tert-butanol ($C_4H_{10}O$)	0.52	3.02	3.13	1.00	13.51	14.29	12.76
"Others" with $T_{r,b}$ > 0.7							

Species	Average A%Err for $T_r < T_{r,b}$ Segment						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R \mid R(\omega)]$	$F_{w,j}^{(2)}$ $[R \mid R(\omega)]$	$F_{w,j}^{(3)}$ $[R \mid R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b) \mid R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b) \mid R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b) \mid R(\omega)]$
Helium (He normal)	3.33	6.42	7.95	6.08	5.22	7.28	8.91
Eicosane ($C_{20}H_{42}$)	7.02	7.90	12.67	15.29	3.03	1.96	5.87
Nonadecane ($C_{19}H_{40}$)	5.85	6.54	11.14	13.77	2.80	1.61	4.95
Octadecane ($C_{18}H_{38}$)	5.11	2.94	6.46	11.07	4.49	1.69	0.95
Heptadecane ($C_{17}H_{36}$)	4.26	2.74	6.40	10.11	3.20	0.59	1.73
Hexadecane ($C_{16}H_{34}$)	5.08	2.33	5.94	10.17	1.62	0.34	0.97
Pentadecane ($C_{15}H_{32}$)	3.79	2.60	7.73	10.96	1.73	0.99	3.14
n-Tetradecane ($C_{14}H_{30}$)	4.73	0.82	4.83	9.10	1.19	0.70	2.09
Tridecane ($C_{13}H_{28}$)	2.92	0.86	5.11	8.48	0.16	0.12	0.48
Dodecane ($C_{12}H_{26}$)	3.33	2.19	3.47	7.26	0.37	0.48	1.07
Undecane ($C_{11}H_{24}$)	3.04	4.21	3.77	7.49	0.05	0.06	0.31
Decane ($C_{10}H_{22}$)	1.00	5.57	3.05	5.52	1.56	0.39	1.12
Nonane (C_9H_{20})	0.85	7.12	3.89	6.07	4.87	0.19	1.81
Octane (C_8H_{18})	30.29	26.07	2.21	21.11	21.38	0.64	14.20
Organic Acids with $T_{r,b}$ < 0.7							
Propanoic acid ($C_3H_6O_2$)	4.04	13.81	6.20	1.95	0.49	3.27	5.02
Acetic Acid ($C_2H_4O_2$)	1.58	14.17	9.08	0.36	18.56	13.55	3.29
Formic acid (CH_2O_2)	3.96	0.61	0.58	1.57	12.68	10.94	6.67
Alcohols with $T_{r,b}$ < 0.7							
Isopropyl alcohol (C_3H_8O)	14.65	43.66	28.44	18.14	22.64	14.43	14.05
1-Pentanol ($C_5H_{12}O$)	296.78	50.00	2.44	87.62	101.13	188.67	215.86
2-Butanol ($C_4H_{10}O$)	1.93	18.27	33.91	31.71	115,394,974.79	689.61	223.97
1-Butanol ($C_4H_{10}O$)	16.27	31.72	17.97	12.88	23,024.32	80.08	12.57
Propanol (C_3H_8O)	42.53	53.79	46.67	42.09	10,772.48	26.21	34.50
Ethanol (C_2H_6O)	36.02	58.23	50.50	40.60	32.06	35.43	36.72

Species	**Average A%Err for $T_r < T_{r,b}$ Segment**						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R \vert R(\omega)]$	$F_{w,j}^{(2)}$ $[R \vert R(\omega)]$	$F_{w,j}^{(3)}$ $[R \vert R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b) \vert R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b) \vert R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b) \vert R(\omega)]$
Benzyl alcohol (C_7H_8O)	1.04	43.33	24.75	9.14	1,164.63	101.08	34.42
Cyclohexanol ($C_6H_{12}O$)	7.31	1.61	4.46	8.17	169.94	71.27	22.20
Methanol (CH_4O)	18.83	62.97	54.59	37.79	45.67	37.59	30.03
"Others" with $T_{r,b} < 0.7$ (Normal)							
Pentafluorotoluene ($C_7H_3F_5$)	1.72	10.94	4.76	0.94	6.07	4.61	3.55
n-Heptane (C_7H_{16})	11.94	22.67	4.75	13.38	12.78	0.58	3.70
Acetic Anhydride ($C_4H_6O_3$)	13.91	26.90	6.43	13.42	21.36	6.08	0.67
Pentafluorobenzene (C_6HF_5)	3.46	7.31	1.73	4.28	1.48	0.53	1.30
n-Hexane (C_6H_{14})	5.61	15.10	3.20	8.14	5.30	0.35	1.54
m-Xylene (C_8H_{10})	2.59	12.85	3.13	5.76	3.20	1.43	0.77
p-Xylene (C_8H_{10})	1.04	7.49	3.06	1.26	3.80	2.26	0.55
Ethylbenzene (C_8H_{10})	9.33	15.03	15.08	20.33	10.59	4.90	3.97
o-Xylene (C_8H_{10})	4.47	11.93	2.15	5.40	5.12	1.35	0.80
n-Pentane (C_5H_{12})	3.17	16.70	5.29	9.17	2.52	0.58	0.39
Naphthalene ($C_{10}H_8$)	1.77	5.25	1.49	2.11	1.19	0.46	0.52
Toluene (C_7H_8)	13.00	12.94	12.58	19.02	4.33	5.82	6.61
Cyclopentanone (C_5H_8O)	0.40	7.19	2.98	4.79	0.91	0.55	1.44
Butane (C_4H_{10})	0.72	13.40	2.59	5.76	1.15	1.34	1.59
Benzene (C_6H_6)	0.90	0.59	1.60	1.88	1.88	1.79	1.07
Propane (C_3H_8)	0.57	16.47	8.43	14.00	1.31	0.87	1.62
Hydrogen (H_2 normal)	1.71	3.14	1.73	0.79	3.63	0.45	0.96
Nitrogen (N_2)	0.05	0.42	0.21	0.45	0.20	0.23	0.23
Ethane (C_2H_6)	0.31	2.33	3.67	6.39	0.99	0.68	0.34
Methane (CH_4)	0.47	0.47	0.04	0.20	0.47	0.04	0.03

Species	Average A%Err for $T_r < T_{r,b}$ Segment						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
Argon (Ar)	0.10	0.10	0.08	0.09	0.10	0.09	0.06
"Others" with $T_{r,b} < 0.7$ (Polar)							
Methyl isobutyl ketone ($C_6H_{12}O$)	1.28	1.47	9.83	10.47	23.51	5.12	1.74
Diethyl ether ($C_4H_{10}O$)	4.81	7.95	7.88	11.49	9.67	4.90	3.35
Acetone (C_3H_6O)	1.58	18.93	4.88	1.85	10.74	6.97	4.36
R152a ($C_2H_4F_2$)	0.58	9.79	2.71	1.43	4.17	2.92	1.73
Ammonia (NH_3)	0.29	0.29	0.38	0.08	0.29	1.35	1.01
Water (H_2O)	1.54	1.54	4.05	2.09	1.54	7.24	5.36
Summary							
Acids (9)							
$T_{r,b} > 0.7$ (6)	11.73	22.36	14.69	7.30	207.43	52.78	8,935.10
$T_{r,b} < 0.7$ (3)	3.29	9.53	5.28	1.29	10.58	9.25	4.99
Alcohols (22)							
$T_{r,b} > 0.7$ (13)	79.28	30.41	53.01	68.72	4,0291.43	299.10	342.87
$T_{r,b} < 0.7$ (9)	50.52	40.40	29.30	32.02	12,825,589.74	138.26	69.37
"Others" (41)							
$T_{r,b} > 0.7$ (14)	5.63	5.59	6.05	10.18	3.69	1.22	3.40
$T_{r,b} < 0.7$ (27)	3.94	9.23	4.25	6.11	5.12	2.35	1.82
Normal (21)	4.48	9.96	4.05	6.55	4.21	1.67	1.51
Polar (6)	1.95	6.66	4.96	4.57	8.32	4.75	2.92
Note: The $F_{w,j}$ function with the least average A%Err for a substance subset has its error shaded gray in the Summary section.							

Table D.3. Comparison of Average A%Err of $F_{w,j}$ Functions for T_r > $T_{r,b}$ Segment.

Species	Average A%Err for $T_r > T_{r,b}$ Segment						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
Organic Acids with $T_{r,b}$ > 0.7							
Decanoic acid ($C_{10}H_{20}O_2$)	0.55	0.66	1.00	0.21	0.86	2.02	2.62
Octanoic acid ($C_8H_{16}O_2$)	0.70	0.70	0.64	0.42	0.81	1.88	2.43
3-Methyl butanoic acid ($C_5H_{10}O_2$)	0.89	0.89	0.70	0.65	0.92	1.97	1.98
Pentanoic acid ($C_5H_{10}O_2$)	0.79	0.79	0.48	0.56	0.82	1.81	1.95
2-Methyl propanoic acid ($C_4H_8O_2$)	0.98	0.97	0.62	0.77	1.01	1.73	1.60
Butanoic acid ($C_4H_8O_2$)	1.31	1.31	1.01	0.66	1.35	2.10	25.40
Alcohols with $T_{r,b}$ > 0.7							
1-Eicosanol ($C_{20}H_{42}O$)	0.36	0.46	0.54	0.60	0.37	0.88	0.67
1-Octadecanol ($C_{18}H_{38}O$)	0.42	0.41	0.74	0.63	0.43	0.89	0.71
1-Heptadecanol ($C_{17}H_{36}O$)	0.52	0.52	0.91	0.70	0.52	0.95	0.78
1-Hexadecanol ($C_{16}H_{34}O$)	0.58	0.59	1.10	0.77	0.59	1.00	0.83
1-Dodecanol ($C_{12}H_{26}O$)	0.98	1.05	1.97	1.10	1.02	1.02	0.85
1-Decanol ($C_{10}H_{22}O$)	1.36	1.37	2.57	1.49	1.40	0.96	0.93
1-Nonanol ($C_9H_{20}O$)	1.53	1.57	2.64	1.66	1.62	1.09	1.08
1-Octanol ($C_8H_{18}O$)	1.99	2.00	2.94	2.16	2.05	1.36	1.42
2-Ethyl-1-hexanol ($C_8H_{18}O$)	1.82	1.83	2.98	1.97	1.85	1.28	1.33
1-Heptanol ($C_7H_{16}O$)	1.51	1.52	2.42	1.69	1.50	1.38	1.45
2-Octanol ($C_8H_{18}O$)	1.32	1.35	2.90	1.42	1.31	1.18	1.26
1-Hexanol ($C_6H_{14}O$)	2.06	2.05	2.25	2.32	1.98	1.67	2.25
Tert-butanol ($C_4H_{10}O$)	1.09	1.12	1.33	0.79	1.23	3.70	3.32
"Others" with $T_{r,b}$ > 0.7							

Species	**Average A%Err for $T_r > T_{r,b}$ Segment**						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
Helium (He normal)	0.32	0.33	0.38	0.35	0.32	0.45	0.36
Eicosane ($C_{20}H_{42}$)	0.40	0.40	0.79	0.58	0.40	0.79	0.53
Nonadecane ($C_{19}H_{40}$)	0.30	0.30	0.69	0.47	0.30	0.67	0.42
Octadecane ($C_{18}H_{38}$)	0.24	0.24	0.63	0.40	0.24	0.58	0.39
Heptadecane ($C_{17}H_{36}$)	0.23	0.23	0.61	0.41	0.23	0.54	0.37
Hexadecane ($C_{16}H_{34}$)	0.17	0.17	0.56	0.34	0.17	0.43	0.34
Pentadecane ($C_{15}H_{32}$)	0.18	0.18	0.55	0.36	0.19	0.42	0.28
n-Tetradecane ($C_{14}H_{30}$)	0.06	0.06	0.43	0.22	0.06	0.29	0.18
Tridecane ($C_{13}H_{28}$)	0.10	0.10	0.47	0.28	0.10	0.26	0.24
Dodecane ($C_{12}H_{26}$)	0.03	0.04	0.39	0.18	0.03	0.18	0.14
Undecane ($C_{11}H_{24}$)	0.01	0.02	0.39	0.18	0.01	0.15	0.13
Decane ($C_{10}H_{22}$)	0.06	0.06	0.39	0.21	0.06	0.12	0.17
Nonane (C_9H_{20})	0.07	0.07	0.41	0.23	0.07	0.09	0.19
Octane (C_8H_{18})	1.57	1.52	0.38	1.48	1.52	0.61	1.53
Organic Acids with $T_{r,b}$ < 0.7							
Propanoic acid ($C_3H_6O_2$)	1.27	1.26	0.80	1.10	1.28	1.29	1.14
Acetic Acid ($C_2H_4O_2$)	0.39	0.44	0.67	0.35	0.47	0.73	0.48
Formic acid (CH_2O_2)	0.96	1.01	0.92	0.76	0.96	0.80	1.01
Alcohols with $T_{r,b}$ < 0.7							
Isopropyl alcohol (C_3H_8O)	3.53	3.46	2.10	3.43	3.55	3.77	3.36
1-Pentanol ($C_5H_{12}O$)	4.06	3.91	1.29	4.11	4.05	3.72	3.99
2-Butanol ($C_4H_{10}O$)	1.28	1.28	1.05	1.04	1.41	3.38	0.91
1-Butanol ($C_4H_{10}O$)	1.41	1.39	0.83	1.22	1.52	3.03	1.09
Propanol (C_3H_8O)	1.45	1.43	0.75	1.28	1.53	2.52	1.18
Ethanol (C_2H_6O)	1.26	1.23	1.04	1.19	1.26	1.26	1.11

Species	**Average A%Err for $T_r > T_{r,b}$ Segment**						
	$F_{w,j}[R(\omega)]$	$F_{w,j}^{(1)}$ $[R\|R(\omega)]$	$F_{w,j}^{(2)}$ $[R\|R(\omega)]$	$F_{w,j}^{(3)}$ $[R\|R(\omega)]$	$F_{w,j}^{(1)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(2)}$ $[A\text{-}W(T_b)\|R(\omega)]$	$F_{w,j}^{(3)}$ $[A\text{-}W(T_b)\|R(\omega)]$
Benzyl alcohol (C_7H_8O)	0.57	0.62	0.79	0.52	0.72	1.68	0.32
Cyclohexanol ($C_6H_{12}O$)	0.32	0.32	0.34	0.17	0.53	1.96	0.29
Methanol (CH_4O)	0.89	0.98	1.45	1.09	0.89	0.61	0.92
"Others" with $T_{r,b} < 0.7$ (Normal)							
Pentafluorotoluene ($C_7H_3F_5$)	0.18	0.18	0.56	0.23	0.18	0.27	0.19
n-Heptane (C_7H_{16})	0.53	0.51	0.19	0.41	0.52	0.24	0.45
Acetic Anhydride ($C_4H_6O_3$)	0.12	0.15	0.55	0.07	0.14	0.30	0.06
Pentafluorobenzene (C_6HF_5)	0.23	0.21	0.29	0.09	0.22	0.09	0.14
n-Hexane (C_6H_{14})	0.27	0.27	0.18	0.15	0.27	0.12	0.20
m-Xylene (C_8H_{10})	0.11	0.11	0.39	0.17	0.11	0.16	0.12
p-Xylene (C_8H_{10})	0.08	0.09	0.47	0.15	0.08	0.24	0.11
Ethylbenzene (C_8H_{10})	0.10	0.10	0.26	0.11	0.10	0.05	0.07
o-Xylene (C_8H_{10})	0.15	0.15	0.27	0.04	0.15	0.08	0.09
n-Pentane (C_5H_{12})	0.08	0.08	0.27	0.10	0.08	0.07	0.06
Naphthalene ($C_{10}H_8$)	0.20	0.20	0.21	0.08	0.20	0.08	0.13
Toluene (C_7H_8)	0.17	0.19	0.19	0.06	0.17	0.10	0.11
Cyclopentanone (C_5H_8O)	0.23	0.23	0.16	0.12	0.23	0.17	0.15
Butane (C_4H_{10})	0.19	0.20	0.10	0.08	0.19	0.12	0.12
Benzene (C_6H_6)	0.10	0.09	0.17	0.15	0.10	0.09	0.11
Propane (C_3H_8)	0.15	0.16	0.09	0.04	0.15	0.09	0.07
Hydrogen (H_2 normal)	0.04	0.04	0.07	0.06	0.04	0.13	0.08
Nitrogen (N_2)	0.15	0.14	0.08	0.07	0.15	0.08	0.08
Ethane (C_2H_6)	0.14	0.13	0.06	0.06	0.14	0.08	0.08
Methane (CH_4)	0.12	0.12	0.06	0.06	0.12	0.06	0.07
Argon (Ar)	0.14	0.14	0.07	0.07	0.14	0.07	0.07

"Others" with $T_{r,b} < 0.7$ (Polar)							
Methyl isobutyl ketone ($C_6H_{12}O$)	0.16	0.16	0.23	0.19	0.15	0.12	0.16
Diethyl ether ($C_4H_{10}O$)	0.15	0.14	0.15	0.03	0.15	0.12	0.06
Acetone (C_3H_6O)	0.17	0.20	0.30	0.10	0.18	0.14	0.12
R152a ($C_2H_4F_2$)	0.12	0.14	0.23	0.04	0.12	0.06	0.06
Ammonia (NH_3)	0.23	0.23	0.18	0.16	0.23	0.23	0.23
Water (H_2O)	0.15	0.15	0.14	0.13	0.15	0.22	0.25
Summary							
Acids (9)							
$T_{r,b} > 0.7$ (6)	0.88	0.89	0.74	0.55	0.96	1.92	6.12
$T_{r,b} < 0.7$ (3)	0.87	0.89	0.80	0.73	0.89	0.93	0.88
Alcohols (22)							
$T_{r,b} > 0.7$ (13)	**1.28**	1.30	2.07	1.40	1.31	1.39	1.37
$T_{r,b} < 0.7$ (9)	1.61	1.60	1.06	1.53	1.69	2.41	1.44
"Others" (41)							
$T_{r,b} > 0.7$ (14)	0.28	**0.27**	0.49	0.41	**0.27**	0.37	0.38
$T_{r,b} < 0.7$ (27)	0.16	0.16	0.21	**0.11**	0.16	0.13	0.13
Normal (21)	0.16	0.16	0.21	**0.11**	0.16	0.12	0.12
Polar (6)	0.17	0.17	0.20	**0.11**	0.17	0.15	0.15
Note: The $F_{w,j}$ function with the least average A%Err for a substance subset has its error shaded gray in the Summary section. Bold font means the least error pertains to a different Fw,j function than that indicated for “All Trs” in Table 3.4.							

Table D.4. Minimum Possible Entire-Curve Average Absolute Percent Error Using the Four Correlations.

Species	# of Points			A%Err			
				Least Total $T_r < T_{r,b}$	Least Total $T_r > T_{r,b}$	Minimum Possible for Entire Curve (All T_rs)	
	$T_r < T_{r,b}$	$T_r > T_{r,b}$	Total (All T_rs)			Total	Average
Organic Acids with $T_{r,b} > 0.7$							
Decanoic acid ($C_{10}H_{20}O_2$)	14	9	24	141.68	4.67	146.35	6.10
Octanoic acid ($C_8H_{16}O_2$)	14	9	24	60.79	6.06	66.85	2.79
3-Methyl butanoic acid ($C_5H_{10}O_2$)	14	10	25	122.81	8.64	131.45	5.26
Pentanoic acid ($C_5H_{10}O_2$)	15	10	26	111.51	6.43	117.94	4.54
2-Methyl propanoic acid ($C_4H_8O_2$)	14	10	25	58.00	7.55	65.55	2.62
Butanoic acid ($C_4H_8O_2$)	12	10	23	37.10	12.85	49.95	2.17
Alcohols with $T_{r,b} > 0.7$							
1-Eicosanol ($C_{20}H_{42}O$)	17	6	24	203.35	1.04	204.40	8.52
1-Octadecanol ($C_{18}H_{38}O$)	16	7	24	330.32	1.04	331.36	13.81
1-Heptadecanol ($C_{17}H_{36}O$)	16	7	24	447.50	2.98	450.48	18.77
1-Hexadecanol ($C_{16}H_{34}O$)	16	7	24	531.42	3.58	535.00	22.29
1-Dodecanol ($C_{12}H_{26}O$)	14	9	24	387.39	3.84	391.24	16.30
1-Decanol ($C_{10}H_{22}O$)	14	9	24	349.55	4.16	353.71	14.74
1-Nonanol ($C_9H_{20}O$)	14	10	25	436.70	6.79	443.49	17.74
1-Octanol ($C_8H_{18}O$)	14	10	25	350.88	10.45	361.33	14.45
2-Ethyl-1-hexanol ($C_8H_{18}O$)	17	10	28	2230.30	11.10	2,241.40	80.05
1-Heptanol ($C_7H_{16}O$)	14	10	25	336.80	15.40	352.20	14.09
2-Octanol ($C_8H_{18}O$)	14	10	25	327.63	12.20	339.83	13.59

Species	# of Points			A%Err			
				Least Total $T_r < T_{r,b}$	Least Total $T_r > T_{r,b}$	Minimum Possible for Entire Curve (All T_rs)	
	$T_r < T_{r,b}$	$T_r > T_{r,b}$	Total (All T_rs)			Total	Average
1-Hexanol ($C_6H_{14}O$)	14	10	25	135.21	18.33	153.54	6.14
Tert-butanol ($C_4H_{10}O$)	6	10	17	2.95	10.64	13.59	0.80
"Others" with $T_{r,b} > 0.7$							
Helium (He normal)	17	6	24	65.37	0.95	66.31	2.76
Eicosane ($C_{20}H_{42}$)	17	6	24	16.61	0.05	16.66	0.69
Nonadecane ($C_{19}H_{40}$)	16	7	24	10.72	0.14	10.86	0.45
Octadecane ($C_{18}H_{38}$)	16	7	24	24.08	0.16	24.24	1.01
Heptadecane ($C_{17}H_{36}$)	16	7	24	13.92	0.17	14.09	0.59
Hexadecane ($C_{16}H_{34}$)	16	7	24	2.06	0.20	2.27	0.09
Pentadecane ($C_{15}H_{32}$)	16	8	25	2.22	0.19	2.42	0.10
n-Tetradecane ($C_{14}H_{30}$)	15	8	24	7.58	0.08	7.66	0.32
Tridecane ($C_{13}H_{28}$)	16	8	25	4.59	0.25	4.84	0.19
Dodecane ($C_{12}H_{26}$)	14	9	24	4.61	0.07	4.68	0.20
Undecane ($C_{11}H_{24}$)	15	9	25	1.62	0.08	1.70	0.07
Decane ($C_{10}H_{22}$)	14	10	25	7.22	0.24	7.46	0.30
Nonane (C_9H_{20})	15	10	26	4.55	0.27	4.82	0.19
Octane (C_8H_{18})	14	10	25	0.87	0.33	1.20	0.05
Organic Acids with $T_{r,b} < 0.7$							
Propanoic acid ($C_3H_6O_2$)	12	11	24	12.11	8.50	20.61	0.86
Acetic Acid ($C_2H_4O_2$)	8	12	21	18.82	4.57	23.40	1.11
Formic acid (CH_2O_2)	7	13	21	10.14	11.25	21.38	1.02
Alcohols with $T_{r,b} < 0.7$							
Isopropyl alcohol (C_3H_8O)	14	11	26	155.16	16.72	171.88	6.61
1-Pentanol ($C_5H_{12}O$)	15	11	27	5.30	3.87	9.17	0.34

Species	**# of Points**			**A%Err**			
				Least Total $T_r < T_{r,b}$	**Least Total $T_r > T_{r,b}$**	**Minimum Possible for Entire Curve (All T_rs)**	
	$T_r < T_{r,b}$	**$T_r > T_{r,b}$**	**Total (All T_rs)**			**Total**	**Average**
2-Butanol ($C_4H_{10}O$)	17	11	29	458.42	13.78	472.21	16.28
1-Butanol ($C_4H_{10}O$)	15	11	27	139.98	8.90	148.88	5.51
Propanol (C_3H_8O)	18	11	30	471.71	6.66	478.36	15.95
Ethanol (C_2H_6O)	16	11	28	523.09	13.57	536.66	19.17
Benzyl alcohol (C_7H_8O)	13	12	26	103.22	6.71	109.93	4.23
Cyclohexanol ($C_6H_{12}O$)	9	12	22	33.90	3.64	37.54	1.71
Methanol (CH_4O)	14	12	27	186.70	10.43	197.13	7.30
"Others" with $T_{r,b} < 0.7$ (Normal)							
Pentafluorotoluene ($C_7H_3F_5$)	11	11	23	16.31	1.77	18.08	0.79
n-Heptane (C_7H_{16})	15	11	27	5.85	0.85	6.70	0.25
Acetic Anhydride ($C_4H_6O_3$)	15	11	27	92.52	1.30	93.82	3.48
Pentafluorobenzene (C_6HF_5)	11	11	23	5.46	1.42	6.88	0.30
n-Hexane (C_6H_{14})	13	12	26	4.11	0.44	4.55	0.18
m-Xylene (C_8H_{10})	13	12	26	17.37	1.15	18.52	0.71
p-Xylene (C_8H_{10})	9	12	22	20.49	0.78	21.27	0.97
Ethylbenzene (C_8H_{10})	16	12	29	79.10	0.74	79.85	2.75
o-Xylene (C_8H_{10})	12	12	25	18.05	1.64	19.69	0.79
n-Pentane (C_5H_{12})	15	12	28	7.11	0.85	7.96	0.28
Naphthalene ($C_{10}H_8$)	9	12	22	7.19	2.22	9.41	0.43
Toluene (C_7H_8)	14	13	28	66.81	1.35	68.16	2.43
Cyclopentanone (C_5H_8O)	12	13	26	1.18	2.77	3.95	0.15
Butane (C_4H_{10})	14	13	28	16.69	0.55	17.23	0.62
Benzene (C_6H_6)	7	13	21	9.00	1.11	10.10	0.48
Propane (C_3H_8)	16	14	31	14.99	0.21	15.20	0.49

Species	**# of Points**			**A%Err**			
				Least Total $T_r < T_{r,b}$	**Least Total $T_r > T_{r,b}$**	**Minimum Possible for Entire Curve (All T_rs)**	
	$T_r < T_{r,b}$	**$T_r > T_{r,b}$**	**Total (All T_rs)**			**Total**	**Average**
Hydrogen (H_2 normal)	9	14	24	2.99	0.57	3.56	0.15
Nitrogen (N_2)	5	14	20	1.96	1.93	3.89	0.19
Ethane (C_2H_6)	14	14	29	11.54	0.29	11.83	0.41
Methane (CH_4)	5	15	21	1.17	0.80	1.97	0.09
Argon (Ar)	2	15	18	0.15	2.15	2.30	0.13
"Others" with $T_{r,b} < 0.7$ (Polar)							
Methyl isobutyl ketone ($C_6H_{12}O$)	15	11	27	79.98	1.65	81.63	3.02
Diethyl ether ($C_4H_{10}O$)	14	12	27	69.40	1.10	70.50	2.61
Acetone (C_3H_6O)	12	13	26	82.02	2.02	84.04	3.23
R152a ($C_2H_4F_2$)	10	13	24	34.27	1.34	35.61	1.48
Ammonia (NH_3)	5	15	21	4.36	3.45	7.81	0.37
Water (H_2O)	8	15	24	15.35	1.97	17.32	0.72
Summary							
Acids (9)							
$T_{r,b} > 0.7$ (6)	83	58	147	531.89	46.20	578.09	3.93
$T_{r,b} < 0.7$ (3)	27	36	66	41.07	24.32	65.39	0.99
Alcohols (22)							
$T_{r,b} > 0.7$ (13)	186	115	314	6,070.02	101.55	6,171.57	19.65
$T_{r,b} < 0.7$ (9)	131	102	242	2,077.48	84.28	2,161.76	8.93
"Others" (41)							
$T_{r,b} > 0.7$ (14)	217	112	343	166.01	3.18	169.19	0.49
$T_{r,b} < 0.7$ (27)	301	345	673	685.40	36.42	721.82	1.07
Normal (21)	237	266	524	400.02	24.89	424.91	0.81
Polar (6)	64	79	149	285.38	11.52	296.90	1.99

Species	**# of Points**			**A%Err**			
				Least Total $T_r < T_{r,b}$	**Least Total** $T_r > T_{r,b}$	**Minimum Possible for Entire Curve (All T_rs)**	
	$T_r < T_{r,b}$	$T_r > T_{r,b}$	**Total (All T_rs)**			**Total**	**Average**
Example Calculation: Minimum entire-curve average A%Err for Helium: the error below $T_{r,b}$ is equal to the number of points in that temperature segment, 17, multiplied by the least average A%Err, 3.845%, which is achieved by the R(ω) correlation as shown in Table 3.3. The error above $T_{r,b}$ is equal to the number of points, 6, multiplied by the least average A%Err, 0.158%, which is achieved by both A-W and A-W(T_b). The minimum possible average A%Err for the entire-curve ("All T_rs") is the error sum, 65.365+0.948 = 66.313%, divided by the total number of points, 17+6+1=24, resulting in a minimum entire-curve average error of 2.763%.							

Table D.5. Wagner Constants Estimated with Subset Best $F_{w,j}$ Functions Indicated in Table 3.5 for "All T_rs," and Corresponding Extrapolation Burden.

Species		Wagner Constants				Extrapolation Burden	
	BestSubset $F_{w,j}$	***a***	***b***	***c***	***d***	**Lowest** T_r	**Δ Log** $P_{v,r}/\Delta\ T_r$
Organic Acids with $T_{r,b}$ **> 0.7**							
Decanoic acid ($C_{10}H_{20}O_2$)	$F_{W,j}^{(3)}[R\|R(\omega)]$	-9.336234	3.652933	-12.592768	0.968327	0.7	19.72975
Octanoic acid ($C_8H_{16}O_2$)		-9.411243	3.306809	-10.345779	-2.010482		19.19087
3-Methyl butanoic acid ($C_5H_{10}O_2$)		-9.156868	2.992206	-8.112095	-2.404724		18.46753
Pentanoic acid ($C_5H_{10}O_2$)		-9.254044	2.983025	-8.073354	-3.161270		20.0958
2-Methyl propanoic acid ($C_4H_8O_2$)		-9.075892	2.816733	-6.916590	-2.895044		18.15688
Butanoic acid ($C_4H_8O_2$)		-9.132629	3.520686	-8.444966	-0.878716		15.45681
Alcohols with $T_{r,b}$ **> 0.7**							
1-Eicosanol ($C_{20}H_{42}O$)	$F_{W,j}^{(1)}[R\|R(\omega)]$	-10.471706	0.832856	-1.423945	-12.373273	0.7	21.33246
1-Octadecanol ($C_{18}H_{38}O$)		-10.576033	2.543372	-5.373623	-6.228728		20.77693
1-Heptadecanol ($C_{17}H_{36}O$)		-10.559583	3.276828	-7.029643	-4.442988		20.44697
1-Hexadecanol ($C_{16}H_{34}O$)		-10.478404	3.678750	-7.924473	-4.247684		20.12536
1-Dodecanol ($C_{12}H_{26}O$)		-9.685483	3.463960	-7.489241	-11.868077		19.84219
1-Decanol ($C_{10}H_{22}O$)		-9.169227	2.834257	-6.406404	-15.553049		19.81489
1-Nonanol ($C_9H_{20}O$)		-8.966112	2.577576	-6.048206	-16.279361		19.98171
1-Octanol ($C_8H_{18}O$)		-8.793790	2.564643	-6.566721	-13.629633		19.92634
2-Ethyl-1-hexanol ($C_8H_{18}O$)		-8.557321	2.298215	-5.792121	-16.755630		27.36288
1-Heptanol ($C_7H_{16}O$)		-8.677391	2.504468	-6.602349	-13.068236		20.93215
2-Octanol ($C_8H_{18}O$)		-8.373002	1.777370	-4.087584	-22.910915		20.69433
1-Hexanol ($C_6H_{14}O$)		-8.658592	3.172615	-9.243657	-2.666598		20.62635
Tert-butanol ($C_4H_{10}O$)		-8.935337	3.663147	-10.739334	3.551533		11.13064
"Others" with $T_{r,b}$ **> 0.7**							
Helium (He normal)	$F_{W,j}^{(2)}[A\text{-}W(T_b)\|R(\omega)]$	-4.025063	0.895170	1.206096	2.005368	0.7	3.772454

Species		**Wagner Constants**				**Extrapolation Burden**	
	***BestSubset* $F_{w,j}$**	***a***	***b***	***c***	***d***	**Lowest T_r**	**Δ Log $P_{v,r}/\Delta\ T_r$**
Eicosane ($C_{20}H_{42}$)	$F_{W,j}^{(2)}[A\text{-}W(T_b)\|R(\omega)]$	-10.638388	3.315417	-7.819432	-5.815914	0.7	20.62657
Nonadecane ($C_{19}H_{40}$)		-10.381684	3.153167	-7.311756	-5.666317		19.95972
Octadecane ($C_{18}H_{38}$)		-10.249744	3.138461	-7.092955	-5.494164		19.31744
Heptadecane ($C_{17}H_{36}$)		-10.022252	2.991269	-6.652861	-5.360778		18.93123
Hexadecane ($C_{16}H_{34}$)		-9.843800	2.899158	-6.326868	-5.220746		18.34345
Pentadecane ($C_{15}H_{32}$)		-9.599214	2.733959	-5.866040	-5.075703		17.98827
n-Tetradecane ($C_{14}H_{30}$)		-9.410321	2.698553	-5.568875	-4.836552		17.24341
Tridecane ($C_{13}H_{28}$)		-9.197514	2.542785	-5.173310	-4.719846		17.07154
Dodecane ($C_{12}H_{26}$)		-8.980381	2.480688	-4.828805	-4.472264		16.2041
Undecane ($C_{11}H_{24}$)		-8.770558	2.383218	-4.482629	-4.277114		16.3055
Decane ($C_{10}H_{22}$)		-8.531165	2.244126	-4.079478	-4.086251		15.3216
Nonane (C_9H_{20})		-8.273387	2.107245	-3.665498	-3.855247		15.92247
Octane (C_8H_{18})		-8.409801	3.018360	-4.419007	-2.831896		14.66129
Organic Acids with $T_{r,b}$ < 0.7							
Propanoic acid ($C_3H_6O_2$)	$F_{W,j}^{(3)}[R\|R(\omega)]$	-8.805434	2.553787	-5.115473	-2.642902	$T_{r,b}$	15.04957
Acetic Acid ($C_2H_4O_2$)		-8.628559	1.956257	-1.506828	-4.217707		11.14838
Formic acid (CH_2O_2)		-7.880104	2.198138	-2.425511	0.520895		10.26626
Alcohols with $T_{r,b}$ < 0.7							
Isopropyl alcohol (C_3H_8O)	$F_{W,j}^{(2)}[R\|R(\omega)]$	-9.727284	4.488092	-10.122450	-1.628257	$T_{r,b}$	19.26901
1-Pentanol ($C_5H_{12}O$)		-9.757294	6.012338	-12.262687	-0.539054		23.50961
2-Butanol ($C_4H_{10}O$)		-8.608172	2.956705	-8.894895	-2.777754		28.16584
1-Butanol ($C_4H_{10}O$)		-8.862874	3.392106	-9.266849	-2.505183		23.09825
Propanol (C_3H_8O)		-9.142061	3.611856	-9.253540	-2.409952		25.80715
Ethanol (C_2H_6O)		-9.653463	4.430644	-9.627932	-2.284199		21.49655
Benzyl alcohol (C_7H_8O)		-7.934130	3.520665	-8.746916	-3.088609		18.91158
Cyclohexanol ($C_6H_{12}O$)		-7.530050	2.909324	-8.530725	-2.742013		14.71258

Species		**Wagner Constants**				**Extrapolation Burden**	
	BestSubset $F_{w,j}$	***a***	***b***	***c***	***d***	**Lowest** T_r	**Δ Log** $P_{v,r}/\Delta\ T_r$
Methanol (CH_4O)	$F_{W,j}^{(2)}[R\|R(\omega)]$	-9.535784	4.483619	-7.785826	-5.364381	$T_{r,b}$	18.22915
"Others" with $T_{r,b}$ < 0.7 (Normal)							
Pentafluorotoluene ($C_7H_3F_5$)	$F_{W,j}^{(3)}[A\text{-}W(T_b)\|R(\omega)]$	-8.178935	2.130704	-3.406157	-3.812138	$T_{r,b}$	12.83999
n-Heptane (C_7H_{16})		-7.858966	1.963130	-2.672465	-3.743164		16.47706
Acetic Anhydride ($C_4H_6O_3$)		-8.422095	2.109332	-3.151541	-4.705476		19.15981
Pentafluorobenzene (C_6HF_5)		-7.975409	2.031953	-2.980893	-3.694758		12.98049
n-Hexane (C_6H_{14})		-7.584953	1.911652	-2.529778	-3.166483		15.28179
m-Xylene (C_8H_{10})		-7.715603	1.975525	-2.827867	-3.197817		15.06272
p-Xylene (C_8H_{10})		-7.715769	1.926860	-2.519378	-3.494559		11.05978
Ethylbenzene (C_8H_{10})		-7.587586	1.962080	-2.793438	-2.890826		19.90904
o-Xylene (C_8H_{10})		-7.661898	1.913430	-2.480863	-3.393043		13.63869
n-Pentane (C_5H_{12})		-7.332078	1.859224	-2.346912	-2.690058		17.45034
Naphthalene ($C_{10}H_8$)		-7.618430	1.884409	-2.389409	-3.351719		10.98263
Toluene (C_7H_8)		-7.403736	1.855128	-2.313349	-2.889262		18.58916
Cyclopentanone (C_5H_8O)		-7.506350	1.946849	-2.787031	-2.715027		15.46669
Butane (C_4H_{10})		-7.062071	1.774220	-2.025198	-2.321292		15.98264
Benzene (C_6H_6)		-7.085725	1.851930	-2.483538	-1.983380		9.995995
Propane (C_3H_8)		-6.813916	1.685810	-1.720094	-2.000173		22.2323
Hydrogen (H_2 normal)		-4.903503	1.107364	0.589057	0.512335		6.03958
Nitrogen (N_2)		-6.214551	1.544632	-1.183427	-1.056009		8.071019
Ethane (C_2H_6)		-6.542678	1.602749	-1.377118	-1.654242		16.06466
Methane (CH_4)		-6.090000	1.472321	-0.850952	-1.032572		8.519146
Argon (Ar)		-6.011251	1.471664	-0.913973	-0.818749		7.221099
"Others" with $T_{r,b}$ < 0.7 (Polar)							
Methyl isobutyl ketone ($C_6H_{12}O$)	$F_{W,j}[R(\omega)]$	-7.868258	2.252544	-3.661345	-2.768379	$T_{r,b}$	17.58682
Diethyl ether ($C_4H_{10}O$)		-7.534614	2.076832	-2.864774	-2.463031		16.31318

Species		**Wagner Constants**				**Extrapolation Burden**	
	***BestSubset* $F_{w,j}$**	***a***	***b***	***c***	***d***	**Lowest T_r**	**Δ Log $P_{v,r}/\Delta T_r$**
Acetone (C_3H_6O)	$F_{W,j}[R(\omega)]$	-7.721787	2.115003	-2.678615	-2.305323	$T_{r,b}$	15.64275
R152a ($C_2H_4F_2$)		-7.536220	2.049946	-2.545677	-2.281967		12.912
Ammonia (NH_3)		-7.452809	2.018413	-2.335659	-2.090503		11.20356
Water (H_2O)		-7.971008	2.162943	-2.534562	-2.244450		14.36959

Note: The “Lowest T_r” refers to the known vapor pressure at the lowest reduced temperature, which is either at 0.7 or the normal reduced boiling point. The lowest T_r of 0.7, obviously, means the extrapolation burden corresponds to that of the Ambrose-Walton equation, and a lowest T_r of $T_{r,b}$ corresponds to that of the Riedel equation.

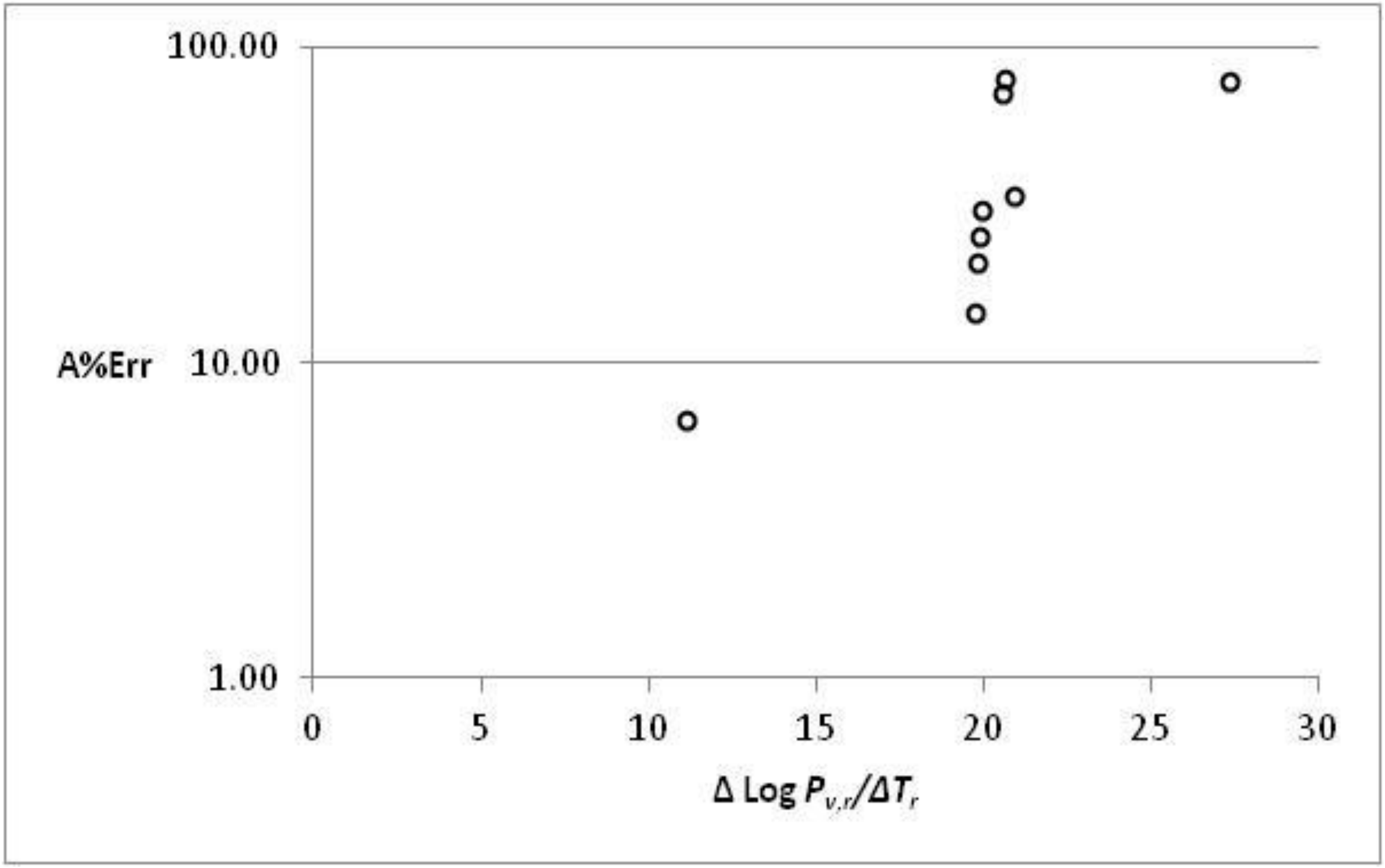

Figure D.1. A%Err @$T_{r,f}$ vs. Extrapolation Burden For Recommended Subset $F_{W,j}^{(1)}[R|R(\omega)]$ (Alcohols with $0.7 < T_{r,b} < 0.76$).

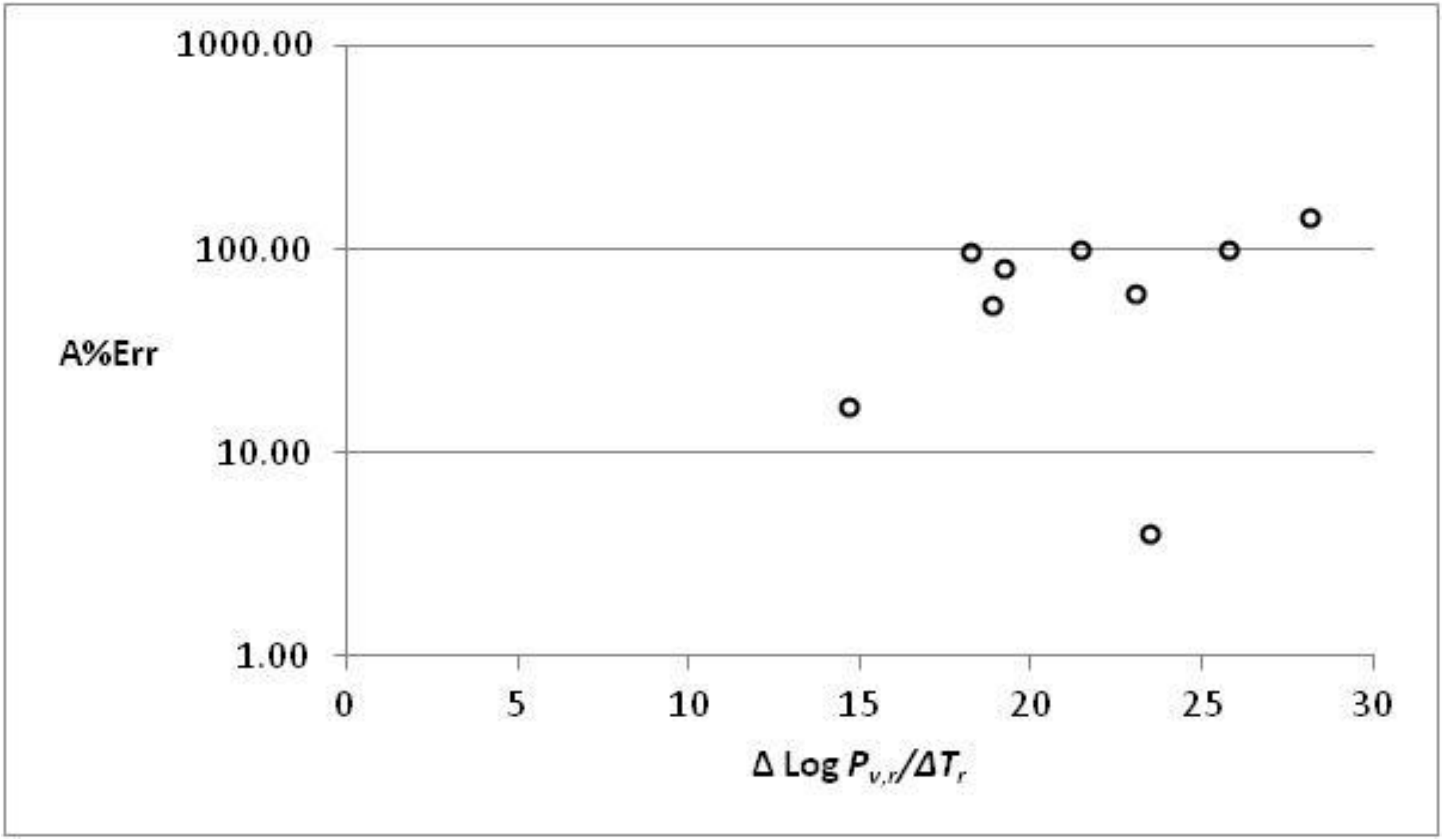

Figure D.2. A%Err @$T_{r,f}$ vs. Extrapolation Burden for Recommended Subset $F_{W,j}^{(2)}[R|R(\omega)]$ (Alcohols with $T_{r,b} < 0.7$).

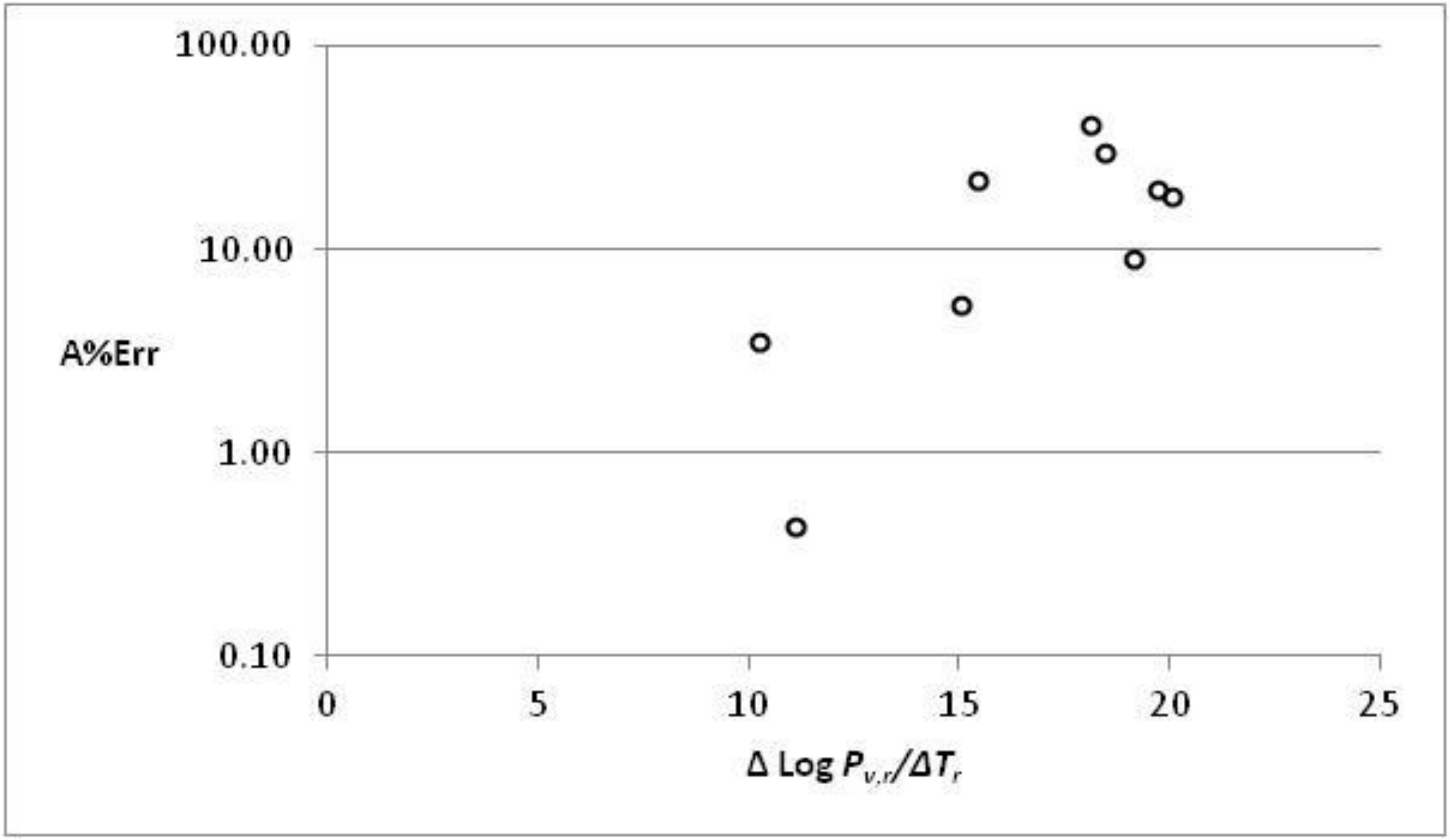

Figure D.3. A%Err @$T_{r,f}$ vs. Extrapolation Burden for Recommended Subset $F_{W,j}^{(3)}[R|R(\omega)]$ (Organic Acids).

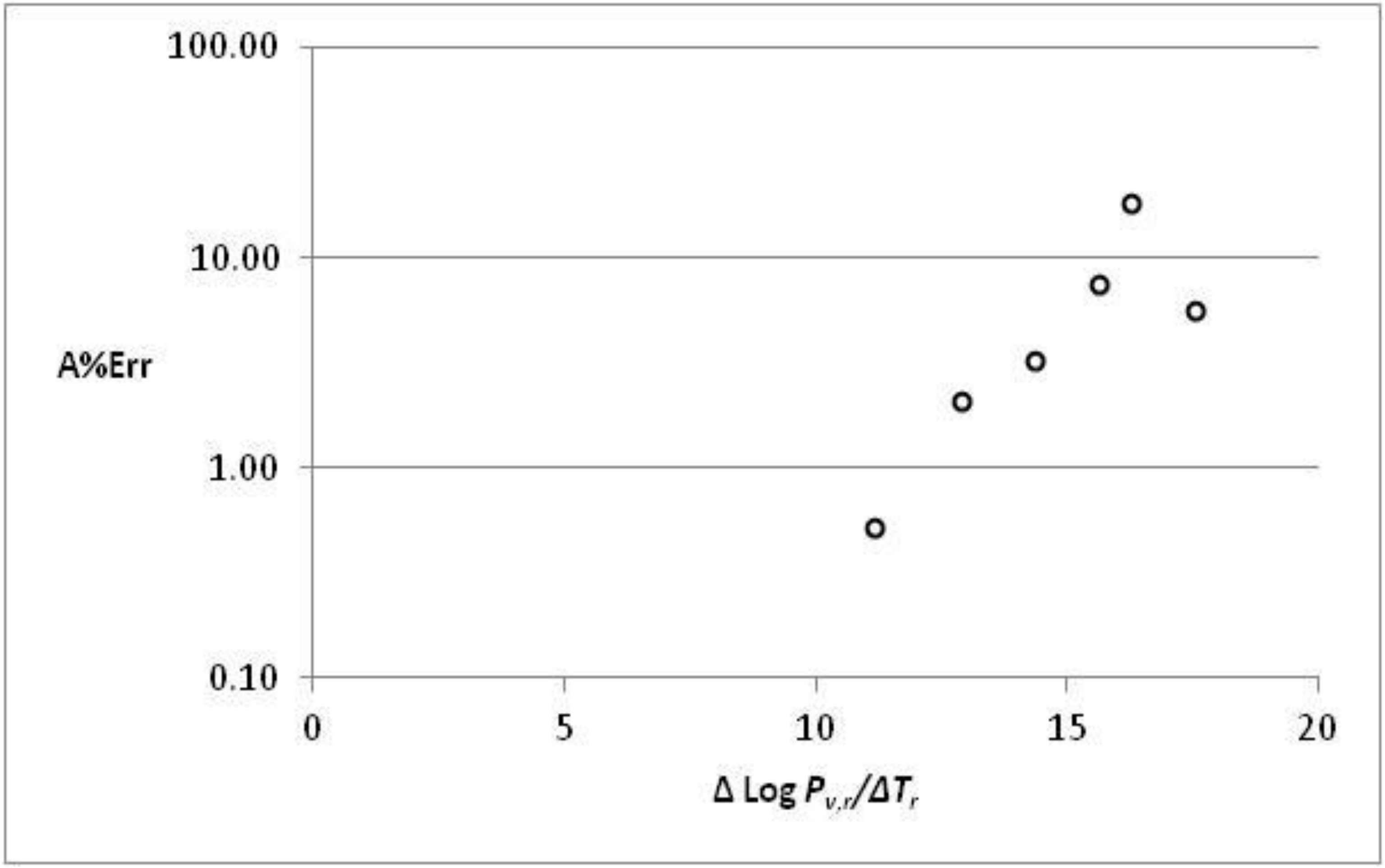

Figure D.4. A%Err @$T_{r,f}$ vs. Extrapolation Burden for Recommended Subset $F_{W,j}[R(\omega)]$ (Polar "Others" with $T_{r,b} < 0.7$).

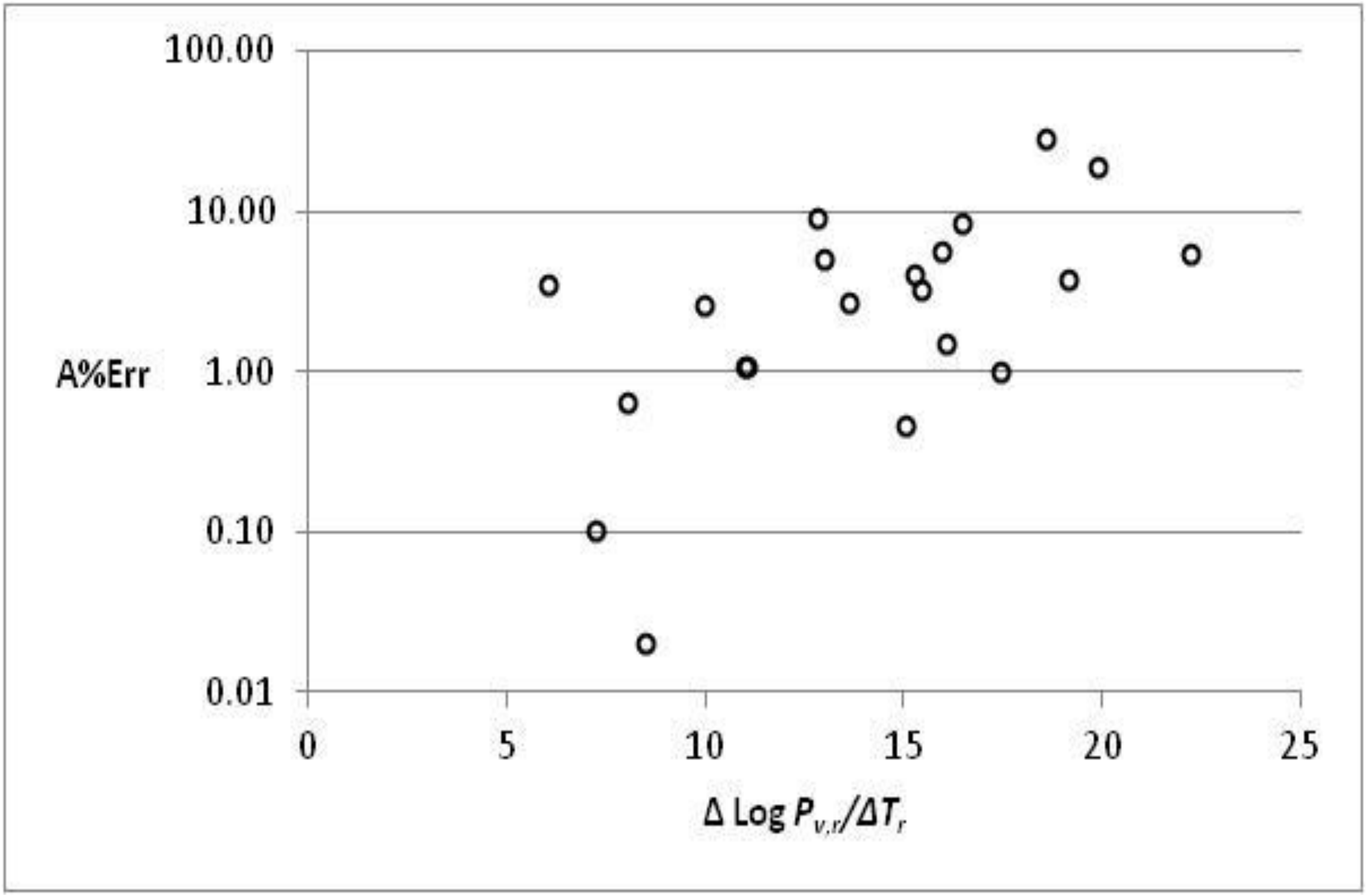

Figure D.5. A%Err @$T_{r,f}$ vs. Extrapolation Burden for Recommended Subset $F_{W,j}^{(3)}[A\text{-}W(T_b)|R(\omega)]$ (Normal "Others" with $T_{r,b} < 0.7$.