PREDICTION AND CORRELATIONS OF RESIDUAL ENTROPY OF SUPERHEATED VAPOR FOR PURE COMPOUNDS

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by

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Abstract

The calculation of the entropy (S) for gases is essential for design process equipments which involve the calculation of the heat and work requirements for industrial processes. Prediction of accurate values of residual entropy (S^R) is necessary step for the calculation of the entropy. In order to obtain accurate values of (S^R), attention has been oriented to calculate it using an **E**quation **O**f **S**tate (EOS).

In this study important equations of state as Lee-Kesler equation and Virial equation truncated to second and to third terms were used to calculate the residual entropy for pure superheated vapor. In addition to those equations, cubic equations of state represented by Soave-Redlich-Kwong (SRK), and Peng-Robison equations were also used. These EOS were tested for the available 2791 experimental data points of 20 pure superheated vapor compounds (14 pure nonpolar compounds + 6 pure polar compounds). The **A**verage **A**bsolute **D**eviation (AAD) for S^R of 2791 experimental data points of the all 20 pure compounds (nonpolar and polar) when using equations of Lee-Kesler, Peng-Robinson, Virial truncated to second and to third terms, and Soave-Redlich-Kwong were 4.0591, 4.5849, 4.9686, 5.0350, and 4.3084 J/mol.K respectively.

It was found from these results that the Lee-Kesler equation was the best (more accurate) one compared with the others, but this equation is sometimes not very preferable, because it needs more time and not easy to apply as cubic equations of state. Noted that SRK equation was the closest one in its accuracy to that of the Lee-Kesler equation in calculating the residual entropy S^R of superheated vapor, but it was developed primarily for calculating vapor-liquid equilibrium and to overcome this problem, efforts

were directed toward possibility of modifying SRK equation to increase its accuracy in predicting the residual entropy as much as possible.

The modification was made by redefining the parameter α in SRK equation to be a function of reduced pressure, acentric factor, and polarity factor for polar compounds in addition to be originally function of reduced temperature and n parameter –which is also function of acentric factor– by using statistical methods. This correlation is as follows:

$$\alpha = [1 + n(\gamma)]^2$$

$$\gamma = -0.920338 \;\; P_r^{-0.34091} + 0.064049 \;\; T_r^{4}\omega + 0.370002 \;\; \omega - P_r^{0.996932} \;\; Tr^{-4}\chi$$

This new modified correlation decreases the deviations in results obtained by using SRK equation in calculating S^R when comparing with the experimental data. The AAD for 2791 experimental data points of 20 pure compounds is 4.3084 J/mol.K while it becomes 2.4621 J/mol.K after modification. Thus SRK equation after this modification gives more accurate results for residual entropy of superheated vapor of pure 20 compounds than the rest of equations mentioned above.

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Notations

Variable Notations

Symbols		Notations	Unit
A, B	=	Constants used in the cubic equations of state, eq.(2-44) and eq. (2-51)	---------
A, B	=	Coefficients of eq.(2-92)	J/mol.K
B, B^{ig}, B^{o}	=	Any derived property, H, S, U …etc used in eq (2-8) and (2-9)	Follows property
B, B′	=	Second Virial Coefficient	cm^3/mol^2
b, c, d	=	Coefficients of eq.(2-62)	-------
C, C′	=	Third Virial Coefficient	Cm^6/mol^3
C	=	Coefficient of eq.(2-92)	K
C_p	=	Heat capacity at constant pressure	J/mol.K
g_1,g_2,..g_5	=	Coefficients of eq. (3-5)	-------
H	=	Enthalpy	J/mol
n	=	Constant used in the cubic equations of state, eq.(2-44) and eq. (2-51)	----
n	=	Coefficient of eq.(2-92)	----
P	=	Pressure	kPa
P*	=	Very low pressure where the real gas approaches ideal gas state used in eq. (2-12).	kPa
R	=	Universal gas constant	J/mol.K
S	=	Entropy	J/mol.K
T	=	Temperature	K
U	=	Internal energy	J/mol
V	=	Volume	m^3
V^o	=	Specified volume of ideal gas at T and P	m^3
Z	=	Compressibility factor	----
Z_c	=	Critical Compressibility factor	----

Abbreviations

AD	=	absolute deviations for residual entropy	J/(mol.K)
AD%	=	absolute percentage deviation for entropy	----
AD/R	=	absolute deviation for residual entropy divided by R	----
AAD	=	Average Absolute Deviation for residual entropy	J/(mol.K)
AAD%	=	Average Absolute Percentage Deviation for entropy	----

AAD/R	=	Average Absolute Deviation per R for residual entropy ----
CSP	=	Corresponding State Principle
EOS	=	Equation Of State
LK	=	Lee-Kesler equation
M.wt.	=	Molecular weight
Pt. no.	=	Point number
PR	=	Peng-Robinson equation
RK	=	Redlich-Kwong equation
Ref.	=	Reference
SRK	=	Soave-Redlich-Kwong equation
TRC	=	Thermodynamics Research Center

Greek Letters

α	=	Constant Used in cubic equations of state
α	=	Riedel's third parameter in eq. (2-35).
β	=	Parameter used in equation (2-57).
Δ	=	Difference
∂	=	Derivative
γ	=	Constant used in equation (2-57)
γ	=	Parameter used in equation (3-4)
ω	=	Acentric factor.
χ	=	Polarity factor of eq. (2-37).

Superscripts

ig	=	Ideal gas
R	=	Residual
sat.	=	Saturated state
(0)	=	Simple Fluid Equation (2-56)
(r)	=	Reference Fluid Equation (2-56)

Subscripts

b	=	Boiling point
c	=	Critical property
cal.	=	Calculated value
exp.	=	Experimental value
g	=	Gas state
l	=	Liquid state
r	=	Reduced property
r	=	Reference fluid
v	=	vaporization

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Chapter One

Introduction

Thermodynamics has been called by many “the science of energy and entropy”. However, unlike energy, the word entropy is seldom heard in everyday conversation, energy and entropy play important roles in thermal systems engineering [8, 38].

Although there are many ways to introduce the concept of entropy, the simplest is just to deal with its utility; namely: a mathematical tool to describe the direction in which things actually occur and if it occurs spontaneously or not, and it is one of the thermodynamic properties of fluids that are essential for design process equipment that calculates the heat and work requirements of industrial process [77], and also the analysis of the performance of compressors or expanders requires knowledge of the entropy behavior [73].

Neither energy nor entropy can be measured directly on energy or entropy meter, so values are usually expressed in relation to an arbitrary reference state by depending on the experimental data of another property that can be measured experimentally as **T**emperature and **P**ressure that denoted by **T** and **P** respectively [8].

One of the important ways to obtain the entropy data for pure substances at various states is the experimental data usually available in graphical or tabular forms, but for graphical it is a more complicated method to practical use comparing with the property tables that provide very accurate information about the properties simply, but they are very bulky and vulnerable to typographical errors [12] and many times some interpolations between two pressures or temperatures is needed to obtain the value of a

thermodynamic property as entropy at certain point. Also for the phase of superheated vapor it is so difficult reaching the conditions of high pressures or temperatures for many compounds in laboratory, thus a more practical and desirable approach a relation based on **E**quation **O**f **S**tate (**EOS**).

Pure gases are categorized into [70]:

1. **Nonpolar gases** which include:

a. Simple fluids with spherical molecules $\omega=0$ as Argon, Krypton,

b. Quantum gases having $\omega<0$ as He, H, and

c. Other nonpolar fluids which are having $\omega>0$ as Benzene, Propane.

2. **Polar gases** that could be subdivided into:

a. Non-hydrogen bonding compounds such as Ketones, and Aldehydes, and

b. Hydrogen bonding compounds (a bond forms between the H atom attached to Oxygen atom in one molecule with the Oxygen atom of another molecule) such as Alcohols, and Water.

In addition to acentricity, the polar compounds are characterized by the presence of dipole moment arises from positive and negative charges that are present in the molecule.

There is no precise recommended method for calculating entropy or residual entropy for superheated vapor. This work involves studying the deviation in calculated entropy values from its actual values (obtained by available experimental data for different compounds: polar and nonpolar gases) then stating which method is more suitable than the others.

The ***aim*** of the present work is to *calculate* the *residual entropy* by using (Lee-Kesler, Peng-Robinson, Virial truncated to B or to C terms, and Soave-Redlich-Kwong equations) by determining the deviation from the actual residual entropy using statistical methods to *modify* the best equation depending on the shape of particle (ω) in addition to the polarity factor (χ) for

the polar gases in order to come out with an equation that predicts the residual entropy for different types of superheated vapor of pure gases with high agreement with experimental data.

Chapter Two

Theories, Definitions, and Literature Review

2.1 General View

A major objective of any field of pure or applied science is to summarize a large amount of experimental informations with a few basic principles. The hope then is that any new experimental measurement can easily understood in terms of these established principles, and these predictions based on these principles will be accurate. The principles of thermodynamics may be summarized as four laws or axioms known as the **Zeroth, First**, **Second, and Third** laws of thermodynamics [51].

Although the formulation of these laws is simple, their implications are remarkably extensive. The **Zeroth law** deals with thermal equilibrium and the possibility of defining the concept of temperature, the **First Law** introduces the concept of internal energy and establishes the principle of conservation of energy. The **Second Law** indicates the natural direction of change of the distribution of energy and introduces the principle of increase of entropy. The concept of entropy describes quantitatively the loss in available energy in all naturally occurring transformations. Finally, the **Third Law** defines the absolute zero of entropy. These laws were deduced from experimental results gathered over centuries and there is no mathematical proof for them but, like all physical laws, thermodynamic laws are based on logical reasoning [50, 77], and the existence of entropy in each one of the laws of thermodynamics appears explicitly or implicitly.

2.2 Ideal and Real Gases

Some thermodynamic properties such as *P*ressure, *V*olume, and *T*emperature can be measured directly; whereas others such as enthalpy and entropy can be indirectly evaluated by relating the measurable properties. An equation that represents the *PVT* behavior of fluid is generally called an equation of state.

The ideal gas is a hypothetical substance that obeys the laws of Boyle and Charles:

$PV = k_1$ (Boyle's law) where k_1 = a constant at a given *T*.

$V = k_2 T$ (Charles's law) where k_2 = a constant at a given P.

Combination of these two equations leads to the relation:

$$PV = kT \tag{2-1}$$

k depends on the units, on the mass, and on the nature of gas; but if one choose one mole of a gas in all cases, then *k* becomes a universal constant independent of the nature of gas and dependent only on the units chosen for P, V, and T [50, 15], thus one can obtain the familiar equation:

$$PV = RT \tag{2-2}$$

Which is called "the ideal gas equation of state" and R is called the gas constant,

The gas constant is the same for all gases, and its value in common unit (SI unit) is 8314.4 J/ (kg-mole. K). The behavior of many fluids in the region of high temperatures and in the region of low pressures can be expressed by the ideal gas equation [12]. Because of its simplicity, the ideal gas equation of state is very convenient to use in thermodynamic calculations, but to indicate over what range of density it will hold with accuracy? Moreover, how much does an actual gas at a given pressure and temperature deviates from ideal gas behavior? The T-V diagram for water shown in Fig. 2-1 presents the approach

in answering these questions. It indicates the error in assuming ideal gas for saturated vapor and superheated vapor regions. As would be expected, at very low pressure or high temperature the error is small but this becomes severe as the density increases (volume decreases) [60].

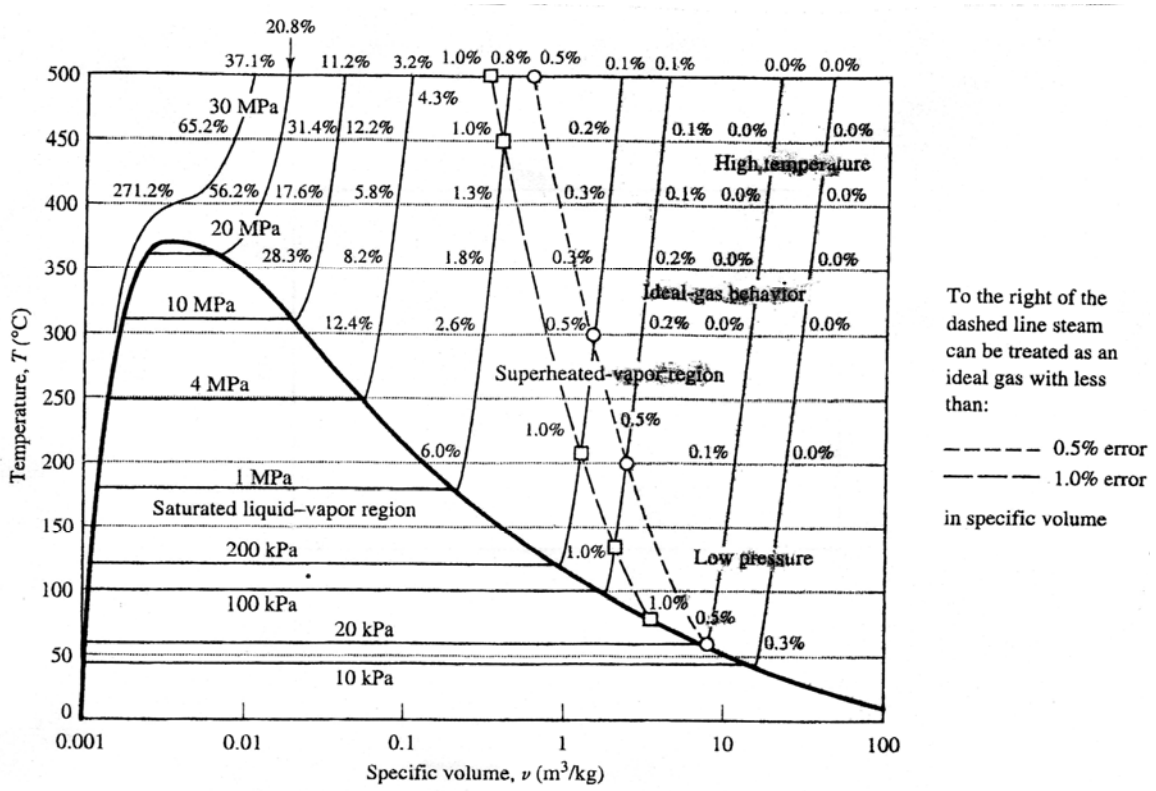

Figure 2-1 T-V diagram for water [60].

Figure 2-1 above shows that steam behaves nearly like an ideal gas at (a) a very low pressure regardless of temperature and (b) a high temperature and moderate pressure. Maximum deviation is near the critical point. It is to point out that ideal gas is hypothetical gas and can exist theoretically only at zero pressure and infinite volume.

2.3 Compressibility factor

To express the deviation of the real gas from the ideal gas the compressibility factor which denoted by Z is introduced, It is defined as the

ratio of the actual volume of the gas to the volume predicted by the ideal gas law at a given temperature and pressure [47]:

Z = actual volume / volume predicted by ideal gas law, or

$$Z = \frac{V}{\left(RT/P\right)} = \frac{PV}{RT} \tag{2-3}$$

For an ideal gas Z = 1, in real gases this seldom the case. Z generally increases with pressure and decreases with temperature. At high pressures or low temperatures, molecules are moving less rapidly and are colliding more often. This allows attractive forces between molecules to dominate, making the volume of the real gas (V_{real}) less than the volume of an ideal gas (V_{ideal}) which causes Z to drop below one. When pressures are lower or temperatures are higher, the molecules are freer to move. In this case repulsive forces dominate, making $Z > 1$. The closer the gas is to its critical point or its boiling point, the more Z deviates from the ideal case [25].

2.4 Critical and Reduced Properties

The **critical temperature**, T_c, the temperature above which distinct liquid and gas phases do not exist. The **critical pressure**, P_c, is the vapor pressure at the critical temperature, and the point at T_c and P_c is called the critical point. The critical molar volume, V_c is the volume of one mole of a substance at the critical temperature and pressure [26].

The critical point represents the state at which vapor and liquid phases in equilibrium becomes indistinguishable from one another, because their properties such as densities are identical. For a pure substance, the critical point is also the highest temperature and pressure at which liquid and vapor phases can exist in equilibrium, so it is a unique point of pressure, temperature, and volume and it is conventional to call the substance in the

superheated region: ***vapor*** if its temperature is below that of the critical point, and **gas** if it above the critical point [50, 81].

The horizontal inflection point exhibited by the critical isotherm at the critical point implies the following mathematical condition:

$$\left(\frac{\partial P}{\partial V}\right)_{T_c} = \left(\frac{\partial^2 P}{\partial V^2}\right)_{T_c} = 0 \tag{2-4}$$

Critical properties vary from substance to another, just as the case for the melting point and boiling point and these properties for many pure substances can be determined experimentally [26, 80, 45] when the critical properties are substituted in eq. (2-3) it will produce the definition of the critical compressibility factor:

$$Z_c = \frac{P_c V_c}{R T_c} \tag{2-5}$$

Z_c can be used as one of the interesting thermodynamic parameters in the prediction method of corresponding states principle, as it will be indicate later.

One of the advantages of the knowledge for the critical properties and the critical point, that they are used as basis for the PVT properties to form general scale factors. The observation of the data for different fluids, exhibits a remarkable uniformity when the thermodynamic coordinates are expressed in suitable dimensionless or reduced form. This fact is the basis for the most generalized correlation which called the theorem of corresponding states [57].

$$\left.\begin{aligned} T_r &= \frac{T}{T_c} \\ P_r &= \frac{P}{P_c} \\ V_r &= \frac{V}{V_c} \end{aligned}\right\} \tag{2-6}$$

2.5 Reference State and Reference Values

The values of thermodynamic properties as enthalpy, and entropy given in the property tables are not obtained by direct measurement but are calculated from other data that can be more readily determined experimentally. Since thermodynamics deal very largely with such properties that have no known absolute values and therefore be concerned with differences of the property between two states. When it gives numerical values of properties of substances and systems; it would be convenient to regard certain states of a substance as reference, or standard, states and the values of properties at these states are considered reference values [16].

The choice of a standard state is purely arbitrary and may vary, depending on the application in question. In many cases, the standard state refers only to an initial state of pressure or concentration along an isotherm and has no reference to any particular temperature. In other cases, a certain temperature is also selected. Thus, in giving values of certain thermodynamic functions such as enthalpy or entropy, the value of the function is considered to be zero at a reference state of 0^{o} C and 1 atm absolute pressure, when the substance is in a state of aggregation that is the commonest one at room temperature, though one may, in special instances, prefer to use other reference states. However, the difference in property between any two states is precisely the same regardless of the datum selected, because the datum cancels in the calculation. A simple standard state would be that of the substance when pure at the given temperature and at pressure of 1 atm, but owing to the fact that only very limited data are available for some compounds so that one can choose satisfactory state depending on the case of the question to be the reference state of calculations [16, 39].

2.6 Superheated Vapor

In the region to the right of the saturated vapor line as in Fig. 2-1, when the vapor is at a temperature greater than the saturation temperature corresponding to the given pressure, it is said to exist as **superheated vapor**, and would be attained by further heating while keeping the pressure constant. Since the superheated region is a single-phase region (vapor phase only), the temperature and pressure of superheated vapor are independent properties, so the temperature may increase while the pressure remains constant. Actually the substances that are called gases are highly superheated vapors [60, 39].

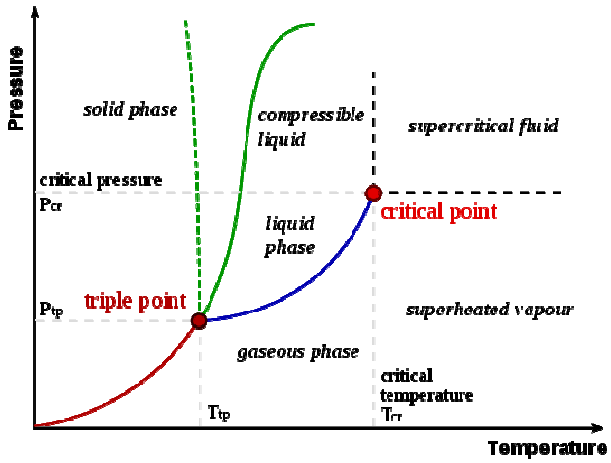

Figure 2-2 A typical phase diagram. The dotted green line gives the anomalous behavior of water [26].

Superheated vapor is characterized by [12]:

Lower pressures ($P < P_{sat}$ at a given T)

Higher temperatures ($T > T_{sat}$ at a given P)

Higher specific volumes ($V > V_g$ at a given P or T)

Higher internal energies ($U > U_g$ at a given P or T)

Higher enthalpies ($H > H_g$ at a given P or T)

Higher entropies ($S > S_g$ at a given P or T)

2.7 Entropy for a Real Gas and Residual Entropy

The concept of entropy was first suggested by the German physicist Clausius. Entropy was conceived as a measure of the change in the ability of the universe to produce work in the future, as a result of past or presently occurring transformations or processes. Also, it will be regarded primarily as a mathematical function that offers the simplest means of making quantitative application of the second law which is merely a generalized statement of experience with spontaneous processes or of tendency of change, also Entropy is a measure of the number of "random" states in which molecules store energy [8, 5]. The calculation of entropy requires knowledge of energy states of molecules. Initially it was considered in a purely macroscopic sense and was related quantitatively to heat, work, and temperature [8].

The entropy of a real gas is a function of two properties, such as temperature and pressure, thus the entropy of a real gas may be expressed as:

$$S = S(T, P) \tag{2-7}$$

Thermodynamic manipulations yield the property changes for the molecular transformations in terms of *departure functions* or *residual functions*. Residual entropy is a thermodynamic property, which depends on the positions of the molecules relative to one another, where In the ideal gas state they are effectively infinitely far apart and therefore a residual property is a property relative to what it would be in the ideal gas state at the same temperature T, pressure P, and composition [2]. Sometime it is convenient to define a residual property as a property relative to ideal gas state at the same T, V and x. In the zero-pressure or infinite-volume limit, all models must give zero for the departure (residual) functions. In the critical region, only those equations that give nonclassical behavior can be satisfactory [45]. There are two equivalent formulations of the departure function:

$$B(T,P) - B^{ig}(T,P) = B(T,P) - B^{o}(T,P) \tag{2-8}$$

$$B(T,V) - B^{ig}\left(T,V^{o}\right) = B(T,V) - B^{o}\left(T,V^{o}\right) \tag{2-9}$$

Where B is any derived property, H, S, U …etc and $V^o = RT/P$ is the specified volume of ideal gas at T and P. So, the residual entropy or entropy departure is a measure of deviation of actual entropy from ideal gas entropy, i.e.

$$S^{R} = S - S^{ig} \tag{2-10}$$

Note that S^{ig} is the entropy of ideal gas. Qualitatively, Fig. 2-3 illustrates how departure functions vary as a function of pressure at a specific temperature [66]:

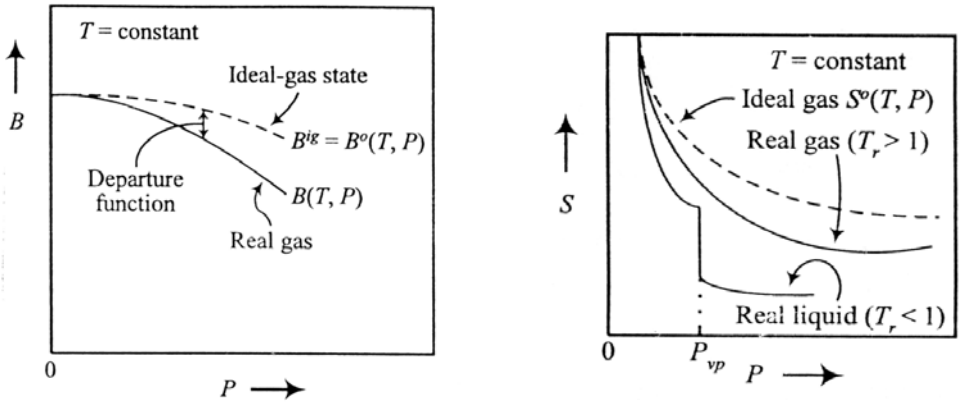

Figure 2-3 Qualitative illustration of isothermal departure function variation with pressure [66].

The starting point for the development of expressions for the residual entropy is the Maxwell relation,

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V \qquad \text{or} \qquad dS = \left(\frac{\partial P}{\partial T}\right)_V dV \tag{2-11}$$

Since the entropy of even ideal gases depends on pressures and becomes infinite as $P \rightarrow 0$ or $V \rightarrow \infty$, the residual property cannot be obtained by direct integration of eq. (2-11). In order to circumvent this problem, it requires a transformation of the integrand $(\partial P/\partial T)_V$ to $((\partial P/\partial T)_V - R/V)$ by using the following identity:

$$\int_{V(T,P_o)}^{V(T,P)} \frac{R}{V} dV = \int_{V(T,P_o)}^{V(T,P^*)} \underset{(ideal)}{\frac{R}{V} dV} + \int_{V(T,P^*)}^{V(T,P)} \underset{(real)}{\frac{R}{V} dV} \tag{2-12}$$

Where P_o is a reference pressure on ideal gas path and P^* is a very low pressure where the real gas approaches ideal gas state.

It should be noted that the integration of the left side of eq. (2-12) results in:

$$\int_{V(T,P_o)}^{V(T,P)} \frac{R}{V} dV = \int_{V^{ig}}^{V} \frac{R}{V} dV = R \ln \frac{V}{V^{ig}} = R \ln \frac{ZRT/P}{RT/P_o} = -R \ln \frac{ZP}{P_o} \tag{2-13}$$

Now, Integrating eq. (2-11) from *V (T, P_o)* to *V (T, P^*)* along ideal gas path and then from *V (T, P^*)* to *V (T, P)* along real gas path gives:

$$S - S_o^{ig} = \int_{V(T,P_o)}^{V(T,P^*)} \underset{(ideal)}{\left(\frac{\partial P}{\partial T}\right)_V} dV + \int_{V(T,P^*)}^{V(T,P)} \underset{(real)}{\left(\frac{\partial P}{\partial T}\right)_V} dV \tag{2-14}$$

Combining equations (2-12), (2-13) and (2-14) gives:

$$S - S_o^{ig} + R \ln \frac{P}{P_o} = -R \ln Z + \int_{V(T,P_o)}^{V(T,P^*)} \underset{(ideal)}{\left[\left(\frac{\partial P}{\partial T}\right)_V - \frac{R}{V}\right]} dV + \int_{V(T,P^*)}^{V(T,P)} \underset{(real)}{\left[\left(\frac{\partial P}{\partial T}\right)_V - \frac{R}{V}\right]} dV \tag{2-15}$$

Now, *V (T, P^*)* can be safely replaced by ∞, as the integrands no longer are infinite at P = 0 (or at V = ∞). The first right-side integrand vanishes, because the integrand is zero as it is known for ideal gas $P = RT/V$ and when differentiating this equation with respect to T at constant V, and combining the resulting equation with it gives:

$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{V} \tag{2-16}$$

Thus, eq. (2-15) reduced to the following when divided through by R:

$$\frac{S - S_o^{ig}}{R} + ln\frac{P}{P_o} = -ln\,Z + \frac{1}{R}\int_{\infty}^{V}\left[\left(\frac{\partial P}{\partial T}\right)_V - \frac{R}{V}\right]dV \qquad (2\text{-}17)$$

The value of S_o^{ig} depends on P_o, for which 1 atmosphere is usually chosen.

With volume explicit equation, the starting point is another Maxwell relation:

$$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P \qquad (2\text{-}18)$$

When this is combined with the corresponding expression for an ideal gas, and integrating the result by manner approximately similar to that for deriving the equation of residual entropy that is pressure explicit equation obtain the next volume explicit equation[18, 73]:

$$\frac{S - S_o^{ig}}{R} + \ln\frac{P}{P_o} = \frac{1}{R}\int_0^P\left[\frac{R}{P} - \left(\frac{\partial V}{\partial T}\right)_P\right]dP \qquad (2\text{-}19)$$

An attractive alternative to the numerical evaluation of integrals in eq. (2-19) is their analytical evaluation by equations of state. This requires an equation which can be directly solved for Z (or V) as a function of P at constant T. such an equation of state is said to be *volume explicit*, the other equations of state are said to be *pressure explicit*; i.e. they can be solved for Z (or P) as a functions of V at constant T [57].

The subsequent sections will partake of explaining the method of calculating the residual entropy by some of the important equations of state.

To evaluate the entropy for a real gas; one can return to the original relation of the entropy for a real gas as expressed before by eq. (2-8):

$$S = S(T, P) \qquad (2\text{-}7)$$

Moreover, its differential is:

$$dS = \left(\frac{\partial S}{\partial T}\right)_P dT + \left(\frac{\partial S}{\partial P}\right)_T dP \tag{2-20}$$

The first term of eq. (2-20) is the heat capacity at constant pressure divided by temperature that can be derived from:

$$H = U + PV \quad \rightarrow \quad dH = dU + PdV + VdP \tag{2-21}$$

and $$dU = TdS - PdV \tag{2-22}$$

By combining the two last equations:

$$dH = TdS + Vdp \tag{2-23}$$

The isobaric form of eq. (2-23) is:

$$\left(\frac{\partial H}{\partial S}\right)_P = T \tag{2-24}$$

And the isobaric effect of temperature on the enthalpy is by definition, the heat capacity at constant pressure, i.e.

$$\left(\frac{\partial H}{\partial T}\right)_P = C_P \tag{2-25}$$

Combining these two equations (2-24) and (2-25) gives the following expression for isobaric effect of temperature on the entropy:

$$\left(\frac{\partial S}{\partial T}\right)_P = \frac{C_P}{T} \tag{2-26}$$

And the second term of eq. (2-20) is to be found from the Maxwell relation that used before by eq (2-18):

$$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P \tag{2-18}$$

When substituting eqs. (2-26) and (2-18) in eq. (2-20) gives:

$$dS = \frac{C_P}{T} dT - \left(\frac{\partial V}{\partial T}\right)_P dP \tag{2-27}$$

and from the ideal gas equation $PV = RT \rightarrow V/T = R/P$, so when applying eq. (2-27) for ideal gas gives:

$$dS^{ig} = \frac{C_P}{T}dT - \frac{R}{P}dP \tag{2-28}$$

General expression for S^{ig} is found by integration of eq. (2-28) from an ideal gas state at reference conditions T_0 and P_0 to the ideal-gas state at T and P:

$$S^{ig} = S_0^{ig} + \int_{T_0}^{T} C_P^{ig}\frac{dT}{T} - R\ln\frac{P}{P_0} \tag{2-29}$$

From eq. (2-10) one can obtain $S = S^{ig} + S^R$ then substituting eq. (2-29) in it gives:

$$S = S_0^{ig} + \int_{T_0}^{T} C_P^{ig}\frac{dT}{T} - R\ln\frac{P}{P_0} + S^R \tag{2-30}$$

The generalized correlations for S^R, together with ideal-gas heat capacities, allow calculation of entropy values of gases at any T and P by eq. (2-30). For a change from state 1 to state 2, by writing eq. (2-30) for both states:

$$\left.\begin{aligned} S_1 &= S_0^{ig} + \int_{T_0}^{T_1} C_P^{ig}\frac{dT}{T} - R\ln\frac{P_1}{P_0} + S_1^R \\ S_2 &= S_0^{ig} + \int_{T_0}^{T_2} C_P^{ig}\frac{dT}{T} - R\ln\frac{P_2}{P_0} + S_2^R \end{aligned}\right\} \tag{2-31}$$

The entropy change for the process, $\Delta S = S_2 - S_1$, is the difference between these two equations:

$$\Delta S = \int_{T_1}^{T_2} C_P^{ig}\frac{dT}{T} - R\ln\frac{P_2}{P_1} + S_2^R - S_1^R \tag{2-32}$$

If one needs to calculate the entropy change between two states when the first state is the reference state at reference conditions T_0 and P_0 which is selected –as it common in many references– at saturated liquid and the second state is at certain T and P then it is necessary to add a new term to the preceding equation to estimate the transformation of saturated liquid into the

saturated vapor at this initial condition which represents the entropy of vaporization (ΔS_v), and eq. (2-32) becomes [50, 57, 30]:

$$\Delta S = \Delta S_v + \int_{T_1}^{T_2} C_P^{ig} \frac{dT}{T} - R \ln \frac{P_2}{P_1} + S_2^R - S_1^R \qquad (2\text{-}33)$$

2.8 (P-V-T) Behavior of Pure Fluids and the Law of Corresponding States Principle (CSP)

The physical and thermodynamic data of chemical compounds and their mixtures are needed for efficient design and operation of chemical processing plants. Because experimental determination of all required data is a formidable proposition, it is usual practice to predict these data by the use of suitable correlations. Of the many creational approaches that have been proposed, the **C**orresponding **S**tates **P**rinciple that denoted always by (**CSP**) has proved to be the most powerful framework for predicting configurational properties of fluids and the best aid in summing up the (P-V-T) behavior [65, 13]. It asserts that suitably dimensionless properties of all substances will follow universal variations of suitably dimensionless variables of state and other dimensionless quantities. The number of parameters characteristic of the substance determines level of CSP [45].

2.8.1 Two-Parameter Corresponding States Principle

Both the van der Waals and Redlich- Kwong (RK) equations of state have been written in the form:

$$Z = f(T_r, P_r) \qquad (2\text{-}34)$$

Expressions such as (2-34) are known as generalized equations, because of their general applicability to all substances. This functional relationship was first recognized by van der Waals in 1873. Thus the prediction of unique

relationship among Z, T_r, and P_r is known as the van der Waals two-parameter theorem of corresponding states. It states that any pure gases at the same reduced temperature and pressure should have the same compressibility factor. Since the van der Waals and RK equations apply to both the liquid and gas phases, the theorem expressed by eq. (2-34) should also apply to both single phases, up to and including the saturated vapor and saturated liquid states [74].

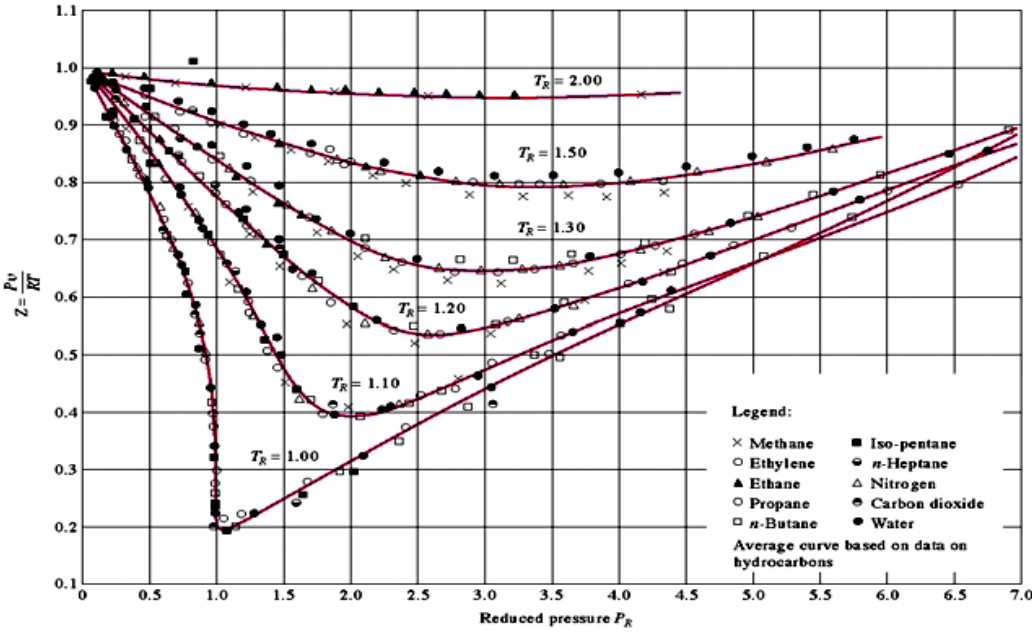

Figure 2-4 Experimental data for Z vs. P_r with T_r as a parameter for different gases [5, 64].

The form of the CSP that involves only two independent parameters is the simplest form and accurately characterizes the behavior of simple mono atomic molecules, that is, molecules with spherically symmetric force fields. The two- parameters CSP led to important generalization of thermodynamic properties, but as more experimental data became available, a great many fluids of non- spherical molecules were found to deviate from this principle. This has necessitated a "third parameter" to account for the deviation [18].

2.8.2 Three-Parameter Corresponding States Principle

The addition of a third parameter extends the practical applicability of the principle to non-polar non-spherical fluids (non-polar gases, for example, inert gases and hydrocarbons, are characterized by a zero dipole moment). A variety of third parameters have been suggested and used in the past [65]:

2.8.2.1 Critical compressibility factor

In 1951, Meissner and Seferian first proposed the use of critical compressibility factor as a third parameter. They have correlated the compressibility factor with T_r, P_r and Z_c using Z_c= 0.27 as a reference. The usefulness of Z_c as a third parameter was again demonstrated by Lydersen et al. [35] in their thermodynamic property correlations [18].

In actuality, the critical compressibility factor can vary greatly between substances. This would suggest that utilizing *Zc* as a third parameter could increase the accuracy of the principle of corresponding states. To calculate *Zc*, V_c must be known. Unfortunately, since the differential compressibility, $(\partial V/\partial P)_T$, approaches infinity at the critical point, the critical volume cannot be accurately measured, and so there is some advantage in avoiding the use of *Zc* [51].

2.8.2.2 Riedel's Parameter

Riedel [18] observed in 1954 that the slope of reduced vapor pressure of a fluid at the critical point could be effectively used to describe the deviation from that of spherical molecular fluids. The observation resulted in a third parameter which is defined as:

$$\alpha_c = \frac{\partial \ln P_r^s}{\partial \ln T_r} = \frac{\partial P_r^s}{\partial T_r} \qquad \text{(At critical point)} \qquad (2\text{-}35)$$

P_r^s is the reduced vapor pressure. The following year, basically the same

parameter was independently introduced by Martin and Hou in 1955[1] in their development of an equation of state.

2.8.2.3 Acentric factor

In this same year in 1955 Pitzer [44] observed that the reduced vapor pressures of molecules with acentric force fields are lower than that of simple fluids; and the difference is greater for molecules of greater acentricity. Pitzer noted that all vapor pressure data for the simple fluids (Ar, Kr, and Xe) lie on the same line when plotted as $\log_{10} P_r^{sat}$ vs. $1/T_r$ and that the line passes through $\log_{10} P_r^{sat} = -1.0$ at $T_r = 0.7$. This is illustrated in Fig. 2-5. Data for other fluids define other lines whose location can be fixed in relation to the line of simple fluids. Thereupon, Pitzer defined the acentric factor ω (a third parameter) of a substance by [57]:

$$\omega = -1 - \log_{10}\left(P_r^s\right)_{T_r=0.7} \tag{2-36}$$

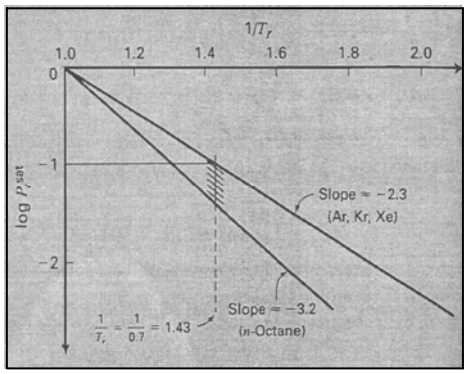

Figure 2-5 Approximate temperature dependence of the reduced vapor pressure [57].

Therefore ω can be determined for any fluid from Tc, Pc, and a single vapor-pressure measurement was made at Tr = 0.7 which is near the normal boiling point of most substances, so the importance of choosing Tr = 0.7 that was adopted by Pitzer not only provides numerical simplicity ($\log_{10} P_r^{sat} = -1$

[1] As cited in reference (Martin, J. J. and Hou, Y. C., AIChE J., 142 (1955)).

for simple fluids) but also beneficial because vapor-pressure data are most commonly available at pressure near atmospheric [57].

Among the third parameters proposed, Pitzer's acentric factor has gained widest acceptance in both academic and industrial areas, because it is of a simple extension of two-parameter corresponding states principle and calculated from experimental data that tend to be accurate as well as accessible and gives good accuracy for normal fluids (nonpolar and weakly polar substances) including hydrocarbons [18,46].

As originally proposed, ω represents the acentricity or nonsphericity of a molecule. For monatomic gases (Ar, Kr, Xe), ω is, therefore, essentially zero and for quantum gases (H_2, He, Ne) and a few others (*e.g.*, Rn) $\omega < 0$. For methane it is still very small. However, for all other species such as higher molecular-weight hydrocarbons ω increases and it is positive values up to 1.5. It also rises with polarity. At present, ω is very widely used as a parameter, which in some manner is supposed to measure the complexity of a molecule with respect to both the geometry and polarity, but the large values of ω for some polar compounds ($\omega > 0.4$) are not meaningful in the context of the original meaning of this property [45, 49]. With three parameter (P_r, T_r, and ω), the principle of corresponding states becomes highly accurate for subcooled and superheated nonpolar and slightly polar substances [54].

2-8-3 Four- Parameter Corresponding States Principle

Polar compounds are characterized by a nonzero dipole moment μ which expresses the effect of electrostatic forces between molecules because it is resulting when the electrical center of a bond does not coincide with its center of mass. Polarity is defined as a magnitude of a dipole moment expressed in debye units (1 debye = 3.162×10^{-25} $(J.m^3)^{1/2}$) as a rough rule [73, 70].

The Pitzer three-parameter CSP excludes systems containing highly polar species and species exhibiting specific interactions like hydrogen bonding. Several attempts have been made to formulate a four-parameter CSP applicable to polar fluid. Notable one among these was the work of Halm and Stiel [23]

2-8-3-1 Polarity Factor of Halm and Stiel

Because the vapor pressure formed the basis for the definition of the acentric factor, this property was chosen as the starting point for the extension of the normal fluid approach to polar fluids to obtaining polarity factor χ which is an empirical parameter for polar substances similar to the acentric factor for normal fluids. The factor χ is defined to be zero for normal fluids and can be expressed for polar fluids as follows:

$$\chi = \log P^s{}_r \Big|_{T_r = 0.6} + 1.552 + 1.7\omega \qquad (2\text{-}37)$$

Values of χ can be obtained from the literatures [23, 31] for some polar compounds. The values of ω, T_c, P_c and χ for number of nonpolar and polar compounds are listed in appendix A.

2.9 Equations of State

The most convenient method of representing the properties or the behavior of a substance, is by a mathematical expression; that is, an equation which represent the (P-V-T) behavior of a fluid. A general form of such an expression is:

$$f(P,V,T) = 0 \qquad (2\text{-}38)$$

This is known as an equation of state (EOS). This is the most convenient way of a large amount of data in a form which is highly useful [47]. A good equation of state is perhaps the best method for handling of (P-V-T) data. More importantly, it provides a most efficient and versatile means of

expressing various thermodynamic functions in terms of (P-V-T) data and make it possible to represent phase equilibria in a compact analytical form. Despite the abundance of such equations of state, and although there have been efforts to establish mathematical forms of equations of state for over 100 years, a truly satisfactory and not-too-complex solution remains to be developed for wide ranges of temperature, pressure, composition -for mixtures- and molecular variety that are very helpful for areas of interest in scientific and engineering applications [18, 4].

The type of equation of state may be written for a pure fluid as:

- Volume explicit form,

$$\left.\begin{array}{l} V = V(P,T) \\ \text{Or} \\ V = \dfrac{RT}{P} Z(P,T) \end{array}\right\} \qquad (2\text{-}39)$$

- Pressure explicit form,

$$\left.\begin{array}{l} P = P(V,T) \\ \text{Or} \\ P = \dfrac{RT}{V} Z(V,T) \end{array}\right\} \qquad (2\text{-}40)$$

- Z - explicit form,

$$Z = Z(T,V) \qquad (2\text{-}41)$$

While, for a mixture of n-components, there are a further independent composition variables. The virial equation is the only common example of a volume-explicit EOS, and the Pitzer-Curl and Lee-Kesler of the *Z*-forms, where there are some common equations of state of pressure-explicit form as van der Waals, Redlich-Kwong, and other cubic equations of state (in which P is given by a cubic function of V) [73, 7]. Equations of state which express Z as a function of T_r and P_r are said to be *generalized*, because of their general

applicability to all gases and liquids. Any equation of state can be put into this form to provide a generalized correlation for the properties of fluids. This allows the estimation of property values from very limited information [57].

For process calculations particularly in petroleum and cryogenic technology, cubic equations of state have proved to be extremely useful. They are simple and can be solved with a straightforward algebraic procedure, so that they lead to robust computer programs for the prediction of thermodynamic data and to relatively short computing times [24].

Many equations of state can represent adequately the properties of the gas phase, some are applied only to the liquid, but the most important category of EOS models contains those that may be applied in the same form to both gaseous and liquid phases. There are no equations of state applicable simultaneously to solid, liquid and gas [7].

Different equations of state have been proposed; the most important equations those are used to calculate S^R in this work are:

2.9.1 Soave-Kwong-Redlich (*SRK*) Equation

Although Redlich-Kwong (*RK*) equation of state [48] which can be considered a modification of the simplest and oldest equation of van der Waals is the one that perhaps received most attention in the last years in the crowd of equations that proposed, but its accuracy when compares with equations containing many more constants regarded very well only when applied to non-polar rather simple fluids. This is because the parameters of *RK* equation are based entirely on the two critical constants T_c and P_c and do not incorporate the acentric factor [7, 55]. Therefore, Soave [59] in 1972 introduced a modification on the *RK* equation of state which has been very successful in extending the applicability of *RK* equation to be applied with

high accuracy for wide range of non-polar and slightly polar components [71, 58]. The temperature dependent term $a/T^{0.5}$ of the *RK* equation was altered to include both the temperature and the acentric factor by Soave; the *SRK* equation is [7]:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)} \tag{2-42}$$

Where the factor α is an empirical function determined from the vapor-pressure data of pure hydrocarbons [74].

The *SRK* equation for residual entropy is:

$$\frac{S^R}{R} = \ln[Z-B] - \frac{BD}{a\alpha A}\ln\left(1+\frac{B}{Z}\right) \tag{2-43}$$

The cubic form in terms of compressibility factor is:

$$Z^3 - (1-B)Z^2 + (A - B^2 - B)Z - AB = 0 \tag{2-44}$$

Where $A = 0.42747\alpha\frac{P_r}{T_r^2}$ $\qquad B = 0.08664\frac{P_r}{T_r}$ (2-45)

$$a = 0.42747\frac{R^2T_c^2}{P_c} \qquad b = 0.08664\frac{RT_c}{P_c} \tag{2-46}$$

$$\alpha = \left[1+n\left(1-T_r^{0.5}\right)\right]^2 \qquad n = 0.48508 + 1.55171\omega - 0.1561\omega^2 \tag{2-47}$$

and $D = na\sqrt{\alpha T_r}$ (2-48)

2.9.2 Peng-Robinson (*PR*) Equation

The equation of Peng and Robinson in 1976 [43] is structurally rather similar to the *SRK* and, like the *SRK*, requires only the critical constants and the acentric factor for its application for a pure fluid. This equation of state was developed primarily for vapor liquid equilibrium predictions. Peng-Robinson modified the standard form as follows [7]:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)+b(V-b)} \tag{2-49}$$

The *SRK* equation for residual entropy is:

$$\frac{S^R}{R} = ln[Z-B] - \frac{BD}{2.828\ a\alpha\ A} ln\left(\frac{Z+2.414B}{Z-0.414B}\right) \tag{2-50}$$

The cubic form in terms of compressibility factor is:

$$Z^3 - (1-B)Z^2 + (A-3B^2-2B)Z - (AB-B^2-B^3) = 0 \tag{2-51}$$

Where $A = 0.45724\alpha \frac{P_r}{T_r^2}$ $\qquad B = 0.07780 \frac{P_r}{T_r}$ (2-52)

$$a = 0.45724 \frac{R^2 T_c^2}{P_c} \qquad b = 0.07780 \frac{RT_c}{P_c} \tag{2-53}$$

$$\alpha = \left[1 + n\left(1 - T_r^{0.5}\right)\right]^2 \qquad n = 0.37464 + 1.5422\omega - 0.26992\omega^2 \tag{2-54}$$

also, $D = na\sqrt{\alpha T_r}$ (2-48)

2.9.3 Lee-Kesler Equation

Lee and Kesler in (1975) [32] developed an analytical correlation, based on Pitzer's three-parameter corresponding states principle [44] to provide increased accuracy and covering the whole range of T_r and Pr of practical interest in hydrocarbon processing. It is to be noted that the original correlations by Pitzer et al., were limited to reduced temperatures above 0.8. Pitzer et al. correlations for the compressibility factor of a fluid whose acentric factor is ω is given by the following equation:

$$Z = Z^{(0)} + \omega Z^{(1)} \tag{2-55}$$

Where $Z^{(0)}$ is the compressibility factor of a simple fluid and $Z^{(1)}$ corrects $Z^{(0)}$ for the effects of nonspherical intermolecular forces (primarily dispersion and overlap) [71]. $Z^{(0)}$ and $Z^{(1)}$ are assumed functions of T_r and Pr. However, Lee and Kesler found that the compressibility factor of any fluid is a function of

the compressibility of a simple fluid ($Z^{(0)}$), the compressibility of a reference fluid ($Z^{(r)}$), and the acentric factor, where $Z^{(0)}$ and $Z^{(r)}$ are functions of T_r and Pr and the correlation of Lee and Kesler takes the form:

$$Z = Z^{(0)} + \frac{\omega}{\omega^r}\left(Z^{(r)} - Z^{(0)}\right) \tag{2-56}$$

Where $\omega^r=0.3978$ and it is the acentric factor for reference fluid, and the correction term $Z^{(1)}$ in eq. (2-56) is obviously equivalent to $(Z^{(r)}- Z^{(0)}) / \omega^r$ this expression is convenient since both $Z^{(r)}$ and $Z^{(0)}$ are given by the same equation with, however, different constants. Lee and Kesler chose n-octane as the heavy reference fluid since it is the heaviest hydrocarbon for which there are accurate (P-V-T) and enthalpy data over a wide range of conditions [32, 33].

The function for both the simple fluid $Z^{(0)}$ and the reference fluid $Z^{(r)}$ are derived through a combination of experimental data and a reduced form of the modified Benedict-Webb-Rubin [9] equation of state with a different set of constants that are scheduled in table 2-1.

$$Z = \left(\frac{P_r V_r}{T_r}\right) = 1 + \frac{B}{V_r} + \frac{C}{V_r^2} + \frac{D}{V_r^5} + \frac{c_4}{T_r^3 V_r^2}\left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right) \tag{2-57}$$

$$B = b_1 - \frac{b_2}{T_r} - \frac{b_3}{T_r^2} - \frac{b_4}{T_r^3} \tag{2-58}$$

$$C = c_1 - \frac{c_2}{T_r} + \frac{c_3}{T_r^3} \tag{2-59}$$

$$D = d_1 + \frac{d_2}{T_r} \tag{2-60}$$

Table 2-1 Constants for Calculating equation (2-57) [32]

constants	Simple Fluid (0)	Reference Fluid (r)
b_1	0.1181193	0.2026579
b_2	0.265729	0.331511
b_3	0.15479	0.027655
b_4	0.030323	0.203488
c_1	0.0236744	0.0313385
c_2	0.0186984	0.0503618
c_3	0.0	0.016901
c_4	0.042724	0.041577
$d_1 \times 10^4$	0.155488	0.48736
$d_2 \times 10^4$	0.623689	0.0740336
β	0.65392	1.226
γ	0.060167	0.03754

For calculating Z for the fluid of interest given at T and P, first the appropriate values of T_r (T/T_c) and P_r (P/P_c) are calculating by using critical properties of the fluid. From the simple fluid constants in Table 2-1 and eq. (2-57) solving for V_r –which is not the correct reduced volume for the fluid of interest, but rather a pseudo-reduced volume– by the trial and error method when V_r is defined as (P_cV/RT_c), which can be considered the initial guess for the calculation, or from the first equality of eq. (2-57) the initial guess can be taken as:

$$V_r = Z\frac{T_r}{P_r} \tag{2-61}$$

the previous equation was depended by Paul and Francis [42] in preparing their computer program for the tables of Lee and Kesler[2]. After trial and error calculation the obtained value of $V_r = V_r^{(0)}$ for simple fluid and when employed in the first equality of eq. (2-57), $Z^{(0)}$ is calculated for simple fluid. This process is then repeated using the reference fluid constants with the same

[2] Paul and Francis [42] took the initial guess for Z of eq. (2-62) equal to 0.2 but for this search which concentrates on the vapor phases especially superheated vapor the initial Z value taken equal to 1 because for vapor phases at high reduced temperatures and pressures the Z value often more than unity [45].

T_r and Pr values of the fluid of interest to find $V_r = V_r^{(r)}$ and $Z^{(r)}$ for the reference fluid. Finally, with $Z^{(0)}$ from the first calculation and from $Z^{(r)}$ from the second, the compressibility factor Z for the fluid of interest is determined from eq. (2-56) [32].

The residual entropy is derived from eq. (2-57):

$$\frac{S - S^{ig}}{R} + \ln\left(\frac{P}{P^*}\right) = \ln(Z) - \frac{b_1 + \left(b_3 / T_r^2\right) + \left(2b_4 / T_r^3\right)}{V_r} - \frac{c_1 - \left(2c_3 / T_r^3\right)}{2V_r^2} - \frac{d_1}{5V_r^5} + 2E \qquad (2\text{-}62)$$

Where: $$E = \frac{c_4}{2T_r^3\gamma}\left\{\beta + 1 - \left(\beta + 1 + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right)\right\} \qquad (2\text{-}63)$$

After determining $V_r^{(0)}$ and $Z^{(0)}$ for the simple fluid at the T_r and P_r appropriate for the fluid of interest, and employing eq. (2-62) with the simple fluid constants in table 2-1, $(S\text{-}S^{ig})/R$ is calculated. This term represents $[(S\text{-}S^{ig})/R]^{(0)}$ in this calculation and Z in eq. (2-62) is $Z^{(0)}$. Then, when repeating the same calculation, using the same T_r and P_r and the values of $V_r^{(r)}$ and $Z^{(r)}$ for the reference fluid which also determined previously, but employing the reference fluid constants from table 2-1. With these, eq. (2-62) allows the calculation of $[(S\text{-}S^{ig})/R]^{(r)}$. Now, determining the residual entropy function for the fluid of interest from:

$$\left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right] = \left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right]^{(0)} + \left(\frac{\omega}{\omega^r}\right)\left\{\left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right]^{(r)} - \left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right]^{(0)}\right\} \qquad (2\text{-}64)$$

2.9.4 Virial Equation

The virial equation of state, also called the virial expansion, is the most interesting and versatile of the equations of state which are used to describe the (P-V-T) properties of a fluid and its importance due to that it has a sound theoretical basis. It is a polynomial series in pressure or in inverse volume whose coefficients are functions only of T for a pure fluid. Virial coefficients are classified into many truncated forms according to the order of the term series [77, 27]. The consistent forms for the initial terms are:

$$Z = \frac{PV}{RT} = 1 + \frac{B(T)}{V} + \frac{C(T)}{V^2} + \frac{D(T)}{V^3} \cdots \quad \text{(2-65a)}$$

$$= 1 + B\rho + C\rho^2 + D\rho^3 \ldots \quad \text{(2-65b)}$$

$$= 1 + B'P + C'P + D'P + \cdots \quad \text{(2-65c)}$$

The coefficient B or B' is called the second virial coefficient, C or C' is called the third virial coefficient, and so on. In practice, since not all of the coefficients of the virial series are known, and only data of the second virial coefficients are plentiful in the literature, terms above the third virial coefficient are rarely used in chemical thermodynamics and the series is usually limited in practice up to moderate pressures. However, the advantages of the virial equation could be increased if quantitative information were available on the third virial coefficient [39, 52].

The word "virial" is related to the Latin word for force. So, this name was taken over for the virial expansion because the terms in that expansion can be calculated from the forces between the molecules [27].

2.9.4.1 Relations between the coefficients

The virial expansion for *P* is:

$$P = \frac{RT}{V}\left(1 + \frac{B(T)}{V} + \frac{C(T)}{V^2} + \frac{D(T)}{V^3}\cdots\right) \tag{2-66}$$

The coefficients of the expansion in pressure are related to the coefficients of the expansion in density (*1/V*) as follows [19]:

$$B = RTB' \;\Rightarrow\; B' = \frac{B}{RT} \tag{2-67a}$$

$$C = (RT)^2\left(C' + B'^2\right) \;\Rightarrow\; C' = \frac{\left(C - B^2\right)}{(RT)^2} \tag{2-67b}$$

The first step of the derivation of these relations is by solving the original virial expansion for *P* above then equating the two virial expansions, and substituting this expression for *P* into the pressure form-side of resulting equation to obtain:

$$1 + B\frac{1}{V} + C\frac{1}{V^2} + \cdots = 1 + B'RT\frac{1}{V} + B'RTB\frac{1}{V^2} + C'(RT)^2\frac{1}{V^2} + \cdots \tag{2-68}$$

Both sides of equation (2-68) are power series in 1/V (third and higher powers of *1/V* have been omitted because the second power is the highest power that are using by the common references). Since the two power series must be equal, the coefficients of each power of *1/V* must be the same on both sides this comparison provides the relations between the coefficients [81, 3].

2.9.4.2 Second Virial Coefficient

Correlation of second virial coefficient of both polar and nonpolar systems is presented by [70, 1].

$$Z = 1 + \frac{B}{V} = 1 + B'P = 1 + \frac{BP}{RT} \tag{2-69}$$

Tsonopoulos correlation for *B*:

$$B = \frac{RT_c}{P_c}\left(B^{(0)} + \omega B^{(1)}\right) \tag{2-70}$$

$$B^{(0)} = 0.1445 - \frac{0.33}{T_r} - \frac{0.1385}{T_r^2} - \frac{0.0121}{T_r^3} - \frac{0.000607}{T_r^8} \tag{2-71}$$

$$B^{(1)} = 0.0637 - \frac{0.331}{T_r^2} - \frac{0.423}{T_r^3} - \frac{0.008}{T_r^8} \tag{2-72}$$

2.9.4.3 Third Virial Coefficient

At high pressures -above 1500 kPa- equations. (2-65a, b, and c) may be truncated after three terms [40]:

$$Z = 1 + \frac{B}{V} + \frac{C}{V^2} = 1 + B'P + C'P^2 \tag{2-73}$$

Orbey-Vera correlation for *C*:

$$C = \left(\frac{RT_c}{P_c}\right)^2 \left(C^{(0)} + \omega C^{(1)}\right) \tag{2-74}$$

$$C^{(0)} = 0.01407 + \frac{0.02432}{T_r^{2.8}} - \frac{0.00313}{T_r^{10.5}} \tag{2-75}$$

$$C^{(1)} = -0.02676 + \frac{0.0177}{T_r^{2.8}} + \frac{0.04}{T_r^3} - \frac{0.003}{T_r^6} - \frac{0.00228}{T_r^{10.5}} \tag{2-76}$$

By using the residual properties, the final expression of the residual entropy after derivation can be expressed as [45]:

$$\frac{S - S^{ig}}{R} = -\left(\frac{dB}{dT}\left(\frac{P}{R}\right) - \frac{1}{2}\left[C - T\frac{dC}{dT} - \left(B^2 - 2BT\frac{dB}{dT}\right)\right]\left(\frac{P}{RT}\right)^2 + \cdots\right) \tag{2-77}$$

2.10 Entropy of Vaporization

Entropy of vaporization (ΔS_v) is the entropy of phase transition of the compound from saturated liquid into saturated vapor at the same condition [30]. The entropy of vaporization is calculated from [11]:

$$\Delta S_{v=} \frac{\Delta H_v}{T} \tag{2-78}$$

(ΔH_v) is the enthalpy of vaporization. As shown in eq. (2-78) the calculation of (ΔS_v) depends essentially on the (ΔH_v), therefore this section will be directed toward the attention to the enthalpy of vaporization and presents some common methods of its estimation. Enthalpy of vaporization is the difference between the enthalpy of the saturated vapor and that of saturated liquid at the same temperature [45] so; the enthalpy change accompanying material transfer between phases is obtained by differencing the enthalpies of each state [53]. For pure substances, the enthalpy of vaporization can be found by empirical methods which are simpler than the application of equations of state to both phases when they are valid [37].

The enthalpy of vaporization can also be calculated from corresponding states methods, Pitzer et al. [44] have shown that ΔH_v can be related to T, T_r and ω and tabulated the entropy change of vaporization. Pitzer et al. proposed the simple correlation:

$$\frac{\Delta H_v}{T} = \Delta S_v = \Delta S_v^{(0)} + \omega \Delta S_v^{(1)} \tag{2-79}$$

Where $\Delta S_v{}^{(0)}$ and $\Delta S_v{}^{(1)}$ are expressed in entropy units, as J/ (mol.K) and are functions only of T_r. Multiplying eq. (2-79) by T_r /R gives:

$$\frac{\Delta H_v}{RT_c} = \frac{T_r}{R}\left(\Delta S_v^{(0)} + \Delta S_v^{(1)}\right) \tag{2-80}$$

Thus ΔH_v /RTc is a function of ω and T_r only. ΔS_v was plotted against ω for several reduced isotherms as illustrated by Fig. 2-6 a) and Fig. 2-6 b) is a plot giving the dependence of the two correlation terms upon T_r [11].

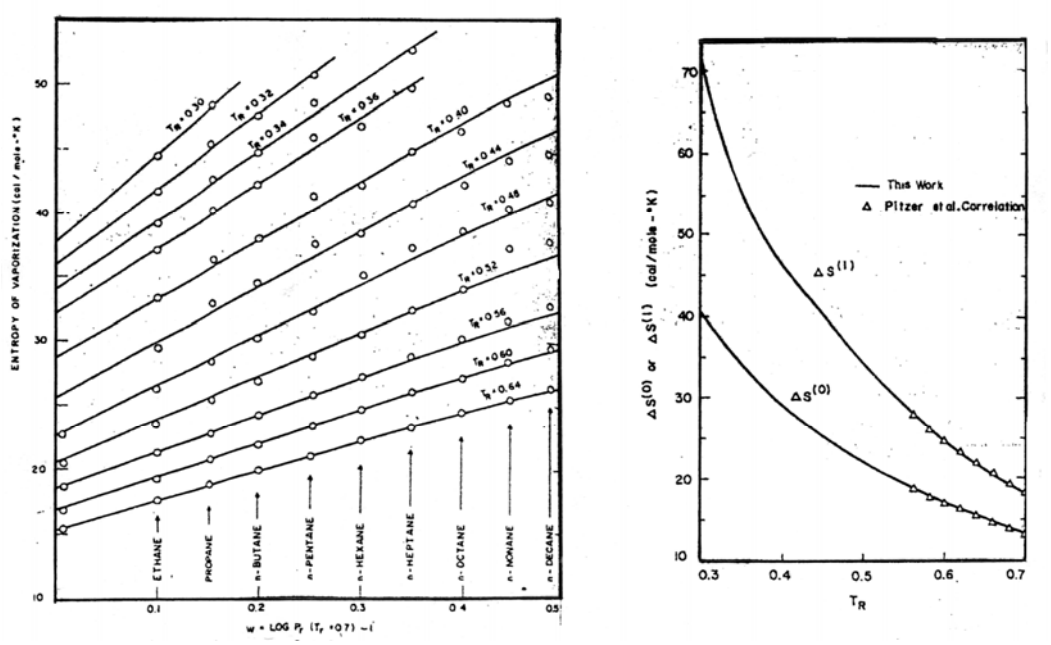

Figure 2-6 a) Dependence of ΔS_v upon ω, b) Dependence of entropy of vaporization functions upon T_r [11].

A pure-component constant that is occasionally used in property correlations is the enthalpy of vaporization at the normal boiling point ΔH_{vb}, where $T = T_b$ (boiling point), P = 101.325 kPa. Several important special estimation methods are summarized below [45, 49]:

1. Giacalone method:

One of the widely used equations to make rapid estimates of ΔH_{vb} has been Giacalone equation:

$$\Delta H_{vb} = RT_c \Delta Z_{vb} T_{br} \frac{\ln(P_c / 1.013)}{1 - T_{br}} \tag{2-81}$$

where P_c is in bar and T_{br} is the reduced boiling point ($T_{br}=T_b/T_c$). Usually, in such cases, ΔZ_{vb} is set equal to unity. Extensive testing of this simplified form indicates that it normally over predicts ΔH_{vb} by a few percent.

2. Kistiakowsky method:

$$\frac{\Delta H_{vb}}{T_b} = \Delta S_{vb} = 36.6 + R \ln T_b \tag{2-82}$$

This method represents another simple equation used in such cases for estimating the ΔH_{vb}. However, better results are obtained with other relations, noted below:

3. Riedel method:

Riedel modified Eq. (2-81) slightly and proposed that:

$$\Delta H_{vb} = 1.093 R T_c T_{br} \frac{\left(\ln P_c - 1.013\right)}{0.930 - T_{br}} \tag{2-83}$$

4. Chen method:

Chen used eq. (2-80) and a similar expression proposed by Pitzer, et al. to correlate vapor pressures so that the acentric factor is eliminated. He obtained the following relation when applied to the normal boiling point:

$$\Delta H_{vb} = R T_c T_{br} \frac{3.978 T_{br} - 3.958 + 1.555 \ln P_c}{1.07 - T_{br}} \tag{2-84}$$

5. Vetere method:

Vetere proposed a relation similar to the one suggested by Chen. When applied to the normal boiling point:

$$\Delta H_{vb} = R T_c T_{br} \frac{0.4343 \ln P_c - 0.69431 + 0.89584 T_{br}}{0.37691 - 0.37306 T_{br} + 0.15075 P_c^{-1} T_{br}^{-2}} \tag{2-85}$$

2.10.1 Variation of ΔH_v with Temperature

The enthalpy of vaporization decreases steadily with increasing temperature and is zero at the critical point. If the enthalpy of vaporization is known at one temperature, the value at another temperature is obtained from a widely used correlation between ΔH_v and T_r which is Watson relation [75]:

$$\frac{\Delta H_{v1}}{\Delta H_{v2}} = \left(\frac{1 - T_{r1}}{1 - Tr_2} \right)^{0.38} \tag{2-86}$$

Eq. (2-86) can be written generally [63] as:

$$\Delta H_{v2} = \Delta H_{v1} \left(\frac{T_2 - T_c}{T_1 - T_c} \right)^n \tag{2-87}$$

Silverberg and Wenzel [56] studied the values of *n* for many different substances. For hydrocarbons, however the original constant of 0.38 appears to be adequate.

Viswanath and Kuloor recommend that *n* be obtained by [49]:

$$n = \left(0.00264 \frac{\Delta H_{vb}}{RT_b} + 0.8794 \right)^{10} \tag{2-88}$$

2.11 Ideal Gas State Thermal Properties

Ideal gas properties are frequently required in correlations of enthalpy, heat capacity, and entropy. In general, these properties are correlated in terms of their deviations from ideality and, thus the accurate predictions of the ideal gas values are required to obtain reliable absolute values [41]. Therefore, it is imperative to know the ideal state properties of pure components for the calculation of thermodynamic properties of real fluids at given temperature and pressure. The most fundamental ideal gas state thermal property is the heat capacity C_p^{ig}. Once this property is accurately known; all other ideal gas state thermal properties can be calculated from the thermodynamic relationships [18].

The molar or specific entropy of a substance may be therefore expressed as a function of two other state variables [57]:

$$S = S(T, P) \tag{2-89}$$

The relationship of C_p^{ig} to S^{ig}_{o} can be obtained by integrating eq. (2-26):

$$\left(\frac{\partial S}{\partial T}\right)_P = \frac{C_P}{T} \tag{2-26}$$

and for ideal gas it becomes:

$$\left(\frac{\partial S_o^{ig}}{\partial T}\right)_P = \frac{C_P^{ig}}{T} \tag{2-90}$$

$$S_o^{ig} = \int_{T_0}^{T} \frac{C_P^{ig}}{T} dT \tag{2-91}$$

Where: $S^{ig}{}_o$= ideal gas entropy at reference pressure (1 atm for API Research Project 44)[3]. Since ideal gas state properties are monatomic functions of temperature, it is a common practice to represent these data, particularly the $C_p{}^{ig}$ by analytical equations. Many such equations have been proposed. The most notable ones are the polynomials with varying number of terms depending on the temperature range covered and the accuracy desired. For relatively short temperature range, the first or second order polynomials are sufficient, but for wide temperature ranges higher order polynomials are needed [18].

Thinh [68] method used a third order polynomial to fit the $C_p{}^{ig}$ data over temperature range of 300-5000 K. Passut and Danner [41] used a fourth order polynomial for $C_p{}^{ig}$ to fit simultaneously the ($H^{ig} - H^{ig}{}_0$), $C_p{}^{ig}$ and $S^{ig}{}_o$ data. Duran et al. [68] showed that the Yuan-moke expression:

$$C_P^{ig} = A + B\exp\left(\frac{-C}{T^n}\right) \tag{2-92}$$

It gave better results than the polynomial with the same number of coefficients. But such exponential expression cannot be analytically integrated to obtain H^{ig} and $S^{ig}{}_o$. From theoretical considerations, Aly and Lee proposed a more accurate but substantially more complex expression

[3] American Petroleum Institute Research Project 44, "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds" Texas A&M Univ. TRC, College Station, 1981 as cited in Reference [18].

involving hyperbolic functions [18]. Thermodynamics Research Center (TRC) [67] fitted ideal gas heat capacity at constant pressure C_p^{ig} data to a following fourth order polynomial:

$$\frac{C_p^{ig}}{R} = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 \tag{2-93}$$

where T in K and the value of C_p^{ig} is obtained by multiplying the result of the above equation by a value of the universal gas constant R and it has the same units as the R used. This polynomial besides it provides simplicity in use, it also covers good range of temperatures. The data related to eq. (2-93) for some pure compounds are listed in Appendix A which is taken from (Appendix A- section c) of ref. [45] that contains data for more than 450 pure compounds that were fitted by TRC.

Chapter Three
Investigation and Development

3.1 Evaluation and Development of Equations of State

The earliest equation of state may be the ideal gas law which does not adequately describe the volumetric behavior of gases except at very low pressure. Consequently, many attempts have been made to develop an equation of state for the real fluids. Since the time of van der Waals first introduced his equation in 1873 and achieved success in qualitatively describing some important features of the volumetric properties of real fluids, there has been a steady outpouring of a rich diversity of equations of state with differing degrees of empiricism, predictive capability and mathematical form to represent the P-V-T behavior of fluids [7, 36].

The development of an accurate and convenient equation presents a challenge to the ingenuity of the investigators because the necessity of fulfilling these criteria limits the mathematical nature of any empirical equation of state. From a practical point of view, the usefulness of a reliable equation exceeds by far the mere description of the P-V-T behavior, for it leads directly to departures from ideal-gas values of thermodynamic properties such as enthalpy, entropy, and free energy, but a convenient equation has yet to be found to give accurate results over a wide range of densities and temperatures. This is of course the reason why generalized correlations are in the form of tables and graphs [13]. So the evolution is expected to continue with more capable equations of state being proposed; approaching, if not reaching, perfection.

From the viewpoint of industrial applications there have been three general forms of equations of state which are based on [18, 45]:

Form 1 Theoretical basis: can be represented by virial equation (1912) which can be derived from molecular theory, but it is limited in its range of applicability; in the same field there are some important equations as: Thiele (1963)→ Carnahan-Starling (1972)→ Beret-Prausnitz (1975) → Donahue-Prausnitz (1978).

Form 2 Semitheoretical basis: can be represented by cubic equations of state. van der Waals equation (1873) was the first equation of state capable of predicting both gaseous and liquid phases and the majority of equation of state models in use today are simple empirical modifications which retain its basic cubic form as:
Redlich-Kwong (1949)→ Wilson (1966)→ Soave (1972)→ Peng-Robinson (1976).

Form 3 Empirical basis: these equations have been utilized for high-precision work, but they usually need many parameters that require fitting to large amounts of experimental data of several properties besides it needs to tedious manipulation and excessive computer storage in lengthy iterative calculations and all of these were limited in practical use. The prominent ones of these long equations are:
Beattie-Bridgeman (1928)→ Benedict-Webb-Rubin (1940)→ Starling (1971)→ Starling-Han (1972)→ Lee-Kesler (1975).

3.2 Experimental Data

The importance of the availability of experimental data for thermodynamic properties of compounds exceeds by far the mere immediate use in the practical applications, but also it has a more essential role in checking the competency of any correlation or prediction by the comparison

of the results of this method with the results of reliable experimental data. So, the accuracy of the method determined by the deviation between the experimental results and the results of correlation or prediction methods which is important in the knowledge of the range of the validity of any equation in such situation to obtain more data by this equation for unavailable compounds. The experimental data of the entropy of superheated vapor, obtained from the literature for the purpose of this investigation consists of some available different **20** compounds with **2791** experimental data points which includes **14** non-polar compounds with **1660** exp. data points and **6** polar compounds with **1131** exp. data points at low to somewhat high pressures as shown in tables 3-1 and 3-2. They have been arranged according to the increasing of acentric factor.

Table 3-1 Experimental entropy data for non polar pure compounds

	Compound	No. of Exp. Data Pts.	Temp. range (K)	Press. Range (kPa)	Ref.
1	Argon	150	100 - 280	101.3 - 12159	[15]
2	Methane	135	300 - 575	400 - 10000	[20]
3	Oxygen	99	280 - 440	200 - 10000	[62]
4	Nitrogen	210	200 - 500	100 - 10000	[28]
5	Ethane	116	400 - 620	300 - 10000	[21]
6	Cyclopropane	18	291.67 - 475	137.9 - 5515.7	[34]
7	Propane	93	260 - 460	50 - 10000	[79]
8	Acetylene	86	210 - 320	202.7 – 6079.5	[15]
9	Neopentane	25	344.45 - 500	34.47 - 3103	[14]
10	Benzene	44	500 - 600	100 - 4500	[72]
11	Carbon dioxide	132	313.15 - 423.15	202.65 - 10130	[15]
12	n-Hexane	199	344.26 - 644.26	6.9 - 4137	[61]
13	n-Heptane	191	410.9 - 644.3	68.95 - 6895	[61]
14	n-Octane	162	399.81 - 644.26	101.33 - 4826	[61]
∑		**1660**			

Table 3-2 Experimental entropy data for polar pure compounds

	Compound	No. of Exp. Data Pts.	Temp. range (K)	Press. Range (kPa)	Ref.
1	Refrigerant 12	117	263.15 - 493.15	25 - 4000	[17]
2	Isopentane	50	477.59-588.71	1013 - 20265	[6]
3	Ammonia	255	243.15 - 713.15	50 - 10000	[22]
4	Refrigerant 152a	156	283.15 - 433.15	100 - 4000	[69]
5	Refrigerant 134a	207	263.15 - 453.15	100 - 6000	[76]
6	Water	346	423.15-1373.15	200 - 60000	[29]
∑		**1131**			

3.3 Calculation of Entropy for Superheated Region

The calculation of entropy for superheated region needing four steps in a calculational path leading from an initial to a final state of a system as obtained in eq. (2-33)

$$\Delta S = \Delta S_v + \int_{T_1}^{T_2} C_P^{ig} \frac{dT}{T} - R \ln \frac{P_2}{P_1} + S_2^R - S_1^R \qquad (2\text{-}33)$$

Thus, in Fig. 2.3 the actual path from state 1 to state 2 – the dashed line – is replaced by a four-step calculational path, these steps visualize as the sum of four changes represented by the sequence of isothermal and isobaric steps:

$$S_2 - S_1 = \left(S_2 - S_2^{ig}\right) + \left(S_2^{ig} - S_1^{ig}\right) + \left(S_1^{ig} - S_1^{v}\right) + \left(S_1^{v} - S_1\right) \qquad (3\text{-}1)$$

- **Step** 1 → 1^{v}: The transformation of saturated liquid at (T_1, P_1) to saturated vapor at T_1 and P_1:

  $S_1^v - S_1 = \Delta S_v$

Saturated entropy of vapor can be calculated by converting saturated liquid at reference T and P to saturated actual gas at the same T and P by using the entropy of vaporization at the normal boiling point ΔS^v after scaling it with the reference temperature by eq. (2-87). Reid, Prausnitz**,** and Poling in

their well known book [49] tested some of the better estimation methods that mentioned in the previous chapter for several different compounds as hydrocarbons, alcohols, rare gases, oxides and other polar compounds and obtaining useful comparison between these methods (Giacalone, Riedel, Chen, and Vetere) and experimental values of ΔH_v. This comparison shows that the average absolute percentage error of Giacalone, Riedel, Chen, and Vetere methods are 2.8, 1.8, 1.7, and 1.6 respectively. Therefore the present investigation employs the more accurate one Vetere method eq. (2-85) to calculate ΔH^v at the normal boiling point and scaled it with eq. (2-87) to obtain ΔH^v at the reference temperature, then calculating ΔS^v by dividing ΔH^v by the reference temperature.

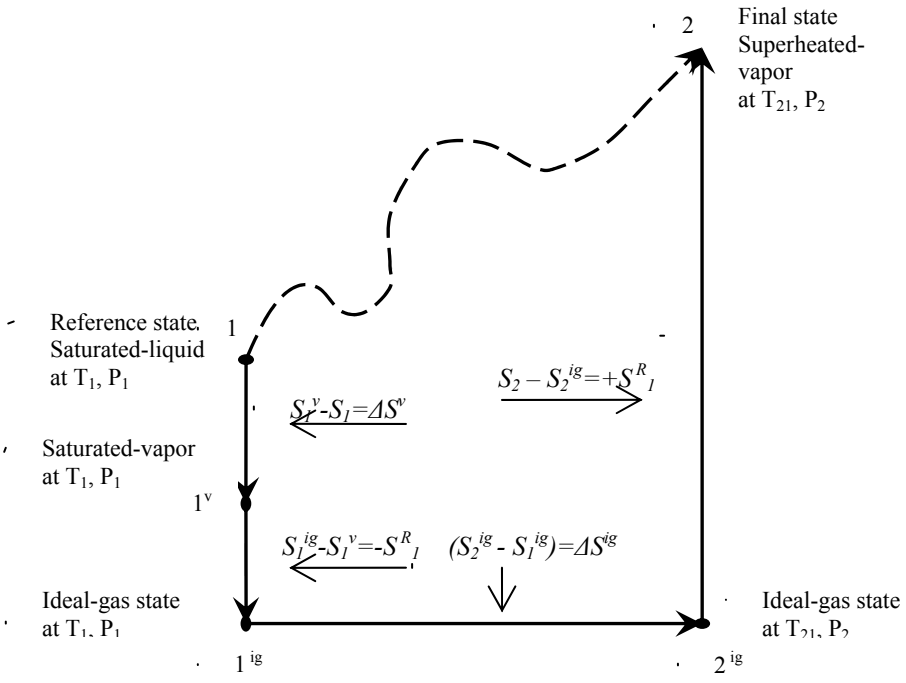

Figure 3-1 Calculational path for entropy change.

- **Step** $1^v \rightarrow 1^{ig}$: A hypothetical process that transforms a real gas into an ideal gas at T_1 and P_1 by using suitable residual entropy of an equation of state.

$$S_1^{ig} - S_1^{v} = -S_1^{R}$$

- **Step** $1^{ig} \rightarrow 2^{ig}$: Changes in the ideal-gas state from (T_1, P_1) to (T_2, P_2). For this process:

$$\Delta S^{ig} = S_2^{ig} - S_1^{ig} = \int_{T_1}^{T_2} C_P^{ig} \frac{dT}{T} - R \ln \frac{P_2}{P_1}$$

In the present work C_p^{ig} is calculated by eq. (2-92)

- **Step** $2^{ig} \rightarrow 2$: Another hypothetical process that transforms the ideal gas back into a real gas at T_2 and P_2:

$$S_2 - S_2^{ig} = S_2^{R}$$

Therefore, Equations (2-33) or (3-1) are results of the totality of the entropy changes for the above four steps.

3.4 Selecting the Optimum EOS for the Present Work

The conflict between accuracy and simplicity is a big dilemma in the development of an equation of state. Despite the wide use of high-speed computers, the simplicity is still highly desired for easy and unequivocal applications of the equation to complex problems. So, for most calculations, the empirical approach is often better than the more complex theoretical approach in view of accuracy as well as minimum data requirements. Often, virial equation – which truncates to second or to third term – can only be considered useful from the first form and employed in the present work. In addition to the Soave-Redlich-Kwong equation (SRK) and Peng-Robinson equation (PR) as the models of cubic equations of state from the second form which have valuable applications in most common use today, Lee and Kesler equation represents –although it is including some complexity– the easiest example of the third form that was also used in the present work.

The **A**verage **A**bsolute **D**eviation for residual entropy AAD in (J/mol.K), which is defined as follows:

$$AAD = \frac{\sum \left| (S^{R}{}_{experimental} - S^{R}{}_{calculated}) \right|}{n} \qquad (3\text{-}2)$$

AAD is considered as a factor for comparison between the different methods that were used for calculating actual residual entropy of superheated vapor for different compounds. It is calculated in (J/mol.K) because when it is calculated in (J/g. K) was being very decimal and the imparity of deviations of using the equations being not perceptible. Also, the dimensionless deviation can be obtained by dividing AAD by R (gas constant) which denoted by AAD/R.

In addition, the **A**verage **A**bsolute **P**ercentage **D**eviation for entropy AAD% is defined as follows:

$$AAD\% = \frac{\sum \left| (S_{experimental} - S_{calculated}) / S_{experimental} \right| \times 100\%}{n} \qquad (3\text{-}3)$$

which is considered as a factor for comparison between the different methods that were associated in determining the actual entropy of superheated vapor for different compounds.

3.5 Application of the EOS for Compounds

3.5.1 Classification of the Application of EOS into Regions

Five different equations of state were applied for calculating residual entropy (S^R) in comparison for all experimental data of pure compounds that supported the present investigation as expressed earlier. To be insight of the precision of these equations with the range of T_r and Pr, summary of results classified into three regions is presented as follows:

Region 1) $T_r < 1$, **and** $P_r < 1$: including 14 compounds involving 859 experimental data points (9 nonpolar compounds with 431 experimental data points and 5 polar compounds with 428 experimental data points) from the 2791 experimental data points of the all 20 compounds.

Region 2) $T_r > 1$, **and** $P_r < 1$: including the 20 compounds involving 1501 experimental data points (14 nonpolar compounds with 921 experimental data points and 6 polar compounds with 580 experimental data points) from the all 2791 experimental data points of the all 20 compounds.

Region 3) $T_r > 1$, **and** $P_r > 1$**:** including 13 compounds involving 431 experimental data points (10 nonpolar compounds with 308 experimental data points and 3 polar compounds with 123 experimental data points) from the all 2791 experimental data points of the all 20 compounds. Although this region represents the supercritical region, but the knowledge of the accuracy of employing these equations in comparison with the accuracy of the modified equation in the present work for this region is advantageous for the some available experimental data.

Table 3-3 The existence of the compounds in the 3 regions.

Non polar compounds		regions			
1	Argon	1, 2, 3	12	n-Hexane	1, 2, 3
2	Methane	2, 3	13	n-Heptane	1, 2, 3
3	Oxygen	2, 3	14	n-Octane	1, 2, 3
4	Nitrogen	2, 3			
5	Ethane	2, 3	Polar compounds		regions
6	Cyclopropane	1, 2	1	Refrigerant 12	1,2
7	Propane	1, 2, 3	2	Isopentane	2, 3
8	Acetylene	1, 2	3	Ammonia	1, 2
9	Neopentane	1, 2	4	Refrigerant 152a	1, 2
10	Benzene	1, 2	5	Refrigerant 134a	1, 2, 3
11	Carbon dioxide	2, 3	6	Water	1, 2, 3

3.5.2 Total Region

This region represents all three regions and consists of 20 compounds involving 2791 experimental data points (14 nonpolar compounds with 1660 experimental data points and 6 polar compounds with 1131 experimental data points).

3.5.3 Summary of the Application of EOS

The application of the equations of state that specified above and employed in the second and fourth steps of the calculational path for estimating S^R for the non-polar and polar compounds are summarized in the followings:

1. **Lee-Kesler equation** it is one of the very important equations of state for calculating thermodynamic properties especially for superheated vapor:

$$\frac{S - S^{ig}}{R} + \ln\left(\frac{P}{P^*}\right) = \ln(Z) - \frac{b_1 + \left(b_3 / T_r^2\right) + \left(2b_4 / T_r^3\right)}{V_r} - \frac{c_1 - \left(2c_3 / T_r^3\right)}{2V_r^2} - \frac{d_1}{5V_r^5} + 2E \qquad (2\text{-}62)$$

As expected it proved that it was the more accurate one than other equations employed for calculating S^R. It was found that the AAD for S^R and AAD% for S were 4.6277 J/mol.K and 1.389 respectively for nonpolar compounds, and the AAD for S^R and AAD% for S were 3.2247 J/mol.K and 2.2096 respectively for polar compounds. So the AAD for S^R and AAD% for S were 4.0591 J/mol.K and 1.7215 respectively for all compounds.

2. **Peng-Robinson equation** was used for calculating residual entropy (S^R) for the experimental data**:**

$$\frac{S^R}{R} = \ln[Z - B] - \frac{BD}{2.828a\alpha A}\ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) \quad (2\text{-}50)$$

this equation was not accurate as Lee-Kesler equation. It was found that the AAD for S^R and AAD% for S were 4.9243 J/mol.K and 1.397 respectively for nonpolar compounds, and the AAD for S^R and AAD% for S were 4.0867 J/mol.K and 2.9399 respectively for polar compounds. So the AAD for S^R and AAD% for S were 4.5849 J/mol.K and 2.0223 respectively for all compounds.

3. **Virial equations** truncation to two terms and also to three terms were applied to the compounds of this investigation:

$$\frac{S - S^{ig}}{R} = \frac{dB}{dT}\left(\frac{P}{R}\right) - \frac{1}{2}\left[C - T\frac{dC}{dT} - \left(B^2 - 2BT\frac{dB}{dT}\right)\right]\left(\frac{P}{RT}\right)^2 + \cdots \quad (2\text{-}77)$$

Both types gave high deviations from the experimental data. It was found that the AAD for S^R and AAD% for S for nonpolar compounds were 4.9782 J/mol.K and 1.4918 respectively of the truncated to two terms equation, while the AAD for S^R and AAD% for S were 4.9501 J/mol.K and 1.5237 respectively of the truncated to three terms equation and the AAD for S^R and AAD% for S for polar compounds were 4.9546 J/mol.K and 3.8575 respectively of the truncated to two terms equation. On the other hand, the AAD for S^R and AAD% for S were 5.1597 J/mol.K and 3.9833 respectively of the truncated to three terms equation. So the AAD for S^R and AAD% for S were 4.9686 J/mol.K and 2.4505 respectively of the truncated to two terms equation for all compounds, while the AAD for S^R and AAD% for S were 5.0350 J/mol.K and 2.5204 respectively of the truncated to three terms equation for all compounds.

4. **Soave-Redlich-Kwong equation**:

$$\frac{S^R}{R} = \ln[Z - B] - \frac{BD}{a\alpha A}\ln\left(1 + \frac{B}{Z}\right) \quad (2\text{-}43)$$

it also was used for calculating residual entropy (S^R) and showed good accuracy that was close to the accuracy of Lee-Kesler equation. It was found that the AAD for S^R and AAD% for S were 4.7665 J/mol.K and 1.3799 respectively for nonpolar compounds, and the AAD for S^R and AAD% for S were 3.6359 J/mol.K and 2.6263 respectively for polar compounds. So the AAD for S^R and AAD% for S were 4.3084 J/mol.K and 1.8850 respectively for all compounds.

5. Soave-Redlich-Kwong equation with modification of its α parameter:

When using new correlation of **α** parameter in this equation that will be discussed in next sections the accuracy of this equation was increased and it is more accurate than Lee-Kesler equation. It was found that the AAD for S^R and AAD% for S were 2.8247 J/mol.K and 0.9592 respectively for nonpolar compounds, and the AAD for S^R and AAD% for S were 2.1235 J/mol.K and 3.2247 respectively for polar compounds by using this new **α** parameter without polarity factor χ, while when adding χ term the AAD for S^R and AAD% for S were 1.9299 J/mol.K and 1.3270 respectively. So the AAD for S^R and AAD% for S were 2.4621 J/mol.K and 1.1083 respectively for all compounds.

Tables 3-4 to 3-6 illustrate the summary of application of these equations of state through the three regions with the total region for nonpolar, polar and both nonpolar and polar compounds.

Table 3-4 Summary of application of EOS through 3 regions and total region for nonpolar compounds.

Region 1 at (Tr < 1 and Pr <1)			No. of points in region 1 is (431)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	7.2542	0.8725	1.7025
Peng-Robinson	7.6357	0.9184	1.7835
Virial (truncated to B)	7.6289	0.9176	1.8469
Virial (truncated to C)	7.5969	0.9138	1.8806
Soave-Redlich-Kwong	7.5950	0.9135	1.7916
This work	4.3948	0.5286	1.1597
Region 2 at (Tr > 1 and Pr <1)			No. of points in region 2 is (921)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	4.1804	0.5028	1.3974
Peng-Robinson	4.2110	0.5065	1.3393
Virial (truncated to B)	4.3024	0.5175	1.4399
Virial (truncated to C)	4.3483	0.5230	1.4831
Soave-Redlich-Kwong	4.1509	0.4993	1.3361
This work	2.6770	0.3220	1.0258
Region 3 at (Tr > 1 and Pr >1)			No. of points in region 3 is (308)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	2.2899	0.2754	0.9253
Peng-Robinson	3.2630	0.3925	1.0290
Virial (truncated to B)	3.2896	0.3957	1.1498
Virial (truncated to C)	3.0457	0.3663	1.1458
Soave-Redlich-Kwong	2.6173	0.3148	0.9166
This work	1.0691	0.1286	0.4798
All regions (1, 2, and 3)			No. of points for all regions (1660)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	4.6277	0.5566	1.3890
Peng-Robinson	4.9243	0.5923	1.3970
Virial (truncated to B)	4.9782	0.5988	1.4918
Virial (truncated to C)	4.9501	0.5954	1.5237
Soave-Redlich-Kwong	4.7665	0.5733	1.3799
This work	2.8247	0.3397	0.9592

Table 3-5 Summary of application of EOS through 3 regions and total region for polar compounds.

Region 1 at (Tr < 1 and Pr <1) No. of points in region 1 is (428)			
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	2.4043	0.2892	1.7041
Peng-Robinson	2.8964	0.3484	2.0294
Virial (truncated to B)	2.9177	0.3509	2.0854
Virial (truncated to C)	2.8258	0.3399	2.0294
Soave-Redlich-Kwong	2.7878	0.3353	1.9536
This work without χ term	1.5487	0.1863	1.1178
This work with χ term	1.4308	0.1721	1.0345
Region 2 at (Tr > 1 and Pr <1) No. of points in region 2 is (580)			
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	3.5325	0.4249	2.4115
Peng-Robinson	4.0331	0.4851	2.7360
Virial (truncated to B)	4.4821	0.5391	3.1450
Virial (truncated to C)	4.4069	0.5301	3.1060
Soave-Redlich-Kwong	3.7976	0.4568	2.5810
This work without χ term	2.0898	0.2514	1.4163
This work with χ term	1.9801	0.2382	1.3408
Region 3 at (Tr > 1 and Pr >1) No. of points in region 3 is (123)			
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	4.6279	0.5566	3.0165
Peng-Robinson	8.4821	1.0202	7.0697
Virial (truncated to B)	14.2703	1.7164	13.3837
Virial (truncated to C)	16.8306	2.0244	14.9193
Soave-Redlich-Kwong	5.8244	0.7006	5.1809
This work without χ term	4.2823	0.5151	3.2432
This work with χ term	3.4304	0.4126	2.2797
All regions (1, 2, and 3) No. of points for all regions (1131)			
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	3.2247	0.3879	2.2096
Peng-Robinson	4.0867	0.4915	2.9399
Virial (truncated to B)	4.9546	0.5959	3.8575
Virial (truncated to C)	5.1597	0.6206	3.9833
Soave-Redlich-Kwong	3.6359	0.4373	2.6263
This work without χ term	2.1235	0.2554	1.5020
This work with χ term	1.9299	0.2321	1.3270

Table 3-6 Summary of application of EOS through 3 regions and all regions for all compounds (polar and non polar).

Region 1 at (Tr < 1 and Pr <1)			No. of points in region 1 is (859)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	4.8377	0.5819	1.7033
Peng-Robinson	5.2743	0.6344	1.9060
Virial (truncated to B)	5.2816	0.6353	1.9657
Virial (truncated to C)	5.2197	0.6278	1.9547
Soave-Redlich-Kwong	5.1998	0.6254	1.8723
This work	2.9180	0.3510	1.0974
Region 2 at (Tr > 1 and Pr <1)			No. of points in region 2 is (1501)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	3.9300	0.4727	1.7892
Peng-Robinson	4.1422	0.4982	1.8790
Virial (truncated to B)	4.3718	0.5258	2.0988
Virial (truncated to C)	4.3709	0.5257	2.1102
Soave-Redlich-Kwong	4.0144	0.4828	1.8171
This work	2.4077	0.2896	1.1475
Region 3 at (Tr > 1 and Pr >1)			No. of points in region 3 is (431)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	2.9571	0.3557	1.5221
Peng-Robinson	4.7524	0.5716	2.7529
Virial (truncated to B)	6.4233	0.7726	4.6412
Virial (truncated to C)	6.9797	0.8395	5.0765
Soave-Redlich-Kwong	3.5325	0.4249	2.1336
This work	1.7430	0.2096	0.9935
All regions (1, 2, and 3)			No. of points for all regions (2791)
Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	4.0591	0.4882	1.7215
Peng-Robinson	4.5849	0.5515	2.0223
Virial (truncated to B)	4.9686	0.5976	2.4505
Virial (truncated to C)	5.0350	0.6056	2.5204
Soave-Redlich-Kwong	4.3084	0.5182	1.8850
This work	2.4621	0.2961	1.1083

3.6 Modification of EOS

3.6.1 Selecting the Optimum EOS for the Modification

Although Lee-Kesler equation proved to be better than Soave-Redlich-Kwong, Peng-Robinson, and Virial equations for the prediction of residual entropy of superheated vapor for the most of compounds that used in this investigation, but it is more useful if the errors can be reduced to value less than those obtained with Lee-Kesler equation.

The modification of any equation is usually done for the equation that proved to be the most accurate. The more accurate one is Lee-Kesler equation, but it is very difficult to modify it, so Soave-Redlich-Kwong equation which is the nearest one in accuracy to the Lee-Kesler equation was selected for modification.

3.6.2 Modification of Soave-Redlich-Kwong Equation

Soave-Redlich-Kwong equation was derived mainly to calculate vapor-liquid equilibria, so all attention was concentrated on that purpose in its derivation, and therefore, there is still room for improving it for superheated vapor.

The modification would be based on modifying α parameter of Soave equation which is function of reduced temperature and also on acentric factor which is included in parameter n:

$$\alpha = \left[1 + n\left(1 - T_r^{0.5}\right)\right]^2 \qquad \text{Soave eq. parameter} \qquad (2\text{-}46)$$

Figures 3-2 to 3-5 show clearly that the values of pressures or reduced pressures influence on the value of α although the temperature is constant. Thus α in Soave equation can be considered a function of temperature, pressure and acentric factor and its equation would be written as:

$$\alpha = \left[1 + n(\gamma)\right]^2 \qquad \text{new form of α parameter} \qquad (3\text{-}4)$$

$$\gamma = g_1 Pr^{g_2} + g_3 Tr^4 \omega + g_4 \omega - Pr^{g_5} Tr^{-4} \chi \qquad (3\text{-}5)$$

The coefficients of this equation had been determined by using statistical methods. These coefficients were calculated with the aid of computer program on non-linear estimation of statistica software that fitting to minimize the error obtained for calculating new α for two selected compounds. In the present work n-octane and water were used in the fitting. By trying many different equations, it was found that equation (3-5) was the optimum equation for predicting γ with lowest error. The coefficients of eq. (3-5) are shown in table 3-7.

Table 3-7 Coefficients of equation (3-5).

coefficient	value	coefficient	value
g_1	-0.920338	g_4	0.370002
g_2	-0.034091	g_5	0.9906321
g_3	0.064049	----	----

The modification was made by comparing the experimental values of residual entropy of superheated vapor with the values calculated by Soave equation which was obtained by using all original parameters of Soave equation except γ parameter which is inserted in the computer program empirically and remain varying until the deviation between the inserted value of γ with the calculated value by Soave equation -for each experimental data point- approached to zero (% error of $(S^R_{exp.}-S^R_{cal.}) \leq 0.00001$).

The new equation of α gives a higher accuracy where the overall **AAD** was 2.4621 J/mol.K for residual entropy and the (**AAD%**) was 1.1083 for entropy, for the all compounds studied in the present work.

The main reason for choosing the mentioned two compounds (n-octane, and water) in the fitting of the experimental data due to their molecular nature

that n-octane represents the normal nonpolar gases which was considered having the highest $\omega > 0$ in comparison with the other used compounds in the present work and thus to be able of controlling the other compounds of less ω and has no polarity properties found ($\chi = 0$). On the other hand water represents the polar compounds which have in addition to $\omega > 0$ the polarity properties $\chi > 0$ and also it has the highest χ among others. The only way for obtaining the experimental values of the parameter γ is by empirically trial and error method which needs great time to obtain any value. Therefore the modification was limited to only these mentioned two types of gases which were used to predict the new α parameter equation that gives more accuracy in calculating S^R and S for all data points (2791) experimental data points for the all 20 nonpolar and polar gases employed in the present work.

Table 3-8 Part of Table 3-6 comparison of the deviations in results for the using compounds with the present work.

Equations used	AAD for S^R (J/mol.K)	AAD/R for S^R	AAD% for S
Lee-Kesler	4.0591	0.4882	1.7215
Peng-Robinson	4.5849	0.5515	2.0223
Virial (truncated to B)	4.9686	0.5976	2.4505
Virial (truncated to C)	5.0350	0.6056	2.5204
Soave-Redlich-Kwong	4.3084	0.5182	1.8850
This work	2.4621	0.2961	1.1083

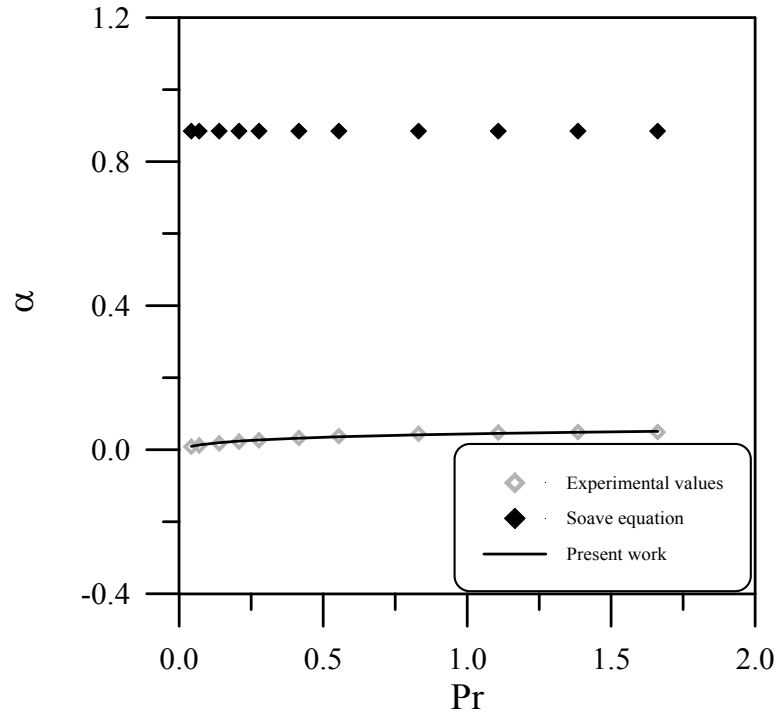

Figure 3-2 The relation between the values of parameter α and reduced pressure for n-octane at T_r =1.3

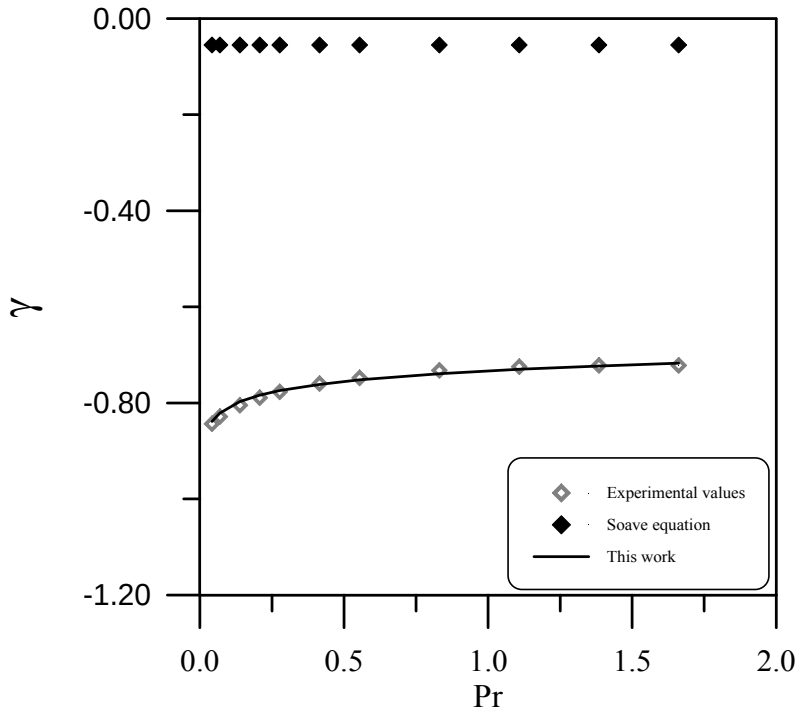

Figure 3-3 The relation between the values of parameter γ and reduced pressure for n-octane at T_r =1.3

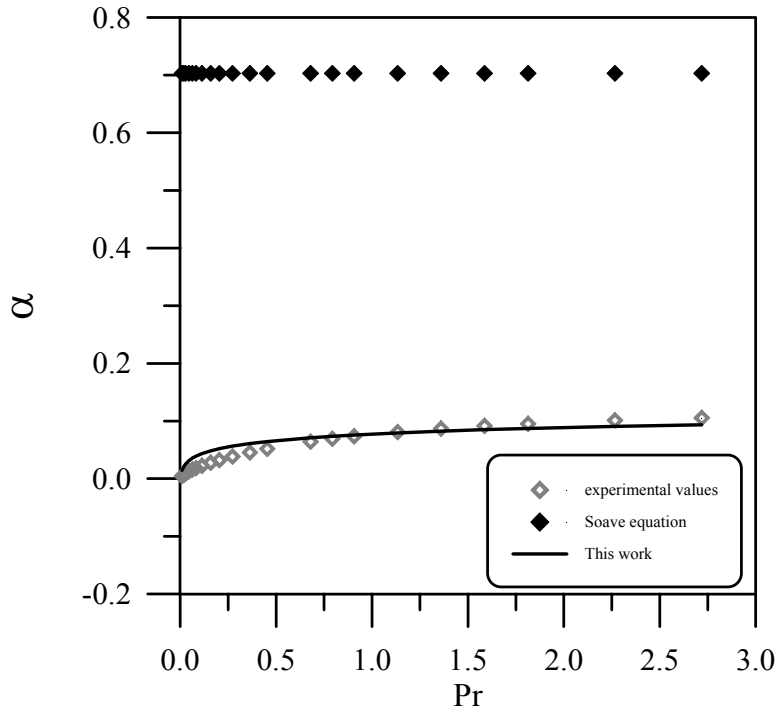

Figure 3-4 The relation between the values of parameter α and reduced pressure for water at T_r =1.349

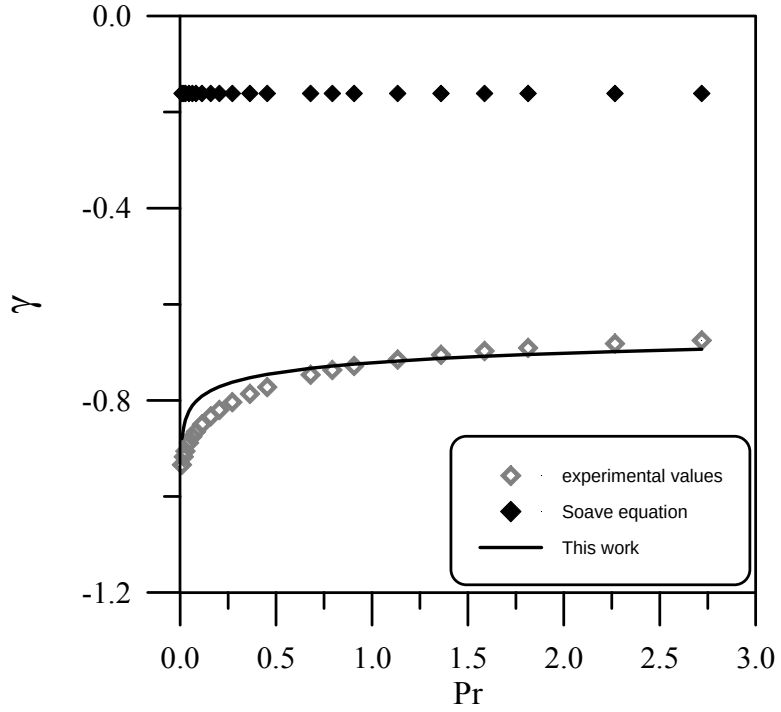

Figure 3-5 The relation between the values of parameter γ and reduced pressure for water at T_r =1.349

3-7 Application of the Developed Correlation

In order to clarify the application of the developed correlation, the detailed calculations are given below for a sample of compounds.

For Water

Calculation of the entropy of superheated vapor for water at 823.15 K and 12500 kPa on the bases that S_0 = 0 J/mol.K at 273.16 K and 0.6113 kPa for saturated liquid.

Data required:

$T_{exp.}$ (K)	$P_{exp.}$ (kPa)	T_c (K)	P_c (kPa)	T_b (K)	M.wt. (g/mol)	R (J/mol.K)	ω	χ
823.15	12500	647.14	22064	373.15	18.015	8.314	0.344	0.023

$$\text{Sat. liq.} \xrightarrow[(1)]{\Delta S^v} \text{Sat. vap.} \xrightarrow[(2)]{-S^R} \text{Ideal gas} \xrightarrow[(3)]{\int_{T_0}^{T} C_p dT/T} \text{Ideal gas}$$

Sat. liq.: T_0= 273.16 K, P_0= 0.6113 kPa

Sat. vap.: T_0=273.16 K, P_0= 0.6113 kPa

Ideal gas: T_0= 273.16 K, P_0=0.6113 kPa

Ideal gas: T=823.15 K, P_0=0.6113 kPa

$$\xrightarrow[(4)]{-R\ln\left(\frac{P}{P_0}\right)} \text{Ideal gas} \xrightarrow[(5)]{+S^R} \text{Actual gas}$$

Ideal gas: T=823.15 K, P=12500 kPa

Actual gas: T=823.15 K, P=12500 kPa

Calculation of the ***entropy of vaporization*** (ΔS^v)by using Vetere method eq. (2-85):

From eq. (2-6): $T_r = \frac{T}{T_c} = 1.27198$, $P_r = \frac{P}{P_c} = 0.56653$ and $T_{br} = \frac{T_b}{T_c} = 0.576614$

$$\Delta H_{vb} = RT_cT_{br}\frac{0.4343\ln P_c - 0.69431 + 0.89584T_{br}}{0.37691 - 0.37306T_{br} + 0.15075P_c^{-1}T_{br}^{-2}} = 41009.85 \text{ J/mol}$$

Then scaling to reference T, and P by eq. (2-87):

$$\Delta H_{v2} = \Delta H_{v1}\left(\frac{T_2 - T_c}{T_1 - T_c}\right)^n \qquad (2\text{-}87)$$

Where $n = \left(0.00264\frac{\Delta H_{vb}}{RT_b} + 0.8794\right)^{10} = 0.4082038$ (2-88)

$\Delta H_{v2} = 46563.13$ J/mol and $\Delta S_{v2} = \Delta H_{v1}/T^r = 170.461$ J/mol.K

Calculation of the ***change of ideal gas entropy*** with changing temperature at constant pressure.

a_0	a_1	a_2	a_3	a_4
4.395	-4.186×10^{-3}	1.405×10^{-5}	-1.564×10^{-8}	0.632×10^{-11}

From eq. (2-92): $\frac{C_p^{ig}}{R} = a_0 + a_1T + a_2T^2 + a_3T^3 + a_4T^4$

From eq. (2-91): $S_T^{ig} = \int_{T_0}^{T} \frac{C_P^{ig}}{T} dT$

So:

$$S_T^{ig} = R \times \left[a_0 \ln\left(\frac{T}{T_0}\right) + a_1(T - T_0) + \frac{a_2}{2}\left(T^2 - T_0^2\right) + \frac{a_3}{3}\left(T^3 - T_0^3\right) + \frac{a_4}{4}\left(T^4 - T_0^4\right)\right]$$

$S_T^{ig} = 39.04844$ J/mol.K

Calculation of the ***change of ideal gas entropy*** with changing pressure and constant temperature.

$S_P^{ig} = -R \ln\frac{P}{P_0} = -82.52187$ J/mol.K

Calculation of the ***residual entropy at reference conditions*** (T_0, and P_0) and at given T and P by using different equations of state:

a. Lee-Kesler equation :

By using the simple fluid constants in table 2-1 in equations (2-58), (2-59), and (2-60):

$$B = b_1 - \frac{b_2}{T_r} - \frac{b_3}{T_r^2} - \frac{b_4}{T_r^3} = -1.78338$$

$$C = c_1 - \frac{c_2}{T_r} + \frac{c_3}{T_r^3} = -0.020623$$

$$D = d_1 + \frac{d_2}{T_r} = 1.6331 \times 10^{-4}$$

From eq. (2-57):

$$Z = \left(\frac{P_r V_r}{T_r}\right) = 1 + \frac{B}{V_r} + \frac{C}{V_r^2} + \frac{D}{V_r^5} + \frac{c_4}{T_r^3 V_r^2}\left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(-\frac{\gamma}{V_r^2}\right)$$

By Newton – Raphson method from the second equating terms finding the value of V_r when assuming the first guess as in eq. (2-61) and continuing iterations until obtaining $V_{r\,new} = V_{r\,old}$. when starting with assuming Z=1 for vapor in eq. (2-61):

$$V_r = Z\frac{T_r}{P_r} = 15233.44$$

Then after knowing the true value of V_r can calculate the true value of Z from the first equating terms.

$$Z = 0.9998829$$

From eq. (2-63):

$$E = \frac{c_4}{2T_r^3\gamma}\left\{\beta + 1 - \left(\beta + 1 + \frac{\gamma}{V_r^2}\right)exp\left(-\frac{\gamma}{V_r^2}\right)\right\} = 8.004 \times 10^{-10}$$

From eq. (2-62):

$$\frac{S - S^{ig}}{R} + ln\left(\frac{P}{P^*}\right) = ln(Z) - \frac{b_1 + \left(b_3 \diagup T_r^2\right) + \left(2b_4 \diagup T_r^3\right)}{V_r} - \frac{c_1 - \left(2c_3 \diagup T_r^3\right)}{2V_r^2} - \frac{d_1}{5V_r^5} + 2E$$

$$\therefore \quad \frac{S - S^{ig}}{R} + ln\left(\frac{P}{P^*}\right) = -2.3479 \times 10^{-4}$$ For simple fluid

Then repeating the same procedures but by using the reference fluid constants in table 2-1 to calculate the residual entropy for reference fluid:

$$\therefore \qquad \frac{S - S^{ig}}{R} + ln\left(\frac{P}{P^*}\right) = -6.0487 \times 10^{-4} \qquad \text{For the reference fluid}$$

Now, determining the residual entropy function for the fluid of interest from eq. (2-64):

$$\left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right] = \left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right]^{(0)} + \left(\frac{\omega}{\omega^r}\right)\left\{\left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right]^{(r)} - \left[\frac{\left(S - S^{ig}\right)}{R} + \ln\left(\frac{P}{P^*}\right)\right]^{(0)}\right\}$$

$$= -0.0000555 \text{ J/mol.K.}$$

$S^R_{\text{at ref. T and P}} = -(S^R/R \times R) = 0.0004614$ J/mol.K. and;

$S^R_{\text{at T and P}} = +(S^R/R \times R) = -2.2932$ J/mol.K.

$$S_{calculated} = \Delta S^v + S^R_{at\ refr.T\ and\ P} + S^{ig}_T + S^{ig}_P + S^R_{at\ T\ and\ P}$$

$$= 170.461 + 0.0004614 + 39.04844 - 82.52187 - 2.2932$$

$$= 124.699 \text{ J/mol.K.}$$

but the experimental value of the entropy is 119.4196 J/mol.K [29].

$$\text{So, } A\%D = \left|\frac{S_{exp.} - S_{cal.}}{S_{exp.}}\right| \times 100\% = \left|\frac{119.4196 - 124.699}{119.4196}\right| \times 100\%$$

$$= \underline{\boldsymbol{4.4208}} \text{ percentage deviation for entropy.}$$

Now, for calculating the accuracy of any equation of state directly for the residual entropy which is the subject of the present investigation, experimental data were needed for residual entropy in the superheated vapor state and it was found that these data were very limited and not available for enough compounds to be the basis for the present evaluation of EOS. Therefore the experimental data of the residual entropy were derived from those experimental data for entropy according to the following relation:

$$S^R_{\text{exp.}} = S^{act.}_{\text{exp.}} - S^{ig} \qquad (3\text{-}6)$$

So, the experimental data for residual entropy were obtained by the above logical relation which was the basis in measuring the accuracy of EOS directly. To complete this example one can calculate AAD for residual entropy as follows:

$S^{R}_{exp.} = S_{exp.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = -7.56797$ J/mol.K.

$S^{R}_{cal.} = S_{cal.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = -2.28859$ J/mol.K.

$AD = \left|S^{R}_{exp.} - S^{R}_{cal.}\right| = \left|-7.56797 - (-2.28859)\right|$

$= \underline{\boldsymbol{5.2794}}$ J/mol.K absolute deviation for S^{R}.

$AD/R = \left|S^{R}_{exp.} - S^{R}_{cal.}\right|/R =$ **0.6350** absolute deviation for S^{R} divided by R.

b. Peng-Robinson equation :

From eq. (2-53): $a = 0.45724\,\dfrac{R^2 T_c^2}{P_c} = 0.5998968$

From eq. (2-54): $n = 0.37464 + 1.5422\omega - 0.26992\omega^2 = 0.873236$

$$\alpha = \left[1 + n\left(1 - T_r^{0.5}\right)\right]^2 = 1.705373$$

So, from eq. (2-52): $A = 0.45724\,\alpha\dfrac{P_r}{T_r^2} = 0.000121254$

$$B = 0.0778\dfrac{P_r}{T_r} = 0.0000051066$$

From eq. (2-48): $D = na\sqrt{\alpha T_r} = 0.444455$

From eq. (2-51): $Z^3 - (1-B)Z^2 + \left(A - 3B^2 - 2B\right)Z - \left(AB - B^2 - B^3\right) = 0$

By Newton – Raphson method finding the value of Z assuming first guess Z_o=1 for vapor and continuing iterations until obtaining $Z_{new} = Z_{old}$.

Z=0.99988 at the reference state conditions, and from eq. (2-50):

$$\frac{S^R}{R} = ln[Z - B] - \frac{BD}{2.828a\alpha A} ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right) = -0.0001214 \text{ J/mol.K.}$$

$S^{R}_{\text{at ref. T and P}} = -(S^{R}/R \times R) = 0.00100912$ J/mol.K. and;

$S^{R}_{\text{at T and P}}$ = + (S^{R}/R × R) = *-1.195654* J/mol.K.

$$S_{calculated} = \Delta S^{v} + S^{R}_{at\ refr.T\ and\ P} + S^{ig}_{T} + S^{ig}_{P} + S^{R}_{at\ T\ and\ P}$$

$$= 125.7929 \text{ J/mol.K.}$$

but the experimental value of the entropy is 119.4196 J/mol.K [29].

So, $$A\%D = \left| \frac{119.4196 - 125.7929}{119.4196} \right| \times 100\%$$

= ***5.3369*** percentage deviation for entropy.

$$S^{R}_{exp.} = S_{exp.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = -7.56797 \text{ J/mol.K.}$$

$$S^{R}_{cal.} = S_{cal.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = -1.19464 \text{ J/mol.K.}$$

$$AD = \left| S^{R}_{exp.} - S^{R}_{cal.} \right| = \left| -7.56797 - (-1.194645) \right|$$

= ***6.3733*** J/mol.K absolute deviation for S^{R}.

AD / R = ***0.7666*** absolute deviation for S^{R} divided by R.

c. Virial equation :

◆ When virial equation truncated to second term, from equations (2-70), (2-71), and (2-72):

$$B^{(0)} = 0.1445 - \frac{0.33}{T_r} - \frac{0.1385}{T_r^2} - \frac{0.0121}{T_r^3} - \frac{0.000607}{T_r^8} = -2.177866$$

$$B^{(1)} = 0.0637 - \frac{0.331}{T_r^2} - \frac{0.423}{T_r^3} - \frac{0.008}{T_r^8} = -11.64155$$

$$B = \frac{RT_c}{P_c}\left(B^{(0)} + \omega B^{(1)}\right) = -0.00150762$$

$$\frac{\partial B}{\partial T} = 1.48455 \times 10^{-8}$$

From equation (2-77)

$$\frac{S - S^{ig}}{R} = -\left(\frac{dB}{dT}\left(\frac{P}{R}\right)\right) = -0.002232 \text{ J/mol.K.}$$

$S^{R}_{\text{reference}}$ = – (S^{R}/R × R) = *0.0185601* J/mol.K

$S^{R}_{\text{at T and P}}$ = + (S^{R}/R × R) = *–1.938784* J/mol.K.

$$S_{calculated} = \Delta S^{v} + S^{R}_{at\ refr.T\ and\ P} + S^{ig}_{T} + S^{ig}_{P} + S^{R}_{at\ T\ and\ P}$$

$= 128.9449$ J/mol.K.

but the experimental value of the entropy is 119.4196 J/mol.K [29].

So, $A\%D = \left| \frac{119.4196 - 128.9449}{119.4196} \right| \times 100\%$

= ***7.9763*** percentage deviation for entropy.

$S^{R}_{exp.} = S_{exp.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v} \right) = -7.56797$ J/mol.K.

$S^{R}_{cal.} = S_{cal.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v} \right) = 1.95733$ J/mol.K.

$AD = \left| S^{R}_{exp.} - S^{R}_{cal.} \right| = \left| -7.56797 - (1.95733) \right|$

= ***9.5253*** J/mol.K absolute deviation for S^R.

$AD / R =$ ***1.1457*** absolute deviation for S^R divided by R.

◆ When virial equation truncated to third term, from equations (2-74), (2-75), and (2-76):

$$C^{(0)} = 0.01407 + \frac{0.02432}{T_r^{2.8}} - \frac{0.00313}{T_r^{10.5}} = -26.54538$$

$$C^{(1)} = -0.02676 + \frac{0.0177}{T_r^{2.8}} + \frac{0.04}{T_r^{3}} - \frac{0.003}{T_r^{6}} - \frac{0.00228}{T_r^{10.5}} = -19.37229$$

$$C = \left(\frac{RT_c}{P_c} \right)^2 \left(C^{(0)} + \omega\, C^{(1)} \right) = -1.97474 \times 10^{-6}$$

$$\frac{\partial C}{\partial T} = 7.66159 \times 10^{-9}$$

From equation (2-77)

$$\frac{S - S^{ig}}{R} = -\left(\frac{dB}{dT}\left(\frac{P}{R} \right) - \frac{1}{2}\left[C - T\frac{dC}{dT} - \left(B^2 - 2BT\frac{dB}{dT} \right) \right] \left(\frac{P}{RT} \right)^2 \right) = -0.0022342$$

$S^{R}_{\text{reference}} = -(S^R/R \times R) = 0.0185752$ J/mol.K

$S^{R}_{\text{at T and P}} = +(S^R/R \times R) = -2.056865$ J/mol.K.

$S_{calculated} = \Delta S^{v} + S^{R}_{at\ refr.T\ and\ P} + S^{ig}_{T} + S^{ig}_{P} + S^{R}_{at\ T\ and\ P}$

$= 129.0259$ J/mol.K.

but the experimental value of the entropy is 119.4196 J/mol.K [29].

So, $A\%D = \left| \frac{119.4196 - 129.0259}{119.4196} \right| \times 100\%$

= **8.04409** percentage deviation for entropy.

$S^{R}_{exp.} = S_{exp.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = -7.56797$ J/mol.K.

$S^{R}_{cal.} = S_{cal.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = 2.03833$ J/mol.K.

$AD = \left| S^{R}_{exp.} - S^{R}_{cal.} \right| = \left| -7.56797 - (2.03833) \right|$

= ***9.60623*** J/mol.K absolute deviation for S^R.

$AD / R =$ ***1.15543*** absolute deviation for S^R divided by R.

d. ***Soave-Redlich-Kwong equation :***

From eq. (2-46): $a = 0.42747 \frac{R^2 T_c^2}{P_c} = 0.5608387$

From eq. (2-47): $n = 0.48508 + 1.55171\omega - 0.1561\omega^2 = 1.000392$

$$\alpha = \left[1 + n\left(1 - T_r^{0.5}\right)\right]^2 = 1.823695$$

So, from eq. (2-45): $A = 0.42747\alpha \frac{P_r}{T_r^2} = 0.0001212$

$$B = 0.08664 \frac{P_r}{T_r} = 0.00000569$$

From eq. (2-48): $D = na\sqrt{\alpha T_r} = 0.492259$

From eq. (2-44): $Z^3 - (1 - B)Z^2 + \left(A - B^2 - B\right)Z - AB = 0$ (2-43)

By Newton – Raphson method finding the value of Z assuming first guess Z_o=1 for vapor and continuing iterations until obtaining $Z_{new} = Z_{old}$.

Z=0.9998788 at the reference state conditions.

From eq. (2-43): $\frac{S^R}{R} = \ln[Z - B] - \frac{BD}{a\alpha A} \ln\left(1 + \frac{B}{Z}\right) =$ -0.0001271

$S^R_{\text{at ref. T and P}} = -(S^R/R \times R) = 0.00105637$ J/mol.K. and;

$S^R_{\text{at T and P}} = +(S^R/R \times R) =$ -1.55652J/mol.K.

$S_{calculated} = \Delta S^v + S^R_{at\ refr.T\ and\ P} + S^{ig}_T + S^{ig}_P + S^R_{at\ T\ and\ P}$

$= 125.4321$ J/mol.K.

but the experimental value of the entropy is 119.4196 J/mol.K [29].

So, $A\%D = \left| \frac{119.4196 - 125.4321}{119.4196} \right| \times 100\%$

= ***5.03477*** percentage deviation for entropy.

$S^{R}_{exp.} = S_{exp.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = -7.56797$ J/mol.K.

$S^{R}_{cal.} = S_{cal.} - \left(S^{ig}_{T} + S^{ig}_{P} + S_{v}\right) = -1.555464$ J/mol.K.

$AD = \left| S^{R}_{exp.} - S^{R}_{cal.} \right| = \left| -7.56797 - (-1.555464) \right|$

= ***6.012506*** J/mol.K absolute deviation for S^R.

$AD / R =$ ***0.723179*** absolute deviation for S^R divided by R.

e. ***new modification of Soave-Redlich-Kwong equation:***

$S^{R}_{\text{at ref. T and P}} = -(S^R/R \times R) = 0.00105637$ J/mol.K.

(the same value of original equation of SRK because it is at saturated conditions.)

From eq. (3-4): $\alpha = [1 + n(\gamma)]^2$ (3-4)

where $\gamma = g_1 Pr^{g_2} + g_3 Tr^4 \omega + g_4 \omega - Pr^{g_5} Tr^{-4} \chi$ (3-5)

by using the coefficients of eq. (3-5) listed in table 3-7 to become:

$\gamma = -0.7583697$ and $\alpha = 0.058241$

From eq. (2-46) and (2-47):

$a = 0.5608387$ and $n = 1.000392$

also, from eq. (2-45): $A = 0.42747 \alpha_{new} \frac{P_r}{T_r^2} = 0.008718$

$$B = 0.08664 \frac{P_r}{T_r} = 0.038589$$

From eq. (2-48): $D = na\sqrt{\alpha T_r} = 0.1527091$

From eq. (2-44): $Z^3 - (1 - B)Z^2 + \left(A - B^2 - B\right)Z - AB = 0$ (2-43)

By Newton – Raphson method finding the value of Z assuming first guess Z_o=1 for vapor and continuing iterations until obtaining $Z_{new} = Z_{old}$.

Z=0.9933231 at the reference state conditions.

From eq. (2-43): $\frac{S^R}{R} = ln[Z - B] - \frac{BD}{a\alpha A} ln\left(1 + \frac{B}{Z}\right) = -0.8350486$

$S^R_{\text{at T, P}} = +S^R = -6.942594$ J/mol.K

$S_{calculated} = \Delta S^v - S^R_{at\ refr.T\ and\ P} + S^{ig}_T + S^{ig}_P + S^R_{at\ T\ and\ P}$

$= 120.046$ J/mol.K

While the experimental value of the entropy is 119.4196 J/mol.K [29].

$$A\%D = \left|\frac{119.4196 - 120.046}{119.4196}\right| \times 100\%$$

= ***0.52454*** percentage deviation for entropy.

$S^R_{exp.} = S_{exp.} - \left(S^{ig}_T + S^{ig}_P + S_v\right) = -7.56797$

$S^R_{cal.} = S_{cal.} - \left(S^{ig}_T + S^{ig}_P + S_v\right) = -6.94157$

$AD = \left|S^R_{exp.} - S^R_{cal.}\right| = \left|-7.56797 - (-6.94157)\right|$

= ***0.6264*** J/mol.K absolute deviation for S^R.

$AD / R =$ ***0.0753*** absolute deviation for S^R divided by R.

Comparison of the deviations in results for the selecting point of temperature and pressure of water with the present work.

Equations used	AD% for S	AD for S^R (J/mol.K)	AD/R for S^R
Lee-Kesler	4.4208	5.2793	0.6349
Peng-Robinson	5.3368	6.3733	0.7665
Virial (truncated to B)	7.9763	9.5253	1.1456
Virial (truncated to C)	8.0440	9.6062	1.1554
Soave-Redlich-Kwong	5.0347	6.0124	0.7232
This work	0.5245	0.6264	0.0753

Chapter Four

Discussion of Results

4.1 Discussion

The entropy of a pure compound cannot be directly measured but is calculated from other properties. It is a function of both temperature and pressure; in general, it increases with the increase in temperature and decreases with the increase in pressure at constant temperature. At zero pressure, all gases behave ideally, and the ideal gas state entropy is remaining dependent on pressure.

The residual entropy term S-S^{ig}, is the difference between the entropy of a compound at certain P and T and that of an ideal gas state at the same conditions. In the absence of P-V-T data for the compounds of interest, or if the data do not cover the conditions under which engineering calculations are to be made, generalized correlations which express Z as a function of T_r and P_r have been found to be of great value in estimating residual properties as residual entropy which are based on a modified theory of corresponding states.

The usual method available for predicting the residual entropy of superheated vapor for pure compounds is by employing the equation of state. In the present work the equations of state employed were: Lee-Kesler, Peng-Robinson, Soave-Redlich-Kwong, and Virial truncated to second and to third terms equations. It is well known that the evaluation of any correlation or prediction method is done by comparison of the calculated values for any equation used with those of the experimental data which normally limited and

mostly not covering wide range of temperatures and pressures for any certain compound. The deviation between the experimental data and results of prediction or correlation method determines the accuracy of the method and this accuracy in the present work was represented as mentioned in the previous chapter by AAD% for entropy and AAD J/mol.K for residual entropy. Tables 4-1 to 4-3 show the AAD% and the AAD in J/mol.K for the calculated entropy and calculated residual entropy respectively of the superheated vapor for nonpolar and polar compounds as compared with experimental values.

4.1.1 Comparison of the Results with the Experimental Data

Comparing the results that are shown in Tables 4-1 to 4-3, indicate that the Lee-Kesler equation gives higher accuracy for predicting S^R as compared with the Peng-Robinson, Virial truncated to second or third terms, and Soave-Redlich-Kwong equations using the experimental data points of the present study.

The AAD% for calculating the entropy of superheated vapor for 14 nonpolar compounds of 1660 data points are 1.389%, 1.397%, 1.4918%, 1.5237%, and 1.3799% when using Lee-Kesler, Peng-Robinson, Virial truncated to second or third terms, Soave-Redlich-Kwong respectively, while the AAD for calculating the residual entropy of superheated vapor of these compounds by using these equations are 4.6277, 4.9243, 4.9782, 4.9501, and 4.7665 J/mol.K respectively. Further more the AAD% for calculating the entropy of superheated vapor for 6 polar compounds of 1131 data points are 2.2096%, 2.9399%, 3.8575%, 3.9833, and 2.6263% when using Lee-Kesler, Peng-Robinson, Virial truncated to second or third terms, Soave-Redlich-

Kwong respectively, while the AAD for calculating the residual entropy of superheated vapor of these compounds by using these equations are 3.2247, 4.0867, 4.9546, 5.1597, and 3.6359 J/mol.K respectively.

The AAD% for calculating the entropy of superheated vapor for the all compounds of 2791 data points are 1.7215%, 2.0223%, 2.4505%, 2.5204%, and 1.8850% when using Lee-Kesler, Peng-Robinson, Virial truncated to second or third terms, Soave-Redlich-Kwong respectively, while the AAD for calculating the residual entropy of superheated vapor of these compounds by using these equations are 4.0591, 4.5849, 4.9686, 5.0350, and 4.3084 J/mol.K respectively.

4.1.2 The Modified Equation

Although of the better results were obtained by Lee-Kesler equation, but this equation is sometimes not very preferable, because it needs more time and not easy to apply as cubic equations of state. Soave-Redlich-Kwong equation showed also a very good accuracy closest to that of the Lee-Kesler equation in calculating the residual entropy S^R of superheated vapor. Thus efforts were directed to modify Soave-Redlich-Kwong equation to increase its accuracy as much as possible and to be more accurate than the original Soave-Redlich-Kwong and even the Lee-Kesler equation. This may be done by using a statistical program and statistical methods that give the suitable form of correlation.

Many attempts were done to develop Soave-Redlich-Kwong equation to this purpose, and the best correlation of this modification was obtained in chapter three which proved a very good accuracy for most compounds under study.

Table 4-1 Summary of results of S^R and deviations for nonpolar compounds

Compounds	Pts.	AAD%						AAD					
		L&K	P&R	Virial B	Virial C	Soave	This work	L&K	P&R	Virial B	Virial C	Soave	This work
Argon	150	0.5555	0.4288	0.4617	0.5150	0.8001	0.4822	0.6552	0.5218	0.5504	0.6042	0.9385	0.5745
Methane	135	0.7593	0.7433	0.7732	0.7868	0.5252	0.5007	1.3063	1.2670	1.3306	1.3561	0.9070	0.8578
Oxygen	99	0.7236	0.7611	1.2173	1.2154	0.6064	0.5475	1.3470	1.4109	2.2086	2.2052	1.1385	1.0325
Nitrogen	210	0.5998	0.5126	0.6160	0.6368	0.4308	0.2925	1.0030	0.8510	1.0322	1.0667	0.7276	0.4956
Ethane	116	1.0350	1.1217	1.0398	1.0331	1.0283	0.9694	2.4919	2.6933	2.5023	2.4871	2.4743	2.3318
Cyclopropane	18	0.9061	1.4623	2.5156	2.9977	1.5671	1.1571	0.7078	1.1635	1.8625	2.2033	1.2437	0.9572
Propane	93	2.0487	1.7837	1.9106	1.9863	1.9116	1.7389	5.5518	4.8568	5.1947	5.3903	5.1873	4.7455
Acetylene	86	1.0753	0.7836	1.5093	1.6558	1.0777	0.9068	2.0440	1.5193	2.9078	3.1808	2.0350	1.7308
Neopentane	25	1.2072	2.2324	2.4907	2.9344	2.2187	2.0851	1.0956	1.9778	2.1842	2.4908	1.9878	1.9338
Benzene	44	0.2246	0.1487	0.1426	0.1475	0.2166	0.2123	0.6945	0.4667	0.4488	0.4652	0.6646	0.6565
Carbon dioxide	132	3.8848	3.2322	3.5382	3.7996	3.2123	2.8853	7.5619	6.2557	6.8665	7.3855	6.2325	5.5966
n-Hexane	199	1.9352	2.0886	2.0369	2.0030	2.0401	1.6176	9.0552	9.7804	9.5384	9.3783	9.5464	7.5307
n-Heptane	191	1.4163	1.7492	1.6427	1.5559	1.6281	0.7301	7.5960	9.3988	8.8259	8.3555	8.7377	3.8807
n-Octane	162	1.8176	2.1173	2.0047	1.9370	2.0085	0.3711	10.867	12.677	12.004	11.594	12.016	2.1418
Overall	**1660**	**1.3890**	**1.3970**	**1.4918**	**1.5237**	**1.3799**	**0.9592**	**4.6277**	**4.9243**	**4.9782**	**4.9501**	**4.7665**	**2.8247**

Table 4-2 Summary of results of S^R and deviations for polar compounds

Compounds	Pts.	AAD%						AAD					
		L&K	P&R	Virial B	Virial C	Soave	This work	L&K	P&R	Virial B	Virial C	Soave	This work
Refrigerant 12	117	0.7826	0.5462	0.5984	0.6164	0.5724	0.7385	0.8192	0.5670	0.6280	0.6532	0.5958	0.7510
Isopentane	50	1.0768	1.0726	0.9843	2.2235	0.4973	0.9544	4.0340	3.9788	3.6402	8.1391	1.8053	3.5397
Ammonia	255	0.9136	1.0305	1.0680	1.0352	0.9484	0.5815	0.9304	1.0272	1.0886	1.0626	0.9512	0.5747
Refrigerant152a	156	1.0637	1.5181	1.3615	1.2579	1.4147	0.7231	1.6562	2.3204	2.0967	1.9475	2.1678	1.0996
Refrigerant134a	207	2.4911	3.4005	3.1510	2.9013	3.0307	1.2397	4.8482	6.5411	6.0567	5.6011	5.8645	2.3752
Water	346	4.1592	5.7919	8.9788	9.4250	5.1695	2.4539	5.3479	6.8755	10.086	10.457	6.2356	3.2028
Overall	**1131**	**2.2096**	**2.9399**	**3.8575**	**3.9833**	**2.6263**	**1.3270**	**3.2247**	**4.0867**	**4.9546**	**5.1597**	**3.6359**	**1.9299**

Table 4-3 Summary of results of S^R and deviations for nonpolar and polar compounds

Compounds	Pts	AAD%						AAD					
		L&K	P&R	Virial B	Virial C	Soave	This work	L&K	P&R	Virial B	Virial C	Soave	This work
Argon	150	0.5555	0.4288	0.4617	0.5150	0.8001	0.4822	0.6552	0.5218	0.5504	0.6042	0.9385	0.5745
Methane	135	0.7593	0.7433	0.7732	0.7868	0.5252	0.5007	1.3063	1.2670	1.3306	1.3561	0.9070	0.8578
Oxygen	99	0.7236	0.7611	1.2173	1.2154	0.6064	0.5475	1.3470	1.4109	2.2086	2.2052	1.1385	1.0325
Nitrogen	210	0.5998	0.5126	0.6160	0.6368	0.4308	0.2925	1.0030	0.8510	1.0322	1.0667	0.7276	0.4956
Ethane	116	1.0350	1.1217	1.0398	1.0331	1.0283	0.9694	2.4919	2.6933	2.5023	2.4871	2.4743	2.3318
Cyclopropane	18	0.9061	1.4623	2.5156	2.9977	1.5671	1.1571	0.7078	1.1635	1.8625	2.2033	1.2437	0.9572
Propane	93	2.0487	1.7837	1.9106	1.9863	1.9116	1.7389	5.5518	4.8568	5.1947	5.3903	5.1873	4.7455
Acetylene	86	1.0753	0.7836	1.5093	1.6558	1.0777	0.9068	2.0440	1.5193	2.9078	3.1808	2.0350	1.7308
Neopentane	25	1.2072	2.2324	2.4907	2.9344	2.2187	2.0851	1.0956	1.9778	2.1842	2.4908	1.9878	1.9338
Benzene	44	0.2246	0.1487	0.1426	0.1475	0.2166	0.2123	0.6945	0.4667	0.4488	0.4652	0.6646	0.6565
Carbon dioxide	132	3.8848	3.2322	3.5382	3.7996	3.2123	2.8853	7.5619	6.2557	6.8665	7.3855	6.2325	5.5966
n-Hexane	199	1.9352	2.0886	2.0369	2.0030	2.0401	1.6176	9.0552	9.7804	9.5384	9.3783	9.5464	7.5307
n-Heptane	191	1.4163	1.7492	1.6427	1.5559	1.6281	0.7301	7.5960	9.3988	8.8259	8.3555	8.7377	3.8807
n-Octane	162	1.8176	2.1173	2.0047	1.9370	2.0085	0.3711	10.8673	12.6769	12.0037	11.5943	12.0160	2.1418
Refrigerant 12	117	0.7826	0.5462	0.5984	0.6164	0.5724	0.7385	0.8192	0.5670	0.6280	0.6532	0.5958	0.7510
Isopentane	50	1.0768	1.0726	0.9843	2.2235	0.4973	0.9544	4.0340	3.9788	3.6402	8.1391	1.8053	3.5397
Ammonia	255	0.9136	1.0305	1.0680	1.0352	0.9484	0.5815	0.9304	1.0272	1.0886	1.0626	0.9512	0.5747
Refrigerant 152a	156	1.0637	1.5181	1.3615	1.2579	1.4147	0.7231	1.6562	2.3204	2.0967	1.9475	2.1678	1.0996
Refrigerant 134a	207	2.4911	3.4005	3.1510	2.9013	3.0307	1.2397	4.8482	6.5411	6.0567	5.6011	5.8645	2.3752
Water	346	4.1592	5.7919	8.9788	9.4250	5.1695	2.4539	5.3479	6.8755	10.0860	10.4567	6.2356	3.2028
Overall	**2791**	**1.7215**	**2.0223**	**2.4505**	**2.5204**	**1.8850**	**1.1083**	**4.0591**	**4.5849**	**4.9686**	**5.0350**	**4.3084**	**2.4621**

The modification was applied for 20 pure compounds of 2791 experimental data points (nonpolar and polar compounds). It reduced the AAD% and AAD of Soave-Redlich-Kwong equation for 1660 experimental data points of 14 nonpolar compounds from 1.3799% to 0.9592% and from 4.7665 to 2.8247 J/mol.K respectively. While it reduced the AAD% and AAD of Soave-Redlich-Kwong equation for 1131 experimental data points of 6 polar compounds from 2.6263% to 1.3270% and from 3.6359 to 1.9299 J/mol.K respectively. On the other hand it reduced the AAD% and AAD of Soave-Redlich-Kwong equation for all the 20 pure compounds under study from 1.8850% to 1.1083% and from 4.3084 to 2.4621 J/mol.K respectively as shown in tables 4-1 to 4-3.

Examples of nonpolar compounds: for octane the AAD% and AAD by using SRK equation were 2.0085% and 12.0160 J/mol.K respectively, while they were 0.3711% and 2.1418 J/mol.K respectively when using the modified SRK equation. For nitrogen the AAD% and AAD by using SRK equation were 0.4308% and 0.7276 J/mol.K respectively, while they were 0.2925% and 0.4956 J/mol.K respectively when using the modified SRK equation.

Examples of polar compounds: for water the AAD% and AAD by using SRK equation were 5.1695% and 6.2356 J/mol.K respectively, while they were 2.4539% and 3.2028 J/mol.K respectively when using the modified SRK equation. For refrigerant (134a) the AAD% and AAD by using SRK equation were 3.0307% and 5.8645 J/mol.K respectively, while they were 1.2397 % and 2.3752 J/mol.K respectively when using the modified SRK equation.

For polar compounds when applying the modified SRK equation without considering polarity effect term the deviation from the experimental data was more than that when considering polarity effect term as shown in

Table 3-5. Although this increase was not very significant, but in practical use more accuracy is desirable.

The interesting features of the developed equation in the present work for calculating the residual entropy are:

1. It is a rather simple equation that achieved good results for both nonpolar and polar compounds.
2. It needs only well-known properties of pure compounds (T_c, P_c, ω, and for polar compounds χ) for each compound.

The new correlation gives very good accuracy for calculating S^R of the compounds shown in Table 4-3 by comparison with the experimental data approximately over the whole temperature and pressure ranges tested. Where the conditions tested for temperature up to $T_r > 2$ and for pressure raised for some compounds up to $P_r > 2$.

Figures 4-1 to 4-10 show the relation either between residual entropy with pressure at constant temperature or between residual entropy with temperature at constant pressure for the results obtained using this new method of correlation and other equations used comparing with the experimental data.

Tables 4-4 and 4-5 show the comparison of results of deviations from the experimental data of n-octane and water when using Lee-Kesler, Peng-Robinson, Soave-Redlich-Kwong equations of state, and the new correlation of this work. Although virial equation was employed in this study but its results were not listed due to the high deviations from the experimental values obtained comparing with deviations of other equations that employed.

Appendix C, contains the comparison between the results obtained using the Lee-Kesler, Peng-Robinson, Soave-Redlich-Kwong equations, and the corresponding counterparts obtained from the new modified SRK equation for the rest of nonpolar and polar compounds employed in this study.

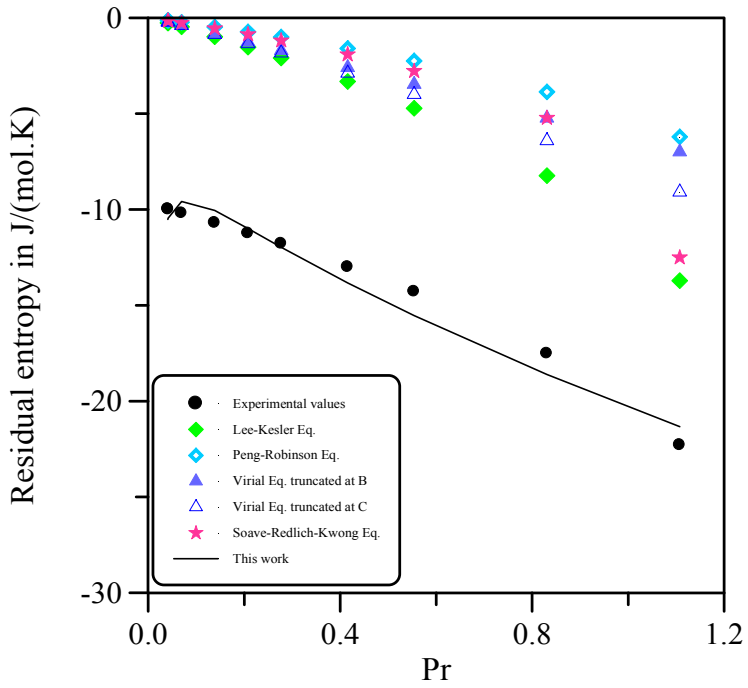

Figure 4-1 The relation between S^R and P_r for n-octane at T_r=1.01564

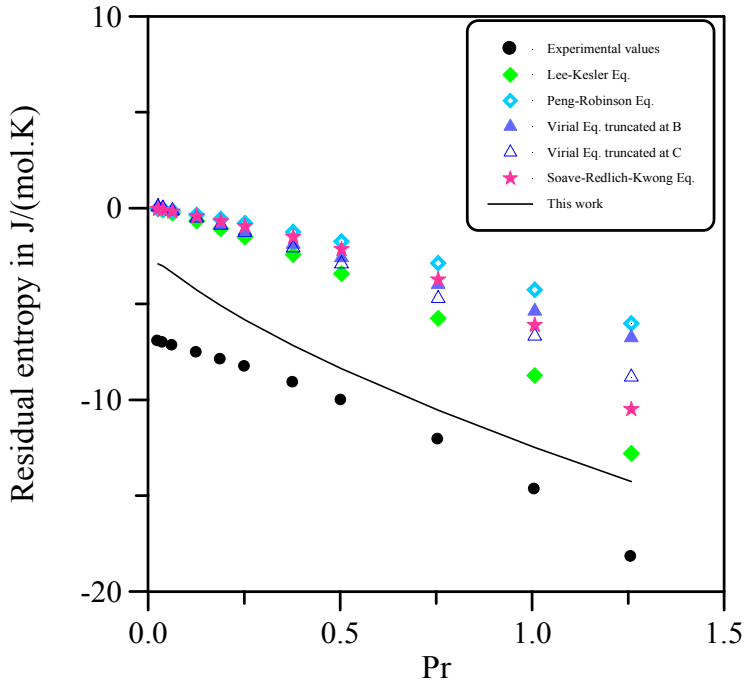

Figure 4-2 The relation between S^R and P_r for n-heptane at T_r=1.089792

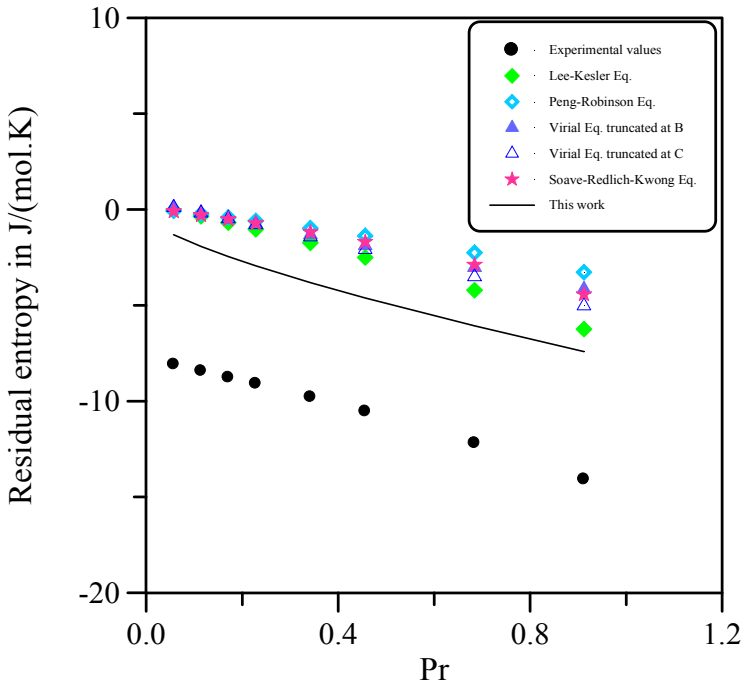

Figure 4-3 The relation between S^R and P_r for n-hexane at T_r=1.116003

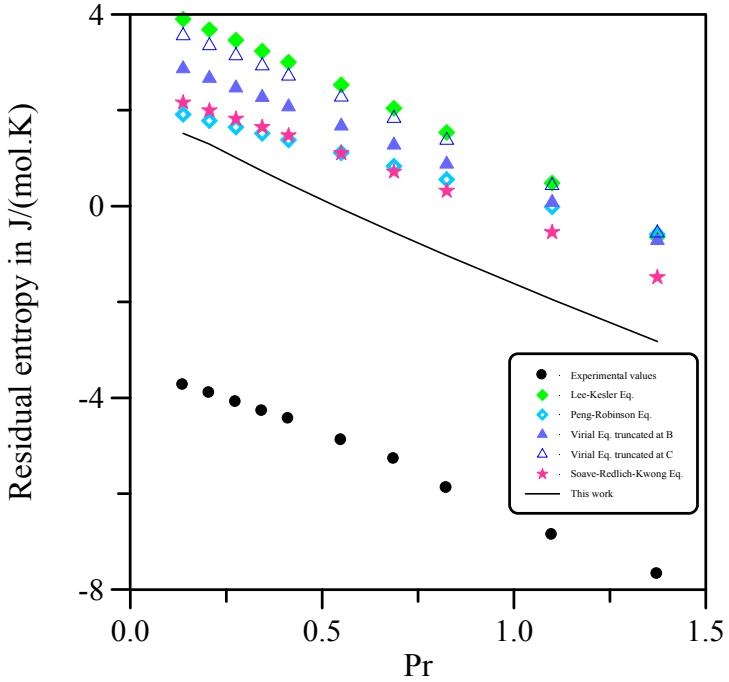

Figure 4-4 The relation between S^R and P_r for carbon dioxide at T_r=1.3256

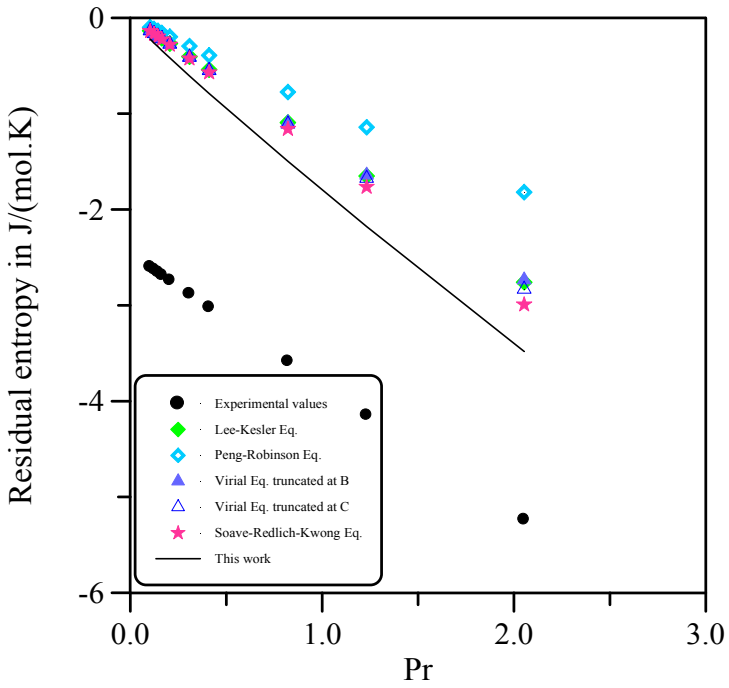

Figure 4-5 The relation between S^R and P_r for ethane at T_r=1.7686

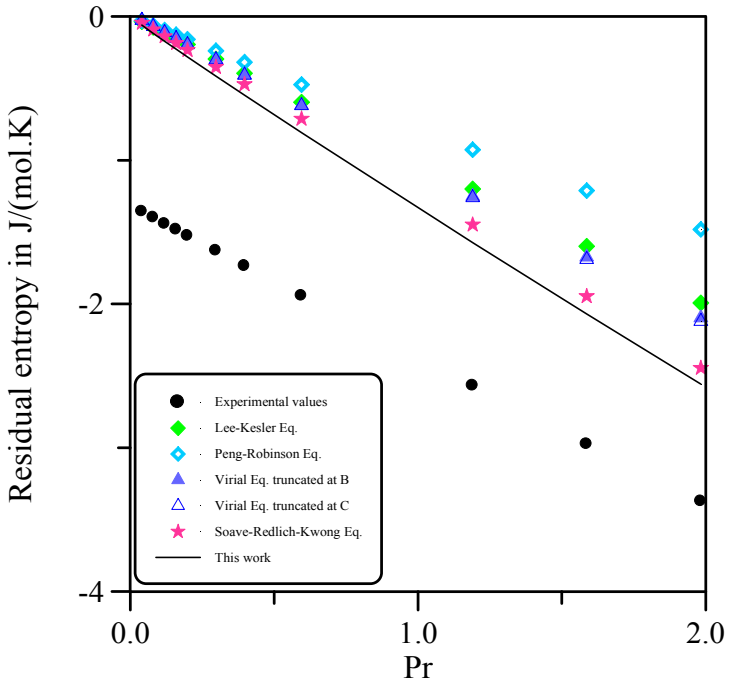

Figure 4-6 The relation between S^R and P_r for oxygen at T_r=1.9407

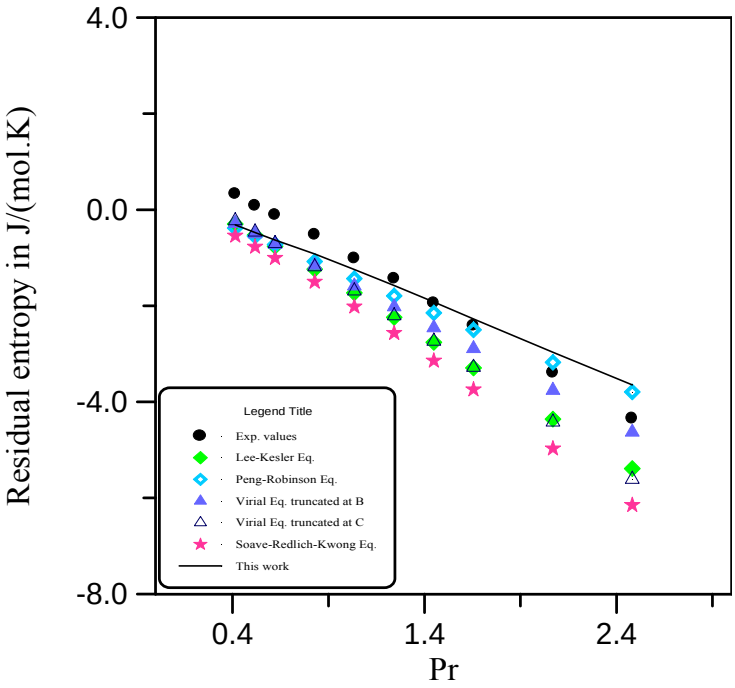

Figure 4-7 The relation between S^R and P_r for argon at T_r=1.45831

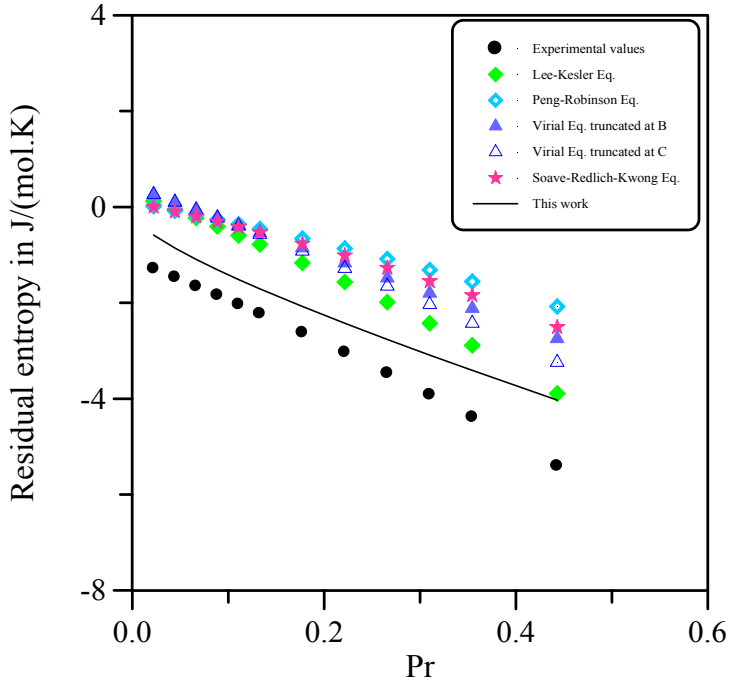

Figure 4-8 The relation between S^R and P_r for refrigerant (152a) at T_r=0.9916

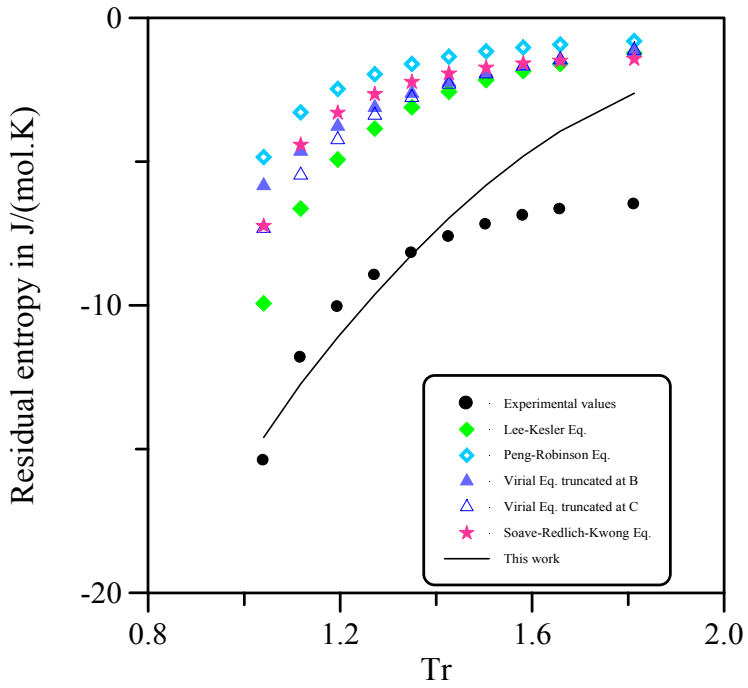

Figure 4-9 The relation between S^R and T_r for water at P_r=0.90645

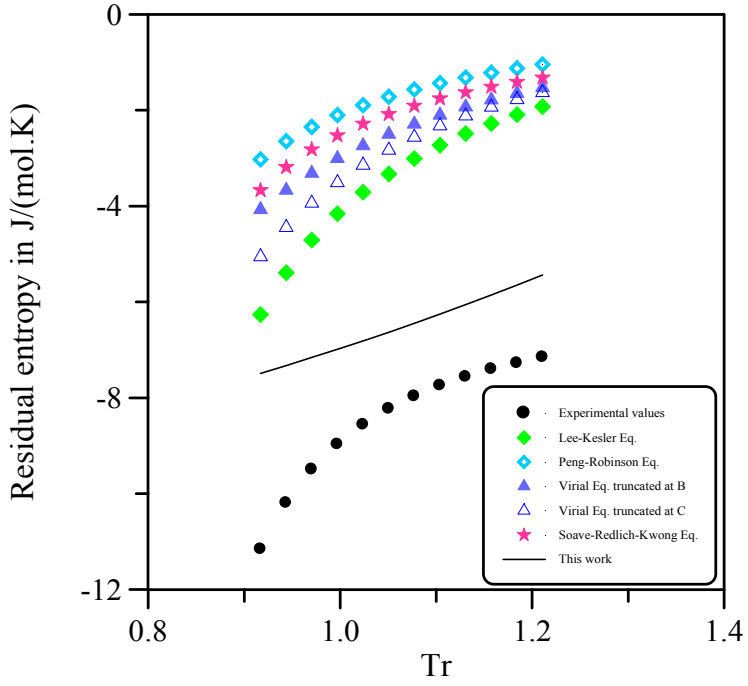

Figure 4-10 The relation between S^R and T_r for refrigerant (134a) at *Pr*=0.4435

Table 4-4 the comparison of deviations in results of **n-octane** from the experimental data [61] when using different EOS[1].

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	399.82	101.4	525.37	2.6743	2.8152	2.8087	2.2997	14.0499	14.7902	14.7562	12.0818	1.6899	1.7789	1.7749	1.4532
2	399.82	103.4	525.18	2.6747	2.8188	2.8122	2.1988	14.0471	14.8039	14.7691	11.5478	1.6896	1.7806	1.7764	1.3890
3	410.93	101.4	531.92	2.6753	2.7986	2.7925	2.1266	14.2306	14.8863	14.8538	11.3119	1.7116	1.7905	1.7866	1.3606
4	410.93	103.4	531.73	2.6763	2.8023	2.7961	2.0319	14.2305	14.9008	14.8675	10.8045	1.7116	1.7923	1.7883	1.2995
5	422.04	101.4	538.52	2.6584	2.7666	2.7609	1.9607	14.3158	14.8991	14.8679	10.5587	1.7219	1.7920	1.7883	1.2700
6	422.04	103.4	538.33	2.6597	2.7705	2.7645	1.8723	14.3181	14.9143	14.8824	10.0791	1.7222	1.7939	1.7900	1.2123
7	422.04	172.4	533.31	2.6925	2.8885	2.8777	0.4707	14.3595	15.4048	15.3469	2.5101	1.7272	1.8529	1.8459	0.3019
8	433.15	101.4	545.22	2.6157	2.7112	2.7057	1.8112	14.2611	14.7819	14.7519	9.8751	1.7153	1.7780	1.7743	1.1878
9	433.15	103.4	545.03	2.6174	2.7150	2.7094	1.7291	14.2653	14.7976	14.7670	9.4242	1.7158	1.7798	1.7762	1.1335
10	433.15	172.4	540.10	2.6449	2.8171	2.8069	0.4369	14.2850	15.2153	15.1600	2.3596	1.7182	1.8301	1.8234	0.2838
11	444.26	101.4	551.91	2.5664	2.6510	2.6458	1.6617	14.1645	14.6312	14.6023	9.1714	1.7037	1.7598	1.7564	1.1031
12	444.26	103.4	551.72	2.5684	2.6549	2.6495	1.5859	14.1706	14.6476	14.6181	8.7497	1.7044	1.7618	1.7582	1.0524
13	444.26	172.4	546.89	2.5888	2.7409	2.7312	0.4025	14.1581	14.9897	14.9368	2.2014	1.7029	1.8030	1.7966	0.2648
14	455.37	101.4	558.71	2.4937	2.5688	2.5638	1.5303	13.9324	14.3521	14.3242	8.5498	1.6758	1.7263	1.7229	1.0284
15	455.37	103.4	558.51	2.4959	2.5727	2.5676	1.4606	13.9400	14.3690	14.3404	8.1576	1.6767	1.7283	1.7249	0.9812
16	455.37	172.4	553.73	2.5165	2.6514	2.6422	0.3766	13.9349	14.6814	14.6305	2.0855	1.6761	1.7659	1.7597	0.2508
17	455.37	344.7	546.41	2.5581	2.8572	2.8347	0.2312	13.9780	15.6124	15.4894	1.2634	1.6813	1.8778	1.8630	0.1520
18	466.48	101.4	565.50	2.4159	2.4829	2.4781	1.4009	13.6620	14.0406	14.0136	7.9219	1.6433	1.6888	1.6855	0.9528
19	466.48	103.4	565.31	2.4183	2.4868	2.4819	1.3372	13.6710	14.0579	14.0303	7.5591	1.6443	1.6909	1.6875	0.9092
20	466.48	172.4	560.57	2.4379	2.5579	2.5491	0.3509	13.6662	14.3388	14.2897	1.9669	1.6438	1.7247	1.7187	0.2366
21	466.48	344.7	553.40	2.4788	2.7427	2.7217	0.1880	13.7175	15.1782	15.0617	1.0402	1.6499	1.8256	1.8116	0.1251
22	477.59	101.4	572.29	2.3335	2.3934	2.3888	1.2747	13.3546	13.6972	13.6709	7.2950	1.6063	1.6475	1.6443	0.8774
23	477.59	103.4	572.10	2.3361	2.3973	2.3926	1.2168	13.3647	13.7148	13.6880	6.9615	1.6075	1.6496	1.6464	0.8373

[1] Results of virial equation were not listed in tables due to the high deviations from the experimental values obtained comparing with other equations that employed.

24	477.59	172.4	567.41	2.3535	2.4607	2.4524	0.3258	13.3543	13.9624	13.9149	1.8487	1.6062	1.6794	1.6737	0.2224
25	477.59	344.7	560.38	2.3898	2.6239	2.6041	0.1453	13.3919	14.7040	14.5931	0.8142	1.6108	1.7686	1.7552	0.0979
26	477.59	517.1	555.55	2.4164	2.7996	2.7635	0.3155	13.4243	15.5534	15.3524	1.7530	1.6147	1.8707	1.8466	0.2108
27	488.71	101.4	579.08	2.2468	2.3005	2.2961	1.1531	13.0109	13.3217	13.2962	6.6773	1.5649	1.6023	1.5992	0.8031
28	488.71	103.4	578.89	2.2495	2.3044	2.2999	1.1008	13.0222	13.3398	13.3137	6.3723	1.5663	1.6045	1.6014	0.7664
29	488.71	172.4	574.25	2.2640	2.3601	2.3521	0.3020	13.0012	13.5528	13.5068	1.7344	1.5638	1.6301	1.6246	0.2086
30	488.71	344.7	567.31	2.3012	2.5099	2.4912	0.1114	13.0552	14.2392	14.1330	0.6318	1.5703	1.7127	1.6999	0.0760
31	488.71	517.1	562.68	2.3192	2.6576	2.6241	0.2362	13.0495	14.9535	14.7651	1.3289	1.5696	1.7986	1.7759	0.1598
32	488.71	689.5	558.80	2.3323	2.8249	2.7694	0.3508	13.0328	15.7855	15.4752	1.9601	1.5676	1.8987	1.8613	0.2358
33	499.82	101.4	585.87	2.1561	2.2043	2.2001	1.0372	12.6318	12.9145	12.8896	6.0765	1.5193	1.5533	1.5503	0.7309
34	499.82	103.4	585.68	2.1589	2.2082	2.2038	0.9902	12.6440	12.9329	12.9075	5.7992	1.5208	1.5556	1.5525	0.6975
35	499.82	172.4	581.09	2.1697	2.2561	2.2484	0.2802	12.6081	13.1100	13.0653	1.6279	1.5165	1.5769	1.5715	0.1958
36	499.82	344.7	574.25	2.2053	2.3921	2.3744	0.0772	12.6640	13.7368	13.6349	0.4431	1.5232	1.6523	1.6400	0.0533
37	499.82	517.1	569.75	2.2191	2.5197	2.4885	0.1663	12.6432	14.3561	14.1782	0.9472	1.5207	1.7267	1.7053	0.1139
38	499.82	689.5	566.02	2.2375	2.6702	2.6198	0.2498	12.6649	15.1139	14.8289	1.4142	1.5233	1.8179	1.7836	0.1701
39	510.93	101.4	592.66	2.0615	2.1050	2.1009	0.9281	12.2176	12.4754	12.4510	5.5005	1.4695	1.5005	1.4976	0.6616
40	510.93	103.4	592.47	2.0643	2.1088	2.1046	0.8861	12.2306	12.4941	12.4692	5.2499	1.4711	1.5028	1.4998	0.6315
41	510.93	172.4	587.88	2.0794	2.1573	2.1499	0.2527	12.2242	12.6821	12.6386	1.4855	1.4703	1.5254	1.5202	0.1787
42	510.93	344.7	581.14	2.1113	2.2792	2.2623	0.0505	12.2698	13.2455	13.1473	0.2936	1.4758	1.5932	1.5813	0.0353
43	510.93	517.1	576.74	2.1262	2.3947	2.3654	0.1134	12.2624	13.8113	13.6424	0.6541	1.4749	1.6612	1.6409	0.0787
44	510.93	689.5	573.20	2.1354	2.5184	2.4722	0.1588	12.2399	14.4355	14.1707	0.9103	1.4722	1.7363	1.7044	0.1095
45	510.93	1034	566.88	2.1496	2.8300	2.7180	0.3529	12.1858	16.0430	15.4082	2.0005	1.4657	1.9296	1.8533	0.2406
46	522.04	101.4	599.36	1.9795	2.0188	2.0148	0.8111	11.8643	12.0999	12.0761	4.8613	1.4270	1.4554	1.4525	0.5847
47	522.04	103.4	599.21	1.9743	2.0145	2.0104	0.7817	11.8302	12.0711	12.0468	4.6839	1.4229	1.4519	1.4490	0.5634
48	522.04	172.4	594.62	1.9929	2.0633	2.0562	0.2206	11.8501	12.2691	12.2267	1.3114	1.4253	1.4757	1.4706	0.1577
49	522.04	344.7	587.98	2.0197	2.1711	2.1550	0.0307	11.8753	12.7658	12.6709	0.1808	1.4283	1.5355	1.5240	0.0217
50	522.04	517.1	583.67	2.0330	2.2740	2.2464	0.0685	11.8659	13.2729	13.1116	0.3995	1.4272	1.5964	1.5770	0.0481
51	522.04	689.5	580.23	2.0456	2.3870	2.3442	0.0934	11.8692	13.8501	13.6018	0.5421	1.4276	1.6659	1.6360	0.0652
52	522.04	1034	574.35	2.0554	2.6461	2.5503	0.2072	11.8050	15.1976	14.6477	1.1903	1.4199	1.8279	1.7618	0.1432
53	533.15	101.4	606.05	1.8936	1.9292	1.9254	0.7032	11.4764	11.6923	11.6689	4.2617	1.3804	1.4063	1.4035	0.5126

54	533.15	103.4	605.91	1.8886	1.9250	1.9211	0.6781	11.4430	11.6637	11.6399	4.1084	1.3764	1.4029	1.4000	0.4942
55	533.15	172.4	601.32	1.9102	1.9741	1.9672	0.1846	11.4865	11.8708	11.8294	1.1101	1.3816	1.4278	1.4228	0.1335
56	533.15	344.7	594.77	1.9306	2.0677	2.0522	0.0171	11.4827	12.2981	12.2061	0.1020	1.3811	1.4792	1.4681	0.0123
57	533.15	517.1	590.56	1.9403	2.1576	2.1314	0.0307	11.4589	12.7421	12.5874	0.1814	1.3783	1.5326	1.5140	0.0218
58	533.15	689.5	587.21	1.9531	2.2591	2.2191	0.0361	11.4686	13.2654	13.0308	0.2121	1.3794	1.5955	1.5673	0.0255
59	533.15	1034	581.66	1.9584	2.4777	2.3934	0.0888	11.3914	14.4121	13.9217	0.5167	1.3701	1.7335	1.6745	0.0622
60	533.15	1379	576.26	1.9560	2.7773	2.5760	0.3050	11.2717	16.0042	14.8442	1.7574	1.3557	1.9250	1.7854	0.2114
61	544.26	101.4	612.70	1.8119	1.8443	1.8406	0.5975	11.1018	11.3000	11.2771	3.6609	1.3353	1.3592	1.3564	0.4403
62	544.26	103.4	612.51	1.8150	1.8480	1.8442	0.5685	11.1168	11.3195	11.2961	3.4824	1.3371	1.3615	1.3587	0.4189
63	544.26	172.4	608.01	1.8233	1.8814	1.8747	0.1536	11.0859	11.4393	11.3987	0.9337	1.3334	1.3759	1.3710	0.1123
64	544.26	344.7	601.51	1.8443	1.9688	1.9539	0.0090	11.0937	11.8425	11.7530	0.0543	1.3343	1.4244	1.4136	0.0065
65	544.26	517.1	597.35	1.8570	2.0537	2.0287	0.0075	11.0929	12.2675	12.1186	0.0450	1.3342	1.4755	1.4576	0.0054
66	544.26	689.5	594.10	1.8673	2.1430	2.1054	0.0058	11.0938	12.7312	12.5082	0.0343	1.3344	1.5313	1.5045	0.0041
67	544.26	1034	588.79	1.8739	2.3349	2.2591	0.0043	11.0333	13.7476	13.3014	0.0255	1.3271	1.6535	1.5999	0.0031
68	544.26	1379	583.91	1.8695	2.5757	2.4180	0.1274	10.9163	15.0395	14.1188	0.7438	1.3130	1.8089	1.6982	0.0895
69	555.37	101.4	619.30	1.7343	1.7637	1.7601	0.4949	10.7405	10.9228	10.9003	3.0651	1.2919	1.3138	1.3111	0.3687
70	555.37	103.4	619.11	1.7374	1.7675	1.7637	0.4696	10.7561	10.9426	10.9196	2.9075	1.2937	1.3162	1.3134	0.3497
71	555.37	172.4	614.61	1.7481	1.8011	1.7947	0.1124	10.7443	11.0700	11.0302	0.6909	1.2923	1.3315	1.3267	0.0831
72	555.37	344.7	608.16	1.7688	1.8822	1.8679	0.0136	10.7574	11.4469	11.3597	0.0826	1.2939	1.3768	1.3663	0.0099
73	555.37	517.1	604.05	1.7832	1.9618	1.9379	0.0020	10.7712	11.8500	11.7061	0.0122	1.2955	1.4253	1.4080	0.0015
74	555.37	689.5	600.89	1.7892	2.0386	2.0031	0.0332	10.7512	12.2496	12.0364	0.1993	1.2931	1.4734	1.4477	0.0240
75	555.37	1034	595.77	1.7973	2.2097	2.1406	0.0559	10.7081	13.1646	12.7528	0.3333	1.2880	1.5834	1.5339	0.0401
76	555.37	1379	591.28	1.7899	2.4080	2.2759	0.0015	10.5834	14.2381	13.4569	0.0087	1.2730	1.7125	1.6186	0.0010
77	566.48	101.4	625.81	1.6683	1.6951	1.6916	0.3887	10.4401	10.6081	10.5859	2.4323	1.2557	1.2759	1.2733	0.2926
78	566.48	103.4	625.62	1.6714	1.6988	1.6952	0.3667	10.4563	10.6281	10.6054	2.2940	1.2577	1.2783	1.2756	0.2759
79	566.48	172.4	621.12	1.6843	1.7328	1.7265	0.0622	10.4618	10.7625	10.7235	0.3861	1.2583	1.2945	1.2898	0.0464
80	566.48	344.7	614.76	1.6961	1.7996	1.7858	0.0221	10.4269	11.0634	10.9784	0.1358	1.2541	1.3307	1.3205	0.0163
81	566.48	517.1	610.69	1.7109	1.8736	1.8508	0.0067	10.4481	11.4419	11.3024	0.0408	1.2567	1.3762	1.3594	0.0049
82	566.48	689.5	607.58	1.7191	1.9456	1.9120	0.0470	10.4453	11.8214	11.6168	0.2856	1.2563	1.4219	1.3973	0.0343
83	566.48	1034	602.66	1.7232	2.0942	2.0305	0.1012	10.3848	12.6212	12.2368	0.6099	1.2491	1.5181	1.4718	0.0734

84	566.48	1379	598.45	1.7138	2.2614	2.1464	0.0912	10.2562	13.5334	12.8453	0.5459	1.2336	1.6278	1.5450	0.0657
85	566.48	2068	589.41	1.6563	2.7838	0.3434	0.3325	9.7622	16.4082	2.0243	1.9601	1.1742	1.9736	0.2435	0.2358
86	577.59	101.4	632.26	1.6058	1.6303	1.6268	0.2871	10.1527	10.3078	10.2859	1.8151	1.2212	1.2398	1.2372	0.2183
87	577.59	103.4	632.07	1.6089	1.6340	1.6305	0.2681	10.1693	10.3280	10.3057	1.6944	1.2232	1.2422	1.2396	0.2038
88	577.59	172.4	627.62	1.6161	1.6604	1.6543	0.0189	10.1428	10.4211	10.3827	0.1187	1.2200	1.2534	1.2488	0.0143
89	577.59	344.7	621.26	1.6339	1.7287	1.7153	0.0417	10.1509	10.7400	10.6568	0.2588	1.2209	1.2918	1.2818	0.0311
90	577.59	517.1	617.25	1.6482	1.7969	1.7750	0.0007	10.1735	11.0915	10.9560	0.0044	1.2237	1.3341	1.3178	0.0005
91	577.59	689.5	614.23	1.6495	1.8560	1.8239	0.0559	10.1319	11.4000	11.2027	0.3434	1.2187	1.3712	1.3474	0.0413
92	577.59	1034	609.45	1.6532	1.9889	1.9295	0.1324	10.0752	12.1211	11.7592	0.8068	1.2118	1.4579	1.4144	0.0970
93	577.59	1379	605.38	1.6561	2.1457	2.0432	0.1445	10.0258	12.9899	12.3690	0.8745	1.2059	1.5624	1.4877	0.1052
94	577.59	2068	597.54	1.6080	2.5489	2.1449	0.0773	9.6086	15.2305	12.8166	0.4621	1.1557	1.8319	1.5416	0.0556
95	588.71	101.4	638.62	1.5543	1.5767	1.5734	0.1832	9.9260	10.0694	10.0478	1.1699	1.1939	1.2111	1.2085	0.1407
96	588.71	103.4	638.43	1.5574	1.5804	1.5769	0.1669	9.9430	10.0897	10.0677	1.0653	1.1959	1.2136	1.2109	0.1281
97	588.71	172.4	633.98	1.5664	1.6071	1.6011	0.0395	9.9308	10.1888	10.1509	0.2506	1.1945	1.2255	1.2209	0.0301
98	588.71	344.7	627.67	1.5820	1.6691	1.6561	0.0715	9.9300	10.4764	10.3948	0.4485	1.1944	1.2601	1.2503	0.0539
99	588.71	517.1	623.75	1.5873	1.7236	1.7024	0.0116	9.9007	10.7511	10.6190	0.0724	1.1909	1.2931	1.2772	0.0087
100	588.71	689.5	620.74	1.5964	1.7852	1.7545	0.0451	9.9095	11.0816	10.8907	0.2800	1.1919	1.3329	1.3099	0.0337
101	588.71	1034	616.10	1.5964	1.9015	1.8458	0.1426	9.8355	11.7153	11.3720	0.8789	1.1830	1.4091	1.3678	0.1057
102	588.71	1379	612.22	1.5967	2.0376	1.9445	0.1835	9.7753	12.4745	11.9045	1.1232	1.1758	1.5004	1.4319	0.1351
103	588.71	2068	605.10	1.5606	2.3728	2.0926	0.0782	9.4434	14.3578	12.6622	0.4732	1.1358	1.7269	1.5230	0.0569
104	588.71	2758	596.01	1.4270	2.9921	1.4874	0.5818	8.5049	17.8331	8.8651	3.4677	1.0230	2.1450	1.0663	0.4171
105	599.82	101.4	644.94	1.5058	1.5264	1.5231	0.0850	9.7117	9.8445	9.8232	0.5485	1.1681	1.1841	1.1815	0.0660
106	599.82	103.4	644.75	1.5090	1.5301	1.5267	0.0711	9.7291	9.8650	9.8432	0.4581	1.1702	1.1865	1.1839	0.0551
107	599.82	172.4	640.30	1.5196	1.5570	1.5512	0.0973	9.7300	9.9697	9.9324	0.6230	1.1703	1.1991	1.1947	0.0749
108	599.82	344.7	634.03	1.5325	1.6126	1.6000	0.1031	9.7167	10.2245	10.1444	0.6539	1.1687	1.2298	1.2202	0.0786
109	599.82	517.1	630.11	1.5437	1.6690	1.6485	0.0407	9.7269	10.5164	10.3875	0.2563	1.1699	1.2649	1.2494	0.0308
110	599.82	689.5	627.19	1.5441	1.7173	1.6878	0.0309	9.6845	10.7707	10.5855	0.1939	1.1648	1.2955	1.2732	0.0233
111	599.82	1034	622.60	1.5535	1.8320	1.7793	0.1331	9.6722	11.4058	11.0782	0.8286	1.1634	1.3719	1.3325	0.0997
112	599.82	1379	618.92	1.5463	1.9456	1.8600	0.2015	9.5701	12.0415	11.5116	1.2470	1.1511	1.4483	1.3846	0.1500
113	599.82	2068	612.32	1.5158	2.2302	2.0070	0.1776	9.2814	13.6561	12.2893	1.0877	1.1164	1.6425	1.4781	0.1308

114	599.82	2758	605.15	1.4187	2.6591	1.6174	0.1605	8.5852	16.0911	9.7879	0.9713	1.0326	1.9354	1.1773	0.1168
115	610.93	101.4	651.15	1.4678	1.4867	1.4835	0.0145	9.5575	9.6807	9.6596	0.0945	1.1496	1.1644	1.1618	0.0114
116	610.93	103.4	650.96	1.4709	1.4903	1.4870	0.0264	9.5753	9.7013	9.6798	0.1721	1.1517	1.1669	1.1643	0.0207
117	610.93	172.4	646.52	1.4830	1.5175	1.5118	0.1613	9.5881	9.8111	9.7743	1.0427	1.1533	1.1801	1.1756	0.1254
118	610.93	344.7	640.30	1.4929	1.5668	1.5545	0.1437	9.5591	10.0321	9.9533	0.9199	1.1498	1.2066	1.1972	0.1107
119	610.93	517.1	636.42	1.5017	1.6171	1.5973	0.0719	9.5571	10.2917	10.1655	0.4575	1.1495	1.2379	1.2227	0.0550
120	610.93	689.5	633.51	1.5082	1.6675	1.6391	0.0013	9.5545	10.5638	10.3836	0.0082	1.1492	1.2706	1.2489	0.0010
121	610.93	1034	629.06	1.5093	1.7643	1.7143	0.1200	9.4944	11.0984	10.7842	0.7546	1.1420	1.3349	1.2971	0.0908
122	610.93	1379	625.47	1.5065	1.8700	1.7904	0.1996	9.4228	11.6961	11.1985	1.2484	1.1334	1.4068	1.3469	0.1502
123	610.93	2068	619.25	1.4828	2.1192	1.9304	0.2312	9.1821	13.1234	11.9540	1.4319	1.1044	1.5785	1.4378	0.1722
124	610.93	2758	613.04	1.4129	2.4588	1.9152	0.0480	8.6616	15.0736	11.7410	0.2945	1.0418	1.8130	1.4122	0.0354
125	610.93	3447	605.48	1.2553	3.0109	1.9997	0.4913	7.6005	18.2303	12.1078	2.9750	0.9142	2.1927	1.4563	0.3578
126	622.04	101.4	657.28	1.4398	1.4571	1.4540	0.1151	9.4631	9.5775	9.5566	0.7568	1.1382	1.1520	1.1495	0.0910
127	622.04	103.4	657.08	1.4429	1.4607	1.4575	0.1252	9.4811	9.5982	9.5769	0.8230	1.1404	1.1545	1.1519	0.0990
128	622.04	172.4	652.64	1.4564	1.4882	1.4827	0.2309	9.5051	9.7129	9.6764	1.5070	1.1433	1.1683	1.1639	0.1813
129	622.04	344.7	646.47	1.4629	1.5312	1.5192	0.1924	9.4574	9.8987	9.8211	1.2437	1.1375	1.1906	1.1813	0.1496
130	622.04	517.1	642.59	1.4765	1.5831	1.5638	0.1196	9.4876	10.1726	10.0489	0.7689	1.1412	1.2236	1.2087	0.0925
131	622.04	689.5	639.72	1.4808	1.6277	1.6002	0.0430	9.4729	10.4129	10.2370	0.2751	1.1394	1.2524	1.2313	0.0331
132	622.04	1034	635.37	1.4797	1.7140	1.6663	0.0888	9.4013	10.8900	10.5873	0.5639	1.1308	1.3098	1.2734	0.0678
133	622.04	1379	631.88	1.4784	1.8107	1.7362	0.1789	9.3420	11.4414	10.9704	1.1304	1.1236	1.3762	1.3195	0.1360
134	622.04	2068	626.00	1.4547	2.0269	1.8615	0.2563	9.1064	12.6885	11.6529	1.6045	1.0953	1.5262	1.4016	0.1930
135	622.04	2758	620.40	1.4006	2.3087	1.9231	0.1693	8.6894	14.3231	11.9311	1.0503	1.0452	1.7228	1.4351	0.1263
136	622.04	3447	614.28	1.2873	2.7088	1.8751	0.1330	7.9075	16.6399	11.5184	0.8172	0.9511	2.0014	1.3854	0.0983
137	622.04	4137	607.87	1.0702	3.2093	2.3725	0.5779	6.5057	19.5082	14.4220	3.5129	0.7825	2.3464	1.7347	0.4225
138	633.15	101.4	663.30	1.4214	1.4374	1.4343	0.2166	9.4282	9.5345	9.5139	1.4368	1.1340	1.1468	1.1443	0.1728
139	633.15	103.4	663.11	1.4246	1.4410	1.4378	0.2252	9.4465	9.5554	9.5343	1.4932	1.1362	1.1493	1.1468	0.1796
140	633.15	172.4	658.71	1.4320	1.4614	1.4560	0.2984	9.4327	9.6266	9.5905	1.9653	1.1346	1.1579	1.1535	0.2364
141	633.15	344.7	652.54	1.4423	1.5055	1.4938	0.2487	9.4118	9.8242	9.7477	1.6225	1.1320	1.1817	1.1724	0.1952
142	633.15	517.1	648.72	1.4526	1.5513	1.5326	0.1683	9.4235	10.0635	9.9419	1.0921	1.1334	1.2104	1.1958	0.1314
143	633.15	689.5	645.89	1.4543	1.5901	1.5635	0.0862	9.3930	10.2704	10.0984	0.5568	1.1298	1.2353	1.2146	0.0670

144	633.15	1034	641.59	1.4571	1.6730	1.6274	0.0479	9.3485	10.7338	10.4409	0.3071	1.1244	1.2910	1.2558	0.0369
145	633.15	1379	638.19	1.4551	1.7600	1.6897	0.1478	9.2866	11.2323	10.7834	0.9435	1.1170	1.3510	1.2970	0.1135
146	633.15	2068	632.55	1.4368	1.9549	1.8066	0.2543	9.0883	12.3658	11.4275	1.6084	1.0931	1.4874	1.3745	0.1935
147	633.15	2758	627.38	1.3954	2.1978	1.8904	0.2299	8.7544	13.7884	11.8600	1.4425	1.0530	1.6585	1.4265	0.1735
148	633.15	3447	622.12	1.3062	2.5091	1.8838	0.0643	8.1261	15.6100	11.7195	0.3999	0.9774	1.8776	1.4096	0.0481
149	633.15	4137	616.62	1.1605	2.9077	2.1159	0.2299	7.1557	17.9296	13.0469	1.4175	0.8607	2.1566	1.5693	0.1705
150	644.26	101.4	669.23	1.4124	1.4272	1.4241	0.3188	9.4524	9.5513	9.5308	2.1336	1.1369	1.1488	1.1464	0.2566
151	644.26	103.4	669.09	1.41	1.42	1.42	0.32	9.42	9.52	9.50	2.13	1.13	1.15	1.14	0.26
152	644.26	172.4	664.69	1.4170	1.4443	1.4389	0.3706	9.4186	9.5999	9.5641	2.4635	1.1329	1.1547	1.1504	0.2963
153	644.26	344.7	658.52	1.4308	1.4895	1.4780	0.3119	9.4223	9.8085	9.7329	2.0541	1.1333	1.1798	1.1707	0.2471
154	644.26	517.1	654.74	1.4376	1.5291	1.5109	0.2249	9.4129	10.0119	9.8922	1.4724	1.1322	1.2042	1.1898	0.1771
155	644.26	689.5	651.92	1.4437	1.5695	1.5436	0.1451	9.4114	10.2319	10.0633	0.9460	1.1320	1.2307	1.2104	0.1138
156	644.26	1034	647.66	1.4492	1.6487	1.6048	0.0094	9.3858	10.6780	10.3938	0.0610	1.1289	1.2843	1.2502	0.0073
157	644.26	1379	644.36	1.4448	1.7255	1.6587	0.0998	9.3097	11.1183	10.6881	0.6429	1.1198	1.3373	1.2856	0.0773
158	644.26	2068	638.91	1.4321	1.9040	1.7688	0.2264	9.1498	12.1650	11.3009	1.4465	1.1005	1.4632	1.3593	0.1740
159	644.26	2758	634.13	1.3908	2.1084	1.8489	0.2551	8.8198	13.3701	11.7241	1.6178	1.0608	1.6081	1.4102	0.1946
160	644.26	3447	629.39	1.3247	2.3696	1.8860	0.1688	8.3376	14.9140	11.8705	1.0622	1.0028	1.7938	1.4278	0.1278
161	644.26	4137	624.61	1.2152	2.6880	1.9930	0.0114	7.5900	16.7893	12.4482	0.0711	0.9129	2.0194	1.4973	0.0086
162	644.26	4826	620.16	1.0636	3.0212	2.2929	0.2039	6.5962	18.7365	14.2198	1.2648	0.7934	2.2536	1.7103	0.1521
∑				294.45	343.01	325.37	60.12	1760.51	2053.66	1946.59	346.97	211.75	247.01	234.13	41.73
Average (Overall)				**1.8176**	**2.1173**	**2.0085**	**0.3711**	**10.8673**	**12.6769**	**12.0160**	**2.1418**	**1.3071**	**1.5248**	**1.4453**	**0.2576**

Table 4-5 The comparison of deviations in results of **water** from the experimental data [29] when using different EOS.

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	423.15	200	131.14	4.3420	4.4895	4.4837	2.2083	5.6941	5.8875	5.8799	2.8959	0.6849	0.7081	0.7072	0.3483
2	473.15	200	135.23	4.1357	4.2249	4.2201	1.6475	5.5927	5.7134	5.7070	2.2279	0.6727	0.6872	0.6864	0.2680
3	523.15	200	138.87	4.0092	4.0663	4.0622	0.9252	5.5675	5.6468	5.6411	1.2849	0.6697	0.6792	0.6785	0.1545

4	573.15	200	142.19	3.9142	3.9524	3.9487	0.1289	5.5654	5.6197	5.6145	0.1832	0.6694	0.6759	0.6753	0.0220
5	673.15	200	148.11	3.7643	3.7832	3.7801	1.3723	5.5755	5.6035	5.5989	2.0326	0.6706	0.6740	0.6734	0.2445
6	773.15	200	153.37	3.6255	3.6358	3.6330	2.4073	5.5603	5.5761	5.5717	3.6920	0.6688	0.6707	0.6702	0.4441
7	873.15	200	158.12	3.4924	3.4982	3.4955	2.9350	5.5220	5.5312	5.5270	4.6407	0.6642	0.6653	0.6648	0.5582
8	973.15	200	162.48	3.3727	3.3759	3.3732	3.1327	5.4801	5.4853	5.4809	5.0901	0.6591	0.6598	0.6592	0.6122
9	1073.2	200	166.55	3.2932	3.2947	3.2918	3.1922	5.4848	5.4872	5.4824	5.3165	0.6597	0.6600	0.6594	0.6395
10	1173.2	200	170.36	3.2981	3.2982	3.2949	3.2552	5.6186	5.6187	5.6131	5.5456	0.6758	0.6758	0.6751	0.6670
11	1273.2	200	173.96	3.4404	3.4393	3.4355	3.4215	5.9849	5.9830	5.9763	5.9520	0.7199	0.7196	0.7188	0.7159
12	423.15	400	124.84	4.7335	5.0520	5.0395	0.8978	5.9094	6.3070	6.2914	1.1208	0.7108	0.7586	0.7567	0.1348
13	473.15	400	129.18	4.3898	4.5817	4.5714	0.7975	5.6706	5.9185	5.9052	1.0303	0.6821	0.7119	0.7103	0.1239
14	523.15	400	132.93	4.2094	4.3324	4.3235	0.9441	5.5955	5.7590	5.7472	1.2550	0.6730	0.6927	0.6913	0.1510
15	573.15	400	136.30	4.0907	4.1735	4.1657	1.2213	5.5758	5.6887	5.6780	1.6647	0.6707	0.6842	0.6829	0.2002
16	673.15	400	142.29	3.9167	3.9588	3.9522	1.9288	5.5731	5.6330	5.6236	2.7444	0.6703	0.6775	0.6764	0.3301
17	773.15	400	147.56	3.7659	3.7898	3.7838	2.5701	5.5571	5.5924	5.5836	3.7925	0.6684	0.6726	0.6716	0.4562
18	873.15	400	152.33	3.6218	3.6364	3.6307	2.9835	5.5171	5.5393	5.5306	4.5448	0.6636	0.6663	0.6652	0.5466
19	973.15	400	156.71	3.4931	3.5021	3.4964	3.1807	5.4740	5.4880	5.4791	4.9844	0.6584	0.6601	0.6590	0.5995
20	1073.2	400	160.77	3.4097	3.4150	3.4089	3.2648	5.4819	5.4903	5.4805	5.2489	0.6594	0.6604	0.6592	0.6313
21	1173.2	400	164.59	3.4118	3.4142	3.4074	3.3462	5.6154	5.6193	5.6081	5.5075	0.6754	0.6759	0.6745	0.6624
22	1273.2	400	168.19	3.5570	3.5568	3.5488	3.5271	5.9824	5.9821	5.9686	5.9321	0.7196	0.7195	0.7179	0.7135
23	473.15	500	127.17	4.4933	4.7392	4.7259	1.1641	5.7142	6.0269	6.0100	1.4805	0.6873	0.7249	0.7229	0.1781
24	523.15	500	130.98	4.2835	4.4408	4.4295	1.2090	5.6106	5.8167	5.8019	1.5836	0.6748	0.6996	0.6978	0.1905
25	573.15	500	134.39	4.1527	4.2587	4.2487	1.4074	5.5808	5.7232	5.7098	1.8914	0.6713	0.6884	0.6868	0.2275
26	623.15	500	137.50	4.0548	4.1292	4.1202	1.6877	5.5756	5.6779	5.6654	2.3206	0.6706	0.6829	0.6814	0.2791
27	673.15	500	140.40	3.9686	4.0226	4.0142	1.9987	5.5720	5.6479	5.6361	2.8063	0.6702	0.6793	0.6779	0.3375
28	773.15	500	145.69	3.8127	3.8437	3.8361	2.5819	5.5548	5.5999	5.5889	3.7616	0.6681	0.6735	0.6722	0.4524
29	873.15	500	150.46	3.6647	3.6837	3.6765	2.9828	5.5140	5.5426	5.5317	4.4880	0.6632	0.6667	0.6654	0.5398
30	973.15	500	154.84	3.5345	3.5465	3.5392	3.1897	5.4729	5.4914	5.4802	4.9391	0.6583	0.6605	0.6592	0.5941
31	1073.2	500	158.91	3.4483	3.4555	3.4478	3.2842	5.4798	5.4912	5.4790	5.2190	0.6591	0.6605	0.6590	0.6277
32	1173.2	500	162.73	3.4495	3.4530	3.4444	3.3738	5.6132	5.6190	5.6050	5.4901	0.6752	0.6758	0.6742	0.6603
33	1273.2	500	166.33	3.5961	3.5965	3.5863	3.5613	5.9814	5.9820	5.9651	5.9234	0.7194	0.7195	0.7175	0.7125

34	473.15	600	125.50	4.5888	4.8902	4.8738	1.4046	5.7591	6.1372	6.1168	1.7628	0.6927	0.7382	0.7357	0.2120
35	523.15	600	129.38	4.3485	4.5409	4.5270	1.3703	5.6259	5.8749	5.8569	1.7729	0.6767	0.7066	0.7045	0.2132
36	573.15	600	132.81	4.2061	4.3356	4.3234	1.5144	5.5862	5.7582	5.7420	2.0113	0.6719	0.6926	0.6906	0.2419
37	673.15	600	138.86	4.0124	4.0787	4.0684	2.0313	5.5715	5.6635	5.6493	2.8206	0.6701	0.6812	0.6795	0.3393
38	773.15	600	144.16	3.8522	3.8903	3.8811	2.5798	5.5532	5.6080	5.5948	3.7189	0.6679	0.6745	0.6729	0.4473
39	873.15	600	148.94	3.7007	3.7242	3.7154	2.9763	5.5116	5.5467	5.5336	4.4328	0.6629	0.6671	0.6656	0.5332
40	973.15	600	153.32	3.5670	3.5820	3.5732	3.1918	5.4690	5.4919	5.4784	4.8936	0.6578	0.6606	0.6589	0.5886
41	1073.2	600	157.39	3.4796	3.4888	3.4794	3.2974	5.4765	5.4910	5.4763	5.1898	0.6587	0.6605	0.6587	0.6242
42	1173.2	600	161.21	3.4811	3.4858	3.4754	3.3958	5.6117	5.6194	5.6025	5.4743	0.6750	0.6759	0.6739	0.6584
43	1273.2	600	164.81	3.6291	3.6300	3.6176	3.5895	5.9811	5.9825	5.9622	5.9158	0.7194	0.7196	0.7171	0.7115
44	473.15	800	122.79	4.7720	5.1887	5.1659	1.7299	5.8593	6.3711	6.3430	2.1241	0.7048	0.7663	0.7629	0.2555
45	523.15	800	126.80	4.4640	4.7289	4.7097	1.5593	5.6603	5.9962	5.9718	1.9771	0.6808	0.7212	0.7183	0.2378
46	573.15	800	130.30	4.2965	4.4744	4.4576	1.6229	5.5982	5.8301	5.8081	2.1147	0.6733	0.7012	0.6986	0.2543
47	673.15	800	136.40	4.0840	4.1751	4.1611	2.0439	5.5706	5.6948	5.6757	2.7879	0.6700	0.6850	0.6827	0.3353
48	773.15	800	141.73	3.9148	3.9674	3.9548	2.5534	5.5484	5.6229	5.6051	3.6189	0.6674	0.6763	0.6742	0.4353
49	873.15	800	146.52	3.7586	3.7913	3.7794	2.9534	5.5070	5.5551	5.5376	4.3273	0.6624	0.6682	0.6661	0.5205
50	973.15	800	150.91	3.6213	3.6425	3.6305	3.1895	5.4650	5.4969	5.4788	4.8133	0.6573	0.6612	0.6590	0.5789
51	1073.2	800	154.99	3.5307	3.5440	3.5313	3.3150	5.4722	5.4928	5.4731	5.1378	0.6582	0.6607	0.6583	0.6180
52	1173.2	800	158.81	3.5308	3.5380	3.5239	3.4277	5.6072	5.6187	5.5961	5.4434	0.6744	0.6758	0.6731	0.6547
53	1273.2	800	162.41	3.6803	3.6822	3.6655	3.6317	5.9772	5.9804	5.9532	5.8982	0.7189	0.7193	0.7160	0.7094
54	473.15	1000	120.59	4.9520	5.4900	5.4602	1.9708	5.9716	6.6204	6.5845	2.3767	0.7183	0.7963	0.7920	0.2859
55	523.15	1000	124.75	4.5684	4.9085	4.8836	1.6709	5.6990	6.1232	6.0921	2.0844	0.6855	0.7365	0.7328	0.2507
56	573.15	1000	128.32	4.3723	4.6002	4.5785	1.6678	5.6104	5.9028	5.8750	2.1400	0.6748	0.7100	0.7066	0.2574
57	673.15	1000	134.48	4.1411	4.2576	4.2397	2.0236	5.5691	5.7257	5.7016	2.7214	0.6698	0.6887	0.6858	0.3273
58	773.15	1000	139.83	3.9654	4.0327	4.0167	2.5146	5.5449	5.6392	5.6168	3.5163	0.6669	0.6783	0.6756	0.4229
59	873.15	1000	144.64	3.8040	3.8462	3.8310	2.9231	5.5022	5.5632	5.5412	4.2279	0.6618	0.6691	0.6665	0.5085
60	973.15	1000	149.04	3.6640	3.6913	3.6761	3.1798	5.4608	5.5016	5.4789	4.7392	0.6568	0.6617	0.6590	0.5700
61	1073.2	1000	153.12	3.5720	3.5894	3.5732	3.3251	5.4694	5.4960	5.4714	5.0914	0.6579	0.6611	0.6581	0.6124
62	1173.2	1000	156.94	3.5709	3.5806	3.5626	3.4510	5.6042	5.6195	5.5913	5.4161	0.6741	0.6759	0.6725	0.6514
63	1273.2	1000	160.55	3.7216	3.7246	3.7034	3.6644	5.9749	5.9797	5.9457	5.8830	0.7187	0.7192	0.7151	0.7076

64	473.15	1200	118.72	5.1354	5.8006	5.7632	2.1836	6.0965	6.8862	6.8418	2.5923	0.7333	0.8283	0.8229	0.3118
65	523.15	1200	123.03	4.6665	5.0843	5.0534	1.7500	5.7411	6.2552	6.2172	2.1530	0.6905	0.7524	0.7478	0.2590
66	573.15	1200	126.67	4.4396	4.7188	4.6920	1.6850	5.6239	5.9774	5.9435	2.1345	0.6764	0.7190	0.7149	0.2567
67	673.15	1200	132.90	4.1894	4.3318	4.3099	1.9890	5.5678	5.7571	5.7279	2.6434	0.6697	0.6925	0.6889	0.3179
68	773.15	1200	138.28	4.0079	4.0903	4.0708	2.4702	5.5421	5.6561	5.6291	3.4158	0.6666	0.6803	0.6771	0.4108
69	873.15	1200	143.10	3.8420	3.8938	3.8753	2.8896	5.4979	5.5720	5.5456	4.1350	0.6613	0.6702	0.6670	0.4974
70	973.15	1200	147.51	3.6984	3.7321	3.7136	3.1652	5.4554	5.5051	5.4778	4.6689	0.6562	0.6622	0.6589	0.5616
71	1073.2	1200	151.59	3.6042	3.6257	3.6062	3.3280	5.4637	5.4964	5.4668	5.0450	0.6572	0.6611	0.6575	0.6068
72	1173.2	1200	155.42	3.6033	3.6155	3.5937	3.4675	5.6002	5.6192	5.5853	5.3891	0.6736	0.6759	0.6718	0.6482
73	1273.2	1200	159.03	3.7550	3.7591	3.7334	3.6896	5.9714	5.9780	5.9371	5.8674	0.7182	0.7190	0.7141	0.7057
74	473.15	1400	117.05	5.3278	6.1263	6.0808	2.3927	6.2364	7.1710	7.1177	2.8007	0.7501	0.8625	0.8561	0.3369
75	523.15	1400	121.54	4.7604	5.2586	5.2213	1.8139	5.7859	6.3914	6.3461	2.2046	0.6959	0.7688	0.7633	0.2652
76	573.15	1400	125.26	4.5007	4.8324	4.8003	1.6883	5.6378	6.0533	6.0131	2.1148	0.6781	0.7281	0.7232	0.2544
77	673.15	1400	131.55	4.2325	4.4013	4.3752	1.9482	5.5680	5.7901	5.7557	2.5629	0.6697	0.6964	0.6923	0.3083
78	773.15	1400	136.96	4.0430	4.1408	4.1176	2.4213	5.5373	5.6712	5.6395	3.3163	0.6660	0.6821	0.6783	0.3989
79	873.15	1400	141.80	3.8731	3.9346	3.9127	2.8527	5.4919	5.5791	5.5481	4.0451	0.6606	0.6710	0.6673	0.4865
80	973.15	1400	146.21	3.7288	3.7689	3.7471	3.1492	5.4518	5.5105	5.4786	4.6044	0.6557	0.6628	0.6590	0.5538
81	1073.2	1400	150.30	3.6326	3.6584	3.6354	3.3285	5.4598	5.4986	5.4640	5.0028	0.6567	0.6614	0.6572	0.6017
82	1173.2	1400	154.13	3.6320	3.6468	3.6211	3.4810	5.5979	5.6208	5.5812	5.3651	0.6733	0.6761	0.6713	0.6453
83	1273.2	1400	157.74	3.7847	3.7899	3.7597	3.7114	5.9698	5.9780	5.9304	5.8542	0.7180	0.7190	0.7133	0.7041
84	523.15	1600	120.22	4.8538	5.4350	5.3910	1.8728	5.8352	6.5338	6.4809	2.2515	0.7018	0.7859	0.7795	0.2708
85	573.15	1600	124.02	4.5575	4.9430	4.9055	1.6844	5.6523	6.1305	6.0839	2.0890	0.6799	0.7374	0.7318	0.2513
86	673.15	1600	130.38	4.2693	4.4649	4.4346	1.9020	5.5663	5.8214	5.7818	2.4798	0.6695	0.7002	0.6954	0.2983
87	773.15	1600	135.81	4.0737	4.1870	4.1602	2.3711	5.5327	5.6866	5.6501	3.2202	0.6655	0.6840	0.6796	0.3873
88	873.15	1600	140.66	3.9015	3.9728	3.9475	2.8162	5.4878	5.5881	5.5526	3.9613	0.6601	0.6721	0.6679	0.4765
89	973.15	1600	145.08	3.7542	3.8009	3.7756	3.1302	5.4467	5.5144	5.4778	4.5414	0.6551	0.6633	0.6589	0.5462
90	1073.2	1600	149.18	3.6575	3.6876	3.6610	3.3267	5.4562	5.5011	5.4615	4.9627	0.6563	0.6617	0.6569	0.5969
91	1173.2	1600	153.01	3.6561	3.6735	3.6439	3.4904	5.5941	5.6208	5.5755	5.3406	0.6729	0.6761	0.6706	0.6424
92	1273.2	1600	156.62	3.8097	3.8160	3.7812	3.7287	5.9667	5.9766	5.9221	5.8398	0.7177	0.7189	0.7123	0.7024
93	523.15	1800	119.02	4.9471	5.6138	5.5628	1.9305	5.8880	6.6815	6.6207	2.2977	0.7082	0.8036	0.7963	0.2764

94	573.15	1800	122.91	4.6119	5.0526	5.0092	1.6776	5.6685	6.2101	6.1568	2.0619	0.6818	0.7469	0.7405	0.2480
95	673.15	1800	129.34	4.3031	4.5260	4.4913	1.8544	5.5654	5.8537	5.8088	2.3984	0.6694	0.7041	0.6987	0.2885
96	773.15	1800	134.80	4.1019	4.2309	4.2003	2.3210	5.5291	5.7031	5.6619	3.1285	0.6650	0.6860	0.6810	0.3763
97	873.15	1800	139.66	3.9262	4.0074	3.9787	2.7786	5.4832	5.5967	5.5565	3.8806	0.6595	0.6732	0.6683	0.4667
98	973.15	1800	144.09	3.7761	3.8294	3.8007	3.1095	5.4410	5.5177	5.4764	4.4805	0.6544	0.6637	0.6587	0.5389
99	1073.2	1800	148.19	3.6791	3.7136	3.6834	3.3225	5.4520	5.5031	5.4584	4.9235	0.6558	0.6619	0.6565	0.5922
100	1173.2	1800	152.02	3.6770	3.6970	3.6635	3.4970	5.5898	5.6203	5.5693	5.3162	0.6723	0.6760	0.6699	0.6394
101	1273.2	1800	155.63	3.8326	3.8401	3.8007	3.7441	5.9648	5.9765	5.9151	5.8270	0.7174	0.7188	0.7115	0.7009
102	523.15	2000	117.91	5.0438	5.7987	5.7402	1.9922	5.9472	6.8373	6.7683	2.3490	0.7153	0.8224	0.8141	0.2825
103	573.15	2000	121.89	4.6658	5.1627	5.1134	1.6709	5.6874	6.2931	6.2330	2.0367	0.6841	0.7569	0.7497	0.2450
104	673.15	2000	128.39	4.3341	4.5847	4.5455	1.8060	5.5646	5.8864	5.8360	2.3187	0.6693	0.7080	0.7020	0.2789
105	723.15	2000	131.23	4.2259	4.4140	4.3776	2.0242	5.5456	5.7924	5.7446	2.6563	0.6670	0.6967	0.6910	0.3195
106	773.15	2000	133.88	4.1276	4.2726	4.2382	2.2710	5.5260	5.7201	5.6741	3.0404	0.6647	0.6880	0.6825	0.3657
107	873.15	2000	138.76	3.9487	4.0400	4.0077	2.7411	5.4791	5.6058	5.5610	3.8034	0.6590	0.6743	0.6689	0.4575
108	973.15	2000	143.20	3.7974	3.8573	3.8252	3.0896	5.4377	5.5235	5.4775	4.4242	0.6540	0.6644	0.6588	0.5321
109	1073.2	2000	147.30	3.6976	3.7364	3.7026	3.3160	5.4466	5.5038	5.4540	4.8845	0.6551	0.6620	0.6560	0.5875
110	1173.2	2000	151.14	3.6960	3.7187	3.6812	3.5022	5.5860	5.6204	5.5636	5.2931	0.6719	0.6760	0.6692	0.6367
111	1273.2	2000	154.75	3.8525	3.8611	3.8170	3.7566	5.9617	5.9751	5.9068	5.8133	0.7171	0.7187	0.7105	0.6992
112	523.15	2500	115.45	5.2957	6.2836	6.2045	2.1659	6.1137	7.2543	7.1630	2.5005	0.7354	0.8725	0.8616	0.3008
113	573.15	2500	119.69	4.7921	5.4353	5.3699	1.6528	5.7355	6.5053	6.4270	1.9781	0.6899	0.7824	0.7730	0.2379
114	673.15	2500	126.37	4.4024	4.7240	4.6730	1.6845	5.5633	5.9697	5.9052	2.1286	0.6691	0.7180	0.7103	0.2560
115	723.15	2500	129.25	4.2845	4.5254	4.4784	1.8934	5.5377	5.8490	5.7883	2.4472	0.6661	0.7035	0.6962	0.2943
116	773.15	2500	131.93	4.1807	4.3662	4.3219	2.1446	5.5155	5.7603	5.7019	2.8293	0.6634	0.6928	0.6858	0.3403
117	873.15	2500	136.84	3.9947	4.1115	4.0702	2.6450	5.4664	5.6262	5.5697	3.6194	0.6575	0.6767	0.6699	0.4353
118	973.15	2500	141.30	3.8396	3.9163	3.8754	3.0343	5.4253	5.5338	5.4759	4.2874	0.6526	0.6656	0.6586	0.5157
119	1073.2	2500	145.42	3.7384	3.7883	3.7454	3.2973	5.4362	5.5089	5.4464	4.7948	0.6539	0.6626	0.6551	0.5767
120	1173.2	2500	149.26	3.7366	3.7660	3.7184	3.5095	5.5772	5.6212	5.5500	5.2382	0.6708	0.6761	0.6675	0.6300
121	1273.2	2500	152.88	3.8955	3.9072	3.8512	3.7818	5.9553	5.9731	5.8876	5.7815	0.7163	0.7184	0.7082	0.6954
122	523.15	3000	113.26	5.5766	6.8170	6.7141	2.3878	6.3162	7.7210	7.6046	2.7044	0.7597	0.9287	0.9147	0.3253
123	573.15	3000	117.80	4.9168	5.7142	5.6311	1.6456	5.7919	6.7313	6.6333	1.9385	0.6966	0.8096	0.7979	0.2332

124	673.15	3000	124.68	4.4607	4.8556	4.7921	1.5648	5.5617	6.0541	5.9749	1.9511	0.6690	0.7282	0.7187	0.2347
125	723.15	3000	127.61	4.3343	4.6295	4.5713	1.7658	5.5308	5.9075	5.8333	2.2532	0.6652	0.7105	0.7016	0.2710
126	773.15	3000	130.32	4.2256	4.4527	4.3982	2.0217	5.5066	5.8026	5.7315	2.6346	0.6623	0.6979	0.6894	0.3169
127	873.15	3000	135.26	4.0335	4.1764	4.1258	2.5510	5.4558	5.6492	5.5807	3.4506	0.6562	0.6795	0.6712	0.4150
128	973.15	3000	139.74	3.8739	3.9678	3.9178	2.9771	5.4135	5.5448	5.4749	4.1603	0.6511	0.6669	0.6585	0.5004
129	1073.2	3000	143.87	3.7718	3.8331	3.7808	3.2745	5.4266	5.5147	5.4395	4.7110	0.6527	0.6633	0.6543	0.5666
130	1173.2	3000	147.72	3.7699	3.8063	3.7483	3.5112	5.5690	5.6227	5.5371	5.1867	0.6698	0.6763	0.6660	0.6239
131	1273.2	3000	151.34	3.9301	3.9447	3.8768	3.7993	5.9478	5.9701	5.8673	5.7499	0.7154	0.7181	0.7057	0.6916
132	523.15	3500	111.24	5.8996	7.4147	7.2843	2.6755	6.5627	8.2481	8.1030	2.9762	0.7894	0.9921	0.9746	0.3580
133	573.15	3500	116.12	5.0435	6.0037	5.9008	1.6544	5.8567	6.9718	6.8523	1.9211	0.7044	0.8386	0.8242	0.2311
134	673.15	3500	123.23	4.5112	4.9817	4.9050	1.4482	5.5592	6.1390	6.0444	1.7846	0.6687	0.7384	0.7270	0.2146
135	723.15	3500	126.20	4.3760	4.7270	4.6571	1.6403	5.5224	5.9653	5.8771	2.0700	0.6642	0.7175	0.7069	0.2490
136	773.15	3500	128.94	4.2632	4.5329	4.4677	1.9010	5.4968	5.8445	5.7604	2.4511	0.6611	0.7030	0.6929	0.2948
137	873.15	3500	133.92	4.0658	4.2354	4.1752	2.4579	5.4450	5.6720	5.5915	3.2916	0.6549	0.6822	0.6725	0.3959
138	973.15	3500	138.42	3.9022	4.0137	3.9545	2.9187	5.4016	5.5558	5.4739	4.0400	0.6497	0.6683	0.6584	0.4859
139	1073.2	3500	142.56	3.7984	3.8712	3.8093	3.2474	5.4150	5.5188	5.4307	4.6295	0.6513	0.6638	0.6532	0.5568
140	1173.2	3500	146.42	3.7979	3.8413	3.7729	3.5087	5.5608	5.6243	5.5241	5.1373	0.6688	0.6765	0.6644	0.6179
141	1273.2	3500	150.04	3.9591	3.9769	3.8968	3.8117	5.9404	5.9671	5.8469	5.7192	0.7145	0.7177	0.7033	0.6879
142	1373.2	3500	153.47	4.3626	4.3554	4.2563	4.2836	6.6954	6.6843	6.5322	6.5741	0.8053	0.8040	0.7857	0.7907
143	573.15	4000	114.60	5.1755	6.3074	6.1827	1.6825	5.9311	7.2284	7.0854	1.9282	0.7134	0.8694	0.8522	0.2319
144	673.15	4000	121.94	4.5591	5.1075	5.0167	1.3381	5.5594	6.2281	6.1174	1.6317	0.6687	0.7491	0.7358	0.1963
145	723.15	4000	124.96	4.4145	4.8227	4.7405	1.5203	5.5162	6.0262	5.9235	1.8997	0.6635	0.7248	0.7125	0.2285
146	773.15	4000	127.73	4.2954	4.6086	4.5322	1.7828	5.4863	5.8864	5.7889	2.2772	0.6599	0.7080	0.6963	0.2739
147	873.15	4000	132.75	4.0921	4.2888	4.2188	2.3647	5.4323	5.6933	5.6004	3.1391	0.6534	0.6848	0.6736	0.3776
148	973.15	4000	137.27	3.9264	4.0557	3.9870	2.8598	5.3898	5.5672	5.4730	3.9257	0.6483	0.6696	0.6583	0.4722
149	1073.2	4000	141.42	3.8223	3.9068	3.8353	3.2197	5.4056	5.5251	5.4239	4.5534	0.6502	0.6645	0.6524	0.5477
150	1173.2	4000	145.29	3.8208	3.8713	3.7923	3.5022	5.5511	5.6244	5.5096	5.0881	0.6677	0.6765	0.6627	0.6120
151	1273.2	4000	148.91	3.9856	4.0065	3.9141	3.8219	5.9351	5.9663	5.8287	5.6914	0.7139	0.7176	0.7011	0.6846
152	1373.2	4000	152.35	4.3919	4.3841	4.2698	4.3034	6.6909	6.6790	6.5049	6.5561	0.8048	0.8033	0.7824	0.7886
153	573.15	4500	113.18	5.3158	6.6293	6.4800	1.7335	6.0165	7.5032	7.3343	1.9620	0.7237	0.9025	0.8822	0.2360

154	673.15	4500	120.78	4.6015	5.2301	5.1244	1.2310	5.5578	6.3171	6.1894	1.4869	0.6685	0.7598	0.7445	0.1788
155	723.15	4500	123.84	4.4488	4.9155	4.8205	1.4036	5.5096	6.0876	5.9699	1.7382	0.6627	0.7322	0.7181	0.2091
156	773.15	4500	126.65	4.3254	4.6830	4.5952	1.6693	5.4779	5.9308	5.8196	2.1140	0.6589	0.7134	0.7000	0.2543
157	873.15	4500	131.71	4.1169	4.3411	4.2610	2.2750	5.4223	5.7175	5.6120	2.9963	0.6522	0.6877	0.6750	0.3604
158	973.15	4500	136.25	3.9480	4.0953	4.0170	2.8016	5.3791	5.5798	5.4732	3.8172	0.6470	0.6711	0.6583	0.4591
159	1073.2	4500	140.41	3.8426	3.9389	3.8576	3.1902	5.3955	5.5308	5.4165	4.4795	0.6490	0.6652	0.6515	0.5388
160	1173.2	4500	144.28	3.8415	3.8991	3.8094	3.4942	5.5426	5.6258	5.4963	5.0416	0.6667	0.6767	0.6611	0.6064
161	1273.2	4500	147.92	4.0072	4.0314	3.9266	3.8277	5.9273	5.9631	5.8081	5.6619	0.7129	0.7172	0.6986	0.6810
162	1373.2	4500	151.35	4.4175	4.4090	4.2795	4.3196	6.6859	6.6731	6.4770	6.5377	0.8042	0.8026	0.7790	0.7864
163	573.15	5000	111.84	5.4654	6.9713	6.7945	1.8089	6.1126	7.7969	7.5991	2.0231	0.7352	0.9378	0.9140	0.2433
164	673.15	5000	119.72	4.6417	5.3529	5.2313	1.1293	5.5573	6.4087	6.2632	1.3521	0.6684	0.7708	0.7533	0.1626
165	723.15	5000	122.84	4.4791	5.0057	4.8972	1.2894	5.5019	6.1488	6.0155	1.5839	0.6618	0.7396	0.7235	0.1905
166	773.15	5000	125.67	4.3506	4.7535	4.6537	1.5567	5.4674	5.9737	5.8483	1.9563	0.6576	0.7185	0.7034	0.2353
167	823.15	5000	128.30	4.2396	4.5555	4.4614	1.8695	5.4393	5.8446	5.7239	2.3986	0.6542	0.7030	0.6885	0.2885
168	873.15	5000	130.77	4.1376	4.3898	4.2994	2.1855	5.4107	5.7405	5.6222	2.8579	0.6508	0.6905	0.6762	0.3437
169	973.15	5000	135.33	3.9659	4.1315	4.0434	2.7424	5.3671	5.5912	5.4720	3.7114	0.6455	0.6725	0.6582	0.4464
170	1073.2	5000	139.51	3.8594	3.9677	3.8763	3.1587	5.3841	5.5353	5.4078	4.4066	0.6476	0.6658	0.6504	0.5300
171	1173.2	5000	143.39	3.8587	3.9237	3.8231	3.4836	5.5329	5.6261	5.4818	4.9950	0.6655	0.6767	0.6593	0.6008
172	1273.2	5000	147.02	4.0267	4.0542	3.9368	3.8317	5.9202	5.9606	5.7880	5.6335	0.7121	0.7169	0.6962	0.6776
173	1373.2	5000	150.46	4.4407	4.4317	4.2867	4.3335	6.6815	6.6678	6.4497	6.5201	0.8036	0.8020	0.7758	0.7842
174	573.15	6000	109.30	5.8076	7.7360	7.4925	2.0524	6.3479	8.4556	8.1894	2.2434	0.7635	1.0170	0.9850	0.2698
175	673.15	6000	117.83	4.7162	5.5996	5.4434	0.9402	5.5571	6.5980	6.4140	1.1078	0.6684	0.7936	0.7715	0.1332
176	723.15	6000	121.05	4.5343	5.1850	5.0476	1.0729	5.4886	6.2762	6.1100	1.2987	0.6602	0.7549	0.7349	0.1562
177	773.15	6000	123.95	4.3961	4.8923	4.7672	1.3415	5.4489	6.0639	5.9088	1.6628	0.6554	0.7294	0.7107	0.2000
178	823.15	6000	126.62	4.2784	4.6667	4.5496	1.6700	5.4174	5.9090	5.7608	2.1146	0.6516	0.7107	0.6929	0.2543
179	873.15	6000	129.12	4.1730	4.4825	4.3705	2.0111	5.3884	5.7880	5.6434	2.5969	0.6481	0.6962	0.6788	0.3123
180	973.15	6000	133.73	3.9965	4.1995	4.0912	2.6257	5.3446	5.6161	5.4713	3.5114	0.6428	0.6755	0.6581	0.4223
181	1073.2	6000	137.93	3.8882	4.0211	3.9093	3.0947	5.3632	5.5464	5.3922	4.2686	0.6451	0.6671	0.6486	0.5134
182	1173.2	6000	141.83	3.8888	3.9687	3.8460	3.4597	5.5154	5.6287	5.4546	4.9068	0.6634	0.6770	0.6561	0.5902
183	1273.2	6000	145.47	4.0599	4.0942	3.9513	3.8345	5.9061	5.9559	5.7480	5.5782	0.7104	0.7164	0.6914	0.6709

184	1373.2	6000	148.91	4.4797	4.4696	4.2934	4.3541	6.6710	6.6559	6.3934	6.4838	0.8024	0.8006	0.7690	0.7799
185	573.15	7000	106.84	6.2313	8.6446	8.3124	2.4557	6.6573	9.2355	8.8807	2.6236	0.8007	1.1108	1.0682	0.3156
186	673.15	7000	116.16	4.7858	5.8514	5.6562	0.7703	5.5589	6.7967	6.5700	0.8948	0.6686	0.8175	0.7902	0.1076
187	723.15	7000	119.49	4.5807	5.3611	5.1922	0.8672	5.4733	6.4058	6.2039	1.0361	0.6583	0.7705	0.7462	0.1246
188	773.15	7000	122.46	4.4342	5.0272	4.8749	1.1355	5.4299	6.1561	5.9696	1.3905	0.6531	0.7404	0.7180	0.1673
189	823.15	7000	125.18	4.3099	4.7728	4.6313	1.4773	5.3951	5.9745	5.7975	1.8493	0.6489	0.7186	0.6973	0.2224
190	873.15	7000	127.72	4.2005	4.5690	4.4345	1.8407	5.3647	5.8353	5.6635	2.3509	0.6453	0.7019	0.6812	0.2828
191	973.15	7000	132.37	4.0203	4.2616	4.1325	2.5096	5.3216	5.6410	5.4700	3.3219	0.6401	0.6785	0.6579	0.3996
192	1073.2	7000	136.59	3.9110	4.0688	3.9361	3.0287	5.3421	5.5578	5.3765	4.1370	0.6425	0.6685	0.6467	0.4976
193	1173.2	7000	140.50	3.9130	4.0081	3.8629	3.4319	5.4978	5.6315	5.4273	4.8219	0.6613	0.6773	0.6528	0.5800
194	1273.2	7000	144.16	4.0873	4.1284	3.9596	3.8322	5.8920	5.9514	5.7080	5.5244	0.7087	0.7158	0.6865	0.6645
195	1373.2	7000	147.60	4.5125	4.5013	4.2934	4.3685	6.6605	6.6441	6.3372	6.4480	0.8011	0.7991	0.7622	0.7756
196	573.15	8000	104.32	6.7847	9.7682	9.3120	3.0919	7.0775	10.1898	9.7139	3.2254	0.8513	1.2256	1.1684	0.3879
197	673.15	8000	114.63	4.8516	6.1103	5.8708	0.6190	5.5616	7.0045	6.7300	0.7095	0.6689	0.8425	0.8095	0.0853
198	723.15	8000	118.09	4.6234	5.5392	5.3357	0.6744	5.4597	6.5412	6.3008	0.7964	0.6567	0.7868	0.7579	0.0958
199	773.15	8000	121.13	4.4668	5.1601	4.9787	0.9379	5.4107	6.2505	6.0308	1.1361	0.6508	0.7518	0.7254	0.1366
200	823.15	8000	123.90	4.3374	4.8773	4.7101	1.2922	5.3742	6.0432	5.8360	1.6011	0.6464	0.7269	0.7020	0.1926
201	873.15	8000	126.47	4.2250	4.6541	4.4959	1.6768	5.3435	5.8863	5.6862	2.1208	0.6427	0.7080	0.6839	0.2551
202	973.15	8000	131.17	4.0406	4.3211	4.1704	2.3960	5.3001	5.6681	5.4704	3.1429	0.6375	0.6818	0.6580	0.3780
203	1073.2	8000	135.42	3.9292	4.1127	3.9585	2.9615	5.3211	5.5696	5.3607	4.0106	0.6400	0.6699	0.6448	0.4824
204	1173.2	8000	139.35	3.9330	4.0437	3.8754	3.4016	5.4805	5.6348	5.4002	4.7399	0.6592	0.6777	0.6495	0.5701
205	1273.2	8000	143.01	4.1104	4.1587	3.9635	3.8264	5.8782	5.9474	5.6682	5.4722	0.7070	0.7153	0.6818	0.6582
206	1373.2	8000	146.46	4.5420	4.5300	4.2899	4.3799	6.6522	6.6346	6.2830	6.4148	0.8001	0.7980	0.7557	0.7716
207	673.15	9000	113.23	4.9129	6.3763	6.0864	0.4844	5.5629	7.2199	6.8916	0.5485	0.6691	0.8684	0.8289	0.0660
208	723.15	9000	116.81	4.6607	5.7182	5.4767	0.4913	5.4444	6.6797	6.3975	0.5739	0.6549	0.8034	0.7695	0.0690
209	773.15	9000	119.93	4.4942	5.2915	5.0788	0.7470	5.3901	6.3464	6.0913	0.8959	0.6483	0.7633	0.7327	0.1078
210	823.15	9000	122.76	4.3614	4.9808	4.7863	1.1135	5.3539	6.1142	5.8755	1.3668	0.6440	0.7354	0.7067	0.1644
211	873.15	9000	125.36	4.2454	4.7368	4.5539	1.5170	5.3222	5.9382	5.7089	1.9018	0.6401	0.7142	0.6867	0.2287
212	923.15	9000	127.80	4.1423	4.5376	4.3616	1.9141	5.2940	5.7992	5.5742	2.4463	0.6368	0.6975	0.6705	0.2942
213	973.15	9000	130.11	4.0564	4.3770	4.2040	2.2830	5.2776	5.6947	5.4697	2.9704	0.6348	0.6850	0.6579	0.3573

214	1073.2	9000	134.39	3.9434	4.1530	3.9768	2.8931	5.2994	5.5810	5.3442	3.8880	0.6374	0.6713	0.6428	0.4676
215	1173.2	9000	138.32	3.9492	4.0758	3.8840	3.3687	5.4626	5.6377	5.3725	4.6597	0.6570	0.6781	0.6462	0.5605
216	1273.2	9000	142.00	4.1296	4.1853	3.9634	3.8173	5.8639	5.9430	5.6278	5.4204	0.7053	0.7148	0.6769	0.6520
217	1373.2	9000	145.45	4.5661	4.5534	4.2808	4.3860	6.6415	6.6230	6.2265	6.3795	0.7988	0.7966	0.7489	0.7673
218	673.15	10000	111.91	4.9735	6.6545	6.3068	0.3703	5.5658	7.4468	7.0577	0.4143	0.6694	0.8957	0.8489	0.0498
219	723.15	10000	115.64	4.6943	5.8997	5.6165	0.3182	5.4284	6.8222	6.4947	0.3679	0.6529	0.8206	0.7812	0.0443
220	773.15	10000	118.84	4.5198	5.4247	5.1786	0.5648	5.3711	6.4465	6.1540	0.6711	0.6460	0.7754	0.7402	0.0807
221	823.15	10000	121.71	4.3807	5.0818	4.8586	0.9385	5.3318	6.1851	5.9134	1.1423	0.6413	0.7439	0.7113	0.1374
222	873.15	10000	124.35	4.2620	4.8172	4.6085	1.3603	5.3000	5.9904	5.7309	1.6916	0.6375	0.7205	0.6893	0.2035
223	923.15	10000	126.82	4.1579	4.6041	4.4040	1.7806	5.2730	5.8389	5.5852	2.2582	0.6342	0.7023	0.6718	0.2716
224	973.15	10000	129.14	4.0693	4.4307	4.2348	2.1715	5.2552	5.7220	5.4691	2.8043	0.6321	0.6882	0.6578	0.3373
225	1073.2	10000	133.45	3.9565	4.1926	3.9940	2.8260	5.2799	5.5951	5.3300	3.7713	0.6351	0.6730	0.6411	0.4536
226	1173.2	10000	137.40	3.9616	4.1044	3.8889	3.3333	5.4435	5.6396	5.3435	4.5801	0.6547	0.6783	0.6427	0.5509
227	1273.2	10000	141.08	4.1466	4.2098	3.9607	3.8063	5.8502	5.9394	5.5880	5.3701	0.7037	0.7144	0.6721	0.6459
228	1373.2	10000	144.55	4.5878	4.5745	4.2690	4.3898	6.6315	6.6122	6.1706	6.3452	0.7976	0.7953	0.7422	0.7632
229	673.15	12500	108.84	5.1211	7.4113	6.8754	0.1784	5.5738	8.0665	7.4832	0.1942	0.6704	0.9702	0.9001	0.0234
230	723.15	12500	112.99	4.7671	6.3727	5.9657	0.0703	5.3862	7.2003	6.7404	0.0795	0.6478	0.8660	0.8107	0.0096
231	773.15	12500	116.41	4.5692	5.7603	5.4194	0.1347	5.3189	6.7054	6.3085	0.1568	0.6398	0.8065	0.7588	0.0189
232	823.15	12500	119.42	4.4208	5.3369	5.0347	0.5245	5.2793	6.3733	6.0125	0.6264	0.6350	0.7666	0.7232	0.0753
233	873.15	12500	122.16	4.2936	5.0155	4.7373	0.9840	5.2450	6.1270	5.7871	1.2021	0.6309	0.7369	0.6961	0.1446
234	923.15	12500	124.70	4.1835	4.7618	4.4980	1.4537	5.2166	5.9378	5.6089	1.8127	0.6275	0.7142	0.6746	0.2180
235	973.15	12500	127.07	4.0924	4.5598	4.3037	1.8993	5.2002	5.7942	5.4687	2.4134	0.6255	0.6969	0.6578	0.2903
236	1073.2	12500	131.45	3.9762	4.2809	4.0240	2.6540	5.2265	5.6271	5.2894	3.4886	0.6286	0.6768	0.6362	0.4196
237	1173.2	12500	135.44	3.9861	4.1706	3.8938	3.2423	5.3987	5.6487	5.2738	4.3914	0.6493	0.6794	0.6343	0.5282
238	1273.2	12500	139.14	4.1783	4.2613	3.9429	3.7697	5.8139	5.9293	5.4862	5.2453	0.6993	0.7132	0.6599	0.6309
239	1373.2	12500	142.62	4.6316	4.6172	4.2278	4.3887	6.6054	6.5848	6.0296	6.2590	0.7945	0.7920	0.7252	0.7528
240	673.15	15000	105.95	5.2603	8.2793	7.4547	0.1433	5.5731	8.7716	7.8980	0.1519	0.6703	1.0550	0.9500	0.0183
241	723.15	15000	110.62	4.8235	6.8788	6.3122	0.3984	5.3356	7.6092	6.9825	0.4407	0.6418	0.9152	0.8398	0.0530
242	773.15	15000	114.29	4.6050	6.1084	5.6544	0.2592	5.2630	6.9813	6.4624	0.2962	0.6330	0.8397	0.7773	0.0356
243	823.15	15000	117.45	4.4476	5.5943	5.2021	0.1347	5.2239	6.5708	6.1101	0.1582	0.6283	0.7903	0.7349	0.0190

244	873.15	15000	120.30	4.3150	5.2140	4.8587	0.6270	5.1907	6.2722	5.8448	0.7543	0.6243	0.7544	0.7030	0.0907
245	923.15	15000	122.90	4.2009	4.9184	4.5854	1.1417	5.1630	6.0449	5.6356	1.4032	0.6210	0.7271	0.6778	0.1688
246	973.15	15000	125.33	4.1049	4.6834	4.3627	1.6345	5.1448	5.8699	5.4679	2.0486	0.6188	0.7060	0.6577	0.2464
247	1073.2	15000	129.78	3.9873	4.3635	4.0455	2.4835	5.1747	5.6630	5.2502	3.2230	0.6224	0.6811	0.6315	0.3877
248	1173.2	15000	133.81	4.0001	4.2283	3.8879	3.1457	5.3527	5.6580	5.2026	4.2094	0.6438	0.6805	0.6258	0.5063
249	1273.2	15000	137.54	4.2013	4.3051	3.9153	3.7261	5.7784	5.9211	5.3851	5.1248	0.6950	0.7122	0.6477	0.6164
250	1373.2	15000	141.03	4.6660	4.6513	4.1762	4.3785	6.5802	6.5594	5.8894	6.1747	0.7915	0.7890	0.7084	0.7427
251	673.15	17500	103.07	5.3856	9.3040	7.9846	0.3213	5.5508	9.5894	8.2295	0.3311	0.6676	1.1534	0.9898	0.0398
252	723.15	17500	108.42	4.8625	7.4270	6.6507	0.6637	5.2718	8.0522	7.2105	0.7196	0.6341	0.9685	0.8673	0.0866
253	773.15	17500	112.38	4.6273	6.4720	5.8830	0.6214	5.2002	7.2733	6.6113	0.6983	0.6255	0.8748	0.7952	0.0840
254	823.15	17500	115.71	4.4645	5.8587	5.3640	0.2335	5.1659	6.7790	6.2066	0.2701	0.6213	0.8154	0.7465	0.0325
255	873.15	17500	118.66	4.3272	5.4138	4.9735	0.2849	5.1345	6.4239	5.9014	0.3380	0.6176	0.7727	0.7098	0.0407
256	923.15	17500	121.34	4.2096	5.0735	4.6655	0.8398	5.1080	6.1562	5.6613	1.0191	0.6144	0.7405	0.6809	0.1226
257	973.15	17500	123.83	4.1107	4.8053	4.4158	1.3774	5.0902	5.9504	5.4680	1.7057	0.6122	0.7157	0.6577	0.2052
258	1023.2	17500	126.15	4.0379	4.5986	4.2170	1.8738	5.0939	5.8012	5.3198	2.3638	0.6127	0.6978	0.6399	0.2843
259	1073.2	17500	128.35	3.9909	4.4414	4.0593	2.3132	5.1222	5.7004	5.2100	2.9690	0.6161	0.6856	0.6267	0.3571
260	1173.2	17500	132.42	4.0074	4.2808	3.8748	3.0461	5.3067	5.6687	5.1311	4.0337	0.6383	0.6818	0.6172	0.4852
261	1273.2	17500	136.17	4.2163	4.3420	3.8790	3.6758	5.7415	5.9126	5.2822	5.0054	0.6906	0.7112	0.6353	0.6020
262	1373.2	17500	139.67	4.6923	4.6779	4.1152	4.3599	6.5537	6.5336	5.7477	6.0895	0.7883	0.7859	0.6913	0.7324
263	673.15	20000	100.05	5.4725	10.555	8.1628	0.8106	5.4754	10.5602	8.1672	0.8111	0.6586	1.2702	0.9823	0.0976
264	723.15	20000	106.32	4.8799	8.0262	6.9679	0.8614	5.1881	8.5333	7.4081	0.9158	0.6240	1.0264	0.8910	0.1101
265	773.15	20000	110.61	4.6392	6.8578	6.1070	0.9511	5.1315	7.5855	6.7551	1.0520	0.6172	0.9124	0.8125	0.1265
266	823.15	20000	114.12	4.4735	6.1328	5.5219	0.5819	5.1051	6.9987	6.3015	0.6641	0.6140	0.8418	0.7579	0.0799
267	873.15	20000	117.18	4.3323	5.6175	5.0836	0.0439	5.0768	6.5828	5.9571	0.0515	0.6106	0.7918	0.7165	0.0062
268	923.15	20000	119.95	4.2118	5.2292	4.7406	0.5470	5.0519	6.2723	5.6862	0.6562	0.6076	0.7544	0.6839	0.0789
269	973.15	20000	122.49	4.1120	4.9278	4.4651	1.1278	5.0368	6.0361	5.4693	1.3814	0.6058	0.7260	0.6578	0.1662
270	1023.2	20000	124.86	4.0361	4.6933	4.2429	1.6647	5.0394	5.8600	5.2976	2.0785	0.6061	0.7048	0.6372	0.2500
271	1073.2	20000	127.09	3.9903	4.5178	4.0690	2.1453	5.0711	5.7414	5.1711	2.7264	0.6099	0.6906	0.6220	0.3279
272	1173.2	20000	131.20	4.0099	4.3301	3.8563	2.9447	5.2611	5.6812	5.0596	3.8635	0.6328	0.6833	0.6086	0.4647
273	1273.2	20000	134.98	4.2253	4.3739	3.8360	3.6205	5.7033	5.9038	5.1778	4.8869	0.6860	0.7101	0.6228	0.5878

274	1373.2	20000	138.49	4.7123	4.6991	4.0471	4.3350	6.5260	6.5076	5.6048	6.0034	0.7849	0.7827	0.6741	0.7221
275	673.15	25000	92.63	5.1817	14.445	5.1735	3.7711	4.7998	13.3801	4.7922	3.4932	0.5773	1.6093	0.5764	0.4202
276	698.15	25000	98.58	4.9922	11.042	7.4319	0.1608	4.9213	10.8858	7.3265	0.1585	0.5919	1.3093	0.8812	0.0191
277	723.15	25000	102.22	4.8248	9.4286	7.4322	1.0137	4.9320	9.6381	7.5974	1.0363	0.5932	1.1593	0.9138	0.1246
278	773.15	25000	107.36	4.6177	7.6977	6.5215	1.5273	4.9573	8.2639	7.0012	1.6396	0.5963	0.9940	0.8421	0.1972
279	823.15	25000	111.27	4.4658	6.7137	5.8232	1.2302	4.9690	7.4702	6.4793	1.3688	0.5977	0.8985	0.7793	0.1646
280	873.15	25000	114.58	4.3268	6.0432	5.2950	0.6659	4.9576	6.9243	6.0669	0.7629	0.5963	0.8328	0.7297	0.0918
281	923.15	25000	117.51	4.2037	5.5503	4.8822	0.0125	4.9398	6.5221	5.7371	0.0147	0.5942	0.7845	0.6901	0.0018
282	973.15	25000	120.17	4.1003	5.1735	4.5515	0.6435	4.9275	6.2171	5.4697	0.7733	0.5927	0.7478	0.6579	0.0930
283	1073.2	25000	124.93	3.9757	4.6650	4.0748	1.8121	4.9666	5.8278	5.0904	2.2637	0.5974	0.7010	0.6123	0.2723
284	1173.2	25000	129.13	4.0033	4.4220	3.8068	2.7377	5.1694	5.7101	4.9157	3.5352	0.6218	0.6868	0.5913	0.4252
285	1273.2	25000	132.95	4.2339	4.4314	3.7387	3.5028	5.6290	5.8917	4.9707	4.6570	0.6771	0.7086	0.5979	0.5601
286	1373.2	25000	136.49	4.7410	4.7322	3.8972	4.2732	6.4711	6.4591	5.3193	5.8325	0.7783	0.7769	0.6398	0.7015
287	673.15	30000	80.58	4.6599	24.380	18.134	13.732	3.7548	19.6452	14.6118	11.0652	0.4516	2.3629	1.7575	1.3309
288	698.15	30000	92.78	4.5295	14.166	7.6072	1.9536	4.2026	13.1431	7.0582	1.8126	0.5055	1.5808	0.8490	0.2180
289	723.15	30000	98.04	4.5984	11.228	7.4860	0.7501	4.5084	11.0084	7.3395	0.7354	0.5423	1.3241	0.8828	0.0885
290	773.15	30000	104.31	4.5370	8.6605	6.8871	1.9881	4.7327	9.0341	7.1842	2.0739	0.5692	1.0866	0.8641	0.2494
291	823.15	30000	108.71	4.4258	7.3476	6.1075	1.8224	4.8111	7.9873	6.6392	1.9811	0.5787	0.9607	0.7986	0.2383
292	873.15	30000	112.29	4.3023	6.4978	5.4971	1.2492	4.8309	7.2962	6.1726	1.4027	0.5811	0.8776	0.7424	0.1687
293	923.15	30000	115.40	4.1806	5.8860	5.0143	0.5452	4.8244	6.7923	5.7865	0.6292	0.5803	0.8170	0.6960	0.0757
294	973.15	30000	118.19	4.0748	5.4250	4.6270	0.1768	4.8160	6.4118	5.4686	0.2090	0.5793	0.7712	0.6578	0.0251
295	1073.2	30000	123.10	3.9522	4.8135	4.0716	1.4868	4.8651	5.9254	5.0122	1.8303	0.5852	0.7127	0.6029	0.2201
296	1173.2	30000	127.40	3.9856	4.5087	3.7448	2.5274	5.0776	5.7439	4.7707	3.2199	0.6107	0.6909	0.5738	0.3873
297	1273.2	30000	131.27	4.2305	4.4809	3.6273	3.3754	5.5534	5.8821	4.7616	4.4309	0.6680	0.7075	0.5727	0.5329
298	1373.2	30000	134.83	4.7590	4.7575	3.7337	4.1994	6.4167	6.4146	5.0343	5.6623	0.7718	0.7715	0.6055	0.6811
299	673.15	35000	75.89	0.8272	28.361	23.705	15.035	0.6278	21.5224	17.9886	11.4095	0.0755	2.5887	2.1637	1.3723
300	698.15	35000	86.02	4.3286	19.228	13.223	5.3674	3.7233	16.5391	11.3735	4.6169	0.4478	1.9893	1.3680	0.5553
301	723.15	35000	93.61	4.2631	13.657	8.5155	0.0370	3.9907	12.7845	7.9714	0.0347	0.4800	1.5377	0.9588	0.0042
302	773.15	35000	101.39	4.3954	9.7748	7.2362	2.3421	4.4565	9.9107	7.3368	2.3746	0.5360	1.1921	0.8825	0.2856
303	823.15	35000	106.33	4.3575	8.0453	6.3850	2.3674	4.6334	8.5549	6.7893	2.5174	0.5573	1.0290	0.8166	0.3028

304	873.15	35000	110.21	4.2585	6.9823	5.6917	1.8048	4.6934	7.6954	6.2729	1.9891	0.5645	0.9256	0.7545	0.2392
305	923.15	35000	113.51	4.1444	6.2382	5.1396	1.0575	4.7044	7.0811	5.8341	1.2004	0.5658	0.8517	0.7017	0.1444
306	973.15	35000	116.43	4.0415	5.6881	4.6977	0.2728	4.7057	6.6228	5.4697	0.3176	0.5660	0.7966	0.6579	0.0382
307	1073.2	35000	121.51	3.9186	4.9614	4.0585	1.1651	4.7615	6.0286	4.9316	1.4157	0.5727	0.7251	0.5932	0.1703
308	1173.2	35000	125.90	3.9597	4.5926	3.6734	2.3151	4.9853	5.7821	4.6248	2.9147	0.5996	0.6955	0.5563	0.3506
309	1273.2	35000	129.82	4.2208	4.5277	3.5079	3.2433	5.4796	5.8779	4.5540	4.2105	0.6591	0.7070	0.5478	0.5064
310	1373.2	35000	133.41	4.7690	4.7774	3.5601	4.1166	6.3624	6.3736	4.7496	5.4920	0.7653	0.7666	0.5713	0.6606
311	673.15	40000	74.10	1.3759	29.494	25.354	12.007	1.0196	21.8562	18.7884	8.8972	0.1226	2.6288	2.2598	1.0701
312	698.15	40000	81.12	3.4163	23.466	18.254	6.9761	2.7712	19.0352	14.8071	5.6588	0.3333	2.2895	1.7810	0.6806
313	723.15	40000	89.10	4.0824	16.775	11.462	1.1463	3.6375	14.9463	10.2131	1.0214	0.4375	1.7977	1.2284	0.1229
314	773.15	40000	98.54	4.2218	11.069	7.7410	2.6084	4.1602	10.9072	7.6280	2.5703	0.5004	1.3119	0.9175	0.3092
315	823.15	40000	104.10	4.2659	8.8123	6.6782	2.8778	4.4407	9.1734	6.9518	2.9957	0.5341	1.1034	0.8362	0.3603
316	873.15	40000	108.29	4.2006	7.5011	5.8881	2.3382	4.5490	8.1232	6.3764	2.5322	0.5471	0.9770	0.7669	0.3046
317	923.15	40000	111.79	4.0993	6.6100	5.2636	1.5524	4.5826	7.3893	5.8842	1.7354	0.5512	0.8888	0.7077	0.2087
318	973.15	40000	114.85	3.9999	5.9611	4.7639	0.7107	4.5937	6.8460	5.4711	0.8162	0.5525	0.8234	0.6581	0.0982
319	1073.2	40000	120.09	3.8809	5.1142	4.0418	0.8503	4.6607	6.1417	4.8538	1.0212	0.5606	0.7387	0.5838	0.1228
320	1173.2	40000	124.57	3.9295	4.6773	3.5969	2.1035	4.8951	5.8267	4.4807	2.6204	0.5888	0.7008	0.5389	0.3152
321	1273.2	40000	128.55	4.2042	4.5709	3.3801	3.1056	5.4044	5.8758	4.3451	3.9922	0.6500	0.7067	0.5226	0.4802
322	1373.2	40000	132.17	4.7718	4.7927	3.3776	4.0255	6.3066	6.3343	4.4640	5.3203	0.7586	0.7619	0.5369	0.6399
323	673.15	50000	72.11	3.5972	30.640	26.733	3.0870	2.5941	22.0958	19.2781	2.2262	0.3120	2.6577	2.3187	0.2678
324	698.15	50000	76.98	0.3753	26.585	22.062	2.8598	0.2889	20.4660	16.9843	2.2016	0.0348	2.4616	2.0428	0.2648
325	723.15	50000	82.66	3.0267	21.864	16.952	0.7957	2.5018	18.0722	14.0120	0.6577	0.3009	2.1737	1.6853	0.0791
326	773.15	50000	93.18	3.9270	14.104	9.8142	3.1553	3.6592	13.1429	9.1451	2.9402	0.4401	1.5808	1.1000	0.3536
327	823.15	50000	99.96	4.0555	10.546	7.4701	3.8681	4.0537	10.5411	7.4668	3.8664	0.4876	1.2679	0.8981	0.4650
328	873.15	50000	104.81	4.0590	8.6395	6.3303	3.3711	4.2541	9.0547	6.6345	3.5331	0.5117	1.0891	0.7980	0.4250
329	923.15	50000	108.71	3.9891	7.4098	5.5236	2.5101	4.3364	8.0549	6.0045	2.7287	0.5216	0.9688	0.7222	0.3282
330	973.15	50000	112.03	3.9038	6.5432	4.8982	1.5564	4.3735	7.3305	5.4877	1.7437	0.5260	0.8817	0.6601	0.2097
331	1073.2	50000	117.62	3.7947	5.4326	3.9997	0.2357	4.4634	6.3899	4.7044	0.2772	0.5368	0.7686	0.5658	0.0333
332	1173.2	50000	122.29	3.8596	4.8512	3.4329	1.6832	4.7199	5.9326	4.1980	2.0584	0.5677	0.7136	0.5049	0.2476
333	1273.2	50000	126.37	4.1615	4.6573	3.1121	2.8241	5.2588	5.8853	3.9327	3.5688	0.6325	0.7079	0.4730	0.4293

334	1373.2	50000	130.04	4.7684	4.8218	2.9998	3.8315	6.2007	6.2702	3.9009	4.9824	0.7458	0.7542	0.4692	0.5993
335	673.15	60000	70.83	4.8917	31.383	27.378	7.7801	3.4648	22.2284	19.3918	5.5106	0.4167	2.6736	2.3324	0.6628
336	698.15	60000	74.99	1.4601	27.845	23.442	4.6056	1.0949	20.8804	17.5786	3.4536	0.1317	2.5115	2.1143	0.4154
337	723.15	60000	79.48	1.2813	24.189	19.477	3.5828	1.0184	19.2254	15.4806	2.8477	0.1225	2.3124	1.8620	0.3425
338	773.15	60000	88.85	3.5434	17.011	12.402	4.5312	3.1483	15.1142	11.0195	4.0260	0.3787	1.8179	1.3254	0.4842
339	823.15	60000	96.27	3.8580	12.436	8.6618	4.9952	3.7142	11.9727	8.3389	4.8090	0.4467	1.4401	1.0030	0.5784
340	873.15	60000	101.70	3.9107	9.8826	6.9082	4.4228	3.9770	10.0502	7.0254	4.4978	0.4784	1.2088	0.8450	0.5410
341	923.15	60000	105.98	3.8698	8.2755	5.8325	3.4528	4.1012	8.7704	6.1814	3.6593	0.4933	1.0549	0.7435	0.4401
342	973.15	60000	109.57	3.7980	7.1664	5.0494	2.3797	4.1616	7.8525	5.5329	2.6076	0.5006	0.9445	0.6655	0.3136
343	1073.2	60000	115.49	3.7022	5.7706	3.9568	0.3605	4.2758	6.6647	4.5699	0.4164	0.5143	0.8016	0.5497	0.0501
344	1173.2	60000	120.35	3.7833	5.0340	3.2621	1.2696	4.5532	6.0584	3.9259	1.5280	0.5477	0.7287	0.4722	0.1838
345	1273.2	60000	124.53	4.1123	4.7479	2.8353	2.5402	5.1211	5.9126	3.5308	3.1633	0.6160	0.7112	0.4247	0.3805
346	1373.2	60000	128.26	4.7538	4.8487	2.6082	3.6241	6.0971	6.2187	3.3452	4.6481	0.7333	0.7480	0.4024	0.5591
∑				1439.1	2004.0	1788.6	849.0	1850.4	2378.9	2157.5	1108.2	222.6	286.1	259.5	133.3
Average (Overall)				**4.1592**	**5.7919**	**5.1695**	**2.4539**	**5.3479**	**6.8755**	**6.2356**	**3.2028**	**0.6432**	**0.8270**	**0.7500**	**0.3852**

Chapter Five

Conclusions and Recommendations

5-1 Conclusions

1. Different equations of state were used to predict the residual entropy of superheated vapor for pure compounds. They are Lee-Kesler, Peng-Robinson, Soave-Redlich-Kwong and Virial truncated to second and to third terms equations of state. The results indicate that Lee-Kesler equation is the most accurate equation among these five equations, SRK equation is the closest one in its accuracy to the Lee-Kesler, and the virial equation (truncated to second or to third terms) gave highest deviations from the experimental values which proscribed the need to listing its results in tables.

2. New modification was made by redefining the parameter α in Soave equation to be a function of reduced pressure, acentric factor, and polarity factor for polar compounds in addition to be originally function of reduced temperature and n parameter –which is also function of acentric factor– by using statistical methods. This correlation is as follows:

$$\alpha = [1 + n(\gamma)]^2$$

$$\gamma = -0.920338 \;\; P_r^{-0.34091} + 0.064049 \;\; T_r^{4}\omega - 0.370002 \;\; \omega - P_r^{0.996932} \;\; Tr^{-4}\chi$$

The results of this correlation were compared with the results obtained from Lee-Kesler, Peng-Robinson, Virial truncated to second and to third terms, and Soave-Redlich-Kwong methods.

a. The AAD of 1660 experimental data points of 14 pure nonpolar compounds obtained from this correlation was 2.8247 J/mol.K in comparison with those obtained from Lee-Kesler, Peng-Robinson, Virial truncated to

second and to third terms, and Soave-Redlich-Kwong methods were 4.6277, 4.9243, 4.9782, 4.9501, and 4.7665 J/mol.K respectively.

b. The AAD of 1131 experimental data points of 6 pure polar compounds obtained from this correlation was 1.9299 J/mol.K in comparison with those obtained when using the same equations above were 3.2247, 4.0867, 4.9546, 5.1597, and 3.6359 J/mol.K respectively.

c. The AAD of 2791 experimental data points of all the 20 pure compounds obtained from this correlation was 2.4621 J/mol.K in comparison with those obtained from Lee-Kesler, Peng-Robinson, Virial truncated to second and to third terms, and Soave-Redlich-Kwong methods were 4.0591, 4.5849, 4.9686, 5.0350, and 4.3084 J/mol.K respectively.

5-2 Recommendations

For those who would carry future work on related subject, the following recommendations can be taken into consideration:

1. Applying this correlation to study other thermodynamic properties such as compressibility factor, Gibes free energy for different conditions.
2. Applying this correlation for other polar compounds after obtaining reliable experimental data for them.
3. Studying the possibility of applying this method to binary and to ternary mixtures when obtaining reliable experimental data for them.

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Appendix A

Physical Properties of Pure Compounds

Table A-1 Physical Properties of Pure Non Polar Compounds [45]

Compounds	formula	M. wt. (g/g.mol)	T_b (K)	T_c (K)	P_c (kPa)	Z_c	ω
Argon	Ar	39.948	87.27	150.86	4898	0.291	-0.002
Methane	CH_4	16.043	111.66	190.56	4599	0.286	0.011
Oxygen	O_2	31.999	90.17	154.58	5043	0.288	0.025
Nitrogen	N_2	28.014	77.35	126.20	3398	0.289	0.037
Ethane	C_2H_6	30.070	184.55	305.32	4872	0.279	0.099
Cyclopropane	C_3H_6	42.081	240.34	398.25	5575	0.274	0.130
Propane	C_3H_8	44.097	231.02	369.83	4248	0.276	0.152
Acetylene	C_2H_2	26.038	188.40	308.30	6114	0.268	0.189
Neopentane	C_5H_{12}	72.150	282.65	433.75	3199	0.269	0.197
Benzene	C_6H_6	78.114	353.24	562.05	4895	0.268	0.210
Carbon dioxide	CO_2	44.010	194.65	304.12	7374	0.274	0.225
n-Hexane	C_6H_{14}	86.177	341.88	507.60	3025	0.261	0.300
n-Heptane	C_7H_{16}	100.204	371.57	540.20	2740	0.261	0.350
n-Octane	C_8H_{18}	114.231	398.82	568.70	2490	0.259	0.399

Table A-2 Physical Properties of Pure Polar Compounds [45, 31]

Compounds	formula	M. wt. (g/g.mol)	T_b (K)	T_c (K)	P_c (kPa)	Z_c	ω	χ
Refrigerant 12	CCl_2F_2	120.913	243.45	385.10	4130	0.280	0.179	0.0069
Isopentane	C_5H_{12}	72.150	300.99	460.39	3381	0.272	0.229	0.0095
Ammonia	NH_3	17.031	239.82	405.40	11353	0.255	0.257	0.0090
Refrigerant 152a	$C_2H_4F_2$	66.051	249.10	386.41	4516	0.252	0.276	0.0132
Refrigerant 134a	$C_2H_2F_4$	102.032	247.04	374.26	4059	0.262	0.326	0.0114
Water	H_2O	18.015	373.15	647.14	22064	0.229	0.344	0.0230

Table A-3 Coefficients of eq. (2-93) of Ideal Gas Heat Capacity for pure nonpolar compounds [45]

Compounds	T range (K)	a_0	$a_1\times10^3$	$a_2\times10^5$	$a_3\times10^8$	$a_4\times10^{11}$
Argon	—	2.500	0.000	0.000	0.000	0.000
Methane	50-1000	4.568	-8.975	3.631	-3.407	1.091
Oxygen	50-1000	3.630	-1.794	0.658	-0.601	0.179
Nitrogen	50-1000	3.539	-0.261	0.007	0.157	-0.099
Ethane	50-1000	4.178	-4.427	5.660	-6.651	2.487
Cyclopropane	50-1000	4.493	-18.097	12.744	-16.049	6.426
Propane	50-1000	3.847	5.131	6.011	-7.893	3.079
Acetylene	50-1000	2.410	10.926	-0.255	-0.790	0.524
Neopentane	200-1000	-11.428	156.037	-33.383	40.127	-17.806
Benzene	50-1000	3.551	-6.184	14.365	-19.807	8.234
Carbon dioxide	50-1000	3.259	1.356	1.502	-2.374	1.056
n-Hexane	200-1000	8.831	-0.166	14.302	-18.314	7.124
n-Heptane	200-1000	9.634	4.156	15.494	-20.066	7.770
n-Octane	200-1000	10.824	4.983	17.751	-23.137	8.980

Table A-4 Coefficients of eq. (2-93) of Ideal Gas Heat Capacity for pure polar compounds [45]

Compounds	T range (K)	a_0	$a_1\times10^3$	$a_2\times10^5$	$a_3\times10^8$	$a_4\times10^{11}$
Refrigerant 12	50-1000	2.185	31.251	-3.724	1.930	-0.323
Isopentane	200-1000	1.959	38.191	2.434	-5.175	2.165
Ammonia	50-1000	4.238	-4.215	2.041	-2.126	0.761
Refrigerant 152a	50-1000	3.292	11.749	2.835	-4.645	1.941
Refrigerant 134a	50-1000	3.064	25.420	0.586	-3.339	1.716
Water	50-1000	4.395	-4.186	1.405	-1.564	0.632

Appendix B

Computer Program for Calculating the Residual Entropy of Superheated Vapor for Pure Compounds

This program in QBASIC Language:

```
CLS
REM  "*****************************************************"
REM "Computer Program for Calculation of the Residual Entropy of Superheated Vapor for H2O Using Equation of State"
REM  "*****************************************************"

REM  "*****************************************************"
REM  "R; the Universal Gas Constant in J/mol.K"
REM  "Tc; the Critical Temperature in K"
REM  "Pc; the Critical Pressure in Pa"
REM  "Tb; the Atmospheric (1 atm = 101325 Pa) Boiling Point in K"
REM  "To; the Reference Temperature in K"
REM  ″Po; the Reference Pressure in Pa"
REM  "w; the Acentric Factor"
REM  " χ; the Stiel Polarity Factor"
REM  "T; the Experimental System Temperature in K"
REM  "P; the Experimental System Pressure in Pa"
REM  "Se; the Experimental System Entropy in J/mol.K"
REM  "*****************************************************"
```

```
READ R, Tc, Pc, Tb, To, Po, w, χ
DATA 8.314, 647.14, 22064000, 373.15, 273.16, 611.3, 0.344, 0.023
Tor = To/Tc: Por = Po/Pc: Tbr =Tb/Tc

REM  "*******************************************************"
REM  "Step (1): Calculating the Entropy of Vaporization by Vetere Method"
REM  "*******************************************************"

Hb = R * Tc * Tbr * ((0.4343 * LOG (Pc / 100000) - 0.69431 + 0.89584 *
Tbr) / (0.37691 - 0.37306 * Tbr + 0.15075 * Pc ^ -1 * 100000 * Tbr ^ -2))
u = (0.00264 * (Hb / (R * Tb)) + 0.8794) ^ 10
Hv = Hb * ((1 - Tor) / (1 - Tbr)) ^ u
Sv= Hv / To

REM  "*******************************************************"
REM "Step (2): Calculation of the Residual Entropy at Reference
Temperature and Reference Pressure"
REM  "*******************************************************"

g = 0.42747 * ((R * Tc) ^ 2) / Pc
n = 0.48508 + 1.55171 * w - .15613 * w ^ 2
m = (1 + (n * (1 - Tor ^ 0.5))) ^ 2
A = 0.42747 * m * (Por / (Tor) ^ 2)
B = 0.08664 * (Por / Tor)
D = n * (g * m) * (Tor / m) ^ 0.5
Z = 1
10 F = Z ^ 3 - (1 - B) * Z ^ 2 + (A - B ^ 2 - B) * Z - (A * B)
DF = 3 * Z ^ 2 - 2 * (1 - B) * Z + (A - B ^ 2 - B)
```

```
Z1 = Z - (F / DF)
IF ABS (Z1 - Z) >= .00000001 THEN Z = Z1: GOTO 10
Z1 = Z
Sr = R * (LOG (Z1 - B) - (B * D / (g * m * A)) * LOG (1 + B / Z1))
Sro = -Sr

FOR I = 1 To 1
READ T (I), P (I), S (I)
DATA 823.15, 12500000, 119.4196
Tr (I) = T (I)/Tc: Pr (I) = P (I)/Pc

REM  "*****************************************************"
REM "Step (3): Calculating the Ideal Gas Entropy with Chang of Temperature at Constant Pressure and with Change of Pressure at Constant Temperature"
REM  "*****************************************************"

a0 = 4.395: a1 = -4.186 * 10 ^ -3: a2 = 1.405 * 10 ^ -5: a3 = -1.564 * 10^ -8:
a4 = .632 * 10 ^ -11
ST (I) = R * ((a0 * LOG (T (I) / To) + (a1) * (T (I) - To) + (a2) / 2 * (T (I) ^2
-To ^ 2) + (a3) / 3 * (T (I) ^ 3 - To ^ 3) + (a4) / 4 * (T (I) ^ 4 - To ^4)))
SP (I) = -R*LOG (P (I)/Po)
Sig (I) = ST (I) + SP (I)

REM  "*****************************************************"
REM "Step (4): Calculation of the Residual Entropy at System Temperature and Pressure"
REM  "*****************************************************"
```

```
g (I) = 0.42747 * ((R * Tc) ^ 2) / Pc
m (I) = (1 + n * (-0.920338 * Pr (I) ^ -0.034091 + 0.064049 * w * Tr(I) ^ 4 +
0.370002 * w - Pr(I) ^ 0.996932 * Tr(I) ^ -4*χ)) ^ 2
A (I) = 0.42747 * m (I) * (Pr (I) / (Tr (I)) ^ 2)
B (I) = 0.08664 * (Pr (I) / Tr (I))
D (I) = n * (g (I) * m (I)) * (Tr (I) / m (I)) ^0.5

12 F (I) = Z ^ 3 - (1 - B (I))* Z ^ 2 + (A (I) - B (I) ^ 2 - B (I))*Z-(A (I)*B (I))
dF (I) = 3 * Z ^ 2 - 2 * (1 - B (I)) * Z + (A (I) - B (I) ^ 2 - B (I))
Z1 (I) = Z - (F (I) / dF (I))
IF ABS (Z1 (I) - Z) >= .00000001THEN Z = Z1 (I): GOTO 12
Z1 (I) = Z
Sr (I) = R * (LOG (Z1 (I) - B (I)) - (B (I) * D (I) / (g (I) * m (I) * A (I))) *
LOG (1 + B (I) / Z1 (I)))

REM  "*******************************************************"
REM "Calculation of Entropy of Superheated Vapor"
REM  "*******************************************************"

Scal (I) = Sv + Sro + Sig(I) + Sr (I)

REM  "*******************************************************"
REM "Experimental and Calculated Residual Entropy of Superheated Vapor"
REM  "*******************************************************"

Sre (I) = Se (I) - Sig (I) - Sv
Srcal (I) = Scal (I) - Sig (I) - Sv
```

```
REM  "*****************************************************"
REM "Calculating the Deviations for the Calculated Values from the Experimental Values of Entropy and Residual Entropy"
REM  "ADP; Absolute Percentage Deviation in Entropy"
REM  "AD; Absolute Deviation in Residual Entropy in J/ (mol.K)"
REM  "ADR; Absolute Deviation in Residual Entropy divided by R (gas constant in J/ (mol.K)) to be dimensionless term"
REM  "*****************************************************"

ADP (I) = ABS ((Se (I)-Scal (I))/S (I))*100
AD (I) = ABS (Sre (I)-Srcal (I))
ADR (I) = AD (I)/R

REM  "*****************************************************"
REM "Printing the Results of the Computer Program"
REM  "*****************************************************"

PRINT "T(I)="; T(I), "P(I)="; P(I), "ADP (I)="; ADP(I), "AD (I)"; AD (I), "ADR (I)"; ADR (I)

NEXT I
END
```

Appendix C

Results for Superheated Vapors of Pure Compounds

Pt. no. = Point number, **T =** Temperature in Kelvin, **P =** Pressure in kPa.

$\mathbf{S_{(exp)}}$ = Experimental value for superheated entropy in J/(mol.K).

AD% = absolute percentage deviations for entropy.

AD = absolute deviations for residual entropy in J / (mol.K).

AD/R = absolute deviations for residual entropy divided by R (gas constant).

L&K = Lee-Kesler equation, **P&R** = Peng-Robinson equation, **Soave** = Soave-Redlich-Kwong equation.

This work = the new modification of Soave-Redlich-Kwong equation.

Table C-1 Argon [15]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	100	101.3	131.48	0.5037	0.5919	0.5884	0.4696	0.6622	0.7782	0.7736	0.6175	0.0797	0.0936	0.0930	0.0743
2	100	304.0	121.79	0.7627	0.5622	0.5945	0.1766	0.9289	0.6847	0.7241	0.2151	0.1117	0.0824	0.0871	0.0259
3	110	101.3	133.50	0.4552	0.5803	0.5751	0.4853	0.6077	0.7747	0.7678	0.6479	0.0731	0.0932	0.0923	0.0779
4	110	304.0	123.89	0.5942	0.5325	0.5563	0.2469	0.7362	0.6598	0.6892	0.3059	0.0886	0.0794	0.0829	0.0368
5	110	506.6	119.18	0.7861	0.5002	0.5633	0.0161	0.9369	0.5961	0.6713	0.0192	0.1127	0.0717	0.0807	0.0023
6	120	101.3	135.34	0.4252	0.5726	0.5662	0.4971	0.5754	0.7749	0.7662	0.6727	0.0692	0.0932	0.0922	0.0809
7	120	304.0	125.80	0.5016	0.5233	0.5413	0.3068	0.6309	0.6584	0.6810	0.3859	0.0759	0.0792	0.0819	0.0464
8	120	506.6	121.17	0.6123	0.4847	0.5341	0.1031	0.7419	0.5873	0.6472	0.1249	0.0892	0.0706	0.0778	0.0150

9	130	101.3	137.03	0.4061	0.5675	0.5602	0.5064	0.5565	0.7776	0.7676	0.6939	0.0669	0.0935	0.0923	0.0835
10	130	304.0	127.55	0.4496	0.5241	0.5379	0.3571	0.5734	0.6685	0.6861	0.4555	0.0690	0.0804	0.0825	0.0548
11	130	506.6	122.99	0.5223	0.4929	0.5331	0.2049	0.6424	0.6062	0.6556	0.2520	0.0773	0.0729	0.0789	0.0303
12	130	1013	116.26	0.6307	0.2929	0.4264	0.3744	0.7332	0.3406	0.4957	0.4353	0.0882	0.0410	0.0596	0.0524
13	135	101.3	137.83	0.4022	0.5685	0.5608	0.5132	0.5543	0.7835	0.7729	0.7073	0.0667	0.0942	0.0930	0.0851
14	135	304.0	128.37	0.4308	0.5244	0.5366	0.3770	0.5530	0.6731	0.6888	0.4840	0.0665	0.0810	0.0828	0.0582
15	135	506.6	123.84	0.4923	0.4981	0.5347	0.2466	0.6097	0.6168	0.6622	0.3054	0.0733	0.0742	0.0796	0.0367
16	135	1013.3	117.20	0.5630	0.3106	0.4307	0.2609	0.6598	0.3640	0.5047	0.3058	0.0794	0.0438	0.0607	0.0368
17	140	101.3	138.59	0.3919	0.5621	0.5541	0.5119	0.5431	0.7790	0.7680	0.7095	0.0653	0.0937	0.0924	0.0853
18	140	304.0	129.16	0.4175	0.5266	0.5373	0.3963	0.5392	0.6801	0.6940	0.5118	0.0649	0.0818	0.0835	0.0616
19	140	506.6	124.66	0.4734	0.5078	0.5414	0.2876	0.5902	0.6331	0.6749	0.3586	0.0710	0.0761	0.0812	0.0431
20	140	1013	118.10	0.5190	0.3350	0.4443	0.1567	0.6130	0.3957	0.5248	0.1851	0.0737	0.0476	0.0631	0.0223
21	145	101.3	139.33	0.3879	0.5613	0.5531	0.5156	0.5405	0.7821	0.7706	0.7184	0.0650	0.0941	0.0927	0.0864
22	145	304.0	129.92	0.4068	0.5286	0.5381	0.4132	0.5285	0.6868	0.6992	0.5368	0.0636	0.0826	0.0841	0.0646
23	145	506.6	125.45	0.4615	0.5195	0.5504	0.3263	0.5790	0.6517	0.6905	0.4094	0.0696	0.0784	0.0831	0.0492
24	145	1013	118.96	0.4897	0.3612	0.4616	0.0633	0.5826	0.4297	0.5491	0.0753	0.0701	0.0517	0.0660	0.0091
25	150	101.3	140.05	0.3887	0.5645	0.5561	0.5228	0.5443	0.7906	0.7788	0.7322	0.0655	0.0951	0.0937	0.0881
26	150	304.0	130.66	0.4041	0.5365	0.5449	0.4340	0.5280	0.7009	0.7119	0.5670	0.0635	0.0843	0.0856	0.0682
27	150	506.6	126.20	0.4456	0.5230	0.5517	0.3533	0.5623	0.6600	0.6962	0.4459	0.0676	0.0794	0.0837	0.0536
28	150	1013	119.79	0.4764	0.3934	0.4863	0.0260	0.5706	0.4712	0.5825	0.0312	0.0686	0.0567	0.0701	0.0038
29	150	1519.9	115.66	0.4590	0.1890	0.3709	0.4252	0.5308	0.2185	0.4290	0.4918	0.0638	0.0263	0.0516	0.0592
30	155	101.3	140.05	0.1052	0.0736	0.0648	0.0351	0.1474	0.1030	0.0908	0.0492	0.0177	0.0124	0.0109	0.0059
31	155	304.0	131.37	0.3997	0.5408	0.5483	0.4498	0.5251	0.7105	0.7203	0.5909	0.0632	0.0855	0.0866	0.0711
32	155	506.6	126.93	0.4386	0.5323	0.5590	0.3831	0.5568	0.6757	0.7095	0.4863	0.0670	0.0813	0.0853	0.0585
33	155	1013	120.58	0.4653	0.4200	0.5065	0.1017	0.5611	0.5065	0.6108	0.1226	0.0675	0.0609	0.0735	0.0148
34	155	1520	116.53	0.4490	0.2427	0.4096	0.2831	0.5232	0.2828	0.4774	0.3299	0.0629	0.0340	0.0574	0.0397
35	160	304.0	132.06	0.3996	0.5480	0.5546	0.4671	0.5277	0.7237	0.7324	0.6168	0.0635	0.0870	0.0881	0.0742
36	160	506.6	127.63	0.4306	0.5379	0.5628	0.4068	0.5496	0.6865	0.7183	0.5192	0.0661	0.0826	0.0864	0.0624
37	160	1013	121.33	0.4524	0.4386	0.5196	0.1626	0.5489	0.5321	0.6304	0.1973	0.0660	0.0640	0.0758	0.0237
38	160	1520	117.36	0.4478	0.2942	0.4488	0.1567	0.5255	0.3453	0.5267	0.1839	0.0632	0.0415	0.0634	0.0221

39	170	506.6	128.97	0.4274	0.5558	0.5777	0.4547	0.5512	0.7169	0.7451	0.5864	0.0663	0.0862	0.0896	0.0705
40	170	1013	122.76	0.4490	0.4841	0.5562	0.2773	0.5512	0.5943	0.6828	0.3405	0.0663	0.0715	0.0821	0.0410
41	170	1520	118.91	0.4580	0.3856	0.5208	0.0540	0.5446	0.4585	0.6193	0.0643	0.0655	0.0551	0.0745	0.0077
42	170	2027	115.98	0.4376	0.2452	0.4596	0.2326	0.5075	0.2843	0.5330	0.2698	0.0610	0.0342	0.0641	0.0324
43	180	506.6	130.22	0.4234	0.5672	0.5867	0.4898	0.5514	0.7386	0.7640	0.6379	0.0663	0.0888	0.0919	0.0767
44	180	1013	124.09	0.4534	0.5240	0.5892	0.3708	0.5626	0.6503	0.7312	0.4601	0.0677	0.0782	0.0879	0.0553
45	180	1520	120.33	0.4727	0.4588	0.5797	0.2173	0.5688	0.5521	0.6976	0.2614	0.0684	0.0664	0.0839	0.0314
46	180	2027	117.51	0.4717	0.3638	0.5521	0.0208	0.5542	0.4275	0.6488	0.0244	0.0667	0.0514	0.0780	0.0029
47	180	2533	115.17	0.4373	0.2261	0.4959	0.2330	0.5036	0.2604	0.5711	0.2683	0.0606	0.0313	0.0687	0.0323
48	180	3040	113.21	0.4560	0.1315	0.5002	0.4592	0.5163	0.1489	0.5662	0.5198	0.0621	0.0179	0.0681	0.0625
49	190	1013	125.33	0.4589	0.5559	0.6156	0.4448	0.5752	0.6967	0.7716	0.5575	0.0692	0.0838	0.0928	0.0671
50	190	1520	121.64	0.4866	0.5159	0.6259	0.3439	0.5919	0.6276	0.7613	0.4184	0.0712	0.0755	0.0916	0.0503
51	190	2027	118.90	0.4976	0.4519	0.6209	0.2107	0.5917	0.5373	0.7383	0.2505	0.0712	0.0646	0.0888	0.0301
52	190	2533	116.65	0.4784	0.3505	0.5888	0.0313	0.5581	0.4089	0.6869	0.0366	0.0671	0.0492	0.0826	0.0044
53	190	3040	114.78	0.5047	0.2874	0.6067	0.1189	0.5792	0.3298	0.6964	0.1364	0.0697	0.0397	0.0838	0.0164
54	190	4053	111.62	0.5447	0.1246	0.6510	0.4852	0.6080	0.1391	0.7266	0.5416	0.0731	0.0167	0.0874	0.0651
55	190	5066	108.91	0.5677	0.0930	0.7206	0.9490	0.6183	0.1013	0.7849	1.0335	0.0744	0.0122	0.0944	0.1243
56	200	1013	126.49	0.4628	0.5796	0.6350	0.5023	0.5854	0.7332	0.8032	0.6353	0.0704	0.0882	0.0966	0.0764
57	200	1520	122.86	0.5008	0.5628	0.6641	0.4455	0.6153	0.6914	0.8159	0.5474	0.0740	0.0832	0.0981	0.0658
58	200	2027	120.17	0.5112	0.5122	0.6665	0.3498	0.6143	0.6155	0.8009	0.4204	0.0739	0.0740	0.0963	0.0506
59	200	2533	117.99	0.5047	0.4391	0.6541	0.2263	0.5954	0.5181	0.7718	0.2670	0.0716	0.0623	0.0928	0.0321
60	200	3040	116.19	0.5391	0.4014	0.6858	0.1328	0.6264	0.4664	0.7968	0.1543	0.0753	0.0561	0.0958	0.0186
61	200	4053	113.18	0.5896	0.2901	0.7436	0.1066	0.6673	0.3283	0.8416	0.1207	0.0803	0.0395	0.1012	0.0145
62	200	5066	110.63	0.6073	0.1198	0.7928	0.4274	0.6719	0.1325	0.8770	0.4728	0.0808	0.0159	0.1055	0.0569
63	200	6080	108.47	0.7080	0.0029	0.9575	0.7153	0.7680	0.0031	1.0386	0.7759	0.0924	0.0004	0.1249	0.0933
64	200	7093	106.43	0.7405	0.2163	1.0941	1.1235	0.7881	0.2302	1.1645	1.1958	0.0948	0.0277	0.1401	0.1438
65	210	1013	127.58	0.4647	0.5968	0.6485	0.5468	0.5929	0.7614	0.8274	0.6976	0.0713	0.0916	0.0995	0.0839
66	210	1520	123.99	0.5041	0.5912	0.6857	0.5179	0.6251	0.7331	0.8502	0.6421	0.0752	0.0882	0.1023	0.0772
67	210	2027	121.34	0.5141	0.5511	0.6939	0.4510	0.6239	0.6687	0.8420	0.5472	0.0750	0.0804	0.1013	0.0658
68	210	2533	119.21	0.5134	0.4956	0.6929	0.3656	0.6120	0.5908	0.8260	0.4358	0.0736	0.0711	0.0993	0.0524

69	210	3040	117.46	0.5507	0.4737	0.7320	0.3107	0.6468	0.5564	0.8598	0.3650	0.0778	0.0669	0.1034	0.0439
70	210	4053	114.57	0.6156	0.4068	0.8093	0.1686	0.7053	0.4660	0.9272	0.1932	0.0848	0.0561	0.1115	0.0232
71	210	5066	112.13	0.6261	0.2662	0.8476	0.0590	0.7021	0.2985	0.9504	0.0661	0.0844	0.0359	0.1143	0.0080
72	210	6080	110.10	0.7208	0.1890	0.9890	0.2328	0.7937	0.2081	1.0889	0.2564	0.0955	0.0250	0.1310	0.0308
73	210	7093	108.21	0.7509	0.0242	1.0880	0.5021	0.8125	0.0261	1.1773	0.5433	0.0977	0.0031	0.1416	0.0653
74	210	8106	106.52	0.8228	0.1218	1.2507	0.7557	0.8764	0.1297	1.3323	0.8050	0.1054	0.0156	0.1602	0.0968
75	210	10133	103.44	0.9217	0.5217	1.5649	1.3603	0.9534	0.5397	1.6188	1.4071	0.1147	0.0649	0.1947	0.1692
76	220	1013	128.60	0.4582	0.6022	0.6510	0.5746	0.5893	0.7744	0.8372	0.7390	0.0709	0.0931	0.1007	0.0889
77	220	1520	125.04	0.4964	0.6032	0.6921	0.5654	0.6208	0.7542	0.8654	0.7069	0.0747	0.0907	0.1041	0.0850
78	220	2027	122.43	0.5122	0.5772	0.7109	0.5272	0.6271	0.7067	0.8704	0.6454	0.0754	0.0850	0.1047	0.0776
79	220	2533	120.33	0.5077	0.5272	0.7106	0.4630	0.6109	0.6344	0.8551	0.5571	0.0735	0.0763	0.1029	0.0670
80	220	3040	118.62	0.5475	0.5178	0.7561	0.4377	0.6495	0.6143	0.8969	0.5192	0.0781	0.0739	0.1079	0.0624
81	220	4053	115.82	0.6208	0.4820	0.8470	0.3652	0.7190	0.5583	0.9810	0.4230	0.0865	0.0671	0.1180	0.0509
82	220	5066	113.47	0.6326	0.3699	0.8870	0.2108	0.7179	0.4197	1.0065	0.2391	0.0863	0.0505	0.1211	0.0288
83	220	6080	111.53	0.7191	0.3170	1.0140	0.1114	0.8021	0.3536	1.1309	0.1242	0.0965	0.0425	0.1360	0.0149
84	220	7093	109.74	0.7423	0.1843	1.0916	0.0704	0.8146	0.2022	1.1980	0.0773	0.0980	0.0243	0.1441	0.0093
85	220	8106	108.16	0.8088	0.0786	1.2263	0.2249	0.8748	0.0851	1.3264	0.2432	0.1052	0.0102	0.1595	0.0293
86	220	10133	105.33	0.9181	0.2018	1.5011	0.5907	0.9670	0.2126	1.5811	0.6222	0.1163	0.0256	0.1902	0.0748
87	220	12159	102.86	1.0150	0.5372	1.7534	0.9730	1.0440	0.5526	1.8036	1.0009	0.1256	0.0665	0.2169	0.1204
88	230	1520	126.03	0.4871	0.6095	0.6939	0.6009	0.6139	0.7682	0.8745	0.7573	0.0738	0.0924	0.1052	0.0911
89	230	2027	123.45	0.5052	0.5926	0.7189	0.5832	0.6236	0.7316	0.8875	0.7199	0.0750	0.0880	0.1067	0.0866
90	230	2533	121.38	0.5022	0.5514	0.7238	0.5402	0.6096	0.6693	0.8786	0.6557	0.0733	0.0805	0.1057	0.0789
91	230	3040	119.69	0.5339	0.5418	0.7644	0.5278	0.6390	0.6485	0.9149	0.6317	0.0769	0.0780	0.1100	0.0760
92	230	4053	116.95	0.6038	0.5203	0.8568	0.4987	0.7061	0.6085	1.0020	0.5832	0.0849	0.0732	0.1205	0.0701
93	230	5066	114.68	0.6252	0.4385	0.9084	0.4070	0.7169	0.5029	1.0417	0.4667	0.0862	0.0605	0.1253	0.0561
94	230	6080	112.79	0.6893	0.3875	1.0114	0.3450	0.7775	0.4370	1.1407	0.3891	0.0935	0.0526	0.1372	0.0468
95	230	7093	111.09	0.7212	0.2918	1.0916	0.2386	0.8012	0.3242	1.2127	0.2651	0.0964	0.0390	0.1459	0.0319
96	230	8106	109.58	0.7742	0.2051	1.2024	0.1431	0.8484	0.2248	1.3175	0.1568	0.1020	0.0270	0.1585	0.0189
97	230	10133	106.92	0.8787	0.0037	1.4448	0.0706	0.9395	0.0039	1.5447	0.0755	0.1130	0.0005	0.1858	0.0091
98	230	12159	104.62	0.9813	0.2491	1.6926	0.2915	1.0266	0.2606	1.7708	0.3050	0.1235	0.0313	0.2130	0.0367

99	240	1520	126.97	0.4788	0.6138	0.6944	0.6293	0.6079	0.7793	0.8817	0.7990	0.0731	0.0937	0.1060	0.0961
100	240	2027	124.41	0.4948	0.6003	0.7206	0.6243	0.6155	0.7468	0.8965	0.7767	0.0740	0.0898	0.1078	0.0934
101	240	2533	122.36	0.4892	0.5624	0.7259	0.5943	0.5985	0.6881	0.8882	0.7272	0.0720	0.0828	0.1068	0.0875
102	240	3040	120.69	0.5171	0.5554	0.7655	0.5950	0.6241	0.6703	0.9238	0.7181	0.0751	0.0806	0.1111	0.0864
103	240	4053	117.99	0.5769	0.5380	0.8523	0.5922	0.6807	0.6347	1.0056	0.6988	0.0819	0.0763	0.1210	0.0840
104	240	5066	115.78	0.6024	0.4766	0.9105	0.5454	0.6975	0.5518	1.0542	0.6314	0.0839	0.0664	0.1268	0.0759
105	240	6080	113.93	0.6499	0.4276	0.9972	0.5116	0.7405	0.4872	1.1362	0.5829	0.0891	0.0586	0.1367	0.0701
106	240	7093	112.29	0.6799	0.3515	1.0734	0.4524	0.7635	0.3947	1.2053	0.5080	0.0918	0.0475	0.1450	0.0611
107	240	8106	110.83	0.7196	0.2756	1.1660	0.3961	0.7975	0.3055	1.2923	0.4390	0.0959	0.0367	0.1554	0.0528
108	240	10133	108.29	0.8118	0.1106	1.3815	0.2828	0.8790	0.1198	1.4960	0.3062	0.1057	0.0144	0.1799	0.0368
109	240	12159	106.10	0.8973	0.0893	1.6017	0.1586	0.9520	0.0947	1.6994	0.1683	0.1145	0.0114	0.2044	0.0202
110	250	1520	127.86	0.4671	0.6124	0.6899	0.6481	0.5973	0.7830	0.8822	0.8287	0.0718	0.0942	0.1061	0.0997
111	250	2027	125.32	0.4838	0.6041	0.7195	0.6558	0.6063	0.7571	0.9017	0.8219	0.0729	0.0911	0.1085	0.0989
112	250	2533	123.29	0.4786	0.5715	0.7278	0.6391	0.5901	0.7047	0.8973	0.7880	0.0710	0.0848	0.1079	0.0948
113	250	3040	121.63	0.4981	0.5613	0.7613	0.6448	0.6058	0.6827	0.9259	0.7842	0.0729	0.0821	0.1114	0.0943
114	250	4053	118.96	0.5473	0.5447	0.8414	0.6604	0.6510	0.6480	1.0009	0.7856	0.0783	0.0779	0.1204	0.0945
115	250	5066	116.80	0.5770	0.5006	0.9066	0.6497	0.6739	0.5848	1.0589	0.7588	0.0811	0.0703	0.1274	0.0913
116	250	6080	114.98	0.6095	0.4515	0.9797	0.6355	0.7008	0.5192	1.1264	0.7307	0.0843	0.0624	0.1355	0.0879
117	250	7093	113.39	0.6400	0.3927	1.0560	0.6141	0.7257	0.4453	1.1974	0.6963	0.0873	0.0536	0.1440	0.0838
118	250	8106	111.96	0.6611	0.3169	1.1282	0.5788	0.7401	0.3548	1.2632	0.6480	0.0890	0.0427	0.1519	0.0779
119	250	10133	109.50	0.7311	0.1724	1.3142	0.5272	0.8005	0.1888	1.4390	0.5773	0.0963	0.0227	0.1731	0.0694
120	250	12159	107.38	0.7873	0.0090	1.4980	0.4591	0.8454	0.0097	1.6085	0.4930	0.1017	0.0012	0.1935	0.0593
121	260	2027	127.18	1.2506	1.3823	1.4928	1.4566	1.5905	1.7580	1.8985	1.8525	0.1913	0.2114	0.2284	0.2228
122	260	2533	124.17	0.4656	0.5749	0.7253	0.6722	0.5781	0.7139	0.9006	0.8347	0.0695	0.0859	0.1083	0.1004
123	260	3040	122.52	0.4793	0.5632	0.7551	0.6831	0.5872	0.6901	0.9251	0.8369	0.0706	0.0830	0.1113	0.1007
124	260	4053	119.88	0.5238	0.5515	0.8341	0.7175	0.6279	0.6611	0.9999	0.8601	0.0755	0.0795	0.1203	0.1035
125	260	5066	117.75	0.5474	0.5121	0.8960	0.7261	0.6446	0.6030	1.0550	0.8550	0.0775	0.0725	0.1269	0.1028
126	260	6080	115.96	0.5724	0.4675	0.9633	0.7318	0.6638	0.5421	1.1170	0.8486	0.0798	0.0652	0.1344	0.1021
127	260	7093	114.40	0.5942	0.4134	1.0316	0.7306	0.6797	0.4729	1.1801	0.8359	0.0818	0.0569	0.1419	0.1005
128	260	8106	113.00	0.6056	0.3427	1.0937	0.7162	0.6843	0.3872	1.2359	0.8093	0.0823	0.0466	0.1487	0.0973

129	260	10133	110.60	0.6544	0.2106	1.2552	0.7079	0.7238	0.2329	1.3883	0.7829	0.0871	0.0280	0.1670	0.0942
130	260	12159	108.54	0.6907	0.0468	1.4150	0.6855	0.7497	0.0508	1.5359	0.7441	0.0902	0.0061	0.1847	0.0895
131	270	2027	127.01	0.4598	0.6028	0.7110	0.6973	0.5840	0.7657	0.9030	0.8856	0.0702	0.0921	0.1086	0.1065
132	270	2533	125.01	0.4542	0.5773	0.7229	0.6994	0.5678	0.7217	0.9036	0.8743	0.0683	0.0868	0.1087	0.1052
133	270	3040	123.37	0.4642	0.5656	0.7508	0.7158	0.5727	0.6978	0.9263	0.8831	0.0689	0.0839	0.1114	0.1062
134	270	4053	120.75	0.5004	0.5535	0.8248	0.7612	0.6042	0.6684	0.9959	0.9191	0.0727	0.0804	0.1198	0.1106
135	270	5066	118.64	0.5147	0.5138	0.8800	0.7811	0.6106	0.6095	1.0440	0.9267	0.0734	0.0733	0.1256	0.1115
136	270	6080	116.88	0.5377	0.4772	0.9473	0.8068	0.6285	0.5578	1.1072	0.9430	0.0756	0.0671	0.1332	0.1134
137	270	7093	115.35	0.5569	0.4315	1.0142	0.8261	0.6424	0.4977	1.1699	0.9529	0.0773	0.0599	0.1407	0.1146
138	270	8106	113.97	0.5565	0.3611	1.0651	0.8241	0.6342	0.4115	1.2139	0.9392	0.0763	0.0495	0.1460	0.1130
139	270	10133	111.62	0.5892	0.2399	1.2097	0.8501	0.6577	0.2677	1.3503	0.9488	0.0791	0.0322	0.1624	0.1141
140	270	12159	109.62	0.6195	0.1002	1.3614	0.8731	0.6791	0.1099	1.4924	0.9571	0.0817	0.0132	0.1795	0.1151
141	280	2027	127.80	0.4482	0.6001	0.7056	0.7111	0.5728	0.7669	0.9018	0.9088	0.0689	0.0922	0.1085	0.1093
142	280	2533	125.82	0.4488	0.5837	0.7254	0.7268	0.5647	0.7344	0.9127	0.9144	0.0679	0.0883	0.1098	0.1100
143	280	3040	124.19	0.4570	0.5733	0.7532	0.7489	0.5676	0.7120	0.9354	0.9301	0.0683	0.0856	0.1125	0.1119
144	280	4053	121.58	0.4805	0.5554	0.8175	0.7977	0.5842	0.6753	0.9939	0.9698	0.0703	0.0812	0.1195	0.1167
145	280	5066	119.49	0.4895	0.5180	0.8700	0.8294	0.5849	0.6189	1.0396	0.9910	0.0704	0.0744	0.1250	0.1192
146	280	6080	117.75	0.5066	0.4838	0.9334	0.8669	0.5965	0.5697	1.0991	1.0208	0.0717	0.0685	0.1322	0.1228
147	280	7093	116.24	0.5192	0.4407	0.9953	0.8984	0.6035	0.5122	1.1570	1.0443	0.0726	0.0616	0.1392	0.1256
148	280	8106	114.89	0.5207	0.3821	1.0490	0.9176	0.5982	0.4390	1.2052	1.0543	0.0719	0.0528	0.1450	0.1268
149	280	10133	112.58	0.5391	0.2688	1.1799	0.9696	0.6069	0.3026	1.3284	1.0916	0.0730	0.0364	0.1598	0.1313
150	280	12159	110.63	0.5646	0.1491	1.3265	1.0289	0.6247	0.1650	1.4676	1.1383	0.0751	0.0198	0.1765	0.1369
∑				83.33	64.32	120.01	72.33	98.28	78.27	140.78	86.18	11.82	9.41	16.93	10.37
Average (Overall)				**0.5555**	**0.4288**	**0.8001**	**0.4822**	**0.6552**	**0.5218**	**0.9385**	**0.5745**	**0.0788**	**0.0628**	**0.1129**	**0.0691**

Table C-2: Methane [20]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	300	400	174.92	0.7233	0.6543	0.6405	0.6482	1.2651	1.1444	1.1204	1.1338	0.1522	0.1376	0.1348	0.1364
2	300	600	171.47	0.7392	0.6785	0.6544	0.6681	1.2675	1.1634	1.1222	1.1457	0.1525	0.1399	0.1350	0.1378
3	300	800	169.00	0.7515	0.6999	0.6650	0.6856	1.2700	1.1829	1.1239	1.1586	0.1528	0.1423	0.1352	0.1394
4	300	1000	167.07	0.7620	0.7201	0.6739	0.7019	1.2730	1.2030	1.1258	1.1726	0.1531	0.1447	0.1354	0.1410
5	300	1500	163.50	0.7813	0.7655	0.6891	0.7384	1.2774	1.2517	1.1267	1.2074	0.1536	0.1506	0.1355	0.1452
6	300	2000	160.92	0.7965	0.8091	0.6997	0.7739	1.2816	1.3020	1.1259	1.2453	0.1542	0.1566	0.1354	0.1498
7	300	3000	157.15	0.8200	0.8955	0.7114	0.8454	1.2887	1.4073	1.1179	1.3285	0.1550	0.1693	0.1345	0.1598
8	300	4000	154.35	0.8372	0.9832	0.7123	0.9195	1.2923	1.5176	1.0995	1.4193	0.1554	0.1825	0.1322	0.1707
9	300	5000	152.09	0.8495	1.0738	0.7032	0.9968	1.2919	1.6331	1.0695	1.5161	0.1554	0.1964	0.1286	0.1824
10	300	6000	150.16	0.8585	1.1690	0.6853	1.0785	1.2891	1.7555	1.0291	1.6195	0.1551	0.2111	0.1238	0.1948
11	300	8000	146.95	0.8652	1.3719	0.6214	1.2488	1.2715	2.0160	0.9131	1.8352	0.1529	0.2425	0.1098	0.2207
12	300	10000	144.28	0.8632	1.5943	0.5311	1.4248	1.2455	2.3004	0.7663	2.0558	0.1498	0.2767	0.0922	0.2473
13	325	400	177.85	0.7159	0.6437	0.6308	0.6298	1.2732	1.1448	1.1218	1.1200	0.1531	0.1377	0.1349	0.1347
14	325	600	174.41	0.7320	0.6656	0.6430	0.6433	1.2767	1.1610	1.1214	1.1221	0.1536	0.1396	0.1349	0.1350
15	325	800	171.96	0.7437	0.6840	0.6511	0.6535	1.2789	1.1761	1.1196	1.1237	0.1538	0.1415	0.1347	0.1352
16	325	1000	170.04	0.7538	0.7010	0.6576	0.6625	1.2817	1.1920	1.1182	1.1265	0.1542	0.1434	0.1345	0.1355
17	325	1500	166.51	0.7732	0.7396	0.6683	0.6811	1.2875	1.2315	1.1128	1.1342	0.1549	0.1481	0.1338	0.1364
18	325	2000	163.96	0.7884	0.7757	0.6744	0.6975	1.2926	1.2718	1.1057	1.1437	0.1555	0.1530	0.1330	0.1376
19	325	3000	160.27	0.8124	0.8460	0.6784	0.7284	1.3021	1.3559	1.0872	1.1675	0.1566	0.1631	0.1308	0.1404
20	325	4000	157.56	0.8304	0.9157	0.6734	0.7581	1.3083	1.4427	1.0609	1.1945	0.1574	0.1735	0.1276	0.1437
21	325	5000	155.38	0.8445	0.9868	0.6613	0.7881	1.3121	1.5333	1.0275	1.2246	0.1578	0.1844	0.1236	0.1473
22	325	6000	153.54	0.8563	1.0608	0.6434	0.8193	1.3147	1.6287	0.9879	1.2580	0.1581	0.1959	0.1188	0.1513
23	325	8000	150.51	0.8724	1.2163	0.5900	0.8825	1.3130	1.8306	0.8881	1.3282	0.1579	0.2202	0.1068	0.1598
24	325	10000	148.03	0.8789	1.3801	0.5156	0.9423	1.3011	2.0429	0.7632	1.3948	0.1565	0.2457	0.0918	0.1678

25	350	400	180.64	0.7097	0.6354	0.6230	0.6158	1.2819	1.1478	1.1254	1.1124	0.1542	0.1381	0.1354	0.1338
26	350	600	177.21	0.7248	0.6547	0.6329	0.6239	1.2845	1.1602	1.1216	1.1056	0.1545	0.1395	0.1349	0.1330
27	350	800	174.77	0.7358	0.6704	0.6389	0.6285	1.2860	1.1717	1.1166	1.0985	0.1547	0.1409	0.1343	0.1321
28	350	1000	172.86	0.7461	0.6858	0.6443	0.6329	1.2898	1.1855	1.1137	1.0941	0.1551	0.1426	0.1340	0.1316
29	350	1500	169.36	0.7648	0.7186	0.6507	0.6383	1.2952	1.2170	1.1020	1.0810	0.1558	0.1464	0.1325	0.1300
30	350	2000	166.83	0.7797	0.7490	0.6531	0.6413	1.3007	1.2496	1.0895	1.0699	0.1565	0.1503	0.1310	0.1287
31	350	3000	163.20	0.8034	0.8073	0.6505	0.6442	1.3112	1.3174	1.0617	1.0513	0.1577	0.1585	0.1277	0.1264
32	350	4000	160.54	0.8217	0.8641	0.6404	0.6444	1.3192	1.3873	1.0281	1.0346	0.1587	0.1669	0.1237	0.1244
33	350	5000	158.43	0.8367	0.9215	0.6245	0.6436	1.3255	1.4598	0.9894	1.0196	0.1594	0.1756	0.1190	0.1226
34	350	6000	156.65	0.8496	0.9804	0.6042	0.6424	1.3309	1.5358	0.9466	1.0064	0.1601	0.1847	0.1139	0.1210
35	350	8000	153.74	0.8687	1.1017	0.5499	0.6372	1.3356	1.6938	0.8455	0.9796	0.1606	0.2037	0.1017	0.1178
36	350	10000	151.38	0.8817	1.2290	0.4812	0.6282	1.3347	1.8606	0.7285	0.9509	0.1605	0.2238	0.0876	0.1144
37	375	400	183.32	0.7017	0.6261	0.6139	0.6025	1.2863	1.1477	1.1254	1.1044	0.1547	0.1380	0.1354	0.1328
38	375	600	179.90	0.7164	0.6436	0.6223	0.6067	1.2888	1.1578	1.1195	1.0914	0.1550	0.1393	0.1347	0.1313
39	375	800	177.46	0.7280	0.6585	0.6277	0.6085	1.2919	1.1685	1.1140	1.0798	0.1554	0.1406	0.1340	0.1299
40	375	1000	175.56	0.7371	0.6713	0.6309	0.6082	1.2941	1.1785	1.1075	1.0679	0.1557	0.1418	0.1332	0.1284
41	375	1500	172.08	0.7549	0.6994	0.6336	0.6038	1.2991	1.2036	1.0904	1.0391	0.1563	0.1448	0.1312	0.1250
42	375	2000	169.58	0.7693	0.7253	0.6328	0.5970	1.3046	1.2299	1.0731	1.0124	0.1569	0.1479	0.1291	0.1218
43	375	3000	165.99	0.7918	0.7735	0.6238	0.5792	1.3143	1.2838	1.0354	0.9615	0.1581	0.1544	0.1245	0.1156
44	375	4000	163.37	0.8107	0.8212	0.6094	0.5597	1.3244	1.3416	0.9957	0.9143	0.1593	0.1614	0.1198	0.1100
45	375	5000	161.30	0.8250	0.8672	0.5887	0.5368	1.3307	1.3988	0.9496	0.8658	0.1601	0.1682	0.1142	0.1041
46	375	6000	159.57	0.8379	0.9145	0.5647	0.5133	1.3370	1.4592	0.9011	0.8191	0.1608	0.1755	0.1084	0.0985
47	375	8000	156.75	0.8591	1.0118	0.5069	0.4635	1.3467	1.5859	0.7945	0.7266	0.1620	0.1908	0.0956	0.0874
48	375	10000	154.48	0.8744	1.1119	0.4368	0.4086	1.3508	1.7176	0.6748	0.6312	0.1625	0.2066	0.0812	0.0759
49	400	400	185.90	0.6927	0.6162	0.6041	0.5897	1.2877	1.1456	1.1231	1.0963	0.1549	0.1378	0.1351	0.1319
50	400	600	182.50	0.7069	0.6321	0.6110	0.5910	1.2901	1.1536	1.1151	1.0785	0.1552	0.1388	0.1341	0.1297
51	400	800	180.07	0.7181	0.6455	0.6151	0.5898	1.2930	1.1623	1.1076	1.0620	0.1555	0.1398	0.1332	0.1277
52	400	1000	178.17	0.7269	0.6568	0.6169	0.5867	1.2951	1.1703	1.0992	1.0453	0.1558	0.1408	0.1322	0.1257
53	400	1500	174.71	0.7440	0.6813	0.6166	0.5751	1.2999	1.1903	1.0773	1.0047	0.1564	0.1432	0.1296	0.1208
54	400	2000	172.22	0.7580	0.7035	0.6130	0.5611	1.3053	1.2116	1.0556	0.9663	0.1570	0.1457	0.1270	0.1162

55	400	3000	168.66	0.7800	0.7444	0.5989	0.5290	1.3156	1.2555	1.0101	0.8923	0.1582	0.1510	0.1215	0.1073
56	400	4000	166.08	0.7970	0.7827	0.5783	0.4932	1.3237	1.3000	0.9605	0.8191	0.1592	0.1564	0.1155	0.0985
57	400	5000	164.04	0.8119	0.8211	0.5541	0.4558	1.3318	1.3469	0.9089	0.7478	0.1602	0.1620	0.1093	0.0899
58	400	6000	162.34	0.8245	0.8593	0.5262	0.4168	1.3386	1.3950	0.8542	0.6766	0.1610	0.1678	0.1027	0.0814
59	400	8000	159.59	0.8458	0.9371	0.4620	0.3353	1.3498	1.4956	0.7373	0.5351	0.1623	0.1799	0.0887	0.0644
60	400	10000	157.39	0.8619	1.0164	0.3877	0.2489	1.3566	1.5997	0.6101	0.3917	0.1632	0.1924	0.0734	0.0471
61	425	400	188.42	0.6834	0.6064	0.5942	0.5778	1.2877	1.1425	1.1196	1.0888	0.1549	0.1374	0.1347	0.1310
62	425	600	185.01	0.6974	0.6211	0.5999	0.5770	1.2902	1.1491	1.1099	1.0675	0.1552	0.1382	0.1335	0.1284
63	425	800	182.59	0.7074	0.6324	0.6020	0.5728	1.2917	1.1548	1.0992	1.0460	0.1554	0.1389	0.1322	0.1258
64	425	1000	180.70	0.7161	0.6427	0.6027	0.5677	1.2940	1.1613	1.0892	1.0258	0.1556	0.1397	0.1310	0.1234
65	425	1500	177.25	0.7326	0.6640	0.5996	0.5506	1.2985	1.1769	1.0628	0.9759	0.1562	0.1416	0.1278	0.1174
66	425	2000	174.78	0.7459	0.6831	0.5931	0.5312	1.3037	1.1938	1.0367	0.9284	0.1568	0.1436	0.1247	0.1117
67	425	3000	171.24	0.7663	0.7167	0.5731	0.4874	1.3123	1.2273	0.9813	0.8346	0.1578	0.1476	0.1180	0.1004
68	425	4000	168.69	0.7829	0.7485	0.5479	0.4407	1.3207	1.2626	0.9242	0.7434	0.1588	0.1519	0.1112	0.0894
69	425	5000	166.68	0.7965	0.7791	0.5184	0.3915	1.3276	1.2986	0.8641	0.6525	0.1597	0.1562	0.1039	0.0785
70	425	6000	165.00	0.8091	0.8102	0.4866	0.3415	1.3350	1.3369	0.8030	0.5635	0.1606	0.1608	0.0966	0.0678
71	425	8000	162.31	0.8292	0.8718	0.4145	0.2369	1.3459	1.4150	0.6728	0.3845	0.1619	0.1702	0.0809	0.0462
72	425	10000	160.15	0.8461	0.9351	0.3349	0.1287	1.3550	1.4976	0.5363	0.2061	0.1630	0.1801	0.0645	0.0248
73	450	400	190.87	0.6736	0.5961	0.5836	0.5663	1.2857	1.1378	1.1140	1.0808	0.1546	0.1368	0.1340	0.1300
74	450	600	187.47	0.6867	0.6092	0.5877	0.5632	1.2874	1.1421	1.1018	1.0559	0.1548	0.1374	0.1325	0.1270
75	450	800	185.05	0.6969	0.6200	0.5891	0.5579	1.2897	1.1472	1.0901	1.0323	0.1551	0.1380	0.1311	0.1242
76	450	1000	183.17	0.7049	0.6287	0.5883	0.5506	1.2911	1.1516	1.0776	1.0086	0.1553	0.1385	0.1296	0.1213
77	450	1500	179.72	0.7203	0.6468	0.5819	0.5289	1.2945	1.1625	1.0457	0.9505	0.1557	0.1398	0.1258	0.1143
78	450	2000	177.26	0.7336	0.6636	0.5731	0.5058	1.3003	1.1762	1.0160	0.8966	0.1564	0.1415	0.1222	0.1078
79	450	3000	173.75	0.7521	0.6906	0.5470	0.4528	1.3068	1.2000	0.9503	0.7867	0.1572	0.1443	0.1143	0.0946
80	450	4000	171.22	0.7680	0.7167	0.5169	0.3979	1.3150	1.2271	0.8850	0.6813	0.1582	0.1476	0.1064	0.0819
81	450	5000	169.23	0.7810	0.7413	0.4828	0.3405	1.3217	1.2544	0.8170	0.5762	0.1590	0.1509	0.0983	0.0693
82	450	6000	167.57	0.7931	0.7662	0.4466	0.2823	1.3290	1.2839	0.7483	0.4730	0.1598	0.1544	0.0900	0.0569
83	450	8000	164.92	0.8132	0.8153	0.3670	0.1619	1.3410	1.3446	0.6053	0.2670	0.1613	0.1617	0.0728	0.0321
84	450	10000	162.80	0.8286	0.8639	0.2792	0.0367	1.3491	1.4065	0.4546	0.0597	0.1623	0.1692	0.0547	0.0072

85	475	400	193.27	0.6640	0.5861	0.5732	0.5556	1.2832	1.1328	1.1079	1.0737	0.1543	0.1363	0.1333	0.1291
86	475	600	189.87	0.6768	0.5983	0.5761	0.5512	1.2850	1.1360	1.0939	1.0466	0.1546	0.1366	0.1316	0.1259
87	475	800	187.45	0.6859	0.6072	0.5756	0.5438	1.2857	1.1383	1.0790	1.0193	0.1546	0.1369	0.1298	0.1226
88	475	1000	185.57	0.6945	0.6160	0.5746	0.5362	1.2889	1.1430	1.0663	0.9950	0.1550	0.1375	0.1283	0.1197
89	475	1500	182.14	0.7096	0.6319	0.5656	0.5115	1.2925	1.1509	1.0303	0.9317	0.1555	0.1384	0.1239	0.1121
90	475	2000	179.69	0.7209	0.6446	0.5527	0.4838	1.2953	1.1583	0.9931	0.8693	0.1558	0.1393	0.1195	0.1046
91	475	3000	176.19	0.7392	0.6673	0.5218	0.4252	1.3024	1.1758	0.9195	0.7492	0.1566	0.1414	0.1106	0.0901
92	475	4000	173.68	0.7540	0.6879	0.4864	0.3638	1.3095	1.1948	0.8447	0.6319	0.1575	0.1437	0.1016	0.0760
93	475	5000	171.70	0.7670	0.7078	0.4480	0.3009	1.3169	1.2154	0.7692	0.5166	0.1584	0.1462	0.0925	0.0621
94	475	6000	170.07	0.7780	0.7268	0.4066	0.2362	1.3231	1.2361	0.6916	0.4017	0.1591	0.1487	0.0832	0.0483
95	475	8000	167.44	0.7960	0.7636	0.3171	0.1027	1.3329	1.2786	0.5310	0.1720	0.1603	0.1538	0.0639	0.0207
96	475	10000	165.36	0.8120	0.8016	0.2223	0.0330	1.3428	1.3255	0.3676	0.0546	0.1615	0.1594	0.0442	0.0066
97	500	400	195.61	0.6558	0.5777	0.5642	0.5469	1.2829	1.1301	1.1037	1.0698	0.1543	0.1359	0.1328	0.1287
98	500	600	192.22	0.6681	0.5887	0.5657	0.5413	1.2841	1.1317	1.0874	1.0404	0.1545	0.1361	0.1308	0.1251
99	500	800	189.81	0.6775	0.5974	0.5646	0.5335	1.2860	1.1339	1.0716	1.0125	0.1547	0.1364	0.1289	0.1218
100	500	1000	187.93	0.6849	0.6041	0.5614	0.5238	1.2871	1.1353	1.0550	0.9844	0.1548	0.1366	0.1269	0.1184
101	500	1500	184.50	0.6998	0.6182	0.5499	0.4971	1.2911	1.1405	1.0147	0.9172	0.1553	0.1372	0.1220	0.1103
102	500	2000	182.06	0.7109	0.6291	0.5346	0.4674	1.2943	1.1453	0.9733	0.8510	0.1557	0.1378	0.1171	0.1024
103	500	3000	178.58	0.7283	0.6472	0.4982	0.4041	1.3006	1.1557	0.8897	0.7217	0.1564	0.1390	0.1070	0.0868
104	500	4000	176.08	0.7423	0.6630	0.4573	0.3381	1.3070	1.1674	0.8052	0.5952	0.1572	0.1404	0.0969	0.0716
105	500	5000	174.12	0.7535	0.6770	0.4126	0.2695	1.3119	1.1788	0.7185	0.4693	0.1578	0.1418	0.0864	0.0564
106	500	6000	172.49	0.7646	0.6919	0.3669	0.2011	1.3189	1.1934	0.6330	0.3468	0.1586	0.1435	0.0761	0.0417
107	500	8000	169.90	0.7818	0.7187	0.2679	0.0591	1.3282	1.2211	0.4552	0.1004	0.1598	0.1469	0.0547	0.0121
108	500	10000	167.85	0.7966	0.7461	0.1636	0.0854	1.3371	1.2522	0.2746	0.1433	0.1608	0.1506	0.0330	0.0172
109	525	400	197.92	0.6496	0.5713	0.5570	0.5406	1.2857	1.1307	1.1025	1.0699	0.1546	0.1360	0.1326	0.1287
110	525	600	194.52	0.6619	0.5818	0.5576	0.5346	1.2876	1.1318	1.0847	1.0399	0.1549	0.1361	0.1305	0.1251
111	525	800	192.11	0.6707	0.5892	0.5549	0.5256	1.2886	1.1319	1.0660	1.0097	0.1550	0.1361	0.1282	0.1214
112	525	1000	190.24	0.6783	0.5955	0.5509	0.5156	1.2903	1.1329	1.0481	0.9810	0.1552	0.1363	0.1261	0.1180
113	525	1500	186.82	0.6924	0.6073	0.5363	0.4870	1.2936	1.1345	1.0019	0.9098	0.1556	0.1365	0.1205	0.1094
114	525	2000	184.38	0.7030	0.6159	0.5179	0.4554	1.2961	1.1356	0.9549	0.8396	0.1559	0.1366	0.1148	0.1010

115	525	3000	180.91	0.7200	0.6303	0.4762	0.3892	1.3026	1.1402	0.8615	0.7040	0.1567	0.1371	0.1036	0.0847
116	525	4000	178.42	0.7328	0.6413	0.4292	0.3193	1.3074	1.1442	0.7658	0.5697	0.1573	0.1376	0.0921	0.0685
117	525	5000	176.47	0.7437	0.6514	0.3794	0.2480	1.3124	1.1495	0.6695	0.4376	0.1579	0.1383	0.0805	0.0526
118	525	6000	174.86	0.7536	0.6611	0.3276	0.1757	1.3178	1.1561	0.5729	0.3072	0.1585	0.1391	0.0689	0.0370
119	525	8000	172.29	0.7701	0.6793	0.2185	0.0280	1.3269	1.1704	0.3764	0.0482	0.1596	0.1408	0.0453	0.0058
120	525	10000	170.26	0.7850	0.6982	0.1049	0.1215	1.3366	1.1887	0.1787	0.2068	0.1608	0.1430	0.0215	0.0249
121	550	1000	192.50	0.6746	0.5899	0.5430	0.5113	1.2986	1.1356	1.0452	0.9844	0.1562	0.1366	0.1257	0.1184
122	550	1500	189.09	0.6876	0.5991	0.5246	0.4808	1.3002	1.1328	0.9920	0.9092	0.1564	0.1362	0.1193	0.1094
123	550	2000	186.65	0.6979	0.6060	0.5033	0.4482	1.3027	1.1310	0.9395	0.8366	0.1567	0.1360	0.1130	0.1006
124	550	3000	183.20	0.7146	0.6167	0.4559	0.3800	1.3092	1.1298	0.8353	0.6962	0.1575	0.1359	0.1005	0.0837
125	550	4000	180.72	0.7271	0.6241	0.4033	0.3083	1.3139	1.1279	0.7288	0.5571	0.1580	0.1357	0.0877	0.0670
126	550	5000	178.78	0.7377	0.6304	0.3478	0.2350	1.3188	1.1270	0.6218	0.4202	0.1586	0.1356	0.0748	0.0505
127	550	6000	177.18	0.7463	0.6353	0.2895	0.1599	1.3224	1.1257	0.5130	0.2834	0.1591	0.1354	0.0617	0.0341
128	550	8000	174.63	0.7620	0.6453	0.1690	0.0083	1.3307	1.1268	0.2952	0.0144	0.1601	0.1355	0.0355	0.0017
129	550	10000	172.61	0.7758	0.6554	0.0442	0.1452	1.3392	1.1313	0.0763	0.2506	0.1611	0.1361	0.0092	0.0301
130	575	3000	185.44	0.7127	0.6069	0.4377	0.3768	1.3217	1.1254	0.8116	0.6988	0.1590	0.1354	0.0976	0.0840
131	575	4000	182.97	0.7250	0.6109	0.3790	0.3041	1.3265	1.1178	0.6934	0.5565	0.1596	0.1345	0.0834	0.0669
132	575	5000	181.04	0.7345	0.6129	0.3166	0.2290	1.3298	1.1095	0.5732	0.4146	0.1599	0.1335	0.0689	0.0499
133	575	6000	179.45	0.7439	0.6151	0.2532	0.1539	1.3349	1.1039	0.4543	0.2761	0.1606	0.1328	0.0546	0.0332
134	575	8000	176.91	0.7590	0.6177	0.1206	0.0003	1.3428	1.0927	0.2134	0.0005	0.1615	0.1314	0.0257	0.0001
135	575	10000	174.91	0.7712	0.6190	0.0172	0.1562	1.3489	1.0827	0.0301	0.2732	0.1622	0.1302	0.0036	0.0329
∑				102.50	100.34	70.90	67.59	176.35	171.04	122.45	115.80	21.21	20.57	14.73	13.93
Average (Overall)				**0.7593**	**0.7433**	**0.5252**	**0.5007**	**1.3063**	**1.2670**	**0.9070**	**0.8578**	**0.1571**	**0.1524**	**0.1091**	**0.1032**

Table C-3 Oxygen [62]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	280	200	197.50	0.6690	0.6728	0.6655	0.6598	1.3212	1.3289	1.3144	1.3031	0.1589	0.1598	0.1581	0.1567
2	280	400	191.69	0.6897	0.6988	0.6836	0.6743	1.3220	1.3395	1.3103	1.2926	0.1590	0.1611	0.1576	0.1555
3	280	600	188.27	0.7034	0.7180	0.6945	0.6824	1.3242	1.3517	1.3074	1.2848	0.1593	0.1626	0.1573	0.1545
4	280	800	185.82	0.7138	0.7340	0.7020	0.6877	1.3264	1.3640	1.3045	1.2779	0.1595	0.1641	0.1569	0.1537
5	280	1000	183.92	0.7235	0.7495	0.7087	0.6925	1.3307	1.3785	1.3035	1.2736	0.1601	0.1658	0.1568	0.1532
6	280	1500	180.42	0.7397	0.7807	0.7170	0.6973	1.3345	1.4086	1.2937	1.2581	0.1605	0.1694	0.1556	0.1513
7	280	2000	177.91	0.7520	0.8089	0.7211	0.6994	1.3379	1.4392	1.2828	1.2443	0.1609	0.1731	0.1543	0.1497
8	280	3000	174.29	0.7715	0.8625	0.7224	0.7007	1.3447	1.5032	1.2590	1.2212	0.1617	0.1808	0.1514	0.1469
9	280	6000	167.78	0.8120	1.0231	0.6965	0.6999	1.3623	1.7165	1.1686	1.1742	0.1639	0.2065	0.1406	0.1412
10	280	8000	164.89	0.8297	1.1352	0.6604	0.6977	1.3681	1.8719	1.0889	1.1504	0.1645	0.2251	0.1310	0.1384
11	280	10000	162.55	0.8415	1.2519	0.6114	0.6930	1.3678	2.0349	0.9938	1.1265	0.1645	0.2448	0.1195	0.1355
12	300	200	199.53	0.6621	0.6648	0.6576	0.6501	1.3211	1.3266	1.3121	1.2971	0.1589	0.1596	0.1578	0.1560
13	300	400	193.73	0.6830	0.6897	0.6747	0.6617	1.3231	1.3361	1.3070	1.2820	0.1591	0.1607	0.1572	0.1542
14	300	600	190.31	0.6970	0.7079	0.6848	0.6671	1.3265	1.3472	1.3032	1.2696	0.1595	0.1620	0.1567	0.1527
15	300	800	187.88	0.7062	0.7213	0.6899	0.6680	1.3267	1.3552	1.2961	1.2550	0.1596	0.1630	0.1559	0.1509
16	300	1000	185.98	0.7147	0.7342	0.6942	0.6684	1.3291	1.3656	1.2912	1.2431	0.1599	0.1642	0.1553	0.1495
17	300	1500	182.51	0.7305	0.7616	0.6994	0.6648	1.3332	1.3899	1.2765	1.2133	0.1604	0.1672	0.1535	0.1459
18	300	2000	180.01	0.7446	0.7878	0.7024	0.6603	1.3404	1.4181	1.2643	1.1885	0.1612	0.1706	0.1521	0.1430
19	300	3000	176.43	0.7629	0.8321	0.6971	0.6429	1.3461	1.4682	1.2299	1.1342	0.1619	0.1766	0.1479	0.1364
20	300	6000	170.04	0.8040	0.9644	0.6576	0.5848	1.3671	1.6400	1.1181	0.9944	0.1644	0.1973	0.1345	0.1196
21	300	8000	167.24	0.8227	1.0543	0.6150	0.5413	1.3759	1.7633	1.0285	0.9054	0.1655	0.2121	0.1237	0.1089
22	300	10000	164.99	0.8362	1.1464	0.5620	0.4943	1.3797	1.8915	0.9272	0.8155	0.1660	0.2275	0.1115	0.0981
23	320	200	201.43	0.6575	0.6593	0.6521	0.6434	1.3244	1.3281	1.3135	1.2961	0.1593	0.1597	0.1580	0.1559
24	320	400	195.64	0.6778	0.6826	0.6675	0.6523	1.3259	1.3353	1.3059	1.2761	0.1595	0.1606	0.1571	0.1535
25	320	600	192.23	0.6896	0.6975	0.6745	0.6533	1.3257	1.3409	1.2965	1.2558	0.1594	0.1613	0.1559	0.1510

26	320	800	189.80	0.7000	0.7112	0.6798	0.6531	1.3287	1.3498	1.2904	1.2396	0.1598	0.1624	0.1552	0.1491
27	320	1000	187.91	0.7081	0.7226	0.6828	0.6508	1.3307	1.3578	1.2831	1.2230	0.1601	0.1633	0.1543	0.1471
28	320	1500	184.45	0.7249	0.7480	0.6864	0.6423	1.3370	1.3796	1.2660	1.1847	0.1608	0.1659	0.1523	0.1425
29	320	2000	181.97	0.7365	0.7688	0.6844	0.6293	1.3403	1.3989	1.2454	1.1451	0.1612	0.1683	0.1498	0.1377
30	320	3000	178.42	0.7557	0.8075	0.6751	0.6002	1.3482	1.4408	1.2044	1.0709	0.1622	0.1733	0.1449	0.1288
31	320	6000	172.13	0.7958	0.9166	0.6214	0.5010	1.3699	1.5778	1.0696	0.8624	0.1648	0.1898	0.1286	0.1037
32	320	8000	169.39	0.8151	0.9896	0.5718	0.4295	1.3807	1.6763	0.9685	0.7275	0.1661	0.2016	0.1165	0.0875
33	320	10000	167.20	0.8294	1.0630	0.5128	0.3535	1.3868	1.7774	0.8575	0.5911	0.1668	0.2138	0.1031	0.0711
34	340	200	203.23	0.6520	0.6530	0.6457	0.6364	1.3250	1.3271	1.3123	1.2934	0.1594	0.1596	0.1578	0.1556
35	340	400	197.44	0.6726	0.6758	0.6606	0.6441	1.3280	1.3343	1.3043	1.2716	0.1597	0.1605	0.1569	0.1530
36	340	600	194.04	0.6850	0.6905	0.6672	0.6440	1.3292	1.3398	1.2947	1.2496	0.1599	0.1611	0.1557	0.1503
37	340	800	191.61	0.6944	0.7022	0.6706	0.6412	1.3306	1.3454	1.2850	1.2286	0.1600	0.1618	0.1546	0.1478
38	340	1000	189.73	0.7032	0.7133	0.6733	0.6379	1.3341	1.3534	1.2775	1.2103	0.1605	0.1628	0.1537	0.1456
39	340	1500	186.28	0.7174	0.7339	0.6721	0.6227	1.3364	1.3670	1.2519	1.1599	0.1607	0.1644	0.1506	0.1395
40	340	2000	183.81	0.7302	0.7533	0.6688	0.6064	1.3421	1.3846	1.2294	1.1146	0.1614	0.1665	0.1479	0.1341
41	340	3000	180.29	0.7481	0.7856	0.6538	0.5674	1.3488	1.4164	1.1787	1.0229	0.1622	0.1704	0.1418	0.1230
42	340	6000	174.07	0.7879	0.8764	0.5867	0.4395	1.3715	1.5254	1.0213	0.7651	0.1650	0.1835	0.1228	0.0920
43	340	8000	171.38	0.8062	0.9345	0.5283	0.3472	1.3817	1.6015	0.9053	0.5950	0.1662	0.1926	0.1089	0.0716
44	340	10000	169.24	0.8213	0.9936	0.4629	0.2518	1.3900	1.6816	0.7834	0.4261	0.1672	0.2023	0.0942	0.0513
45	360	200	204.93	0.6472	0.6476	0.6401	0.6307	1.3264	1.3272	1.3119	1.2924	0.1595	0.1596	0.1578	0.1555
46	360	400	199.14	0.6679	0.6696	0.6542	0.6372	1.3300	1.3335	1.3027	1.2690	0.1600	0.1604	0.1567	0.1526
47	360	600	195.74	0.6804	0.6837	0.6600	0.6361	1.3319	1.3383	1.2919	1.2452	0.1602	0.1610	0.1554	0.1498
48	360	800	193.33	0.6899	0.6947	0.6626	0.6323	1.3338	1.3431	1.2810	1.2224	0.1604	0.1615	0.1541	0.1470
49	360	1000	191.44	0.6972	0.7036	0.6629	0.6264	1.3347	1.3470	1.2691	1.1991	0.1605	0.1620	0.1526	0.1442
50	360	1500	188.00	0.7129	0.7236	0.6608	0.6096	1.3403	1.3603	1.2424	1.1460	0.1612	0.1636	0.1494	0.1378
51	360	2000	185.55	0.7237	0.7389	0.6534	0.5883	1.3428	1.3710	1.2123	1.0917	0.1615	0.1649	0.1458	0.1313
52	360	3000	182.04	0.7415	0.7665	0.6335	0.5428	1.3498	1.3954	1.1533	0.9881	0.1623	0.1678	0.1387	0.1189
53	360	6000	175.89	0.7794	0.8403	0.5514	0.3934	1.3708	1.4779	0.9699	0.6920	0.1649	0.1778	0.1167	0.0832
54	360	8000	173.24	0.7978	0.8872	0.4849	0.2876	1.3821	1.5370	0.8400	0.4982	0.1662	0.1849	0.1010	0.0599
55	360	10000	171.14	0.8129	0.9341	0.4117	0.1783	1.3911	1.5985	0.7046	0.3052	0.1673	0.1923	0.0847	0.0367

56	380	200	206.55	0.6440	0.6437	0.6360	0.6267	1.3301	1.3296	1.3137	1.2945	0.1600	0.1599	0.1580	0.1557
57	380	400	200.76	0.6643	0.6648	0.6488	0.6322	1.3336	1.3346	1.3026	1.2693	0.1604	0.1605	0.1567	0.1527
58	380	600	197.37	0.6749	0.6763	0.6518	0.6285	1.3321	1.3347	1.2866	1.2405	0.1602	0.1605	0.1547	0.1492
59	380	800	194.95	0.6842	0.6864	0.6534	0.6237	1.3340	1.3382	1.2738	1.2159	0.1604	0.1610	0.1532	0.1463
60	380	1000	193.07	0.6930	0.6961	0.6543	0.6185	1.3381	1.3440	1.2632	1.1942	0.1609	0.1617	0.1519	0.1436
61	380	1500	189.64	0.7075	0.7130	0.6486	0.5985	1.3418	1.3522	1.2301	1.1350	0.1614	0.1626	0.1480	0.1365
62	380	2000	187.19	0.7172	0.7253	0.6377	0.5741	1.3426	1.3578	1.1938	1.0747	0.1615	0.1633	0.1436	0.1293
63	380	3000	183.70	0.7363	0.7503	0.6145	0.5256	1.3525	1.3783	1.1289	0.9655	0.1627	0.1658	0.1358	0.1161
64	380	6000	177.60	0.7714	0.8081	0.5159	0.3601	1.3700	1.4352	0.9162	0.6396	0.1648	0.1726	0.1102	0.0769
65	380	8000	174.98	0.7891	0.8447	0.4399	0.2444	1.3809	1.4780	0.7697	0.4277	0.1661	0.1778	0.0926	0.0514
66	380	10000	172.91	0.8034	0.8803	0.3574	0.1251	1.3891	1.5222	0.6180	0.2163	0.1671	0.1831	0.0743	0.0260
67	400	200	208.09	0.6403	0.6395	0.6314	0.6227	1.3324	1.3307	1.3140	1.2958	0.1603	0.1601	0.1580	0.1559
68	400	400	202.31	0.6600	0.6593	0.6427	0.6272	1.3352	1.3339	1.3003	1.2689	0.1606	0.1604	0.1564	0.1526
69	400	600	198.92	0.6718	0.6713	0.6460	0.6242	1.3364	1.3354	1.2849	1.2416	0.1607	0.1606	0.1545	0.1493
70	400	800	196.50	0.6807	0.6804	0.6461	0.6185	1.3376	1.3370	1.2696	1.2153	0.1609	0.1608	0.1527	0.1462
71	400	1000	194.63	0.6874	0.6873	0.6439	0.6107	1.3379	1.3378	1.2532	1.1886	0.1609	0.1609	0.1507	0.1430
72	400	1500	191.20	0.7017	0.7024	0.6356	0.5893	1.3417	1.3430	1.2154	1.1267	0.1614	0.1615	0.1462	0.1355
73	400	2000	188.76	0.7130	0.7145	0.6238	0.5651	1.3458	1.3488	1.1776	1.0667	0.1619	0.1622	0.1416	0.1283
74	400	3000	185.28	0.7301	0.7340	0.5938	0.5120	1.3527	1.3599	1.1001	0.9487	0.1627	0.1636	0.1323	0.1141
75	400	6000	179.22	0.7630	0.7778	0.4784	0.3360	1.3675	1.3939	0.8573	0.6022	0.1645	0.1677	0.1031	0.0724
76	400	8000	176.63	0.7804	0.8054	0.3925	0.2142	1.3785	1.4226	0.6933	0.3784	0.1658	0.1711	0.0834	0.0455
77	400	10000	174.58	0.7959	0.8334	0.3020	0.0904	1.3896	1.4549	0.5273	0.1578	0.1671	0.1750	0.0634	0.0190
78	420	200	209.57	0.6369	0.6355	0.6271	0.6192	1.3346	1.3318	1.3141	1.2977	0.1605	0.1602	0.1581	0.1561
79	420	400	203.79	0.6558	0.6540	0.6366	0.6228	1.3364	1.3328	1.2973	1.2691	0.1607	0.1603	0.1560	0.1526
80	420	600	200.40	0.6670	0.6647	0.6381	0.6189	1.3365	1.3321	1.2788	1.2402	0.1608	0.1602	0.1538	0.1492
81	420	800	197.99	0.6752	0.6725	0.6366	0.6123	1.3367	1.3316	1.2603	1.2122	0.1608	0.1602	0.1516	0.1458
82	420	1000	196.11	0.6829	0.6799	0.6344	0.6053	1.3392	1.3333	1.2440	1.1870	0.1611	0.1604	0.1496	0.1428
83	420	1500	192.69	0.6964	0.6926	0.6227	0.5825	1.3420	1.3345	1.2000	1.1224	0.1614	0.1605	0.1443	0.1350
84	420	2000	190.26	0.7070	0.7024	0.6076	0.5570	1.3451	1.3363	1.1560	1.0597	0.1618	0.1607	0.1390	0.1275
85	420	3000	186.79	0.7227	0.7171	0.5709	0.5012	1.3500	1.3395	1.0663	0.9361	0.1624	0.1611	0.1283	0.1126

86	420	6000	180.76	0.7570	0.7513	0.4409	0.3220	1.3683	1.3580	0.7970	0.5820	0.1646	0.1633	0.0959	0.0700
87	420	8000	178.19	0.7734	0.7701	0.3437	0.1961	1.3781	1.3723	0.6124	0.3495	0.1658	0.1651	0.0737	0.0420
88	420	10000	176.17	0.7859	0.7869	0.2400	0.0661	1.3845	1.3864	0.4228	0.1165	0.1665	0.1667	0.0508	0.0140
89	440	200	210.99	0.6322	0.6303	0.6214	0.6147	1.3339	1.3299	1.3111	1.2970	0.1604	0.1600	0.1577	0.1560
90	440	400	205.20	0.6518	0.6489	0.6305	0.6190	1.3376	1.3316	1.2938	1.2701	0.1609	0.1602	0.1556	0.1528
91	440	600	201.81	0.6637	0.6598	0.6317	0.6158	1.3395	1.3316	1.2748	1.2428	0.1611	0.1602	0.1533	0.1495
92	440	800	199.41	0.6711	0.6662	0.6282	0.6084	1.3383	1.3286	1.2527	1.2132	0.1610	0.1598	0.1507	0.1459
93	440	1000	197.54	0.6780	0.6722	0.6241	0.6006	1.3393	1.3278	1.2327	1.1864	0.1611	0.1597	0.1483	0.1427
94	440	1500	194.12	0.6921	0.6838	0.6101	0.5782	1.3435	1.3275	1.1844	1.1224	0.1616	0.1597	0.1425	0.1350
95	440	2000	191.69	0.7015	0.6910	0.5910	0.5515	1.3448	1.3245	1.1329	1.0571	0.1618	0.1593	0.1363	0.1272
96	440	3000	188.24	0.7168	0.7019	0.5480	0.4948	1.3492	1.3213	1.0315	0.9314	0.1623	0.1589	0.1241	0.1120
97	440	6000	182.23	0.7495	0.7243	0.3992	0.3128	1.3658	1.3198	0.7274	0.5701	0.1643	0.1587	0.0875	0.0686
98	440	8000	179.68	0.7647	0.7347	0.2893	0.1849	1.3741	1.3202	0.5199	0.3322	0.1653	0.1588	0.0625	0.0400
99	440	10000	177.68	0.7777	0.7445	0.1748	0.0544	1.3819	1.3228	0.3106	0.0967	0.1662	0.1591	0.0374	0.0116
∑				71.638	75.348	60.033	54.205	133.358	139.684	112.715	102.219	16.040	16.801	13.557	12.295
Average (Overall)				**0.7236**	**0.7611**	**0.6064**	**0.5475**	**1.3470**	**1.4109**	**1.1385**	**1.0325**	**0.1620**	**0.1697**	**0.1369**	**0.1242**

Table C-4 Nitrogen [28]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	200	100	179.94	0.5444	0.4800	0.4772	0.4743	0.9796	0.8636	0.8587	0.8535	0.1178	0.1039	0.1033	0.1027
2	220	100	182.73	0.5329	0.4676	0.4650	0.4590	0.9737	0.8545	0.8498	0.8387	0.1171	0.1028	0.1022	0.1009
3	240	100	185.27	0.5250	0.4593	0.4568	0.4489	0.9726	0.8510	0.8463	0.8317	0.1170	0.1024	0.1018	0.1000
4	260	100	187.60	0.5206	0.4548	0.4522	0.4434	0.9766	0.8532	0.8483	0.8318	0.1175	0.1026	0.1020	0.1000
5	280	100	189.76	0.5148	0.4490	0.4462	0.4372	0.9769	0.8520	0.8468	0.8297	0.1175	0.1025	0.1018	0.0998
6	300	100	191.77	0.5100	0.4442	0.4412	0.4326	0.9781	0.8518	0.8461	0.8296	0.1176	0.1025	0.1018	0.0998
7	320	100	193.65	0.5061	0.4402	0.4369	0.4293	0.9800	0.8525	0.8460	0.8313	0.1179	0.1025	0.1018	0.1000

8	340	100	195.42	0.5009	0.4350	0.4312	0.4250	0.9788	0.8502	0.8426	0.8305	0.1177	0.1023	0.1014	0.0999
9	360	100	197.09	0.4962	0.4303	0.4258	0.4214	0.9779	0.8481	0.8393	0.8306	0.1176	0.1020	0.1009	0.0999
10	380	100	198.67	0.4925	0.4265	0.4213	0.4191	0.9784	0.8474	0.8370	0.8326	0.1177	0.1019	0.1007	0.1001
11	400	100	200.17	0.4895	0.4234	0.4173	0.4175	0.9799	0.8476	0.8353	0.8358	0.1179	0.1020	0.1005	0.1005
12	200	200	174.13	0.5611	0.5014	0.4920	0.4887	0.9770	0.8731	0.8568	0.8509	0.1175	0.1050	0.1030	0.1023
13	220	200	176.92	0.5550	0.4926	0.4836	0.4738	0.9819	0.8715	0.8556	0.8383	0.1181	0.1048	0.1029	0.1008
14	240	200	179.47	0.5452	0.4811	0.4723	0.4586	0.9785	0.8633	0.8476	0.8230	0.1177	0.1038	0.1019	0.0990
15	260	200	181.81	0.5380	0.4727	0.4638	0.4482	0.9782	0.8593	0.8433	0.8149	0.1177	0.1034	0.1014	0.0980
16	280	200	183.98	0.5287	0.4625	0.4534	0.4373	0.9727	0.8508	0.8341	0.8045	0.1170	0.1023	0.1003	0.0968
17	300	200	185.99	0.5254	0.4584	0.4488	0.4336	0.9772	0.8526	0.8348	0.8064	0.1175	0.1026	0.1004	0.0970
18	320	200	187.87	0.5226	0.4549	0.4446	0.4312	0.9817	0.8547	0.8353	0.8100	0.1181	0.1028	0.1005	0.0974
19	340	200	189.64	0.5181	0.4499	0.4386	0.4279	0.9826	0.8532	0.8319	0.8114	0.1182	0.1026	0.1001	0.0976
20	360	200	191.31	0.5140	0.4452	0.4327	0.4254	0.9834	0.8516	0.8277	0.8138	0.1183	0.1024	0.0996	0.0979
21	380	200	192.89	0.5108	0.4413	0.4272	0.4242	0.9853	0.8512	0.8241	0.8182	0.1185	0.1024	0.0991	0.0984
22	400	200	194.39	0.5082	0.4379	0.4220	0.4238	0.9879	0.8513	0.8203	0.8238	0.1188	0.1024	0.0987	0.0991
23	200	400	168.27	0.5789	0.5318	0.5081	0.5061	0.9741	0.8948	0.8549	0.8516	0.1172	0.1076	0.1028	0.1024
24	220	400	171.08	0.5734	0.5193	0.4967	0.4813	0.9810	0.8884	0.8498	0.8234	0.1180	0.1069	0.1022	0.0990
25	240	400	173.64	0.5662	0.5073	0.4853	0.4619	0.9831	0.8809	0.8427	0.8020	0.1182	0.1060	0.1014	0.0965
26	260	400	175.99	0.5592	0.4969	0.4749	0.4474	0.9841	0.8745	0.8358	0.7873	0.1184	0.1052	0.1005	0.0947
27	280	400	178.17	0.5485	0.4835	0.4610	0.4324	0.9773	0.8615	0.8214	0.7705	0.1175	0.1036	0.0988	0.0927
28	300	400	180.19	0.5429	0.4758	0.4523	0.4251	0.9783	0.8572	0.8150	0.7659	0.1177	0.1031	0.0980	0.0921
29	320	400	182.08	0.5371	0.4679	0.4431	0.4193	0.9780	0.8520	0.8068	0.7634	0.1176	0.1025	0.0970	0.0918
30	340	400	183.85	0.5347	0.4636	0.4368	0.4182	0.9831	0.8523	0.8031	0.7689	0.1182	0.1025	0.0966	0.0925
31	360	400	185.53	0.5267	0.4537	0.4245	0.4127	0.9772	0.8417	0.7875	0.7656	0.1175	0.1012	0.0947	0.0921
32	380	400	187.11	0.5248	0.4498	0.4175	0.4139	0.9819	0.8416	0.7811	0.7745	0.1181	0.1012	0.0940	0.0932
33	400	400	188.61	0.5232	0.4462	0.4100	0.4160	0.9868	0.8416	0.7733	0.7846	0.1187	0.1012	0.0930	0.0944
34	200	600	164.79	0.5961	0.5632	0.5243	0.5255	0.9823	0.9281	0.8639	0.8660	0.1182	0.1116	0.1039	0.1042
35	220	600	167.63	0.5856	0.5412	0.5042	0.4847	0.9816	0.9071	0.8452	0.8125	0.1181	0.1091	0.1017	0.0977
36	240	600	170.20	0.5813	0.5291	0.4931	0.4612	0.9894	0.9005	0.8393	0.7850	0.1190	0.1083	0.1009	0.0944
37	260	600	172.57	0.5690	0.5109	0.4751	0.4368	0.9819	0.8817	0.8199	0.7538	0.1181	0.1061	0.0986	0.0907

38	280	600	174.75	0.5629	0.5003	0.4638	0.4237	0.9836	0.8742	0.8105	0.7404	0.1183	0.1052	0.0975	0.0891
39	300	600	176.78	0.5551	0.4886	0.4508	0.4126	0.9813	0.8638	0.7970	0.7294	0.1180	0.1039	0.0959	0.0877
40	320	600	178.67	0.5520	0.4820	0.4422	0.4089	0.9862	0.8613	0.7900	0.7306	0.1186	0.1036	0.0950	0.0879
41	340	600	180.45	0.5461	0.4729	0.4301	0.4046	0.9854	0.8533	0.7762	0.7301	0.1185	0.1026	0.0934	0.0878
42	360	600	182.13	0.5397	0.4633	0.4168	0.4013	0.9829	0.8437	0.7591	0.7309	0.1182	0.1015	0.0913	0.0879
43	380	600	183.72	0.5336	0.4540	0.4027	0.3995	0.9804	0.8340	0.7399	0.7340	0.1179	0.1003	0.0890	0.0883
44	400	600	185.22	0.5332	0.4502	0.3931	0.4041	0.9876	0.8338	0.7281	0.7485	0.1188	0.1003	0.0876	0.0900
45	200	800	162.30	0.6033	0.5857	0.5306	0.5365	0.9792	0.9506	0.8611	0.8708	0.1178	0.1143	0.1036	0.1047
46	220	800	165.15	0.6001	0.5663	0.5143	0.4917	0.9911	0.9352	0.8493	0.8121	0.1192	0.1125	0.1022	0.0977
47	240	800	167.75	0.5871	0.5421	0.4917	0.4522	0.9848	0.9094	0.8248	0.7585	0.1185	0.1094	0.0992	0.0912
48	260	800	170.12	0.5813	0.5281	0.4780	0.4297	0.9889	0.8984	0.8132	0.7310	0.1189	0.1081	0.0978	0.0879
49	280	800	172.31	0.5741	0.5144	0.4636	0.4127	0.9892	0.8864	0.7988	0.7110	0.1190	0.1066	0.0961	0.0855
50	300	800	174.35	0.5641	0.4989	0.4463	0.3978	0.9836	0.8698	0.7782	0.6935	0.1183	0.1046	0.0936	0.0834
51	320	800	176.25	0.5581	0.4879	0.4326	0.3906	0.9837	0.8600	0.7625	0.6884	0.1183	0.1034	0.0917	0.0828
52	340	800	178.03	0.5544	0.4796	0.4204	0.3885	0.9870	0.8537	0.7485	0.6916	0.1187	0.1027	0.0900	0.0832
53	360	800	179.71	0.5497	0.4703	0.4061	0.3876	0.9879	0.8452	0.7299	0.6965	0.1188	0.1017	0.0878	0.0838
54	380	800	181.30	0.5450	0.4610	0.3905	0.3882	0.9882	0.8358	0.7080	0.7037	0.1189	0.1005	0.0852	0.0846
55	400	800	182.81	0.5403	0.4515	0.3731	0.3897	0.9877	0.8255	0.6821	0.7124	0.1188	0.0993	0.0820	0.0857
56	200	1000	160.34	0.6124	0.6109	0.5388	0.5507	0.9819	0.9795	0.8639	0.8830	0.1181	0.1178	0.1039	0.1062
57	220	1000	163.22	0.6047	0.5821	0.5143	0.4896	0.9869	0.9500	0.8395	0.7991	0.1187	0.1143	0.1010	0.0961
58	240	1000	165.83	0.5950	0.5579	0.4925	0.4460	0.9867	0.9252	0.8166	0.7396	0.1187	0.1113	0.0982	0.0890
59	260	1000	168.21	0.5900	0.5421	0.4773	0.4195	0.9924	0.9118	0.8028	0.7057	0.1194	0.1097	0.0966	0.0849
60	280	1000	170.41	0.5818	0.5254	0.4598	0.3985	0.9914	0.8953	0.7835	0.6792	0.1192	0.1077	0.0942	0.0817
61	300	1000	172.46	0.5697	0.5060	0.4383	0.3799	0.9825	0.8726	0.7559	0.6551	0.1182	0.1050	0.0909	0.0788
62	320	1000	174.36	0.5665	0.4963	0.4253	0.3748	0.9878	0.8654	0.7415	0.6536	0.1188	0.1041	0.0892	0.0786
63	340	1000	176.15	0.5594	0.4831	0.4072	0.3694	0.9853	0.8509	0.7173	0.6506	0.1185	0.1023	0.0863	0.0783
64	360	1000	177.83	0.5565	0.4742	0.3921	0.3708	0.9896	0.8433	0.6973	0.6594	0.1190	0.1014	0.0839	0.0793
65	380	1000	179.42	0.5532	0.4650	0.3749	0.3738	0.9926	0.8343	0.6727	0.6707	0.1194	0.1004	0.0809	0.0807
66	400	1000	180.94	0.5441	0.4498	0.3497	0.3722	0.9844	0.8138	0.6328	0.6734	0.1184	0.0979	0.0761	0.0810
67	200	1500	156.71	0.6272	0.6690	0.5509	0.5825	0.9828	1.0483	0.8633	0.9128	0.1182	0.1261	0.1038	0.1098

68	220	1500	159.64	0.6247	0.6324	0.5228	0.4957	0.9973	1.0096	0.8347	0.7914	0.1200	0.1214	0.1004	0.0952
69	240	1500	162.29	0.6150	0.5992	0.4942	0.4327	0.9981	0.9724	0.8021	0.7022	0.1200	0.1170	0.0965	0.0845
70	260	1500	164.71	0.6030	0.5697	0.4665	0.3869	0.9932	0.9384	0.7683	0.6374	0.1195	0.1129	0.0924	0.0767
71	280	1500	166.93	0.5956	0.5484	0.4445	0.3591	0.9942	0.9155	0.7420	0.5995	0.1196	0.1101	0.0892	0.0721
72	300	1500	168.99	0.5870	0.5281	0.4213	0.3397	0.9920	0.8924	0.7120	0.5740	0.1193	0.1073	0.0856	0.0690
73	320	1500	170.91	0.5795	0.5101	0.3984	0.3284	0.9904	0.8718	0.6810	0.5613	0.1191	0.1049	0.0819	0.0675
74	340	1500	172.71	0.5722	0.4931	0.3744	0.3228	0.9883	0.8515	0.6465	0.5576	0.1189	0.1024	0.0778	0.0671
75	360	1500	174.40	0.5682	0.4796	0.3515	0.3245	0.9910	0.8364	0.6129	0.5660	0.1192	0.1006	0.0737	0.0681
76	380	1500	176.00	0.5630	0.4649	0.3247	0.3279	0.9909	0.8182	0.5715	0.5771	0.1192	0.0984	0.0687	0.0694
77	400	1500	177.52	0.5568	0.4491	0.2938	0.3322	0.9885	0.7972	0.5215	0.5898	0.1189	0.0959	0.0627	0.0709
78	200	2000	154.05	0.6420	0.7311	0.5618	0.6194	0.9891	1.1262	0.8655	0.9543	0.1190	0.1355	0.1041	0.1148
79	220	2000	157.05	0.6338	0.6745	0.5195	0.4939	0.9954	1.0593	0.8159	0.7757	0.1197	0.1274	0.0981	0.0933
80	240	2000	159.74	0.6249	0.6324	0.4852	0.4112	0.9982	1.0102	0.7751	0.6569	0.1201	0.1215	0.0932	0.0790
81	260	2000	162.18	0.6187	0.6015	0.4577	0.3584	1.0034	0.9756	0.7423	0.5813	0.1207	0.1173	0.0893	0.0699
82	280	2000	164.43	0.6060	0.5694	0.4253	0.3175	0.9965	0.9362	0.6993	0.5221	0.1199	0.1126	0.0841	0.0628
83	300	2000	166.50	0.6013	0.5481	0.4008	0.2974	1.0011	0.9126	0.6673	0.4952	0.1204	0.1098	0.0803	0.0596
84	320	2000	168.44	0.5893	0.5215	0.3679	0.2797	0.9926	0.8785	0.6197	0.4711	0.1194	0.1057	0.0745	0.0567
85	340	2000	170.25	0.5821	0.5007	0.3378	0.2739	0.9909	0.8525	0.5751	0.4664	0.1192	0.1025	0.0692	0.0561
86	360	2000	171.95	0.5769	0.4825	0.3070	0.2757	0.9920	0.8296	0.5279	0.4741	0.1193	0.0998	0.0635	0.0570
87	380	2000	173.55	0.5755	0.4680	0.2764	0.2851	0.9988	0.8123	0.4798	0.4948	0.1201	0.0977	0.0577	0.0595
88	400	2000	175.08	0.5667	0.4459	0.2340	0.2897	0.9921	0.7807	0.4098	0.5071	0.1193	0.0939	0.0493	0.0610
89	200	2500	151.93	0.6504	0.7903	0.5647	0.6544	0.9881	1.2008	0.8579	0.9942	0.1188	0.1444	0.1032	0.1196
90	220	2500	154.99	0.6443	0.7206	0.5166	0.4959	0.9987	1.1169	0.8007	0.7686	0.1201	0.1343	0.0963	0.0925
91	240	2500	157.72	0.6370	0.6696	0.4776	0.3934	1.0046	1.0561	0.7532	0.6205	0.1208	0.1270	0.0906	0.0746
92	260	2500	160.19	0.6306	0.6310	0.4445	0.3272	1.0102	1.0108	0.7121	0.5241	0.1215	0.1216	0.0856	0.0630
93	280	2500	162.46	0.6190	0.5939	0.4080	0.2791	1.0057	0.9649	0.6629	0.4535	0.1210	0.1161	0.0797	0.0545
94	300	2500	164.55	0.6121	0.5656	0.3761	0.2522	1.0072	0.9307	0.6189	0.4150	0.1211	0.1119	0.0744	0.0499
95	320	2500	166.50	0.6017	0.5363	0.3394	0.2340	1.0019	0.8929	0.5650	0.3896	0.1205	0.1074	0.0680	0.0469
96	340	2500	168.32	0.5945	0.5115	0.3032	0.2279	1.0006	0.8609	0.5103	0.3837	0.1204	0.1036	0.0614	0.0461
97	360	2500	170.03	0.5882	0.4884	0.2644	0.2297	1.0001	0.8304	0.4496	0.3905	0.1203	0.0999	0.0541	0.0470

98	380	2500	171.65	0.5789	0.4624	0.2183	0.2334	0.9938	0.7938	0.3748	0.4006	0.1195	0.0955	0.0451	0.0482
99	400	2500	173.18	0.5732	0.4398	0.1702	0.2439	0.9927	0.7616	0.2948	0.4224	0.1194	0.0916	0.0355	0.0508
100	200	3000	150.15	0.6546	0.8493	0.5617	0.6895	0.9829	1.2753	0.8434	1.0352	0.1182	0.1534	0.1014	0.1245
101	220	3000	153.27	0.6526	0.7668	0.5102	0.4977	1.0002	1.1752	0.7820	0.7628	0.1203	0.1414	0.0941	0.0917
102	240	3000	156.04	0.6474	0.7068	0.4674	0.3751	1.0102	1.1030	0.7294	0.5853	0.1215	0.1327	0.0877	0.0704
103	260	3000	158.55	0.6349	0.6540	0.4230	0.2890	1.0067	1.0370	0.6706	0.4582	0.1211	0.1247	0.0807	0.0551
104	280	3000	160.83	0.6309	0.6183	0.3890	0.2401	1.0147	0.9944	0.6256	0.3861	0.1220	0.1196	0.0753	0.0464
105	300	3000	162.94	0.6218	0.5827	0.3498	0.2062	1.0132	0.9494	0.5699	0.3360	0.1219	0.1142	0.0686	0.0404
106	320	3000	164.91	0.6070	0.5445	0.3031	0.1813	1.0010	0.8979	0.4998	0.2991	0.1204	0.1080	0.0601	0.0360
107	340	3000	166.74	0.5998	0.5157	0.2609	0.1751	1.0002	0.8599	0.4350	0.2919	0.1203	0.1034	0.0523	0.0351
108	360	3000	168.46	0.5924	0.4876	0.2142	0.1767	0.9980	0.8214	0.3609	0.2977	0.1200	0.0988	0.0434	0.0358
109	380	3000	170.08	0.5871	0.4619	0.1643	0.1864	0.9985	0.7855	0.2794	0.3170	0.1201	0.0945	0.0336	0.0381
110	400	3000	171.61	0.5845	0.4387	0.1105	0.2028	1.0031	0.7528	0.1896	0.3480	0.1207	0.0905	0.0228	0.0419
111	220	3500	151.78	0.6621	0.8167	0.5039	0.5026	1.0049	1.2395	0.7648	0.7628	0.1209	0.1491	0.0920	0.0918
112	240	3500	154.60	0.6533	0.7411	0.4518	0.3532	1.0100	1.1458	0.6985	0.5460	0.1215	0.1378	0.0840	0.0657
113	260	3500	157.13	0.6477	0.6867	0.4091	0.2597	1.0177	1.0790	0.6428	0.4081	0.1224	0.1298	0.0773	0.0491
114	280	3500	159.44	0.6387	0.6395	0.3653	0.1973	1.0184	1.0195	0.5824	0.3146	0.1225	0.1226	0.0700	0.0378
115	300	3500	161.57	0.6276	0.5964	0.3189	0.1565	1.0140	0.9636	0.5152	0.2528	0.1220	0.1159	0.0620	0.0304
116	320	3500	163.54	0.6206	0.5614	0.2745	0.1371	1.0149	0.9182	0.4489	0.2242	0.1221	0.1104	0.0540	0.0270
117	340	3500	165.39	0.6073	0.5224	0.2201	0.1243	1.0044	0.8640	0.3641	0.2056	0.1208	0.1039	0.0438	0.0247
118	360	3500	167.12	0.5987	0.4893	0.1655	0.1258	1.0005	0.8177	0.2767	0.2103	0.1203	0.0983	0.0333	0.0253
119	380	3500	168.74	0.5973	0.4637	0.1117	0.1414	1.0078	0.7824	0.1885	0.2386	0.1212	0.0941	0.0227	0.0287
120	400	3500	170.29	0.5861	0.4281	0.0404	0.1519	0.9981	0.7290	0.0688	0.2587	0.1200	0.0877	0.0083	0.0311
121	420	3500	171.75	0.5828	0.3997	0.0326	0.1730	1.0010	0.6864	0.0560	0.2970	0.1204	0.0826	0.0067	0.0357
122	220	4000	150.47	0.6649	0.8621	0.4896	0.5023	1.0004	1.2971	0.7367	0.7558	0.1203	0.1560	0.0886	0.0909
123	240	4000	153.33	0.6596	0.7773	0.4357	0.3324	1.0113	1.1919	0.6681	0.5096	0.1216	0.1434	0.0804	0.0613
124	260	4000	155.89	0.6547	0.7146	0.3888	0.2251	1.0206	1.1140	0.6061	0.3510	0.1228	0.1340	0.0729	0.0422
125	280	4000	158.22	0.6472	0.6621	0.3416	0.1554	1.0241	1.0476	0.5405	0.2459	0.1232	0.1260	0.0650	0.0296
126	300	4000	160.37	0.6340	0.6114	0.2880	0.1075	1.0167	0.9805	0.4619	0.1724	0.1223	0.1179	0.0556	0.0207
127	320	4000	162.36	0.6225	0.5673	0.2338	0.0813	1.0107	0.9210	0.3795	0.1320	0.1216	0.1108	0.0456	0.0159

128	340	4000	164.21	0.6154	0.5302	0.1795	0.0743	1.0106	0.8706	0.2948	0.1219	0.1215	0.1047	0.0355	0.0147
129	360	4000	165.95	0.6056	0.4919	0.1169	0.0755	1.0050	0.8163	0.1941	0.1254	0.1209	0.0982	0.0233	0.0151
130	380	4000	167.58	0.6021	0.4604	0.0533	0.0911	1.0090	0.7715	0.0894	0.1526	0.1214	0.0928	0.0107	0.0184
131	400	4000	169.13	0.5941	0.4242	0.0238	0.1074	1.0048	0.7174	0.0402	0.1816	0.1209	0.0863	0.0048	0.0218
132	420	4000	170.60	0.5876	0.3887	0.1104	0.1282	1.0024	0.6630	0.1883	0.2188	0.1206	0.0797	0.0226	0.0263
133	220	4500	149.28	0.6742	0.9163	0.4805	0.5100	1.0064	1.3678	0.7173	0.7613	0.1211	0.1645	0.0863	0.0916
134	240	4500	152.19	0.6661	0.8154	0.4191	0.3126	1.0138	1.2409	0.6378	0.4757	0.1219	0.1493	0.0767	0.0572
135	260	4500	154.78	0.6622	0.7441	0.3683	0.1914	1.0249	1.1518	0.5701	0.2962	0.1233	0.1385	0.0686	0.0356
136	280	4500	157.14	0.6499	0.6797	0.3115	0.1079	1.0213	1.0680	0.4895	0.1695	0.1228	0.1285	0.0589	0.0204
137	300	4500	159.30	0.6409	0.6275	0.2572	0.0591	1.0209	0.9996	0.4097	0.0941	0.1228	0.1202	0.0493	0.0113
138	320	4500	161.30	0.6312	0.5802	0.1992	0.0322	1.0181	0.9359	0.3213	0.0520	0.1225	0.1126	0.0386	0.0063
139	340	4500	163.16	0.6240	0.5388	0.1390	0.0247	1.0182	0.8792	0.2267	0.0403	0.1225	0.1057	0.0273	0.0048
140	360	4500	164.91	0.6130	0.4952	0.0683	0.0256	1.0108	0.8167	0.1127	0.0423	0.1216	0.0982	0.0136	0.0051
141	380	4500	166.55	0.6074	0.4578	0.0052	0.0410	1.0116	0.7624	0.0086	0.0683	0.1217	0.0917	0.0010	0.0082
142	400	4500	168.11	0.5966	0.4150	0.0940	0.0572	1.0029	0.6976	0.1580	0.0962	0.1206	0.0839	0.0190	0.0116
143	420	4500	169.58	0.5927	0.3782	0.1883	0.0838	1.0052	0.6414	0.3193	0.1420	0.1209	0.0771	0.0384	0.0171
144	440	4500	170.98	0.5889	0.3400	0.2976	0.1115	1.0069	0.5814	0.5089	0.1906	0.1211	0.0699	0.0612	0.0229
145	240	5000	151.15	0.6749	0.8569	0.4037	0.2955	1.0201	1.2953	0.6101	0.4466	0.1227	0.1558	0.0734	0.0537
146	260	5000	153.78	0.6653	0.7703	0.3428	0.1535	1.0231	1.1846	0.5271	0.2361	0.1231	0.1425	0.0634	0.0284
147	280	5000	156.16	0.6547	0.7001	0.2830	0.0626	1.0224	1.0933	0.4419	0.0977	0.1230	0.1315	0.0532	0.0118
148	300	5000	158.33	0.6500	0.6463	0.2280	0.0129	1.0291	1.0234	0.3610	0.0204	0.1238	0.1231	0.0434	0.0024
149	320	5000	160.35	0.6356	0.5895	0.1600	0.0210	1.0193	0.9453	0.2566	0.0337	0.1226	0.1137	0.0309	0.0041
150	340	5000	162.22	0.6285	0.5437	0.0938	0.0290	1.0196	0.8820	0.1522	0.0471	0.1226	0.1061	0.0183	0.0057
151	360	5000	163.98	0.6162	0.4948	0.0152	0.0284	1.0104	0.8114	0.0249	0.0466	0.1215	0.0976	0.0030	0.0056
152	380	5000	165.63	0.6085	0.4513	0.0682	0.0132	1.0078	0.7475	0.1129	0.0219	0.1212	0.0899	0.0136	0.0026
153	400	5000	167.18	0.6069	0.4139	0.1567	0.0148	1.0147	0.6919	0.2620	0.0247	0.1220	0.0832	0.0315	0.0030
154	420	5000	168.66	0.5997	0.3698	0.2648	0.0410	1.0115	0.6238	0.4466	0.0691	0.1217	0.0750	0.0537	0.0083
155	440	5000	170.07	0.5922	0.3239	0.3899	0.0682	1.0071	0.5508	0.6632	0.1159	0.1211	0.0663	0.0798	0.0139
156	460	5000	171.41	0.5886	0.2797	0.5315	0.0986	1.0090	0.4794	0.9111	0.1690	0.1214	0.0577	0.1096	0.0203
157	480	5000	172.70	0.5810	0.2285	0.7020	0.1225	1.0033	0.3947	1.2124	0.2115	0.1207	0.0475	0.1458	0.0254

158	500	5000	173.93	0.5782	0.1787	0.8980	0.1474	1.0056	0.3108	1.5619	0.2564	0.1210	0.0374	0.1879	0.0308
159	260	6000	152.01	0.6763	0.8300	0.2944	0.0829	1.0280	1.2617	0.4475	0.1261	0.1236	0.1518	0.0538	0.0152
160	280	6000	154.43	0.6689	0.7476	0.2288	0.0233	1.0330	1.1545	0.3534	0.0360	0.1242	0.1389	0.0425	0.0043
161	300	6000	156.64	0.6598	0.6772	0.1599	0.0878	1.0335	1.0608	0.2504	0.1375	0.1243	0.1276	0.0301	0.0165
162	320	6000	158.68	0.6488	0.6135	0.0846	0.1233	1.0296	0.9735	0.1343	0.1957	0.1238	0.1171	0.0162	0.0235
163	340	6000	160.58	0.6353	0.5522	0.0002	0.1388	1.0202	0.8868	0.0003	0.2229	0.1227	0.1067	0.0000	0.0268
164	360	6000	162.35	0.6265	0.4986	0.0885	0.1329	1.0172	0.8095	0.1436	0.2157	0.1223	0.0974	0.0173	0.0259
165	380	6000	164.01	0.6205	0.4489	0.1856	0.1122	1.0177	0.7363	0.3043	0.1840	0.1224	0.0886	0.0366	0.0221
166	400	6000	165.58	0.6132	0.3979	0.2977	0.0848	1.0154	0.6589	0.4930	0.1404	0.1221	0.0793	0.0593	0.0169
167	420	6000	167.07	0.6053	0.3454	0.4272	0.0533	1.0113	0.5770	0.7138	0.0891	0.1216	0.0694	0.0859	0.0107
168	440	6000	168.48	0.6022	0.2957	0.5723	0.0155	1.0146	0.4982	0.9643	0.0261	0.1220	0.0599	0.1160	0.0031
169	460	6000	169.83	0.5964	0.2408	0.7446	0.0189	1.0129	0.4090	1.2646	0.0321	0.1218	0.0492	0.1521	0.0039
170	480	6000	171.13	0.5860	0.1779	0.9515	0.0458	1.0029	0.3044	1.6283	0.0783	0.1206	0.0366	0.1959	0.0094
171	500	6000	172.36	0.5860	0.1211	1.1848	0.0785	1.0100	0.2088	2.0421	0.1353	0.1215	0.0251	0.2456	0.0163
172	260	7000	150.48	0.6849	0.8909	0.2414	0.0105	1.0307	1.3406	0.3633	0.0158	0.1240	0.1612	0.0437	0.0019
173	280	7000	152.94	0.6807	0.7951	0.1703	0.1114	1.0410	1.2160	0.2605	0.1704	0.1252	0.1463	0.0313	0.0205
174	300	7000	155.19	0.6670	0.7073	0.0873	0.1912	1.0351	1.0977	0.1355	0.2967	0.1245	0.1320	0.0163	0.0357
175	320	7000	157.25	0.6592	0.6362	0.0049	0.2286	1.0367	1.0004	0.0077	0.3595	0.1247	0.1203	0.0009	0.0432
176	340	7000	159.17	0.6454	0.5653	0.0917	0.2456	1.0272	0.8998	0.1459	0.3909	0.1236	0.1082	0.0176	0.0470
177	360	7000	160.95	0.6401	0.5066	0.1903	0.2345	1.0302	0.8154	0.3063	0.3775	0.1239	0.0981	0.0368	0.0454
178	380	7000	162.63	0.6294	0.4443	0.3074	0.2147	1.0236	0.7225	0.5000	0.3492	0.1231	0.0869	0.0601	0.0420
179	400	7000	164.21	0.6223	0.3857	0.4372	0.1820	1.0219	0.6333	0.7179	0.2989	0.1229	0.0762	0.0864	0.0359
180	420	7000	165.71	0.6135	0.3243	0.5884	0.1456	1.0167	0.5374	0.9750	0.2412	0.1223	0.0646	0.1173	0.0290
181	440	7000	167.13	0.6088	0.2649	0.7594	0.1031	1.0175	0.4427	1.2691	0.1723	0.1224	0.0533	0.1526	0.0207
182	460	7000	168.49	0.6008	0.1992	0.9625	0.0649	1.0122	0.3357	1.6217	0.1093	0.1217	0.0404	0.1951	0.0132
183	480	7000	169.79	0.5935	0.1304	1.2000	0.0293	1.0076	0.2215	2.0375	0.0497	0.1212	0.0266	0.2451	0.0060
184	500	7000	171.03	0.5902	0.0608	1.4765	0.0053	1.0095	0.1041	2.5253	0.0090	0.1214	0.0125	0.3037	0.0011
185	260	8000	149.13	0.6902	0.9513	0.1830	0.0652	1.0293	1.4187	0.2729	0.0973	0.1238	0.1706	0.0328	0.0117
186	280	8000	151.63	0.6887	0.8411	0.1063	0.2034	1.0443	1.2753	0.1612	0.3084	0.1256	0.1534	0.0194	0.0371
187	300	8000	153.91	0.6765	0.7415	0.0157	0.2923	1.0412	1.1412	0.0241	0.4499	0.1252	0.1373	0.0029	0.0541

188	320	8000	156.00	0.6653	0.6559	0.0805	0.3383	1.0379	1.0232	0.1256	0.5277	0.1248	0.1231	0.0151	0.0635
189	340	8000	157.93	0.6573	0.5813	0.1829	0.3507	1.0380	0.9181	0.2889	0.5538	0.1249	0.1104	0.0347	0.0666
190	360	8000	159.73	0.6490	0.5110	0.2978	0.3410	1.0366	0.8163	0.4758	0.5447	0.1247	0.0982	0.0572	0.0655
191	380	8000	161.43	0.6335	0.4358	0.4351	0.3223	1.0227	0.7035	0.7023	0.5203	0.1230	0.0846	0.0845	0.0626
192	400	8000	163.02	0.6266	0.3694	0.5825	0.2844	1.0215	0.6022	0.9496	0.4637	0.1229	0.0724	0.1142	0.0558
193	420	8000	164.53	0.6169	0.2992	0.7553	0.2431	1.0149	0.4922	1.2427	0.3999	0.1221	0.0592	0.1495	0.0481
194	440	8000	165.96	0.6104	0.2299	0.9523	0.1962	1.0130	0.3816	1.5804	0.3256	0.1218	0.0459	0.1901	0.0392
195	460	8000	167.32	0.6060	0.1594	1.1804	0.1483	1.0140	0.2668	1.9750	0.2482	0.1220	0.0321	0.2376	0.0299
196	480	8000	168.62	0.6018	0.0847	1.4486	0.1040	1.0148	0.1428	2.4427	0.1754	0.1221	0.0172	0.2938	0.0211
197	500	8000	169.87	0.5953	0.0022	1.7685	0.0678	1.0113	0.0038	3.0041	0.1152	0.1216	0.0005	0.3613	0.0139
198	260	10000	146.81	0.7001	1.0788	0.0609	0.2181	1.0279	1.5838	0.0894	0.3203	0.1236	0.1905	0.0107	0.0385
199	280	10000	149.39	0.7020	0.9357	0.0285	0.3905	1.0487	1.3978	0.0426	0.5833	0.1261	0.1681	0.0051	0.0702
200	300	10000	151.73	0.6914	0.8099	0.1354	0.4990	1.0491	1.2288	0.2055	0.7571	0.1262	0.1478	0.0247	0.0911
201	320	10000	153.87	0.6786	0.6999	0.2534	0.5569	1.0441	1.0770	0.3899	0.8568	0.1256	0.1295	0.0469	0.1031
202	340	10000	155.84	0.6687	0.6040	0.3806	0.5736	1.0421	0.9413	0.5932	0.8938	0.1253	0.1132	0.0713	0.1075
203	360	10000	157.67	0.6601	0.5159	0.5222	0.5610	1.0408	0.8134	0.8233	0.8845	0.1252	0.0978	0.0990	0.1064
204	380	10000	159.39	0.6471	0.4266	0.6875	0.5327	1.0314	0.6799	1.0958	0.8491	0.1241	0.0818	0.1318	0.1021
205	400	10000	161.00	0.6400	0.3440	0.8705	0.4852	1.0303	0.5539	1.4016	0.7812	0.1239	0.0666	0.1686	0.0940
206	420	10000	162.52	0.6342	0.2618	1.0808	0.4286	1.0306	0.4255	1.7566	0.6966	0.1240	0.0512	0.2113	0.0838
207	440	10000	163.97	0.6239	0.1725	1.3301	0.3735	1.0230	0.2828	2.1809	0.6124	0.1230	0.0340	0.2623	0.0737
208	460	10000	165.35	0.6145	0.0801	1.6201	0.3187	1.0160	0.1324	2.6789	0.5270	0.1222	0.0159	0.3222	0.0634
209	480	10000	166.66	0.6104	0.0125	1.9558	0.2634	1.0172	0.0208	3.2596	0.4389	0.1223	0.0025	0.3921	0.0528
210	500	10000	167.92	0.6031	0.1148	2.3567	0.2184	1.0127	0.1928	3.9573	0.3667	0.1218	0.0232	0.4760	0.0441
∑				125.96	107.64	90.458	61.423	210.629	178.717	152.803	104.066	25.334	21.496	18.379	12.517
Average (Overall)				**0.5998**	**0.5126**	**0.4308**	**0.2925**	**1.0030**	**0.8510**	**0.7276**	**0.4956**	**0.1206**	**0.1024**	**0.0875**	**0.0596**

Table C-5 Ethane [21]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	400	300	237.14	1.0690	1.0932	1.0819	1.0759	2.5349	2.5924	2.5655	2.5513	0.3049	0.3118	0.3086	0.3069
2	400	400	234.68	1.0794	1.1122	1.0967	1.0916	2.5332	2.6101	2.5739	2.5618	0.3047	0.3139	0.3096	0.3081
3	400	500	232.77	1.0880	1.1295	1.1098	1.1061	2.5325	2.6290	2.5832	2.5745	0.3046	0.3162	0.3107	0.3097
4	400	600	231.19	1.0961	1.1464	1.1224	1.1205	2.5341	2.6504	2.5948	2.5905	0.3048	0.3188	0.3121	0.3116
5	400	700	229.85	1.1016	1.1609	1.1324	1.1328	2.5320	2.6682	2.6027	2.6038	0.3045	0.3209	0.3131	0.3132
6	400	800	228.68	1.1075	1.1759	1.1428	1.1459	2.5325	2.6889	2.6132	2.6204	0.3046	0.3234	0.3143	0.3152
7	400	1000	226.70	1.1165	1.2034	1.1608	1.1703	2.5310	2.7281	2.6314	2.6531	0.3044	0.3281	0.3165	0.3191
8	400	1500	223.01	1.1322	1.2676	1.1989	1.2302	2.5250	2.8269	2.6736	2.7434	0.3037	0.3400	0.3216	0.3300
9	400	2000	220.30	1.1429	1.3296	1.2315	1.2919	2.5179	2.9292	2.7130	2.8461	0.3029	0.3523	0.3263	0.3423
10	420	300	240.42	1.0482	1.0685	1.0576	1.0467	2.5200	2.5689	2.5427	2.5164	0.3031	0.3090	0.3058	0.3027
11	420	400	237.97	1.0590	1.0865	1.0716	1.0597	2.5200	2.5855	2.5502	2.5219	0.3031	0.3110	0.3067	0.3033
12	420	500	236.06	1.0680	1.1028	1.0839	1.0716	2.5212	2.6033	2.5588	2.5296	0.3032	0.3131	0.3078	0.3043
13	420	600	234.49	1.0754	1.1175	1.0946	1.0821	2.5216	2.6206	2.5666	2.5375	0.3033	0.3152	0.3087	0.3052
14	420	700	233.16	1.0815	1.1312	1.1040	1.0918	2.5216	2.6374	2.5740	2.5457	0.3033	0.3172	0.3096	0.3062
15	420	800	231.99	1.0868	1.1441	1.1125	1.1011	2.5213	2.6542	2.5810	2.5544	0.3033	0.3192	0.3104	0.3072
16	420	1000	230.03	1.0961	1.1689	1.1283	1.1190	2.5213	2.6887	2.5955	2.5741	0.3033	0.3234	0.3122	0.3096
17	420	1500	226.39	1.1116	1.2248	1.1600	1.1607	2.5166	2.7728	2.6262	2.6276	0.3027	0.3335	0.3159	0.3160
18	420	2000	223.72	1.1236	1.2794	1.1878	1.2040	2.5137	2.8623	2.6572	2.6936	0.3023	0.3443	0.3196	0.3240
19	420	4000	216.79	1.1482	1.4988	1.2683	1.4005	2.4892	3.2491	2.7496	3.0361	0.2994	0.3908	0.3307	0.3652
20	440	300	243.66	1.0292	1.0464	1.0359	1.0211	2.5077	2.5496	2.5239	2.4881	0.3016	0.3067	0.3036	0.2993
21	440	400	241.22	1.0397	1.0630	1.0487	1.0316	2.5080	2.5642	2.5297	2.4884	0.3017	0.3084	0.3043	0.2993
22	440	500	239.32	1.0474	1.0768	1.0586	1.0396	2.5066	2.5771	2.5335	2.4880	0.3015	0.3100	0.3047	0.2993
23	440	600	237.75	1.0547	1.0904	1.0683	1.0477	2.5075	2.5925	2.5398	2.4909	0.3016	0.3118	0.3055	0.2996
24	440	700	236.43	1.0608	1.1029	1.0767	1.0549	2.5080	2.6075	2.5456	2.4940	0.3017	0.3136	0.3062	0.3000
25	440	800	235.27	1.0662	1.1147	1.0844	1.0616	2.5084	2.6225	2.5511	2.4977	0.3017	0.3154	0.3068	0.3004

26	440	1000	233.32	1.0744	1.1360	1.0972	1.0733	2.5068	2.6505	2.5599	2.5043	0.3015	0.3188	0.3079	0.3012
27	440	1500	229.71	1.0914	1.1870	1.1254	1.1026	2.5071	2.7267	2.5852	2.5327	0.3016	0.3280	0.3109	0.3046
28	440	2000	227.07	1.1046	1.2360	1.1494	1.1321	2.5081	2.8066	2.6101	2.5706	0.3017	0.3376	0.3139	0.3092
29	440	4000	220.30	1.1320	1.4255	1.2150	1.2594	2.4939	3.1404	2.6768	2.7744	0.3000	0.3777	0.3220	0.3337
30	460	300	246.87	1.0095	1.0242	1.0139	0.9964	2.4921	2.5284	2.5031	2.4597	0.2997	0.3041	0.3011	0.2959
31	460	400	244.43	1.0206	1.0405	1.0266	1.0056	2.4947	2.5434	2.5093	2.4580	0.3001	0.3059	0.3018	0.2956
32	460	500	242.54	1.0290	1.0541	1.0365	1.0124	2.4956	2.5566	2.5138	2.4555	0.3002	0.3075	0.3024	0.2953
33	460	600	240.98	1.0358	1.0663	1.0448	1.0181	2.4960	2.5695	2.5177	2.4533	0.3002	0.3091	0.3028	0.2951
34	460	700	239.65	1.0415	1.0774	1.0520	1.0229	2.4959	2.5819	2.5212	2.4514	0.3002	0.3106	0.3032	0.2948
35	460	800	238.50	1.0464	1.0878	1.0585	1.0272	2.4957	2.5944	2.5245	2.4499	0.3002	0.3121	0.3036	0.2947
36	460	1000	236.56	1.0552	1.1078	1.0703	1.0354	2.4963	2.6206	2.5319	2.4494	0.3003	0.3152	0.3045	0.2946
37	460	1500	232.98	1.0723	1.1538	1.0947	1.0540	2.4983	2.6880	2.5504	2.4555	0.3005	0.3233	0.3068	0.2953
38	460	2000	230.37	1.0849	1.1967	1.1142	1.0714	2.4993	2.7569	2.5669	2.4682	0.3006	0.3316	0.3087	0.2969
39	460	4000	223.73	1.1143	1.3625	1.1671	1.1466	2.4930	3.0484	2.6112	2.5652	0.2999	0.3667	0.3141	0.3085
40	480	300	250.04	0.9925	1.0051	0.9951	0.9755	2.4816	2.5132	2.4882	2.4391	0.2985	0.3023	0.2993	0.2934
41	480	400	247.61	1.0027	1.0198	1.0062	0.9823	2.4828	2.5251	2.4914	2.4323	0.2986	0.3037	0.2997	0.2926
42	480	500	245.72	1.0101	1.0317	1.0145	0.9868	2.4821	2.5352	2.4929	2.4248	0.2985	0.3049	0.2998	0.2917
43	480	600	244.17	1.0173	1.0435	1.0226	0.9913	2.4840	2.5479	2.4969	2.4206	0.2988	0.3065	0.3003	0.2911
44	480	700	242.85	1.0235	1.0543	1.0296	0.9951	2.4855	2.5603	2.5004	2.4165	0.2990	0.3079	0.3007	0.2907
45	480	800	241.70	1.0277	1.0632	1.0347	0.9971	2.4839	2.5697	2.5008	2.4100	0.2988	0.3091	0.3008	0.2899
46	480	1000	239.77	1.0376	1.0826	1.0463	1.0032	2.4877	2.5958	2.5086	2.4054	0.2992	0.3122	0.3017	0.2893
47	480	1500	236.21	1.0540	1.1238	1.0667	1.0127	2.4895	2.6545	2.5197	2.3921	0.2994	0.3193	0.3031	0.2877
48	480	2000	233.63	1.0663	1.1621	1.0828	1.0211	2.4912	2.7150	2.5298	2.3855	0.2996	0.3266	0.3043	0.2869
49	480	4000	227.09	1.0970	1.3087	1.1248	1.0565	2.4912	2.9718	2.5542	2.3990	0.2996	0.3574	0.3072	0.2886
50	480	6000	222.92	1.1129	1.4599	1.1448	1.1027	2.4808	3.2545	2.5521	2.4581	0.2984	0.3914	0.3070	0.2957
51	500	400	250.76	0.9866	1.0013	0.9880	0.9622	2.4739	2.5109	2.4774	2.4128	0.2976	0.3020	0.2980	0.2902
52	500	500	248.87	0.9941	1.0127	0.9959	0.9656	2.4741	2.5204	2.4784	2.4032	0.2976	0.3032	0.2981	0.2891
53	500	600	247.33	1.0002	1.0228	1.0023	0.9679	2.4738	2.5296	2.4789	2.3939	0.2975	0.3043	0.2982	0.2879
54	500	700	246.01	1.0065	1.0331	1.0089	0.9706	2.4761	2.5414	2.4820	2.3879	0.2978	0.3057	0.2985	0.2872
55	500	800	244.87	1.0109	1.0415	1.0137	0.9717	2.4754	2.5503	2.4821	2.3793	0.2977	0.3068	0.2985	0.2862

56	500	1000	242.94	1.0200	1.0589	1.0234	0.9745	2.4781	2.5724	2.4862	2.3676	0.2981	0.3094	0.2990	0.2848
57	500	1500	239.40	1.0367	1.0968	1.0413	0.9778	2.4819	2.6258	2.4930	2.3410	0.2985	0.3158	0.2999	0.2816
58	500	2000	236.83	1.0498	1.1322	1.0554	0.9800	2.4862	2.6814	2.4996	2.3210	0.2990	0.3225	0.3007	0.2792
59	500	4000	230.38	1.0813	1.2628	1.0878	0.9849	2.4911	2.9091	2.5060	2.2689	0.2996	0.3499	0.3014	0.2729
60	500	6000	226.31	1.0988	1.3949	1.1002	0.9954	2.4866	3.1567	2.4899	2.2527	0.2991	0.3797	0.2995	0.2710
61	500	10000	220.68	1.1053	1.6747	1.0805	1.0266	2.4393	3.6957	2.3845	2.2656	0.2934	0.4445	0.2868	0.2725
62	520	400	253.88	0.9715	0.9842	0.9711	0.9442	2.4665	2.4988	2.4655	2.3971	0.2967	0.3006	0.2965	0.2883
63	520	500	252.00	0.9790	0.9950	0.9784	0.9466	2.4669	2.5074	2.4656	2.3855	0.2967	0.3016	0.2966	0.2869
64	520	600	250.45	0.9862	1.0057	0.9855	0.9492	2.4699	2.5187	2.4682	2.3772	0.2971	0.3029	0.2969	0.2859
65	520	700	249.14	0.9912	1.0142	0.9904	0.9497	2.4695	2.5266	2.4674	2.3661	0.2970	0.3039	0.2968	0.2846
66	520	800	247.99	0.9968	1.0233	0.9959	0.9510	2.4721	2.5376	2.4697	2.3585	0.2973	0.3052	0.2970	0.2837
67	520	1000	246.08	1.0047	1.0382	1.0034	0.9508	2.4724	2.5549	2.4692	2.3397	0.2974	0.3073	0.2970	0.2814
68	520	1500	242.55	1.0217	1.0736	1.0193	0.9495	2.4781	2.6040	2.4724	2.3029	0.2981	0.3132	0.2974	0.2770
69	520	2000	240.00	1.0341	1.1052	1.0304	0.9457	2.4819	2.6525	2.4730	2.2697	0.2985	0.3190	0.2974	0.2730
70	520	4000	233.62	1.0653	1.2215	1.0533	0.9263	2.4889	2.8536	2.4608	2.1640	0.2994	0.3432	0.2960	0.2603
71	520	6000	229.62	1.0845	1.3382	1.0591	0.9104	2.4902	3.0729	2.4320	2.0904	0.2995	0.3696	0.2925	0.2514
72	520	10000	224.15	1.0979	1.5819	1.0324	0.8831	2.4611	3.5458	2.3141	1.9794	0.2960	0.4265	0.2783	0.2381
73	540	500	255.08	0.9661	0.9800	0.9636	0.9311	2.4644	2.4999	2.4580	2.3751	0.2964	0.3007	0.2956	0.2857
74	540	600	253.54	0.9719	0.9888	0.9688	0.9315	2.4642	2.5069	2.4564	2.3618	0.2964	0.3015	0.2955	0.2841
75	540	700	252.23	0.9779	0.9978	0.9743	0.9324	2.4667	2.5166	2.4574	2.3518	0.2967	0.3027	0.2956	0.2829
76	540	800	251.09	0.9833	1.0062	0.9791	0.9328	2.4691	2.5264	2.4585	2.3422	0.2970	0.3039	0.2957	0.2817
77	540	1000	249.18	0.9909	1.0199	0.9855	0.9308	2.4691	2.5413	2.4556	2.3194	0.2970	0.3057	0.2954	0.2790
78	540	1500	245.67	1.0072	1.0520	0.9986	0.9250	2.4743	2.5844	2.4534	2.2725	0.2976	0.3109	0.2951	0.2733
79	540	2000	243.14	1.0191	1.0805	1.0072	0.9168	2.4779	2.6272	2.4488	2.2291	0.2980	0.3160	0.2945	0.2681
80	540	4000	236.81	1.0516	1.1861	1.0232	0.8805	2.4904	2.8089	2.4231	2.0851	0.2995	0.3378	0.2915	0.2508
81	540	6000	232.88	1.0716	1.2897	1.0224	0.8444	2.4956	3.0034	2.3810	1.9663	0.3002	0.3612	0.2864	0.2365
82	540	10000	227.54	1.0884	1.5016	0.9858	0.7716	2.4765	3.4167	2.2430	1.7557	0.2979	0.4110	0.2698	0.2112
83	560	500	258.14	0.9546	0.9666	0.9503	0.9178	2.4643	2.4952	2.4530	2.3692	0.2964	0.3001	0.2950	0.2850
84	560	600	256.60	0.9612	0.9757	0.9559	0.9186	2.4665	2.5037	2.4529	2.3571	0.2967	0.3011	0.2950	0.2835
85	560	700	255.29	0.9657	0.9828	0.9595	0.9174	2.4653	2.5090	2.4495	2.3421	0.2965	0.3018	0.2946	0.2817

86	560	800	254.16	0.9707	0.9904	0.9636	0.9170	2.4672	2.5173	2.4490	2.3306	0.2968	0.3028	0.2946	0.2803
87	560	1000	252.25	0.9789	1.0038	0.9698	0.9145	2.4692	2.5322	2.4463	2.3069	0.2970	0.3046	0.2942	0.2775
88	560	1500	248.75	0.9949	1.0336	0.9808	0.9058	2.4749	2.5710	2.4398	2.2531	0.2977	0.3092	0.2935	0.2710
89	560	2000	246.23	1.0069	1.0598	0.9875	0.8945	2.4792	2.6096	2.4315	2.2026	0.2982	0.3139	0.2925	0.2649
90	560	4000	239.96	1.0393	1.1551	0.9961	0.8446	2.4939	2.7717	2.3903	2.0266	0.3000	0.3334	0.2875	0.2438
91	560	6000	236.08	1.0583	1.2457	0.9874	0.7917	2.4984	2.9407	2.3310	1.8689	0.3005	0.3537	0.2804	0.2248
92	560	10000	230.85	1.0795	1.4330	0.9426	0.6872	2.4920	3.3081	2.1760	1.5863	0.2997	0.3979	0.2617	0.1908
93	580	600	259.63	0.9506	0.9630	0.9433	0.9066	2.4679	2.5003	2.4490	2.3538	0.2968	0.3007	0.2946	0.2831
94	580	700	258.33	0.9557	0.9704	0.9472	0.9058	2.4689	2.5068	2.4468	2.3399	0.2970	0.3015	0.2943	0.2814
95	580	800	257.19	0.9603	0.9773	0.9505	0.9046	2.4699	2.5134	2.4446	2.3265	0.2971	0.3023	0.2940	0.2798
96	580	1000	255.29	0.9688	0.9902	0.9563	0.9017	2.4732	2.5280	2.4414	2.3020	0.2975	0.3041	0.2936	0.2769
97	580	1500	251.80	0.9840	1.0172	0.9648	0.8902	2.4778	2.5613	2.4294	2.2415	0.2980	0.3081	0.2922	0.2696
98	580	2000	249.29	0.9965	1.0419	0.9702	0.8773	2.4841	2.5974	2.4187	2.1871	0.2988	0.3124	0.2909	0.2631
99	580	4000	243.06	1.0271	1.1265	0.9703	0.8157	2.4964	2.7380	2.3583	1.9827	0.3003	0.3293	0.2837	0.2385
100	580	6000	239.23	1.0479	1.2086	0.9568	0.7530	2.5068	2.8912	2.2890	1.8014	0.3015	0.3477	0.2753	0.2167
101	580	10000	234.09	1.0706	1.3730	0.9017	0.6235	2.5062	3.2140	2.1108	1.4594	0.3014	0.3866	0.2539	0.1755
102	600	600	262.63	0.9423	0.9529	0.9331	0.8978	2.4747	2.5026	2.4506	2.3577	0.2977	0.3010	0.2948	0.2836
103	600	700	261.33	0.9469	0.9594	0.9362	0.8962	2.4746	2.5073	2.4464	2.3421	0.2976	0.3016	0.2943	0.2817
104	600	800	260.20	0.9510	0.9654	0.9386	0.8943	2.4745	2.5120	2.4423	2.3268	0.2976	0.3021	0.2938	0.2799
105	600	1000	258.30	0.9596	0.9778	0.9439	0.8911	2.4785	2.5257	2.4381	2.3016	0.2981	0.3038	0.2933	0.2768
106	600	1500	254.82	0.9746	1.0029	0.9506	0.8781	2.4836	2.5556	2.4223	2.2375	0.2987	0.3074	0.2914	0.2691
107	600	2000	252.32	0.9859	1.0246	0.9532	0.8626	2.4875	2.5853	2.4050	2.1765	0.2992	0.3110	0.2893	0.2618
108	600	4000	246.13	1.0171	1.1019	0.9475	0.7948	2.5034	2.7121	2.3320	1.9561	0.3011	0.3262	0.2805	0.2353
109	600	6000	242.33	1.0369	1.1740	0.9269	0.7228	2.5128	2.8450	2.2461	1.7517	0.3022	0.3422	0.2702	0.2107
110	600	10000	237.27	1.0613	1.3191	0.8618	0.5758	2.5181	3.1298	2.0449	1.3662	0.3029	0.3764	0.2460	0.1643
111	620	1000	261.27	0.9512	0.9666	0.9325	0.8823	2.4852	2.5254	2.4364	2.3053	0.2989	0.3038	0.2930	0.2773
112	620	1500	257.80	0.9657	0.9896	0.9371	0.8681	2.4896	2.5511	2.4158	2.2379	0.2994	0.3068	0.2906	0.2692
113	620	2000	255.31	0.9776	1.0103	0.9388	0.8524	2.4959	2.5794	2.3968	2.1763	0.3002	0.3102	0.2883	0.2618
114	620	4000	249.15	1.0075	1.0792	0.9256	0.7789	2.5103	2.6889	2.3062	1.9405	0.3019	0.3234	0.2774	0.2334
115	620	6000	245.40	1.0278	1.1438	0.8995	0.7019	2.5222	2.8069	2.2074	1.7224	0.3034	0.3376	0.2655	0.2072

116	620	10000	240.40	1.0527	1.2711	0.8237	0.5421	2.5307	3.0557	1.9803	1.3032	0.3044	0.3675	0.2382	0.1567
∑				120.06	130.11	119.28	112.45	289.06	312.42	287.02	270.48	34.77	37.58	34.52	32.53
Average (Overall)				**1.0350**	**1.1217**	**1.0283**	**0.9694**	**2.4919**	**2.6933**	**2.4743**	**2.3318**	**0.2997**	**0.3239**	**0.2976**	**0.2805**

Table C-6 Cyclopropane [34]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	291.67	137.9	73.62	0.6249	1.7480	1.6326	1.4628	0.4601	1.2870	1.2020	1.0770	0.0553	0.1548	0.1446	0.1295
2	291.67	172.4	71.69	0.6804	1.7565	1.6449	1.4192	0.4878	1.2591	1.1791	1.0174	0.0587	0.1514	0.1418	0.1224
3	291.67	206.8	70.10	0.7561	1.7761	1.6693	1.3844	0.5300	1.2451	1.1702	0.9704	0.0637	0.1498	0.1408	0.1167
4	291.67	275.8	67.53	0.8571	1.7454	1.6505	1.2366	0.5788	1.1787	1.1146	0.8350	0.0696	0.1418	0.1341	0.1004
5	291.67	344.7	65.48	0.9572	1.6916	1.6114	1.0551	0.6268	1.1077	1.0552	0.6909	0.0754	0.1332	0.1269	0.0831
6	291.67	413.7	63.74	1.0088	1.5701	1.5072	0.7946	0.6430	1.0008	0.9607	0.5065	0.0773	0.1204	0.1156	0.0609
7	291.67	482.6	62.19	1.0090	1.3789	1.3360	0.4522	0.6275	0.8576	0.8309	0.2812	0.0755	0.1031	0.0999	0.0338
8	291.67	551.6	60.78	0.9727	1.1325	1.1125	0.0415	0.5912	0.6884	0.6762	0.0252	0.0711	0.0828	0.0813	0.0030
9	475.00	137.9	108.68	0.8202	1.7466	1.6619	1.6837	0.8914	1.8983	1.8062	1.8299	0.1072	0.2283	0.2172	0.2201
10	475.00	413.7	99.31	0.8531	1.7967	1.7279	1.7537	0.8472	1.7844	1.7160	1.7416	0.1019	0.2146	0.2064	0.2095
11	475.00	689.5	94.84	0.8621	1.7751	1.7298	1.7431	0.8176	1.6834	1.6405	1.6531	0.0983	0.2025	0.1973	0.1988
12	475.00	965.3	91.81	0.8572	1.7208	1.7036	1.6932	0.7869	1.5798	1.5640	1.5545	0.0947	0.1900	0.1881	0.1870
13	475.00	1378.9	88.51	0.8684	1.6370	1.6692	1.6051	0.7686	1.4489	1.4774	1.4207	0.0925	0.1743	0.1777	0.1709
14	475.00	2068.4	84.60	0.9083	1.4791	1.6134	1.4140	0.7684	1.2514	1.3650	1.1962	0.0924	0.1505	0.1642	0.1439
15	475.00	2757.9	81.66	0.9649	1.2980	1.5622	1.1674	0.7879	1.0599	1.2757	0.9532	0.0948	0.1275	0.1534	0.1147
16	475.00	3447.4	79.23	1.0289	1.0861	1.5145	0.8566	0.8151	0.8605	1.1999	0.6786	0.0980	0.1035	0.1443	0.0816
17	475.00	4136.8	77.09	1.0894	0.8300	1.4664	0.4659	0.8399	0.6399	1.1306	0.3592	0.1010	0.0770	0.1360	0.0432
18	475.00	5515.8	73.32	1.1904	0.1533	1.3950	0.5983	0.8729	0.1124	1.0229	0.4387	0.1050	0.0135	0.1230	0.0528
∑				16.309	26.322	28.209	20.827	12.741	20.943	22.387	17.229	1.533	2.519	2.693	2.072
Average (Overall)				**0.9061**	**1.4623**	**1.5671**	**1.1571**	**0.7078**	**1.1635**	**1.2437**	**0.9572**	**0.0851**	**0.1399**	**0.1496**	**0.1151**

Table C-7 Propane [79]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	260	50	266.25	2.0337	1.9864	1.9898	1.9705	5.4146	5.2889	5.2978	5.2464	0.6513	0.6361	0.6372	0.6310
2	260	100	260.24	2.0810	1.9828	1.9900	1.9429	5.4157	5.1602	5.1787	5.0562	0.6514	0.6207	0.6229	0.6082
3	260	200	253.96	2.1295	1.9214	1.9370	1.8246	5.4080	4.8795	4.9192	4.6338	0.6505	0.5869	0.5917	0.5573
4	280	50	271.37	1.9963	1.9619	1.9649	1.9531	5.4175	5.3240	5.3321	5.3001	0.6516	0.6404	0.6413	0.6375
5	280	100	265.42	2.0428	1.9715	1.9778	1.9465	5.4219	5.2327	5.2494	5.1664	0.6521	0.6294	0.6314	0.6214
6	280	200	259.27	2.0936	1.9441	1.9577	1.8799	5.4281	5.0404	5.0757	4.8739	0.6529	0.6063	0.6105	0.5862
7	280	300	255.48	2.1262	1.8924	1.9145	1.7821	5.4320	4.8349	4.8913	4.5529	0.6534	0.5815	0.5883	0.5476
8	280	400	252.66	2.1524	1.8282	1.8599	1.6651	5.4383	4.6191	4.6993	4.2070	0.6541	0.5556	0.5652	0.5060
9	280	500	250.33	2.1714	1.7492	1.7922	1.5264	5.4356	4.3789	4.4865	3.8211	0.6538	0.5267	0.5396	0.4596
10	300	50	276.39	1.9609	1.9351	1.9378	1.9318	5.4195	5.3483	5.3558	5.3391	0.6519	0.6433	0.6442	0.6422
11	300	100	270.48	2.0057	1.9526	1.9583	1.9389	5.4250	5.2813	5.2966	5.2443	0.6525	0.6352	0.6371	0.6308
12	300	200	264.41	2.0561	1.9454	1.9575	1.9054	5.4367	5.1439	5.1760	5.0383	0.6539	0.6187	0.6226	0.6060
13	300	300	260.73	2.0904	1.9188	1.9381	1.8473	5.4504	5.0028	5.0534	4.8166	0.6556	0.6017	0.6078	0.5793
14	300	400	258.01	2.1163	1.8803	1.9078	1.7728	5.4604	4.8513	4.9223	4.5741	0.6568	0.5835	0.5920	0.5502
15	300	500	255.81	2.1383	1.8342	1.8708	1.6863	5.4700	4.6920	4.7857	4.3137	0.6579	0.5643	0.5756	0.5188
16	300	600	253.93	2.1581	1.7818	1.8288	1.5888	5.4801	4.5246	4.6439	4.0344	0.6591	0.5442	0.5586	0.4852
17	300	700	252.27	2.1756	1.7225	1.7812	1.4792	5.4882	4.3452	4.4934	3.7315	0.6601	0.5226	0.5405	0.4488
18	300	800	250.74	2.1912	1.6559	1.7282	1.3567	5.4942	4.1520	4.3334	3.4018	0.6608	0.4994	0.5212	0.4092
19	320	50	281.33	1.9281	1.9084	1.9108	1.9092	5.4241	5.3687	5.3757	5.3711	0.6524	0.6457	0.6466	0.6460
20	320	100	275.44	1.9705	1.9300	1.9351	1.9250	5.4277	5.3160	5.3302	5.3023	0.6528	0.6394	0.6411	0.6378
21	320	200	269.45	2.0210	1.9369	1.9479	1.9154	5.4454	5.2189	5.2485	5.1610	0.6550	0.6277	0.6313	0.6208
22	320	300	265.83	2.0525	1.9228	1.9402	1.8807	5.4561	5.1114	5.1576	4.9993	0.6563	0.6148	0.6203	0.6013
23	320	400	263.18	2.0787	1.9014	1.9258	1.8352	5.4707	5.0041	5.0683	4.8300	0.6580	0.6019	0.6096	0.5809
24	320	500	261.06	2.1019	1.8749	1.9070	1.7817	5.4872	4.8946	4.9785	4.6513	0.6600	0.5887	0.5988	0.5595
25	320	600	259.27	2.1200	1.8411	1.8818	1.7178	5.4965	4.7735	4.8789	4.4537	0.6611	0.5741	0.5868	0.5357

26	320	700	257.70	2.1389	1.8059	1.8559	1.6492	5.5121	4.6537	4.7828	4.2500	0.6630	0.5597	0.5753	0.5112
27	320	800	256.29	2.1550	1.7651	1.8257	1.5718	5.5230	4.5239	4.6792	4.0283	0.6643	0.5441	0.5628	0.4845
28	340	50	286.20	1.8976	1.8822	1.8845	1.8864	5.4310	5.3869	5.3935	5.3988	0.6532	0.6479	0.6487	0.6494
29	340	100	280.34	1.9403	1.9087	1.9135	1.9105	5.4395	5.3510	5.3644	5.3560	0.6543	0.6436	0.6452	0.6442
30	340	200	274.38	1.9871	1.9218	1.9319	1.9145	5.4522	5.2732	5.3008	5.2532	0.6558	0.6343	0.6376	0.6318
31	340	300	270.81	2.0176	1.9173	1.9331	1.8975	5.4638	5.1923	5.2351	5.1387	0.6572	0.6245	0.6297	0.6181
32	340	400	268.22	2.0433	1.9068	1.9288	1.8719	5.4806	5.1143	5.1734	5.0207	0.6592	0.6151	0.6222	0.6039
33	340	500	266.15	2.0633	1.8891	1.9179	1.8369	5.4914	5.0280	5.1045	4.8889	0.6605	0.6048	0.6140	0.5880
34	340	600	264.42	2.0816	1.8687	1.9047	1.7969	5.5042	4.9411	5.0364	4.7512	0.6620	0.5943	0.6058	0.5715
35	340	700	262.92	2.0991	1.8459	1.8899	1.7525	5.5188	4.8532	4.9688	4.6075	0.6638	0.5837	0.5976	0.5542
36	340	800	261.57	2.1150	1.8203	1.8728	1.7030	5.5323	4.7613	4.8989	4.4545	0.6654	0.5727	0.5892	0.5358
37	340	1000	259.23	2.1439	1.7614	1.8337	1.5896	5.5577	4.5660	4.7535	4.1207	0.6685	0.5492	0.5718	0.4956
38	340	2000	250.27	2.2660	1.2998	1.5847	0.6601	5.6710	3.2529	3.9659	1.6520	0.6821	0.3913	0.4770	0.1987
39	360	200	279.25	1.9561	1.9045	1.9138	1.9083	5.4625	5.3184	5.3444	5.3289	0.6570	0.6397	0.6428	0.6410
40	360	300	275.72	1.9852	1.9061	1.9206	1.9036	5.4735	5.2554	5.2955	5.2485	0.6583	0.6321	0.6369	0.6313
41	360	400	273.16	2.0090	1.9016	1.9217	1.8906	5.4878	5.1943	5.2493	5.1645	0.6601	0.6248	0.6314	0.6212
42	360	500	271.13	2.0280	1.8913	1.9175	1.8703	5.4985	5.1280	5.1989	5.0709	0.6614	0.6168	0.6253	0.6099
43	360	600	269.44	2.0462	1.8796	1.9121	1.8468	5.5133	5.0644	5.1521	4.9759	0.6631	0.6091	0.6197	0.5985
44	360	700	267.98	2.0610	1.8636	1.9030	1.8175	5.5231	4.9939	5.0996	4.8703	0.6643	0.6007	0.6134	0.5858
45	360	800	266.69	2.0765	1.8474	1.8942	1.7865	5.5378	4.9267	5.0515	4.7643	0.6661	0.5926	0.6076	0.5730
46	360	1000	264.45	2.1027	1.8075	1.8707	1.7125	5.5605	4.7799	4.9469	4.5286	0.6688	0.5749	0.5950	0.5447
47	360	2000	256.38	2.2162	1.5199	1.7232	1.1456	5.6819	3.8968	4.4178	2.9371	0.6834	0.4687	0.5314	0.3533
48	380	200	284.06	1.9285	1.8870	1.8957	1.8994	5.4782	5.3603	5.3850	5.3954	0.6589	0.6447	0.6477	0.6490
49	380	300	280.55	1.9561	1.8926	1.9061	1.9035	5.4879	5.3097	5.3476	5.3403	0.6601	0.6386	0.6432	0.6423
50	380	400	278.02	1.9766	1.8905	1.9091	1.8981	5.4953	5.2559	5.3077	5.2772	0.6610	0.6322	0.6384	0.6347
51	380	500	276.02	1.9950	1.8858	1.9098	1.8887	5.5067	5.2051	5.2715	5.2133	0.6623	0.6261	0.6341	0.6270
52	380	600	274.36	2.0107	1.8777	1.9075	1.8747	5.5166	5.1516	5.2334	5.1434	0.6635	0.6196	0.6295	0.6186
53	380	700	272.93	2.0257	1.8684	1.9043	1.8583	5.5286	5.0993	5.1974	5.0718	0.6650	0.6133	0.6251	0.6100
54	380	800	271.67	2.0392	1.8570	1.8994	1.8387	5.5397	5.0450	5.1600	4.9953	0.6663	0.6068	0.6206	0.6008
55	380	1000	269.50	2.0626	1.8291	1.8855	1.7912	5.5587	4.9294	5.0815	4.8272	0.6686	0.5929	0.6112	0.5806

56	380	2000	261.95	2.1648	1.6331	1.7955	1.4296	5.6707	4.2779	4.7034	3.7450	0.6821	0.5145	0.5657	0.4504
57	380	4000	250.27	2.4278	0.8311	5.0151	0.3452	6.0759	2.0799	12.5513	0.8640	0.7308	0.2502	1.5097	0.1039
58	400	300	285.33	1.9280	1.8762	1.8889	1.8976	5.5011	5.3533	5.3895	5.4143	0.6617	0.6439	0.6482	0.6512
59	400	400	282.82	1.9475	1.8774	1.8948	1.8995	5.5080	5.3096	5.3589	5.3722	0.6625	0.6386	0.6446	0.6462
60	400	500	280.84	1.9648	1.8760	1.8984	1.8976	5.5181	5.2685	5.3314	5.3291	0.6637	0.6337	0.6413	0.6410
61	400	600	279.20	1.9791	1.8711	1.8987	1.8912	5.5257	5.2241	5.3013	5.2802	0.6646	0.6284	0.6376	0.6351
62	400	700	277.79	1.9924	1.8648	1.8980	1.8825	5.5347	5.1804	5.2725	5.2293	0.6657	0.6231	0.6342	0.6290
63	400	800	276.55	2.0039	1.8564	1.8953	1.8707	5.5418	5.1340	5.2416	5.1736	0.6666	0.6175	0.6305	0.6223
64	400	1000	274.44	2.0270	1.8385	1.8899	1.8438	5.5629	5.0456	5.1866	5.0603	0.6691	0.6069	0.6238	0.6086
65	400	2000	267.24	2.1154	1.6953	1.8328	1.6104	5.6531	4.5306	4.8979	4.3037	0.6799	0.5449	0.5891	0.5176
66	400	4000	257.54	2.3077	1.2035	1.8695	0.6406	5.9431	3.0993	4.8146	1.6497	0.7148	0.3728	0.5791	0.1984
67	420	300	290.05	1.8998	1.8570	1.8690	1.8865	5.5103	5.3861	5.4209	5.4717	0.6628	0.6478	0.6520	0.6581
68	420	400	287.56	1.9201	1.8621	1.8786	1.8955	5.5213	5.3547	5.4019	5.4505	0.6641	0.6441	0.6497	0.6556
69	420	500	285.59	1.9350	1.8616	1.8827	1.8977	5.5261	5.3167	5.3768	5.4196	0.6647	0.6395	0.6467	0.6519
70	420	600	283.97	1.9482	1.8592	1.8850	1.8971	5.5324	5.2795	5.3530	5.3872	0.6654	0.6350	0.6439	0.6480
71	420	700	282.58	1.9603	1.8553	1.8862	1.8942	5.5394	5.2426	5.3300	5.3528	0.6663	0.6306	0.6411	0.6438
72	420	800	281.37	1.9719	1.8506	1.8868	1.8900	5.5483	5.2070	5.3088	5.3179	0.6673	0.6263	0.6385	0.6396
73	420	1000	279.29	1.9916	1.8369	1.8843	1.8753	5.5623	5.1303	5.2627	5.2375	0.6690	0.6171	0.6330	0.6300
74	420	2000	272.33	2.0705	1.7306	1.8512	1.7314	5.6386	4.7130	5.0413	4.7150	0.6782	0.5669	0.6064	0.5671
75	420	4000	263.60	2.2245	1.3834	1.8254	1.1398	5.8636	3.6467	4.8119	3.0045	0.7053	0.4386	0.5788	0.3614
76	440	300	294.72	1.8743	1.8384	1.8498	1.8742	5.5239	5.4183	5.4519	5.5237	0.6644	0.6517	0.6557	0.6644
77	440	400	292.24	1.8920	1.8436	1.8591	1.8855	5.5292	5.3876	5.4331	5.5102	0.6650	0.6480	0.6535	0.6628
78	440	500	290.30	1.9073	1.8460	1.8659	1.8932	5.5367	5.3588	5.4166	5.4958	0.6660	0.6446	0.6515	0.6610
79	440	600	288.69	1.9194	1.8450	1.8694	1.8967	5.5410	5.3263	5.3968	5.4754	0.6665	0.6406	0.6491	0.6586
80	440	700	287.31	1.9302	1.8426	1.8717	1.8980	5.5456	5.2938	5.3775	5.4532	0.6670	0.6367	0.6468	0.6559
81	440	800	286.11	1.9404	1.8393	1.8733	1.8980	5.5517	5.2624	5.3595	5.4303	0.6678	0.6330	0.6446	0.6532
82	440	1000	284.06	1.9585	1.8298	1.8740	1.8934	5.5633	5.1976	5.3231	5.3784	0.6692	0.6252	0.6403	0.6469
83	440	2000	277.28	2.0283	1.7481	1.8564	1.8121	5.6240	4.8472	5.1475	5.0246	0.6764	0.5830	0.6191	0.6044
84	440	4000	269.14	2.1531	1.4841	1.8274	1.4416	5.7949	3.9943	4.9184	3.8800	0.6970	0.4804	0.5916	0.4667
85	440	10000	251.97	2.6464	0.1873	1.4350	0.9509	6.6684	0.4719	3.6158	2.3961	0.8021	0.0568	0.4349	0.2882

86	460	500	294.94	1.8800	1.8282	1.8472	1.8838	5.5449	5.3921	5.4481	5.5563	0.6669	0.6486	0.6553	0.6683
87	460	600	293.34	1.8905	1.8277	1.8509	1.8898	5.5455	5.3613	5.4294	5.5435	0.6670	0.6449	0.6530	0.6668
88	460	700	291.98	1.9011	1.8271	1.8547	1.8951	5.5507	5.3348	5.4154	5.5333	0.6676	0.6417	0.6514	0.6655
89	460	800	290.79	1.9111	1.8258	1.8579	1.8992	5.5572	5.3091	5.4026	5.5226	0.6684	0.6386	0.6498	0.6642
90	460	1000	288.76	1.9269	1.8184	1.8600	1.9013	5.5642	5.2510	5.3711	5.4904	0.6693	0.6316	0.6460	0.6604
91	460	2000	282.13	1.9896	1.7553	1.8544	1.8664	5.6133	4.9522	5.2317	5.2656	0.6752	0.5956	0.6293	0.6333
92	460	4000	274.39	2.0934	1.5467	1.8332	1.6410	5.7442	4.2441	5.0302	4.5028	0.6909	0.5105	0.6050	0.5416
93	460	10000	259.44	2.4930	0.3486	1.7990	0.1464	6.4677	0.9044	4.6674	0.3799	0.7779	0.1088	0.5614	0.0457
∑				190.53	165.88	177.78	161.72	516.32	451.69	482.42	441.33	62.10	54.33	58.02	53.08
Average (Overall)				**2.0487**	**1.7837**	**1.9116**	**1.7389**	**5.5518**	**4.8568**	**5.1873**	**4.7455**	**0.6678**	**0.5842**	**0.6239**	**0.5708**

Table C-8 Acetylene [15]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	210	202.7	193.58	1.0500	1.0244	1.0288	0.9510	2.0325	1.9830	1.9916	1.8409	0.2445	0.2385	0.2395	0.2214
2	220	202.7	195.44	1.0258	1.0420	1.0454	0.9903	2.0048	2.0365	2.0431	1.9355	0.2411	0.2449	0.2457	0.2328
3	230	202.7	197.25	1.0102	1.0584	1.0609	1.0249	1.9926	2.0876	2.0925	2.0216	0.2397	0.2511	0.2517	0.2432
4	240	202.7	199.00	0.9983	1.0712	1.0729	1.0530	1.9867	2.1316	2.1352	2.0955	0.2390	0.2564	0.2568	0.2520
5	250	202.7	200.70	0.9865	1.0786	1.0798	1.0734	1.9799	2.1647	2.1671	2.1544	0.2381	0.2604	0.2607	0.2591
6	260	202.7	202.35	0.9738	1.0811	1.0818	1.0870	1.9706	2.1877	2.1890	2.1996	0.2370	0.2631	0.2633	0.2646
7	270	202.7	203.96	0.9622	1.0815	1.0818	1.0968	1.9624	2.2059	2.2064	2.2371	0.2360	0.2653	0.2654	0.2691
8	280	202.7	205.53	0.9516	1.0806	1.0805	1.1040	1.9559	2.2210	2.2207	2.2690	0.2353	0.2671	0.2671	0.2729
9	290	202.7	207.07	0.9427	1.0794	1.0789	1.1096	1.9519	2.2350	2.2341	2.2975	0.2348	0.2688	0.2687	0.2763
10	300	202.7	208.57	0.9359	1.0788	1.0781	1.1148	1.9520	2.2501	2.2486	2.3252	0.2348	0.2706	0.2705	0.2797
11	310	202.7	210.05	0.9301	1.0781	1.0771	1.1190	1.9537	2.2645	2.2625	2.3505	0.2350	0.2724	0.2721	0.2827
12	320	202.7	211.50	0.9244	1.0764	1.0753	1.1215	1.9551	2.2767	2.2742	2.3720	0.2352	0.2738	0.2735	0.2853
13	210	304.0	189.80	1.0876	0.9301	0.9432	0.7998	2.0643	1.7652	1.7902	1.5180	0.2483	0.2123	0.2153	0.1826

14	220	304.0	191.73	1.0599	0.9711	0.9824	0.8757	2.0321	1.8618	1.8835	1.6790	0.2444	0.2239	0.2265	0.2019
15	230	304.0	193.58	1.0384	1.0017	1.0115	0.9353	2.0102	1.9392	1.9580	1.8106	0.2418	0.2332	0.2355	0.2178
16	240	304.0	195.37	1.0203	1.0238	1.0322	0.9816	1.9934	2.0001	2.0166	1.9177	0.2398	0.2406	0.2426	0.2307
17	250	304.0	197.10	1.0046	1.0393	1.0467	1.0175	1.9800	2.0484	2.0629	2.0055	0.2381	0.2464	0.2481	0.2412
18	260	304.0	198.78	0.9913	1.0507	1.0572	1.0463	1.9705	2.0886	2.1014	2.0797	0.2370	0.2512	0.2528	0.2501
19	270	304.0	200.41	0.9795	1.0586	1.0643	1.0689	1.9631	2.1216	2.1329	2.1421	0.2361	0.2552	0.2565	0.2576
20	280	304.0	202.00	0.9688	1.0637	1.0687	1.0865	1.9571	2.1487	2.1588	2.1946	0.2354	0.2584	0.2597	0.2640
21	290	304.0	203.55	0.9592	1.0668	1.0712	1.1003	1.9525	2.1716	2.1806	2.2396	0.2349	0.2612	0.2623	0.2694
22	300	304.0	205.07	0.9511	1.0690	1.0730	1.1116	1.9504	2.1923	2.2004	2.2796	0.2346	0.2637	0.2647	0.2742
23	310	304.0	206.56	0.9450	1.0715	1.0749	1.1217	1.9521	2.2132	2.2204	2.3171	0.2348	0.2662	0.2671	0.2787
24	320	304.0	208.03	0.9399	1.0732	1.0763	1.1300	1.9552	2.2326	2.2390	2.3508	0.2352	0.2685	0.2693	0.2827
25	230	506.6	188.69	1.0794	0.8539	0.8808	0.7034	2.0367	1.6112	1.6619	1.3273	0.2450	0.1938	0.1999	0.1596
26	240	506.6	190.57	1.0553	0.9059	0.9298	0.8004	2.0111	1.7264	1.7720	1.5254	0.2419	0.2077	0.2131	0.1835
27	250	506.6	192.38	1.0361	0.9453	0.9669	0.8773	1.9932	1.8186	1.8600	1.6876	0.2397	0.2187	0.2237	0.2030
28	260	506.6	194.12	1.0211	0.9762	0.9957	0.9395	1.9822	1.8950	1.9329	1.8238	0.2384	0.2279	0.2325	0.2194
29	270	506.6	195.80	1.0073	0.9988	1.0166	0.9886	1.9723	1.9556	1.9905	1.9357	0.2372	0.2352	0.2394	0.2328
30	280	506.6	197.43	0.9929	1.0135	1.0299	1.0258	1.9603	2.0009	2.0333	2.0251	0.2358	0.2407	0.2446	0.2436
31	290	506.6	199.02	0.9812	1.0253	1.0405	1.0567	1.9527	2.0406	2.0708	2.1029	0.2349	0.2454	0.2491	0.2529
32	300	506.6	200.56	0.9717	1.0351	1.0492	1.0827	1.9489	2.0760	2.1044	2.1714	0.2344	0.2497	0.2531	0.2612
33	310	506.6	202.08	0.9646	1.0438	1.0570	1.1051	1.9493	2.1092	2.1359	2.2332	0.2345	0.2537	0.2569	0.2686
34	320	506.6	203.56	0.9583	1.0504	1.0628	1.1235	1.9507	2.1383	2.1635	2.2870	0.2346	0.2572	0.2602	0.2751
35	240	709.3	187.18	1.0833	0.7627	0.8056	0.5755	2.0277	1.4276	1.5078	1.0772	0.2439	0.1717	0.1814	0.1296
36	250	709.3	189.07	1.0601	0.8307	0.8692	0.7015	2.0043	1.5707	1.6433	1.3263	0.2411	0.1889	0.1977	0.1595
37	260	709.3	190.88	1.0410	0.8820	0.9168	0.8007	1.9870	1.6835	1.7500	1.5284	0.2390	0.2025	0.2105	0.1838
38	270	709.3	192.61	1.0242	0.9205	0.9524	0.8793	1.9728	1.7731	1.8345	1.6937	0.2373	0.2133	0.2206	0.2037
39	280	709.3	194.29	1.0082	0.9485	0.9779	0.9411	1.9589	1.8429	1.9000	1.8284	0.2356	0.2217	0.2285	0.2199
40	290	709.3	195.91	0.9950	0.9707	0.9980	0.9917	1.9493	1.9018	1.9553	1.9430	0.2345	0.2287	0.2352	0.2337
41	300	709.3	197.50	0.9853	0.9898	1.0153	1.0350	1.9459	1.9549	2.0053	2.0441	0.2340	0.2351	0.2412	0.2459
42	310	709.3	199.04	0.9784	1.0067	1.0306	1.0723	1.9475	2.0037	2.0514	2.1344	0.2342	0.2410	0.2467	0.2567
43	320	709.3	200.55	0.9723	1.0201	1.0428	1.1031	1.9500	2.0459	2.0912	2.2123	0.2345	0.2461	0.2515	0.2661

44	250	1013	185.27	1.0974	0.6332	0.7037	0.3841	2.0331	1.1732	1.3038	0.7116	0.2445	0.1411	0.1568	0.0856
45	260	1013	187.20	1.0708	0.7222	0.7851	0.5520	2.0046	1.3519	1.4698	1.0333	0.2411	0.1626	0.1768	0.1243
46	270	1013	189.04	1.0495	0.7896	0.8466	0.6841	1.9840	1.4926	1.6004	1.2933	0.2386	0.1795	0.1925	0.1556
47	280	1013	190.79	1.0314	0.8411	0.8933	0.7893	1.9678	1.6047	1.7043	1.5060	0.2367	0.1930	0.2050	0.1811
48	290	1013	192.48	1.0155	0.8807	0.9289	0.8738	1.9547	1.6952	1.7880	1.6819	0.2351	0.2039	0.2151	0.2023
49	300	1013	194.11	1.0029	0.9129	0.9578	0.9437	1.9468	1.7721	1.8592	1.8319	0.2342	0.2131	0.2236	0.2203
50	310	1013	195.70	0.9936	0.9402	0.9823	1.0029	1.9446	1.8401	1.9224	1.9626	0.2339	0.2213	0.2312	0.2361
51	320	1013	197.24	0.9867	0.9635	1.0031	1.0529	1.9461	1.9004	1.9786	2.0768	0.2341	0.2286	0.2380	0.2498
52	260	1520	182.48	1.1209	0.3944	0.5254	0.0095	2.0455	0.7197	0.9588	0.0173	0.2460	0.0866	0.1153	0.0021
53	270	1520	184.53	1.0877	0.5265	0.6410	0.2643	2.0071	0.9716	1.1828	0.4876	0.2414	0.1169	0.1423	0.0587
54	280	1520	186.45	1.0625	0.6257	0.7278	0.4617	1.9809	1.1666	1.3570	0.8607	0.2383	0.1403	0.1632	0.1035
55	290	1520	188.26	1.0426	0.7023	0.7948	0.6182	1.9628	1.3222	1.4963	1.1638	0.2361	0.1590	0.1800	0.1400
56	300	1520	190.01	1.0295	0.7656	0.8504	0.7473	1.9561	1.4548	1.6159	1.4200	0.2353	0.1750	0.1944	0.1708
57	310	1520	191.68	1.0194	0.8172	0.8957	0.8535	1.9540	1.5664	1.7169	1.6361	0.2350	0.1884	0.2065	0.1968
58	320	1520	193.30	1.0109	0.8590	0.9323	0.9410	1.9541	1.6603	1.8020	1.8189	0.2350	0.1997	0.2167	0.2188
59	270	2027	180.80	1.1374	0.2038	0.4102	0.2943	2.0563	0.3685	0.7416	0.5320	0.2473	0.0443	0.0892	0.0640
60	280	2027	182.95	1.1022	0.3741	0.5496	0.0418	2.0166	0.6845	1.0055	0.0765	0.2426	0.0823	0.1209	0.0092
61	290	2027	184.94	1.0756	0.4993	0.6529	0.2965	1.9892	0.9233	1.2075	0.5483	0.2393	0.1111	0.1452	0.0659
62	300	2027	186.81	1.0553	0.5956	0.7331	0.4964	1.9714	1.1126	1.3695	0.9273	0.2371	0.1338	0.1647	0.1115
63	310	2027	188.59	1.0408	0.6732	0.7981	0.6582	1.9628	1.2695	1.5051	1.2412	0.2361	0.1527	0.1810	0.1493
64	320	2027	190.29	1.0304	0.7368	0.8518	0.7909	1.9607	1.4020	1.6208	1.5051	0.2358	0.1686	0.1949	0.1810
65	280	2533	179.79	1.1474	0.0615	0.3564	0.5157	2.0628	0.1107	0.6408	0.9272	0.2481	0.0133	0.0771	0.1115
66	290	2533	182.03	1.1115	0.2589	0.5026	0.1139	2.0233	0.4713	0.9148	0.2073	0.2434	0.0567	0.1100	0.0249
67	300	2533	184.07	1.0838	0.4014	0.6112	0.1849	1.9949	0.7389	1.1251	0.3404	0.2399	0.0889	0.1353	0.0409
68	310	2533	185.97	1.0633	0.5112	0.6968	0.4179	1.9774	0.9506	1.2958	0.7771	0.2378	0.1143	0.1559	0.0935
69	320	2533	187.77	1.0502	0.6008	0.7682	0.6064	1.9719	1.1280	1.4424	1.1387	0.2372	0.1357	0.1735	0.1370
70	280	3040	176.62	1.2155	0.3472	0.1896	1.2920	2.1469	0.6132	0.3349	2.2819	0.2582	0.0738	0.0403	0.2745
71	290	3040	179.27	1.1574	0.0303	0.3606	0.6442	2.0749	0.0543	0.6465	1.1549	0.2496	0.0065	0.0778	0.1389
72	300	3040	181.55	1.1172	0.1771	0.4923	0.2023	2.0283	0.3215	0.8937	0.3673	0.2440	0.0387	0.1075	0.0442
73	310	3040	183.63	1.0946	0.3349	0.6025	0.1319	2.0100	0.6149	1.1064	0.2423	0.2418	0.0740	0.1331	0.0291

74	320	3040	185.55	1.0742	0.4525	0.6873	0.3871	1.9931	0.8397	1.2753	0.7183	0.2397	0.1010	0.1534	0.0864
75	290	3546	176.44	1.2240	0.3990	0.2949	1.3658	2.1596	0.7039	0.5203	2.4098	0.2598	0.0847	0.0626	0.2898
76	300	3546	179.12	1.1642	0.0833	0.4018	0.6877	2.0852	0.1492	0.7197	1.2317	0.2508	0.0180	0.0866	0.1482
77	310	3546	181.43	1.1308	0.1336	0.5184	0.2176	2.0516	0.2424	0.9406	0.3948	0.2468	0.0292	0.1131	0.0475
78	320	3546	183.50	1.1056	0.2919	0.6159	0.1294	2.0289	0.5356	1.1303	0.2375	0.2440	0.0644	0.1359	0.0286
79	300	4053	176.64	1.2398	0.3931	0.4302	1.3152	2.1899	0.6944	0.7598	2.3231	0.2634	0.0835	0.0914	0.2794
80	310	4053	179.27	1.1744	0.1008	0.4666	0.6508	2.1053	0.1807	0.8364	1.1667	0.2532	0.0217	0.1006	0.1403
81	320	4053	181.56	1.1430	0.1123	0.5601	0.1783	2.0753	0.2039	1.0169	0.3237	0.2496	0.0245	0.1223	0.0389
82	300	5066	170.28	1.8181	1.3835	7.1429	3.6850	3.0959	2.3558	12.1630	6.2748	0.3724	0.2834	1.4630	0.7547
83	310	5066	174.75	1.3656	0.6789	6.9592	1.8781	2.3865	1.1864	12.1615	3.2821	0.2870	0.1427	1.4628	0.3948
84	320	5066	177.74	1.2642	0.3095	0.6244	0.9844	2.2469	0.5501	1.1099	1.7497	0.2703	0.0662	0.1335	0.2105
85	310	6080	168.38	2.2697	1.5951	4.6707	4.5207	3.8218	2.6858	7.8646	7.6119	0.4597	0.3230	0.9459	0.9156
86	320	6080	173.64	1.5410	0.8487	4.2812	2.1976	2.6758	1.4736	7.4337	3.8158	0.3218	0.1772	0.8941	0.4590
∑				92.472	67.393	92.679	77.987	175.786	130.661	175.012	148.849	21.143	15.716	21.050	17.903
Average (Overall)				**1.0753**	**0.7836**	**1.0777**	**0.9068**	**2.0440**	**1.5193**	**2.0350**	**1.7308**	**0.2459**	**0.1827**	**0.2448**	**0.2082**

Table C-9 Neopentane [14]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	344.44	34.5	81.71	0.8433	2.7595	2.5299	2.5731	0.6890	2.2548	2.0671	2.1024	0.0829	0.2712	0.2486	0.2529
2	344.44	68.9	75.79	0.9097	2.8694	2.6314	2.6601	0.6894	2.1746	1.9943	2.0160	0.0829	0.2616	0.2399	0.2425
3	344.44	103.4	72.28	0.9927	2.9339	2.6950	2.6936	0.7176	2.1208	1.9481	1.9471	0.0863	0.2551	0.2343	0.2342
4	344.44	137.9	69.75	1.0556	2.9476	2.7115	2.6690	0.7362	2.0558	1.8912	1.8615	0.0886	0.2473	0.2275	0.2239
5	344.44	172.4	67.72	1.0856	2.9082	2.6774	2.5845	0.7352	1.9695	1.8132	1.7503	0.0884	0.2369	0.2181	0.2105
6	344.44	206.8	66.06	1.1517	2.8882	2.6650	2.5132	0.7608	1.9080	1.7605	1.6603	0.0915	0.2295	0.2118	0.1997
7	344.44	241.3	64.61	1.1877	2.8255	2.6115	2.3927	0.7674	1.8256	1.6874	1.5460	0.0923	0.2196	0.2030	0.1859
8	344.44	275.8	63.34	1.2437	2.7705	2.5677	2.2738	0.7878	1.7549	1.6264	1.4403	0.0948	0.2111	0.1956	0.1732

9	344.44	344.7	61.17	1.3712	2.6438	2.4683	2.0001	0.8387	1.6172	1.5098	1.2234	0.1009	0.1945	0.1816	0.1472
10	344.44	413.7	59.30	1.4697	2.4476	2.3064	1.6297	0.8715	1.4513	1.3676	0.9663	0.1048	0.1746	0.1645	0.1162
11	344.44	482.6	57.66	1.6191	2.2600	2.1612	1.2388	0.9336	1.3032	1.2463	0.7143	0.1123	0.1568	0.1499	0.0859
12	344.44	551.6	56.18	1.7814	2.0407	1.9937	0.7834	1.0009	1.1466	1.1201	0.4401	0.1204	0.1379	0.1347	0.0529
13	500	68.9	136.65	1.1685	2.3432	2.2082	2.2926	1.5968	3.2020	3.0176	3.1330	0.1921	0.3851	0.3630	0.3768
14	500	137.9	130.79	1.2217	2.4185	2.2856	2.4118	1.5979	3.1633	2.9894	3.1544	0.1922	0.3805	0.3596	0.3794
15	500	275.8	124.84	1.2894	2.4782	2.3567	2.5422	1.6097	3.0939	2.9422	3.1737	0.1936	0.3721	0.3539	0.3817
16	500	413.7	121.31	1.3601	2.5153	2.4097	2.6373	1.6500	3.0513	2.9231	3.1992	0.1985	0.3670	0.3516	0.3848
17	500	551.6	118.74	1.4162	2.5250	2.4382	2.6963	1.6816	2.9983	2.8951	3.2016	0.2023	0.3606	0.3482	0.3851
18	500	689.5	116.66	1.4265	2.4809	2.4155	2.6949	1.6641	2.8942	2.8178	3.1438	0.2002	0.3481	0.3389	0.3781
19	500	1034.2	112.67	1.4165	2.3081	2.3071	2.6049	1.5960	2.6005	2.5994	2.9349	0.1920	0.3128	0.3127	0.3530
20	500	1378.9	109.62	1.3824	2.0798	2.1604	2.4296	1.5153	2.2798	2.3681	2.6633	0.1823	0.2742	0.2848	0.3203
21	500	1723.7	107.02	1.2942	1.7687	1.9516	2.1437	1.3851	1.8929	2.0886	2.2942	0.1666	0.2277	0.2512	0.2759
22	500	2068.4	104.73	1.1991	1.4203	1.7317	1.7924	1.2558	1.4874	1.8135	1.8771	0.1510	0.1789	0.2181	0.2258
23	500	2413.2	102.52	1.0009	0.9351	1.4096	1.2753	1.0261	0.9587	1.4452	1.3074	0.1234	0.1153	0.1738	0.1573
24	500	2757.9	100.22	0.5822	0.1896	0.8743	0.4670	0.5835	0.1900	0.8763	0.4681	0.0702	0.0229	0.1054	0.0563
25	500	3102.6	98.56	0.7103	0.0525	0.9000	0.1270	0.7001	0.0517	0.8871	0.1252	0.0842	0.0062	0.1067	0.0151
∑				30.179	55.810	55.468	52.127	27.390	49.446	49.695	48.344	3.294	5.947	5.977	5.815
Average (Overall)				**1.2072**	**2.2324**	**2.2187**	**2.0851**	**1.0956**	**1.9778**	**1.9878**	**1.9338**	**0.1318**	**0.2379**	**0.2391**	**0.2326**

Table C-10 Benzene [72]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	500	100	325.56	0.0565	0.0422	0.0455	0.0765	0.1838	0.1375	0.1481	0.2491	0.0221	0.0165	0.0178	0.0300
2	500	200	319.65	0.0796	0.0332	0.0405	0.0751	0.2545	0.1062	0.1295	0.2401	0.0306	0.0128	0.0156	0.0289
3	500	400	313.58	0.1245	0.0098	0.0262	0.0526	0.3904	0.0308	0.0821	0.1649	0.0470	0.0037	0.0099	0.0198
4	500	600	309.89	0.1721	0.0157	0.0112	0.0164	0.5332	0.0486	0.0347	0.0509	0.0641	0.0058	0.0042	0.0061

5	500	800	307.16	0.2256	0.0403	0.0011	0.0279	0.6930	0.1238	0.0035	0.0856	0.0833	0.0149	0.0004	0.0103
6	500	1000	304.95	0.2833	0.0665	0.0128	0.0823	0.8638	0.2029	0.0391	0.2511	0.1039	0.0244	0.0047	0.0302
7	500	2000	297.01	0.7065	0.2010	0.0020	0.5224	2.0984	0.5971	0.0060	1.5515	0.2524	0.0718	0.0007	0.1866
8	525	100	332.47	0.0361	0.0273	0.0303	0.0647	0.1200	0.0906	0.1007	0.2152	0.0144	0.0109	0.0121	0.0259
9	525	200	326.58	0.0535	0.0187	0.0255	0.0678	0.1748	0.0612	0.0833	0.2215	0.0210	0.0074	0.0100	0.0266
10	525	400	320.54	0.0856	0.0040	0.0110	0.0551	0.2742	0.0130	0.0352	0.1765	0.0330	0.0016	0.0042	0.0212
11	525	600	316.89	0.1226	0.0250	0.0006	0.0342	0.3886	0.0794	0.0019	0.1083	0.0467	0.0095	0.0002	0.0130
12	525	800	314.21	0.1626	0.0465	0.0113	0.0055	0.5108	0.1462	0.0356	0.0173	0.0614	0.0176	0.0043	0.0021
13	525	1000	312.05	0.2027	0.0713	0.0238	0.0330	0.6325	0.2226	0.0742	0.1029	0.0761	0.0268	0.0089	0.0124
14	525	2000	304.50	0.4719	0.1990	0.0467	0.3329	1.4371	0.6060	0.1422	1.0138	0.1729	0.0729	0.0171	0.1219
15	525	3000	298.50	1.0202	0.3295	0.3543	0.9503	3.0452	0.9837	1.0576	2.8366	0.3663	0.1183	0.1272	0.3412
16	550	100	339.32	0.0138	0.0091	0.0119	0.0487	0.0469	0.0307	0.0403	0.1654	0.0056	0.0037	0.0049	0.0199
17	550	200	333.44	0.0253	0.0008	0.0056	0.0537	0.0842	0.0025	0.0186	0.1790	0.0101	0.0003	0.0022	0.0215
18	550	400	327.44	0.0516	0.0190	0.0051	0.0525	0.1690	0.0623	0.0166	0.1719	0.0203	0.0075	0.0020	0.0207
19	550	600	323.81	0.0767	0.0410	0.0185	0.0388	0.2482	0.1327	0.0599	0.1257	0.0299	0.0160	0.0072	0.0151
20	550	800	321.17	0.1074	0.0595	0.0274	0.0225	0.3450	0.1910	0.0880	0.0723	0.0415	0.0230	0.0106	0.0087
21	550	1000	319.05	0.1363	0.0823	0.0394	0.0033	0.4347	0.2625	0.1258	0.0104	0.0523	0.0316	0.0151	0.0013
22	550	2000	311.78	0.3197	0.2002	0.0759	0.2081	0.9967	0.6240	0.2367	0.6488	0.1199	0.0751	0.0285	0.0780
23	550	3000	306.44	0.5985	0.3411	0.0101	0.5955	1.8341	1.0452	0.0310	1.8248	0.2206	0.1257	0.0037	0.2195
24	550	4000	300.82	1.2362	0.5107	4.4688	1.4305	3.7187	1.5364	13.4429	4.3031	0.4473	0.1848	1.6169	0.5176
25	575	100	346.09	0.0121	0.0137	0.0110	0.0275	0.0417	0.0473	0.0381	0.0951	0.0050	0.0057	0.0046	0.0114
26	575	200	340.22	0.0050	0.0242	0.0183	0.0340	0.0171	0.0825	0.0623	0.1158	0.0021	0.0099	0.0075	0.0139
27	575	400	334.24	0.0143	0.0418	0.0287	0.0391	0.0479	0.1395	0.0959	0.1306	0.0058	0.0168	0.0115	0.0157
28	575	600	330.66	0.0362	0.0585	0.0376	0.0368	0.1196	0.1935	0.1244	0.1218	0.0144	0.0233	0.0150	0.0146
29	575	800	328.03	0.0554	0.0795	0.0499	0.0251	0.1818	0.2607	0.1637	0.0823	0.0219	0.0314	0.0197	0.0099
30	575	1000	325.95	0.0786	0.0982	0.0591	0.0113	0.2561	0.3201	0.1926	0.0370	0.0308	0.0385	0.0232	0.0044
31	575	2000	318.91	0.2129	0.2013	0.0952	0.1204	0.6790	0.6421	0.3035	0.3839	0.0817	0.0772	0.0365	0.0462
32	575	3000	313.94	0.3819	0.3359	0.0986	0.3804	1.1988	1.0544	0.3095	1.1943	0.1442	0.1268	0.0372	0.1436
33	575	4000	309.42	0.6367	0.5106	0.1157	0.8339	1.9701	1.5798	0.3580	2.5803	0.2370	0.1900	0.0431	0.3104
34	575	4500	306.94	0.8240	0.6394	2.8990	1.2110	2.5292	1.9626	8.8982	3.7172	0.3042	0.2361	1.0703	0.4471

35	600	100	352.79	0.0387	0.0379	0.0354	0.0041	0.1365	0.1337	0.1248	0.0145	0.0164	0.0161	0.0150	0.0017
36	600	200	346.94	0.0303	0.0443	0.0387	0.0166	0.1053	0.1536	0.1341	0.0575	0.0127	0.0185	0.0161	0.0069
37	600	400	340.98	0.0176	0.0623	0.0500	0.0252	0.0600	0.2125	0.1707	0.0860	0.0072	0.0256	0.0205	0.0103
38	600	600	337.41	0.0030	0.0799	0.0603	0.0269	0.0102	0.2695	0.2035	0.0909	0.0012	0.0324	0.0245	0.0109
39	600	800	334.81	0.0129	0.0973	0.0698	0.0241	0.0432	0.3257	0.2336	0.0808	0.0052	0.0392	0.0281	0.0097
40	600	1000	332.75	0.0295	0.1152	0.0791	0.0171	0.0981	0.3835	0.2632	0.0569	0.0118	0.0461	0.0317	0.0068
41	600	2000	325.87	0.1249	0.2119	0.1184	0.0667	0.4072	0.6905	0.3860	0.2174	0.0490	0.0831	0.0464	0.0261
42	600	3000	321.18	0.2425	0.3281	0.1381	0.2354	0.7788	1.0536	0.4435	0.7561	0.0937	0.1267	0.0533	0.0909
43	600	4000	317.17	0.3907	0.4786	0.0984	0.5183	1.2392	1.5178	0.3121	1.6438	0.1491	0.1826	0.0375	0.1977
44	600	4500	314.84	0.3679	0.6908	0.1247	0.8375	1.1584	2.1748	0.3926	2.6367	0.1393	0.2616	0.0472	0.3171
∑				9.8838	6.5431	9.5315	9.3419	30.5561	20.5347	29.2437	28.8856	3.6753	2.4699	3.5174	3.4743
Average (Overall)				**0.2246**	**0.1487**	**0.2166**	**0.2123**	**0.6945**	**0.4667**	**0.6646**	**0.6565**	**0.0835**	**0.0561**	**0.0799**	**0.0790**

Table C-11 Carbon dioxide [15]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	313.15	202.7	209.62	3.7114	2.7192	2.8620	2.7595	7.7796	5.6999	5.9992	5.7843	0.9357	0.6856	0.7216	0.6957
2	313.15	608.0	200.11	3.8898	2.9329	3.0670	2.8974	7.7838	5.8689	6.1373	5.7979	0.9362	0.7059	0.7382	0.6974
3	313.15	1013	195.48	3.9786	3.0866	3.2062	3.0022	7.7775	6.0338	6.2675	5.8687	0.9355	0.7257	0.7539	0.7059
4	313.15	1520	191.61	4.0565	3.2635	3.3596	3.1396	7.7728	6.2533	6.4375	6.0160	0.9349	0.7521	0.7743	0.7236
5	313.15	2027	188.74	4.0925	3.4128	3.4797	3.2686	7.7241	6.4413	6.5675	6.1691	0.9291	0.7748	0.7899	0.7420
6	313.15	2533	186.27	4.1736	3.6199	3.6506	3.4724	7.7742	6.7427	6.8000	6.4680	0.9351	0.8110	0.8179	0.7780
7	313.15	3040	184.19	4.2019	3.7875	3.7735	3.6542	7.7394	6.9761	6.9504	6.7305	0.9309	0.8391	0.8360	0.8095
8	313.15	4053	180.63	4.1865	4.0964	3.9547	4.0481	7.5622	7.3993	7.1433	7.3120	0.9096	0.8900	0.8592	0.8795
9	313.15	5066	177.20	4.2536	4.5679	4.2017	4.6989	7.5375	8.0944	7.4456	8.3266	0.9066	0.9736	0.8956	1.0015
10	313.15	6080	173.52	4.4411	5.2891	4.4192	5.7393	7.7061	9.1776	7.6681	9.9587	0.9269	1.1039	0.9223	1.1978
11	323.15	202.7	210.85	3.6765	2.6861	2.8282	2.7239	7.7519	5.6636	5.9632	5.7433	0.9324	0.6812	0.7172	0.6908

12	323.15	608.0	201.38	3.8508	2.8866	3.0205	2.8417	7.7547	5.8130	6.0826	5.7227	0.9327	0.6992	0.7316	0.6883
13	323.15	1013	196.79	3.9381	3.0286	3.1487	2.9264	7.7498	5.9599	6.1964	5.7589	0.9321	0.7169	0.7453	0.6927
14	323.15	1520	192.96	4.0223	3.1971	3.2954	3.0432	7.7613	6.1691	6.3587	5.8721	0.9335	0.7420	0.7648	0.7063
15	323.15	2027	190.10	4.0788	3.3503	3.4217	3.1612	7.7538	6.3690	6.5047	6.0095	0.9326	0.7661	0.7824	0.7228
16	323.15	2533	187.73	4.1441	3.5228	3.5618	3.3128	7.7796	6.6133	6.6864	6.2190	0.9357	0.7954	0.8042	0.7480
17	323.15	3040	185.79	4.1311	3.6277	3.6276	3.4107	7.6752	6.7400	6.7397	6.3367	0.9232	0.8107	0.8106	0.7622
18	323.15	4053	182.42	4.1177	3.8833	3.7779	3.6943	7.5115	7.0839	6.8916	6.7391	0.9035	0.8520	0.8289	0.8106
19	323.15	5066	179.29	4.1720	4.2606	3.9916	4.1631	7.4798	7.6387	7.1563	7.4639	0.8997	0.9188	0.8608	0.8977
20	323.15	6080	176.17	4.2797	4.7674	4.2163	4.8416	7.5396	8.3988	7.4280	8.5296	0.9069	1.0102	0.8934	1.0259
21	333.15	202.7	212.05	3.6480	2.6597	2.8011	2.6958	7.7355	5.6398	5.9397	5.7164	0.9304	0.6783	0.7144	0.6876
22	333.15	608.0	202.61	3.8162	2.8466	2.9802	2.7945	7.7321	5.7676	6.0383	5.6620	0.9300	0.6937	0.7263	0.6810
23	333.15	1013	198.08	3.8898	2.9664	3.0869	2.8502	7.7050	5.8759	6.1146	5.6457	0.9267	0.7067	0.7355	0.6791
24	333.15	1520	194.30	3.9661	3.1151	3.2150	2.9370	7.7062	6.0527	6.2468	5.7067	0.9269	0.7280	0.7514	0.6864
25	333.15	2027	191.48	4.0273	3.2596	3.3346	3.0343	7.7117	6.2415	6.3852	5.8102	0.9276	0.7507	0.7680	0.6989
26	333.15	2533	189.18	4.080	3.405	3.450	3.145	7.719	6.441	6.527	5.949	0.928	0.775	0.785	0.716
27	333.15	3040	187.49	3.9672	3.3930	3.4036	3.1096	7.4380	6.3614	6.3813	5.8300	0.8946	0.7651	0.7675	0.7012
28	333.15	4053	184.04	4.0753	3.7277	3.6484	3.4295	7.5002	6.8605	6.7145	6.3117	0.9021	0.8252	0.8076	0.7592
29	333.15	5066	181.13	4.1139	4.0329	3.8244	3.7657	7.4515	7.3047	6.9272	6.8207	0.8963	0.8786	0.8332	0.8204
30	333.15	6080	178.36	4.1769	4.4127	4.0096	4.2281	7.4502	7.8707	7.1517	7.5414	0.8961	0.9467	0.8602	0.9071
31	343.15	202.7	213.19	3.6355	2.6495	2.7903	2.6846	7.7505	5.6484	5.9486	5.7234	0.9322	0.6794	0.7155	0.6884
32	343.15	608.0	203.81	3.7871	2.8136	2.9469	2.7561	7.7185	5.7345	6.0062	5.6173	0.9284	0.6897	0.7224	0.6756
33	343.15	1013	199.32	3.8548	2.9202	3.0410	2.7931	7.6832	5.8205	6.0612	5.5671	0.9241	0.7001	0.7290	0.6696
34	343.15	1520	195.59	3.9202	3.0482	3.1494	2.8510	7.6677	5.9620	6.1601	5.5764	0.9223	0.7171	0.7409	0.6707
35	343.15	2027	192.83	3.9725	3.1726	3.2505	2.9187	7.6601	6.1177	6.2680	5.6280	0.9214	0.7358	0.7539	0.6769
36	343.15	2533	190.58	4.0187	3.2986	3.3494	2.9986	7.6589	6.2866	6.3833	5.7148	0.9212	0.7561	0.7678	0.6874
37	343.15	3040	188.74	4.0141	3.3812	3.4003	3.0446	7.5762	6.3815	6.4177	5.7463	0.9113	0.7676	0.7719	0.6912
38	343.15	4053	185.57	4.0323	3.5940	3.5343	3.2105	7.4827	6.6694	6.5586	5.9576	0.9000	0.8022	0.7889	0.7166
39	343.15	5066	182.81	4.0698	3.8562	3.6895	3.4599	7.4399	7.0494	6.7446	6.3250	0.8949	0.8479	0.8112	0.7608
40	343.15	6080	180.24	4.1259	4.1728	3.8573	3.7996	7.4366	7.5212	6.9526	6.8485	0.8945	0.9046	0.8363	0.8237
41	353.15	202.7	214.33	3.6126	2.6292	2.7694	2.6641	7.7429	5.6353	5.9357	5.7100	0.9313	0.6778	0.7139	0.6868

42	353.15	608.0	204.99	3.7551	2.7790	2.9119	2.7178	7.6976	5.6967	5.9692	5.5712	0.9259	0.6852	0.7180	0.6701
43	353.15	1013	200.51	3.8246	2.8812	3.0021	2.7460	7.6687	5.7772	6.0197	5.5061	0.9224	0.6949	0.7240	0.6623
44	353.15	1520	196.83	3.8865	2.9972	3.0995	2.7854	7.6497	5.8994	6.1007	5.4825	0.9201	0.7096	0.7338	0.6594
45	353.15	2027	194.10	3.9368	3.1104	3.1907	2.8341	7.6414	6.0373	6.1932	5.5010	0.9191	0.7262	0.7449	0.6617
46	353.15	2533	191.91	3.9728	3.2160	3.2710	2.8847	7.6241	6.1718	6.2774	5.5360	0.9170	0.7423	0.7550	0.6659
47	353.15	3040	190.10	3.9701	3.2892	3.3153	2.9111	7.5472	6.2529	6.3024	5.5340	0.9078	0.7521	0.7580	0.6656
48	353.15	4053	187.01	3.9989	3.4867	3.4421	3.0364	7.4782	6.5203	6.4370	5.6782	0.8995	0.7843	0.7742	0.6830
49	353.15	5066	184.35	4.0382	3.7183	3.5820	3.2228	7.4445	6.8548	6.6035	5.9413	0.8954	0.8245	0.7943	0.7146
50	353.15	6080	181.94	4.0906	3.9901	3.7330	3.4755	7.4424	7.2595	6.7919	6.3233	0.8952	0.8732	0.8169	0.7606
51	363.15	202.7	215.46	3.5889	2.6085	2.7480	2.6436	7.7326	5.6202	5.9208	5.6958	0.9301	0.6760	0.7122	0.6851
52	363.15	608.0	206.13	3.7304	2.7526	2.8851	2.6892	7.6896	5.6739	5.9472	5.5433	0.9249	0.6825	0.7153	0.6667
53	363.15	1013	201.69	3.7908	2.8405	2.9615	2.6998	7.6457	5.7292	5.9731	5.4453	0.9196	0.6891	0.7184	0.6550
54	363.15	1520	198.04	3.8471	2.9437	3.0468	2.7212	7.6189	5.8298	6.0341	5.3892	0.9164	0.7012	0.7258	0.6482
55	363.15	2027	195.35	3.8928	3.0445	3.1268	2.7514	7.6047	5.9476	6.1083	5.3749	0.9147	0.7154	0.7347	0.6465
56	363.15	2533	193.18	3.9354	3.1482	3.2067	2.7929	7.6024	6.0817	6.1947	5.3953	0.9144	0.7315	0.7451	0.6489
57	363.15	3040	191.39	3.9412	3.2206	3.2522	2.8103	7.5432	6.1639	6.2244	5.3787	0.9073	0.7414	0.7487	0.6469
58	363.15	4053	188.35	3.9820	3.4086	3.3761	2.9066	7.5001	6.4202	6.3590	5.4747	0.9021	0.7722	0.7648	0.6585
59	363.15	5066	185.79	4.0209	3.6142	3.5009	3.0423	7.4704	6.7149	6.5044	5.6523	0.8985	0.8077	0.7823	0.6799
60	363.15	6080	183.47	4.0830	3.8642	3.6489	3.2423	7.4910	7.0895	6.6945	5.9486	0.9010	0.8527	0.8052	0.7155
61	363.15	8106	179.53	4.0669	4.2992	3.7906	3.6350	7.3011	7.7182	6.8051	6.5258	0.8782	0.9283	0.8185	0.7849
62	373.15	202.7	216.54	3.5739	2.5965	2.7354	2.6323	7.7391	5.6226	5.9233	5.7002	0.9309	0.6763	0.7124	0.6856
63	373.15	608.0	207.24	3.7136	2.7348	2.8670	2.6706	7.6961	5.6676	5.9414	5.5346	0.9257	0.6817	0.7146	0.6657
64	373.15	1013	202.83	3.7639	2.8083	2.9292	2.6642	7.6345	5.6962	5.9414	5.4040	0.9183	0.6851	0.7146	0.6500
65	373.15	1520	199.20	3.8225	2.9076	3.0113	2.6778	7.6146	5.7921	5.9987	5.3343	0.9159	0.6967	0.7215	0.6416
66	373.15	2027	196.55	3.8619	2.9954	3.0793	2.6902	7.5907	5.8875	6.0523	5.2877	0.9130	0.7081	0.7280	0.6360
67	373.15	2533	194.43	3.8892	3.0767	3.1380	2.7038	7.5619	5.9820	6.1013	5.2570	0.9095	0.7195	0.7339	0.6323
68	373.15	3040	192.64	3.9106	3.1566	3.1928	2.7223	7.5335	6.0810	6.1507	5.2444	0.9061	0.7314	0.7398	0.6308
69	373.15	4053	189.66	3.9563	3.3319	3.3090	2.7907	7.5034	6.3192	6.2759	5.2928	0.9025	0.7601	0.7549	0.6366
70	373.15	5066	187.08	4.0469	3.5681	3.4728	2.9378	7.5709	6.6753	6.4970	5.4961	0.9106	0.8029	0.7814	0.6611
71	373.15	6080	184.91	4.0754	3.7597	3.5756	3.0566	7.5356	6.9519	6.6116	5.6518	0.9064	0.8362	0.7952	0.6798

72	373.15	8106	181.26	4.0182	4.0863	3.6616	3.2809	7.2832	7.4067	6.6370	5.9469	0.8760	0.8909	0.7983	0.7153
73	383.15	202.7	217.61	3.5591	2.5848	2.7230	2.6219	7.7451	5.6248	5.9257	5.7055	0.9316	0.6765	0.7127	0.6863
74	383.15	608.0	208.44	3.6411	2.6625	2.7941	2.5988	7.5893	5.5496	5.8240	5.4168	0.9128	0.6675	0.7005	0.6515
75	383.15	1013	204.00	3.7166	2.7570	2.8778	2.6118	7.5817	5.6242	5.8705	5.3279	0.9119	0.6765	0.7061	0.6408
76	383.15	1520	200.40	3.7661	2.8420	2.9461	2.6081	7.5473	5.6953	5.9041	5.2266	0.9078	0.6850	0.7101	0.6287
77	383.15	2027	197.77	3.8068	2.9253	3.0103	2.6123	7.5286	5.7852	5.9535	5.1664	0.9055	0.6958	0.7161	0.6214
78	383.15	2533	195.67	3.8363	3.0025	3.0662	2.6176	7.5064	5.8749	5.9995	5.1219	0.9029	0.7066	0.7216	0.6161
79	383.15	3040	193.88	3.8707	3.0887	3.1287	2.6376	7.5046	5.9884	6.0659	5.1137	0.9026	0.7203	0.7296	0.6151
80	383.15	4053	190.93	3.9259	3.2586	3.2436	2.6886	7.4957	6.2216	6.1931	5.1335	0.9016	0.7483	0.7449	0.6174
81	383.15	5066	188.50	3.9690	3.4303	3.3494	2.7571	7.4815	6.4660	6.3135	5.1971	0.8999	0.7777	0.7594	0.6251
82	383.15	6080	186.40	3.9953	3.5994	3.4396	2.8361	7.4473	6.7092	6.4114	5.2864	0.8958	0.8070	0.7712	0.6358
83	383.15	8106	182.73	4.0471	3.9824	3.6174	3.0720	7.3954	7.2771	6.6101	5.6136	0.8895	0.8753	0.7951	0.6752
84	383.15	10133	179.51	4.0752	4.4109	3.7633	3.3883	7.3152	7.9178	6.7553	6.0822	0.8799	0.9524	0.8125	0.7316
85	393.15	202.7	218.66	3.5449	2.5738	2.7114	2.6126	7.7514	5.6279	5.9288	5.7127	0.9323	0.6769	0.7131	0.6871
86	393.15	608.0	209.41	3.6693	2.6905	2.8217	2.6283	7.6839	5.6342	5.9090	5.5041	0.9242	0.6777	0.7107	0.6620
87	393.15	1013	205.03	3.7245	2.7615	2.8820	2.6167	7.6361	5.6618	5.9090	5.3650	0.9185	0.6810	0.7107	0.6453
88	393.15	1520	201.47	3.7647	2.8326	2.9371	2.5972	7.5847	5.7069	5.9173	5.2326	0.9123	0.6864	0.7117	0.6294
89	393.15	2027	198.87	3.7964	2.9020	2.9881	2.5849	7.5500	5.7713	5.9424	5.1407	0.9081	0.6942	0.7147	0.6183
90	393.15	2533	196.79	3.8270	2.9750	3.0406	2.5828	7.5313	5.8546	5.9836	5.0828	0.9059	0.7042	0.7197	0.6114
91	393.15	3040	195.08	3.8337	3.0280	3.0711	2.5659	7.4788	5.9070	5.9909	5.0056	0.8995	0.7105	0.7206	0.6021
92	393.15	4053	192.20	3.8741	3.1705	3.1620	2.5809	7.4461	6.0938	6.0775	4.9605	0.8956	0.7330	0.7310	0.5967
93	393.15	5066	189.92	3.8649	3.2757	3.2064	2.5722	7.3402	6.2211	6.0896	4.8851	0.8829	0.7483	0.7324	0.5876
94	393.15	6080	187.74	3.9638	3.5002	3.3595	2.6930	7.4417	6.5713	6.3073	5.0560	0.8951	0.7904	0.7586	0.6081
95	393.15	8106	184.30	3.9694	3.7951	3.4750	2.8088	7.3156	6.9944	6.4044	5.1766	0.8799	0.8413	0.7703	0.6226
96	393.15	10133	181.55	3.8211	3.9897	3.4338	2.8528	6.9373	7.2434	6.2342	5.1793	0.8344	0.8712	0.7498	0.6230
97	403.15	202.7	219.71	3.5230	2.5552	2.6922	2.5960	7.7405	5.6140	5.9151	5.7038	0.9310	0.6753	0.7115	0.6861
98	403.15	608.0	210.46	3.6520	2.6739	2.8046	2.6143	7.6861	5.6275	5.9027	5.5021	0.9245	0.6769	0.7100	0.6618
99	403.15	1013	206.10	3.7038	2.7386	2.8589	2.5960	7.6334	5.6441	5.8920	5.3502	0.9181	0.6789	0.7087	0.6435
100	403.15	1520	202.56	3.7427	2.8043	2.9089	2.5699	7.5812	5.6804	5.8923	5.2055	0.9119	0.6832	0.7087	0.6261
101	403.15	2027	199.98	3.7736	2.8685	2.9554	2.5507	7.5464	5.7365	5.9101	5.1009	0.9077	0.6900	0.7109	0.6135

102	403.15	2533	197.93	3.7943	2.9270	2.9941	2.5318	7.5101	5.7935	5.9263	5.0114	0.9033	0.6968	0.7128	0.6028
103	403.15	3040	196.26	3.7914	2.9656	3.0111	2.4979	7.4410	5.8202	5.9095	4.9024	0.8950	0.7000	0.7108	0.5897
104	403.15	4053	193.42	3.8336	3.0989	3.0957	2.4972	7.4148	5.9939	5.9877	4.8300	0.8918	0.7209	0.7202	0.5809
105	403.15	5066	191.17	3.8288	3.1962	3.1364	2.4724	7.3196	6.1102	5.9959	4.7265	0.8804	0.7349	0.7212	0.5685
106	403.15	6080	189.05	3.9240	3.4029	3.2776	2.5657	7.4183	6.4332	6.1964	4.8506	0.8923	0.7738	0.7453	0.5834
107	403.15	8106	185.68	3.9527	3.6865	3.4009	2.6460	7.3394	6.8451	6.3147	4.9130	0.8828	0.8233	0.7595	0.5909
108	403.15	10133	183.01	3.8423	3.8743	3.3848	2.6535	7.0317	7.0903	6.1945	4.8561	0.8458	0.8528	0.7451	0.5841
109	413.15	202.7	220.74	3.5025	2.5380	2.6744	2.5813	7.7316	5.6025	5.9037	5.6981	0.9299	0.6739	0.7101	0.6854
110	413.15	608.0	211.49	3.6355	2.6584	2.7887	2.6023	7.6889	5.6224	5.8979	5.5038	0.9248	0.6763	0.7094	0.6620
111	413.15	1013	207.13	3.6926	2.7257	2.8457	2.5867	7.6484	5.6457	5.8942	5.3578	0.9199	0.6791	0.7089	0.6444
112	413.15	1520	203.63	3.7200	2.7765	2.8812	2.5453	7.5750	5.6537	5.8669	5.1829	0.9111	0.6800	0.7057	0.6234
113	413.15	2027	201.07	3.7491	2.8351	2.9225	2.5195	7.5382	5.7004	5.8761	5.0658	0.9067	0.6856	0.7068	0.6093
114	413.15	2533	199.04	3.7684	2.8881	2.9564	2.4938	7.5006	5.7485	5.8844	4.9635	0.9022	0.6914	0.7078	0.5970
115	413.15	3040	197.38	3.7647	2.9215	2.9691	2.4529	7.4307	5.7665	5.8604	4.8414	0.8938	0.6936	0.7049	0.5823
116	413.15	4053	194.56	3.8158	3.0543	3.0555	2.4469	7.4241	5.9425	5.9448	4.7607	0.8930	0.7148	0.7150	0.5726
117	413.15	5066	192.35	3.8124	3.1424	3.0903	2.4070	7.3331	6.0443	5.9441	4.6298	0.8820	0.7270	0.7150	0.5569
118	413.15	6080	190.27	3.9102	3.3397	3.2269	2.4838	7.4398	6.3544	6.1397	4.7259	0.8949	0.7643	0.7385	0.5684
119	413.15	8106	186.95	3.9619	3.6177	3.3591	2.5406	7.4068	6.7632	6.2799	4.7496	0.8909	0.8135	0.7553	0.5713
120	413.15	10133	184.33	3.8852	3.8029	3.3640	2.5239	7.1617	7.0101	6.2009	4.6525	0.8614	0.8432	0.7458	0.5596
121	423.15	202.7	221.76	3.4837	2.5225	2.6584	2.5685	7.7253	5.5939	5.8951	5.6959	0.9292	0.6728	0.7091	0.6851
122	423.15	608.0	212.51	3.6202	2.6445	2.7742	2.5926	7.6933	5.6197	5.8953	5.5095	0.9253	0.6759	0.7091	0.6627
123	423.15	1013	208.14	3.6819	2.7140	2.8336	2.5799	7.6637	5.6489	5.8979	5.3699	0.9218	0.6794	0.7094	0.6459
124	423.15	1520	204.66	3.7066	2.7589	2.8635	2.5328	7.5860	5.6464	5.8605	5.1835	0.9124	0.6791	0.7049	0.6235
125	423.15	2027	202.12	3.7332	2.8116	2.8993	2.5008	7.5454	5.6827	5.8600	5.0545	0.9076	0.6835	0.7048	0.6079
126	423.15	2533	200.11	3.7502	2.8588	2.9280	2.4685	7.5045	5.7206	5.8592	4.9397	0.9026	0.6881	0.7047	0.5941
127	423.15	3040	198.47	3.7447	2.8866	2.9358	2.4210	7.4320	5.7289	5.8266	4.8048	0.8939	0.6891	0.7008	0.5779
128	423.15	4053	195.67	3.8025	3.0178	3.0225	2.4104	7.4402	5.9047	5.9141	4.7163	0.8949	0.7102	0.7113	0.5673
129	423.15	5066	193.47	3.8076	3.1051	3.0594	2.3657	7.3668	6.0075	5.9191	4.5770	0.8861	0.7226	0.7119	0.5505
130	423.15	6080	191.41	3.9150	3.3017	3.1990	2.4367	7.4936	6.3197	6.1233	4.6641	0.9013	0.7601	0.7365	0.5610
131	423.15	8106	188.15	3.9816	3.5703	3.3335	2.4714	7.4914	6.7175	6.2719	4.6500	0.9011	0.8080	0.7544	0.5593

132	423.15	10133	185.57	3.9379	3.7586	3.3591	2.4421	7.3075	6.9748	6.2335	4.5319	0.8789	0.8389	0.7498	0.5451
∑				512.80	426.66	424.03	380.86	998.16	825.75	822.69	738.76	120.06	99.32	98.95	88.86
Average (Overall)				**3.8848**	**3.2322**	**3.2123**	**2.8853**	**7.5619**	**6.2557**	**6.2325**	**5.5966**	**0.9095**	**0.7524**	**0.7496**	**0.6732**

Table C-12 n-Hexane [61]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	344.26	6.9	433.54	1.8334	1.8000	1.8008	1.2424	7.9486	7.8036	7.8074	5.3863	0.9561	0.9386	0.9391	0.6479
2	344.26	68.9	413.38	2.0271	2.0798	2.0766	1.8356	8.3797	8.5975	8.5842	7.5878	1.0079	1.0341	1.0325	0.9127
3	344.26	103.4	409.95	1.9728	2.0780	2.0722	1.8282	8.0873	8.5188	8.4949	7.4946	0.9727	1.0246	1.0218	0.9014
4	355.37	6.9	437.77	2.0294	1.9952	1.9960	1.4518	8.8838	8.7341	8.7380	6.3555	1.0685	1.0505	1.0510	0.7644
5	355.37	68.9	418.07	2.1313	2.1714	2.1684	1.9240	8.9102	9.0779	9.0655	8.0435	1.0717	1.0919	1.0904	0.9675
6	355.37	103.4	414.35	2.1592	2.2444	2.2390	1.9880	8.9465	9.2995	9.2771	8.2372	1.0761	1.1185	1.1158	0.9908
7	366.48	6.9	442.24	2.1560	2.1212	2.1221	1.5938	9.5346	9.3809	9.3848	7.0483	1.1468	1.1283	1.1288	0.8478
8	366.48	68.9	422.58	2.2671	2.2968	2.2940	2.0471	9.5802	9.7056	9.6939	8.6507	1.1523	1.1674	1.1660	1.0405
9	366.48	103.4	418.90	2.2951	2.3637	2.3587	2.1024	9.6141	9.9015	9.8803	8.8067	1.1564	1.1909	1.1884	1.0593
10	366.48	172.4	413.99	2.3419	2.4937	2.4835	2.2153	9.6951	10.3237	10.2816	9.1711	1.1661	1.2417	1.2367	1.1031
11	377.59	6.9	446.75	2.2652	2.2300	2.2309	1.7197	10.1196	9.9625	9.9664	7.6829	1.2172	1.1983	1.1988	0.9241
12	377.59	68.9	427.16	2.3740	2.3949	2.3923	2.1441	10.1406	10.2301	10.2191	9.1586	1.2197	1.2305	1.2291	1.1016
13	377.59	103.4	423.51	2.4007	2.4554	2.4507	2.1905	10.1673	10.3991	10.3791	9.2771	1.2229	1.2508	1.2484	1.1158
14	377.59	172.4	418.72	2.4369	2.5634	2.5539	2.2763	10.2038	10.7335	10.6937	9.5313	1.2273	1.2910	1.2862	1.1464
15	388.71	6.9	451.44	2.3250	2.2895	2.2904	1.7978	10.4960	10.3359	10.3400	8.1159	1.2624	1.2432	1.2437	0.9762
16	388.71	68.9	431.88	2.4363	2.4500	2.4476	2.1989	10.5222	10.5811	10.5707	9.4968	1.2656	1.2727	1.2714	1.1423
17	388.71	103.4	428.28	2.4605	2.5036	2.4991	2.2363	10.5375	10.7222	10.7032	9.5777	1.2674	1.2897	1.2874	1.1520
18	388.71	172.4	423.51	2.5010	2.6064	2.5975	2.3126	10.5921	11.0385	11.0007	9.7942	1.2740	1.3277	1.3232	1.1780

19	388.71	344.7	416.33	2.5776	2.8595	2.8363	2.5360	10.7313	11.9049	11.8083	10.5581	1.2907	1.4319	1.4203	1.2699
20	399.82	6.9	456.20	2.3616	2.3259	2.3268	1.8537	10.7735	10.6109	10.6150	8.4565	1.2958	1.2763	1.2768	1.0171
21	399.82	68.9	436.68	2.4731	2.4806	2.4783	2.2302	10.7996	10.8322	10.8224	9.7388	1.2990	1.3029	1.3017	1.1714
22	399.82	103.4	433.11	2.4937	2.5270	2.5228	2.2586	10.8003	10.9446	10.9265	9.7822	1.2990	1.3164	1.3142	1.1766
23	399.82	172.4	428.38	2.5363	2.6240	2.6156	2.3252	10.8651	11.2408	11.2048	9.9610	1.3068	1.3520	1.3477	1.1981
24	399.82	344.7	421.39	2.6026	2.8421	2.8206	2.5019	10.9671	11.9763	11.8856	10.5426	1.3191	1.4405	1.4296	1.2681
25	410.93	6.9	461.04	2.3758	2.3400	2.3409	1.8882	10.9532	10.7885	10.7926	8.7052	1.3174	1.2976	1.2981	1.0471
26	410.93	68.9	441.59	2.4771	2.4794	2.4773	2.2305	10.9387	10.9487	10.9394	9.8495	1.3157	1.3169	1.3158	1.1847
27	410.93	103.4	438.02	2.5017	2.5268	2.5228	2.2582	10.9580	11.0676	11.0504	9.8915	1.3180	1.3312	1.3291	1.1897
28	410.93	172.4	433.36	2.5361	2.6089	2.6009	2.3068	10.9906	11.3058	11.2714	9.9968	1.3219	1.3599	1.3557	1.2024
29	410.93	344.7	426.47	2.6038	2.8082	2.7881	2.4547	11.1046	11.9763	11.8905	10.4687	1.3356	1.4405	1.4302	1.2592
30	410.93	517.1	421.85	2.6536	3.0110	2.9743	2.6417	11.1943	12.7022	12.5472	11.1440	1.3464	1.5278	1.5092	1.3404
31	422.04	6.9	466.02	2.3527	2.3169	2.3178	1.8862	10.9639	10.7972	10.8014	8.7900	1.3187	1.2987	1.2992	1.0573
32	422.04	68.9	446.53	2.4664	2.4642	2.4622	2.2175	11.0132	11.0036	10.9947	9.9019	1.3247	1.3235	1.3224	1.1910
33	422.04	103.4	443.00	2.4859	2.5039	2.5002	2.2362	11.0126	11.0923	11.0758	9.9065	1.3246	1.3342	1.3322	1.1915
34	422.04	172.4	438.38	2.5192	2.5793	2.5718	2.2754	11.0438	11.3071	11.2742	9.9747	1.3283	1.3600	1.3560	1.1997
35	422.04	344.7	431.63	2.5753	2.7503	2.7314	2.3866	11.1157	11.8712	11.7898	10.3013	1.3370	1.4279	1.4181	1.2390
36	422.04	517.1	427.16	2.6210	2.9271	2.8932	2.5358	11.1957	12.5032	12.3584	10.8320	1.3466	1.5039	1.4865	1.3029
37	433.15	6.9	471.00	2.3250	2.2892	2.2901	1.8801	10.9505	10.7822	10.7864	8.8552	1.3171	1.2969	1.2974	1.0651
38	433.15	68.9	451.55	2.4335	2.4275	2.4257	2.1837	10.9882	10.9615	10.9531	9.8606	1.3217	1.3184	1.3174	1.1860
39	433.15	103.4	448.01	2.4557	2.4677	2.4642	2.2017	11.0020	11.0557	11.0398	9.8641	1.3233	1.3298	1.3279	1.1864
40	433.15	172.4	443.47	2.4785	2.5278	2.5206	2.2232	10.9913	11.2098	11.1781	9.8592	1.3220	1.3483	1.3445	1.1859
41	433.15	344.7	436.79	2.5364	2.6867	2.6689	2.3154	11.0786	11.7351	11.6574	10.1133	1.3325	1.4115	1.4021	1.2164
42	433.15	517.1	432.46	2.5726	2.8363	2.8048	2.4279	11.1256	12.2659	12.1297	10.4998	1.3382	1.4753	1.4589	1.2629
43	433.15	689.5	428.96	2.6127	3.0056	2.9557	2.5844	11.2074	12.8928	12.6790	11.0861	1.3480	1.5507	1.5250	1.3334
44	444.26	6.9	476.01	2.2851	2.2495	2.2504	1.8623	10.8775	10.7078	10.7120	8.8645	1.3083	1.2879	1.2884	1.0662
45	444.26	68.9	456.64	2.3793	2.3702	2.3684	2.1299	10.8649	10.8233	10.8152	9.7261	1.3068	1.3018	1.3008	1.1698
46	444.26	103.4	453.10	2.4037	2.4106	2.4072	2.1471	10.8912	10.9223	10.9070	9.7285	1.3100	1.3137	1.3119	1.1701
47	444.26	172.4	448.55	2.4316	2.4716	2.4648	2.1676	10.9071	11.0867	11.0561	9.7231	1.3119	1.3335	1.3298	1.1695
48	444.26	344.7	441.99	2.4801	2.6095	2.5926	2.2329	10.9619	11.5335	11.4591	9.8690	1.3185	1.3872	1.3783	1.1870

49	444.26	517.1	437.73	2.5199	2.7481	2.7187	2.3265	11.0302	12.0294	11.9005	10.1840	1.3267	1.4469	1.4314	1.2249
50	444.26	689.5	434.41	2.5441	2.8831	2.8373	2.4379	11.0517	12.5243	12.3254	10.5907	1.3293	1.5064	1.4825	1.2738
51	455.37	6.9	481.10	2.2260	2.1905	2.1913	1.8253	10.7093	10.5383	10.5425	8.7815	1.2881	1.2675	1.2680	1.0562
52	455.37	68.9	461.72	2.3209	2.3090	2.3073	2.0728	10.7159	10.6613	10.6535	9.5708	1.2889	1.2823	1.2814	1.1512
53	455.37	103.4	458.22	2.3389	2.3414	2.3381	2.0811	10.7174	10.7287	10.7139	9.5363	1.2891	1.2904	1.2887	1.1470
54	455.37	172.4	453.68	2.3710	2.4031	2.3966	2.1007	10.7568	10.9023	10.8728	9.5304	1.2938	1.3113	1.3078	1.1463
55	455.37	344.7	447.18	2.4163	2.5277	2.5117	2.1479	10.8054	11.3036	11.2321	9.6050	1.2997	1.3596	1.3510	1.1553
56	455.37	517.1	443.03	2.4479	2.6463	2.6186	2.2149	10.8448	11.7238	11.6011	9.8128	1.3044	1.4101	1.3954	1.1803
57	455.37	689.5	439.82	2.4684	2.7628	2.7204	2.2992	10.8568	12.1515	11.9649	10.1125	1.3058	1.4616	1.4391	1.2163
58	466.48	6.9	486.15	2.1710	2.1356	2.1365	1.7924	10.5543	10.3822	10.3865	8.7138	1.2695	1.2488	1.2493	1.0481
59	466.48	68.9	466.85	2.2504	2.2363	2.2347	2.0047	10.5060	10.4400	10.4325	9.3590	1.2637	1.2557	1.2548	1.1257
60	466.48	103.4	463.35	2.2699	2.2686	2.2655	2.0122	10.5175	10.5113	10.4970	9.3237	1.2650	1.2643	1.2626	1.1214
61	466.48	172.4	458.84	2.2975	2.3227	2.3164	2.0229	10.5416	10.6573	10.6287	9.2817	1.2679	1.2819	1.2784	1.1164
62	466.48	344.7	452.41	2.3376	2.4337	2.4184	2.0524	10.5758	11.0102	10.9413	9.2854	1.2720	1.3243	1.3160	1.1168
63	466.48	517.1	448.34	2.3668	2.5398	2.5137	2.1017	10.6113	11.3869	11.2697	9.4228	1.2763	1.3696	1.3555	1.1334
64	466.48	689.5	445.20	2.3885	2.6455	2.6059	2.1680	10.6335	11.7776	11.6013	9.6518	1.2790	1.4166	1.3954	1.1609
65	466.48	1034	440.11	2.4271	2.8795	2.8007	2.3690	10.6818	12.6730	12.3261	10.4263	1.2848	1.5243	1.4826	1.2541
66	477.59	6.9	491.27	2.0975	2.0622	2.0631	1.7409	10.3044	10.1313	10.1356	8.5526	1.2394	1.2186	1.2191	1.0287
67	477.59	68.9	471.97	2.1763	2.1602	2.1587	1.9337	10.2717	10.1955	10.1883	9.1266	1.2355	1.2263	1.2254	1.0977
68	477.59	103.4	468.47	2.1969	2.1923	2.1894	1.9405	10.2920	10.2705	10.2566	9.0907	1.2379	1.2353	1.2337	1.0934
69	477.59	172.4	464.00	2.2195	2.2388	2.2328	1.9424	10.2985	10.3881	10.3603	9.0129	1.2387	1.2495	1.2461	1.0841
70	477.59	344.7	457.65	2.2532	2.3359	2.3214	1.9549	10.3115	10.6903	10.6236	8.9465	1.2403	1.2858	1.2778	1.0761
71	477.59	517.1	453.61	2.2861	2.4374	2.4126	1.9951	10.3700	11.0561	10.9436	9.0499	1.2473	1.3298	1.3163	1.0885
72	477.59	689.5	450.54	2.3061	2.5314	2.4942	2.0440	10.3898	11.4050	11.2375	9.2089	1.2497	1.3718	1.3516	1.1076
73	477.59	1034	445.67	2.3361	2.7303	2.6587	2.1924	10.4112	12.1681	11.8487	9.7707	1.2522	1.4636	1.4252	1.1752
74	488.71	6.9	496.36	2.0284	1.9933	1.9942	1.6934	10.0680	9.8940	9.8983	8.4054	1.2110	1.1900	1.1906	1.0110
75	488.71	68.9	477.09	2.0988	2.0809	2.0795	1.8599	10.0131	9.9279	9.9209	8.8737	1.2044	1.1941	1.1933	1.0673
76	488.71	103.4	473.63	2.1125	2.1051	2.1022	1.8583	10.0053	9.9702	9.9567	8.8013	1.2034	1.1992	1.1976	1.0586
77	488.71	172.4	469.16	2.1375	2.1517	2.1459	1.8595	10.0284	10.0948	10.0678	8.7241	1.2062	1.2142	1.2109	1.0493
78	488.71	344.7	462.84	2.1715	2.2427	2.2288	1.8633	10.0504	10.3802	10.3156	8.6243	1.2089	1.2485	1.2408	1.0373

79	488.71	517.1	458.87	2.1985	2.3310	2.3074	1.8868	10.0882	10.6965	10.5881	8.6582	1.2134	1.2866	1.2735	1.0414
80	488.71	689.5	455.88	2.2146	2.4129	2.3778	1.9189	10.0957	10.9997	10.8398	8.7476	1.2143	1.3230	1.3038	1.0522
81	488.71	1034	451.15	2.2450	2.5910	2.5251	2.0325	10.1284	11.6891	11.3918	9.1698	1.2182	1.4060	1.3702	1.1029
82	488.71	1379	447.18	2.2678	2.7905	2.6753	2.2128	10.1410	12.4788	11.9636	9.8952	1.2198	1.5009	1.4390	1.1902
83	499.82	68.9	482.22	2.0179	1.9985	1.9971	1.7835	9.7304	9.6373	9.6306	8.6002	1.1704	1.1592	1.1584	1.0344
84	499.82	103.4	478.75	2.0323	2.0225	2.0197	1.7812	9.7299	9.6827	9.6696	8.5276	1.1703	1.1646	1.1630	1.0257
85	499.82	172.4	474.32	2.0517	2.0614	2.0559	1.7742	9.7317	9.7776	9.7513	8.4153	1.1705	1.1760	1.1729	1.0122
86	499.82	344.7	468.04	2.0848	2.1461	2.1327	1.7697	9.7578	10.0445	9.9817	8.2828	1.1737	1.2081	1.2006	0.9962
87	499.82	517.1	464.14	2.1047	2.2210	2.1985	1.7770	9.7687	10.3087	10.2040	8.2478	1.1750	1.2399	1.2273	0.9920
88	499.82	689.5	461.18	2.1232	2.2983	2.2650	1.8006	9.7918	10.5992	10.4458	8.3041	1.1777	1.2749	1.2564	0.9988
89	499.82	1034	456.60	2.1486	2.4539	2.3927	1.8807	9.8104	11.2043	10.9251	8.5874	1.1800	1.3476	1.3141	1.0329
90	499.82	1379	452.85	2.1629	2.6204	2.5173	2.0098	9.7948	11.8663	11.3995	9.1014	1.1781	1.4273	1.3711	1.0947
91	510.93	68.9	487.34	1.9337	1.9132	1.9118	1.7043	9.4239	9.3237	9.3172	8.3058	1.1335	1.1214	1.1207	0.9990
92	510.93	103.4	483.88	1.9488	1.9368	1.9342	1.7015	9.4299	9.3719	9.3591	8.2333	1.1342	1.1272	1.1257	0.9903
93	510.93	172.4	479.44	1.9700	1.9758	1.9704	1.6941	9.4450	9.4727	9.4469	8.1223	1.1360	1.1394	1.1363	0.9769
94	510.93	344.7	473.20	2.0015	2.0540	2.0411	1.6817	9.4708	9.7194	9.6582	7.9577	1.1391	1.1690	1.1617	0.9571
95	510.93	517.1	469.34	2.0211	2.1233	2.1017	1.6812	9.4857	9.9656	9.8641	7.8905	1.1409	1.1987	1.1864	0.9491
96	510.93	689.5	466.45	2.0327	2.1877	2.1561	1.6890	9.4818	10.2047	10.0569	7.8782	1.1405	1.2274	1.2096	0.9476
97	510.93	1034	461.98	2.0569	2.3276	2.2705	1.7446	9.5025	10.7532	10.4890	8.0596	1.1430	1.2934	1.2616	0.9694
98	510.93	1379	458.37	2.0713	2.4747	2.3810	1.8402	9.4941	11.3432	10.9138	8.4349	1.1419	1.3643	1.3127	1.0145
99	522.04	103.4	488.96	1.8695	1.8557	1.8532	1.6267	9.1413	9.0737	9.0612	7.9541	1.0995	1.0914	1.0899	0.9567
100	522.04	172.4	484.56	1.8847	1.8870	1.8818	1.6115	9.1324	9.1438	9.1186	7.8087	1.0984	1.0998	1.0968	0.9392
101	522.04	344.7	478.36	1.9137	1.9586	1.9461	1.5915	9.1543	9.3690	9.3093	7.6129	1.1011	1.1269	1.1197	0.9157
102	522.04	517.1	474.53	1.9322	2.0221	2.0013	1.5835	9.1687	9.5954	9.4969	7.5140	1.1028	1.1541	1.1423	0.9038
103	522.04	689.5	471.68	1.9437	2.0812	2.0510	1.5836	9.1682	9.8168	9.6740	7.4696	1.1027	1.1808	1.1636	0.8984
104	522.04	1034	467.32	1.9635	2.2045	2.1507	1.6156	9.1757	10.3020	10.0505	7.5500	1.1036	1.2391	1.2089	0.9081
105	522.04	1379	463.82	1.9800	2.3380	2.2518	1.6868	9.1837	10.8441	10.4444	7.8235	1.1046	1.3043	1.2562	0.9410
106	522.04	2068	457.83	1.9885	2.6400	2.4321	1.9490	9.1039	12.0866	11.1348	8.9232	1.0950	1.4538	1.3393	1.0733
107	533.15	172.4	489.65	1.8034	1.8027	1.7977	1.5339	8.8302	8.8271	8.8024	7.5105	1.0621	1.0617	1.0587	0.9034
108	533.15	344.7	483.48	1.8295	1.8676	1.8555	1.5066	8.8451	9.0295	8.9711	7.2841	1.0639	1.0861	1.0790	0.8761

109	533.15	517.1	479.69	1.8460	1.9251	1.9051	1.4914	8.8551	9.2346	9.1386	7.1542	1.0651	1.1107	1.0992	0.8605
110	533.15	689.5	476.84	1.8643	1.9865	1.9575	1.4920	8.8896	9.4724	9.3341	7.1143	1.0692	1.1393	1.1227	0.8557
111	533.15	1034	472.58	1.8771	2.0925	2.0416	1.5012	8.8711	9.8888	9.6482	7.0946	1.0670	1.1894	1.1605	0.8533
112	533.15	1379	469.19	1.8916	2.2110	2.1309	1.5488	8.8754	10.3737	9.9982	7.2670	1.0675	1.2477	1.2026	0.8741
113	533.15	2068	463.53	1.8991	2.4716	2.2922	1.7377	8.8031	11.4564	10.6252	8.0545	1.0588	1.3780	1.2780	0.9688
114	544.26	172.4	494.66	1.7334	1.7302	1.7253	1.4683	8.5747	8.5585	8.5342	7.2633	1.0314	1.0294	1.0265	0.8736
115	544.26	344.7	488.53	1.7562	1.7884	1.7767	1.4343	8.5796	8.7369	8.6797	7.0072	1.0319	1.0509	1.0440	0.8428
116	544.26	517.1	484.78	1.7703	1.8399	1.8205	1.4123	8.5820	8.9193	8.8256	6.8466	1.0322	1.0728	1.0615	0.8235
117	544.26	689.5	482.00	1.7791	1.8879	1.8600	1.3983	8.5754	9.0997	8.9653	6.7397	1.0314	1.0945	1.0783	0.8106
118	544.26	1034	477.78	1.7985	1.9915	1.9431	1.4008	8.5927	9.5148	9.2836	6.6928	1.0335	1.1444	1.1166	0.8050
119	544.26	1379	474.50	1.8078	2.0939	2.0190	1.4257	8.5778	9.9353	9.5799	6.7650	1.0317	1.1950	1.1523	0.8137
120	544.26	2068	469.08	1.8155	2.3230	2.1641	1.5592	8.5163	10.8969	10.1514	7.3138	1.0243	1.3107	1.2210	0.8797
121	544.26	2758	464.18	1.7983	2.6007	2.2570	1.8245	8.3474	12.0720	10.4766	8.4688	1.0040	1.4520	1.2601	1.0186
122	555.37	172.4	499.68	1.6598	1.6542	1.6494	1.3998	8.2935	8.2655	8.2417	6.9946	0.9975	0.9942	0.9913	0.8413
123	555.37	344.7	493.55	1.6862	1.7131	1.7018	1.3667	8.3221	8.4551	8.3990	6.7454	1.0010	1.0170	1.0102	0.8113
124	555.37	517.1	489.83	1.6973	1.7585	1.7398	1.3382	8.3141	8.6136	8.5219	6.5550	1.0000	1.0360	1.0250	0.7884
125	555.37	689.5	487.09	1.7038	1.8008	1.7739	1.3175	8.2992	8.7713	8.6404	6.4175	0.9982	1.0550	1.0393	0.7719
126	555.37	1034	482.94	1.7202	1.8936	1.8475	1.3062	8.3076	9.1451	8.9220	6.3084	0.9992	1.1000	1.0731	0.7588
127	555.37	1379	479.73	1.7295	1.9868	1.9163	1.3168	8.2971	9.5314	9.1928	6.3171	0.9980	1.1464	1.1057	0.7598
128	555.37	2068	474.53	1.7352	2.1883	2.0448	1.4045	8.2340	10.3842	9.7031	6.6646	0.9904	1.2490	1.1671	0.8016
129	555.37	2758	469.99	1.7183	2.4219	2.1395	1.5898	8.0759	11.3824	10.0552	7.4718	0.9714	1.3691	1.2094	0.8987
130	566.48	172.4	504.62	1.5970	1.5894	1.5847	1.3428	8.0589	8.0203	7.9968	6.7761	0.9693	0.9647	0.9618	0.8150
131	566.48	344.7	498.53	1.6194	1.6416	1.6306	1.3036	8.0729	8.1840	8.1288	6.4985	0.9710	0.9844	0.9777	0.7816
132	566.48	517.1	494.81	1.6346	1.6883	1.6701	1.2762	8.0880	8.3536	8.2638	6.3149	0.9728	1.0048	0.9940	0.7595
133	566.48	689.5	492.10	1.6383	1.7247	1.6987	1.2492	8.0620	8.4874	8.3595	6.1474	0.9697	1.0209	1.0055	0.7394
134	566.48	1034	488.03	1.6504	1.8066	1.7623	1.2247	8.0544	8.8166	8.6006	5.9768	0.9688	1.0605	1.0345	0.7189
135	566.48	1379	484.89	1.6578	1.8899	1.8230	1.2215	8.0383	9.1638	8.8396	5.9229	0.9668	1.1022	1.0632	0.7124
136	566.48	2068	479.87	1.6616	2.0685	1.9370	1.2725	7.9735	9.9261	9.2951	6.1064	0.9590	1.1939	1.1180	0.7345
137	566.48	2758	475.58	1.6498	2.2735	2.0308	1.4036	7.8462	10.8121	9.6578	6.6753	0.9437	1.3005	1.1616	0.8029
138	577.59	172.4	509.49	1.5448	1.5353	1.5308	1.2968	7.8707	7.8224	7.7993	6.6072	0.9467	0.9409	0.9381	0.7947

139	577.59	344.7	503.43	1.5629	1.5811	1.5703	1.2518	7.8683	7.9595	7.9052	6.3021	0.9464	0.9574	0.9508	0.7580
140	577.59	517.1	499.75	1.5744	1.6215	1.6038	1.2185	7.8683	8.1033	8.0150	6.0897	0.9464	0.9747	0.9640	0.7325
141	577.59	689.5	497.05	1.5823	1.6594	1.6342	1.1928	7.8647	8.2480	8.1229	5.9288	0.9460	0.9921	0.9770	0.7131
142	577.59	1034	493.04	1.5891	1.7300	1.6875	1.1556	7.8349	8.5298	8.3200	5.6976	0.9424	1.0260	1.0007	0.6853
143	577.59	1379	489.94	1.6004	1.8105	1.7468	1.1466	7.8411	8.8701	8.5583	5.6179	0.9431	1.0669	1.0294	0.6757
144	577.59	2068	485.10	1.5971	1.9642	1.8424	1.1624	7.7474	9.5283	8.9375	5.6390	0.9318	1.1461	1.0750	0.6782
145	577.59	2758	480.99	1.5933	2.1508	1.9361	1.2563	7.6639	10.3449	9.3126	6.0428	0.9218	1.2443	1.1201	0.7268
146	588.71	172.4	514.36	1.4886	1.4775	1.4730	1.2473	7.6567	7.5996	7.5768	6.4155	0.9209	0.9141	0.9113	0.7716
147	588.71	344.7	508.30	1.5094	1.5238	1.5133	1.2039	7.6722	7.7455	7.6919	6.1196	0.9228	0.9316	0.9252	0.7361
148	588.71	517.1	504.66	1.5169	1.5580	1.5408	1.1650	7.6552	7.8624	7.7757	5.8790	0.9208	0.9457	0.9353	0.7071
149	588.71	689.5	501.95	1.5284	1.5972	1.5727	1.1406	7.6719	8.0172	7.8945	5.7251	0.9228	0.9643	0.9495	0.6886
150	588.71	1034	497.98	1.5364	1.6638	1.6227	1.0985	7.6508	8.2852	8.0809	5.4704	0.9202	0.9965	0.9720	0.6580
151	588.71	1379	494.95	1.5428	1.7334	1.6725	1.0768	7.6364	8.5793	8.2781	5.3295	0.9185	1.0319	0.9957	0.6410
152	588.71	2068	490.23	1.5430	1.8756	1.7618	1.0733	7.5643	9.1946	8.6368	5.2615	0.9098	1.1059	1.0388	0.6328
153	588.71	2758	486.29	1.5388	2.0402	1.8466	1.1313	7.4829	9.9213	8.9799	5.5014	0.9000	1.1933	1.0801	0.6617
154	599.82	172.4	519.13	1.4495	1.4370	1.4326	1.2152	7.5248	7.4598	7.4372	6.3086	0.9051	0.8973	0.8945	0.7588
155	599.82	344.7	513.10	1.4657	1.4768	1.4665	1.1667	7.5208	7.5777	7.5248	5.9865	0.9046	0.9114	0.9051	0.7201
156	599.82	517.1	509.46	1.4763	1.5120	1.4953	1.1295	7.5211	7.7032	7.6178	5.7544	0.9046	0.9265	0.9163	0.6921
157	599.82	689.5	506.79	1.4839	1.5452	1.5214	1.0995	7.5201	7.8310	7.7104	5.5719	0.9045	0.9419	0.9274	0.6702
158	599.82	1034	502.86	1.4921	1.6075	1.5678	1.0529	7.5033	8.0832	7.8837	5.2944	0.9025	0.9722	0.9482	0.6368
159	599.82	1379	499.90	1.4928	1.6660	1.6076	1.0188	7.4624	8.3281	8.0362	5.0931	0.8976	1.0017	0.9666	0.6126
160	599.82	2068	495.24	1.5005	1.8028	1.6957	1.0042	7.4309	8.9282	8.3977	4.9734	0.8938	1.0739	1.0101	0.5982
161	599.82	2758	491.49	1.4895	1.9430	1.7658	1.0276	7.3209	9.5495	8.6786	5.0506	0.8805	1.1486	1.0439	0.6075
162	599.82	3447	488.10	1.4752	2.1083	1.8286	1.1042	7.2006	10.2907	8.9254	5.3895	0.8661	1.2378	1.0735	0.6482
163	610.93	172.4	523.85	1.4132	1.3994	1.3951	1.1862	7.4029	7.3306	7.3082	6.2139	0.8904	0.8817	0.8790	0.7474
164	610.93	344.7	517.83	1.4317	1.4398	1.4297	1.1398	7.4139	7.4559	7.4036	5.9024	0.8917	0.8968	0.8905	0.7099
165	610.93	517.1	514.22	1.4379	1.4689	1.4525	1.0974	7.3940	7.5532	7.4689	5.6432	0.8893	0.9085	0.8984	0.6788
166	610.93	689.5	511.55	1.4485	1.5032	1.4800	1.0690	7.4098	7.6894	7.5708	5.4687	0.8912	0.9249	0.9106	0.6578
167	610.93	1034	507.65	1.4564	1.5609	1.5224	1.0183	7.3934	7.9239	7.7286	5.1692	0.8893	0.9531	0.9296	0.6217
168	610.93	1379	504.73	1.4577	1.6154	1.5591	0.9796	7.3573	8.1534	7.8695	4.9442	0.8849	0.9807	0.9465	0.5947

169	610.93	2068	500.19	1.4627	1.7384	1.6369	0.9473	7.3161	8.6950	8.1875	4.7380	0.8800	1.0458	0.9848	0.5699
170	610.93	2758	496.54	1.4553	1.8672	1.7032	0.9517	7.2263	9.2716	8.4569	4.7258	0.8692	1.1152	1.0172	0.5684
171	610.93	3447	493.33	1.4382	2.0092	1.7579	0.9934	7.0950	9.9119	8.6721	4.9009	0.8534	1.1922	1.0431	0.5895
172	610.93	4137	490.34	1.4130	2.1710	1.8007	1.0739	6.9284	10.6450	8.8292	5.2657	0.8333	1.2804	1.0620	0.6334
173	622.04	344.7	522.52	1.4000	1.4055	1.3956	1.1158	7.3155	7.3438	7.2921	5.8305	0.8799	0.8833	0.8771	0.7013
174	622.04	517.1	518.91	1.4088	1.4354	1.4194	1.0755	7.3102	7.4485	7.3652	5.5808	0.8793	0.8959	0.8859	0.6713
175	622.04	689.5	516.28	1.4150	1.4636	1.4409	1.0418	7.3052	7.5563	7.4393	5.3787	0.8787	0.9089	0.8948	0.6469
176	622.04	1034.2	512.42	1.4218	1.5166	1.4792	0.9871	7.2857	7.7713	7.5798	5.0580	0.8763	0.9347	0.9117	0.6084
177	622.04	1379	509.49	1.4301	1.5740	1.5197	0.9512	7.2864	8.0195	7.7426	4.8461	0.8764	0.9646	0.9313	0.5829
178	622.04	2068	505.06	1.4303	1.6823	1.5857	0.9018	7.2240	8.4967	8.0088	4.5547	0.8689	1.0220	0.9633	0.5478
179	622.04	2758	501.52	1.4229	1.7984	1.6451	0.8881	7.1359	9.0193	8.2504	4.4540	0.8583	1.0848	0.9923	0.5357
180	622.04	3447	498.42	1.4118	1.9296	1.7002	0.9106	7.0367	9.6174	8.4742	4.5385	0.8464	1.1568	1.0193	0.5459
181	622.04	4137	495.60	1.3855	2.0676	1.7385	0.9562	6.8668	10.2470	8.6159	4.7387	0.8259	1.2325	1.0363	0.5700
182	633.15	344.7	527.10	1.3845	1.3875	1.3778	1.1085	7.2977	7.3135	7.2622	5.8427	0.8778	0.8797	0.8735	0.7027
183	633.15	517.1	523.53	1.3886	1.4113	1.3956	1.0633	7.2697	7.3888	7.3064	5.5668	0.8744	0.8887	0.8788	0.6696
184	633.15	689.5	520.90	1.3973	1.4405	1.4184	1.0316	7.2787	7.5036	7.3881	5.3735	0.8755	0.9025	0.8886	0.6463
185	633.15	1034	517.07	1.4028	1.4887	1.4523	0.9733	7.2532	7.6979	7.5096	5.0324	0.8724	0.9259	0.9033	0.6053
186	633.15	1379	514.18	1.4102	1.5416	1.4890	0.9332	7.2510	7.9267	7.6560	4.7982	0.8721	0.9534	0.9209	0.5771
187	633.15	2068	509.82	1.4110	1.6419	1.5495	0.8746	7.1936	8.3708	7.8997	4.4586	0.8652	1.0068	0.9502	0.5363
188	633.15	2758	506.39	1.4006	1.7441	1.5998	0.8434	7.0927	8.8322	8.1012	4.2707	0.8531	1.0623	0.9744	0.5137
189	633.15	3447	503.40	1.3912	1.8628	1.6510	0.8474	7.0034	9.3775	8.3109	4.2656	0.8424	1.1279	0.9996	0.5131
190	633.15	4137	500.69	1.3721	1.9896	1.6919	0.8736	6.8701	9.9620	8.4712	4.3742	0.8263	1.1982	1.0189	0.5261
191	644.26	344.7	531.65	1.3709	1.3717	1.3621	1.1033	7.2881	7.2924	7.2415	5.8659	0.8766	0.8771	0.8710	0.7055
192	644.26	517.1	528.08	1.3772	1.3964	1.3809	1.0605	7.2724	7.3739	7.2923	5.6005	0.8747	0.8869	0.8771	0.6736
193	644.26	689.5	525.48	1.3813	1.4195	1.3978	1.0239	7.2582	7.4592	7.3450	5.3804	0.8730	0.8972	0.8834	0.6472
194	644.26	1034	521.65	1.3918	1.4698	1.4343	0.9691	7.2602	7.6674	7.4820	5.0555	0.8733	0.9222	0.8999	0.6081
195	644.26	1379	518.84	1.3908	1.5110	1.4598	0.9181	7.2159	7.8394	7.5740	4.7637	0.8679	0.9429	0.9110	0.5730
196	644.26	2068	514.51	1.3977	1.6097	1.5210	0.8578	7.1915	8.2822	7.8254	4.4132	0.8650	0.9962	0.9412	0.5308
197	644.26	2758	511.15	1.3894	1.7044	1.5676	0.8168	7.1019	8.7124	8.0131	4.1750	0.8542	1.0479	0.9638	0.5022
198	644.26	3447	508.27	1.3783	1.8094	1.6118	0.8030	7.0053	9.1968	8.1923	4.0811	0.8426	1.1062	0.9854	0.4909

199	644.26	4137	505.67	1.3615	1.9233	1.6503	0.8106	6.8845	9.7258	8.3450	4.0991	0.8281	1.1698	1.0037	0.4930
∑				385.11	415.63	405.99	321.91	1801.98	1946.30	1899.74	1498.61	216.74	234.10	228.50	180.25
Average (Overall)				**1.9352**	**2.0886**	**2.0401**	**1.6176**	**9.0552**	**9.7804**	**9.5464**	**7.5307**	**1.0891**	**1.1764**	**1.1482**	**0.9058**

Table C-13 n-Heptane [61]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	410.93	68.9	488.84	2.1838	2.2284	2.2251	1.2051	10.6752	10.8931	10.8772	5.8911	1.2840	1.3102	1.3083	0.7086
2	410.93	103.4	485.23	2.1936	2.2710	2.2657	1.3269	10.6440	11.0195	10.9938	6.4387	1.2802	1.3254	1.3223	0.7744
3	410.93	172.4	480.49	2.2011	2.3480	2.3381	1.4227	10.5761	11.2819	11.2345	6.8361	1.2721	1.3570	1.3513	0.8222
4	422.04	68.9	494.59	2.1753	2.2131	2.2100	1.2160	10.7591	10.9457	10.9304	6.0140	1.2941	1.3165	1.3147	0.7234
5	422.04	101.4	491.19	2.1837	2.2486	2.2437	1.3211	10.7260	11.0448	11.0206	6.4891	1.2901	1.3285	1.3255	0.7805
6	422.04	103.4	490.98	2.1901	2.2568	2.2517	1.3312	10.7531	11.0803	11.0556	6.5360	1.2934	1.3327	1.3298	0.7861
7	422.04	172.4	486.28	2.2001	2.3276	2.3183	1.4136	10.6985	11.3189	11.2736	6.8740	1.2868	1.3614	1.3560	0.8268
8	422.04	344.7	479.32	2.1882	2.4884	2.4652	1.5157	10.4884	11.9273	11.8164	7.2651	1.2615	1.4346	1.4213	0.8738
9	433.15	68.9	500.42	2.1433	2.1752	2.1723	1.2062	10.7257	10.8852	10.8704	6.0363	1.2901	1.3093	1.3075	0.7260
10	433.15	103.4	496.85	2.1535	2.2110	2.2062	1.3061	10.6999	10.9854	10.9615	6.4894	1.2870	1.3213	1.3184	0.7805
11	433.15	172.4	492.20	2.1640	2.2751	2.2663	1.3749	10.6512	11.1982	11.1547	6.7674	1.2811	1.3469	1.3417	0.8140
12	433.15	344.7	485.32	2.1650	2.4260	2.4044	1.4551	10.5071	11.7739	11.6692	7.0620	1.2638	1.4162	1.4036	0.8494
13	444.26	68.9	506.29	2.0973	2.1241	2.1213	1.1851	10.6186	10.7544	10.7401	5.9999	1.2772	1.2935	1.2918	0.7217
14	444.26	103.4	502.73	2.1109	2.1604	2.1559	1.2780	10.6120	10.8612	10.8382	6.4250	1.2764	1.3064	1.3036	0.7728
15	444.26	172.4	498.11	2.1206	2.2177	2.2093	1.3335	10.5631	11.0466	11.0047	6.6424	1.2705	1.3287	1.3236	0.7989
16	444.26	344.7	491.36	2.1207	2.3489	2.3287	1.3837	10.4202	11.5414	11.4420	6.7989	1.2533	1.3882	1.3762	0.8178
17	444.26	517.1	486.83	2.1099	2.4915	2.4547	1.4609	10.2715	12.1293	11.9500	7.1122	1.2354	1.4589	1.4373	0.8555
18	455.37	68.9	512.21	2.0379	2.0604	2.0577	1.1528	10.4385	10.5536	10.5397	5.9045	1.2555	1.2694	1.2677	0.7102
19	455.37	103.4	508.64	2.0543	2.0970	2.0927	1.2388	10.4489	10.6665	10.6442	6.3010	1.2568	1.2830	1.2803	0.7579
20	455.37	172.4	504.07	2.0621	2.1471	2.1391	1.2811	10.3945	10.8230	10.7826	6.4575	1.2502	1.3018	1.2969	0.7767

21	455.37	344.7	497.40	2.0661	2.2665	2.2474	1.3105	10.2766	11.2736	11.1788	6.5182	1.2361	1.3560	1.3446	0.7840
22	455.37	517.1	492.99	2.0586	2.3914	2.3574	1.3596	10.1488	11.7897	11.6219	6.7026	1.2207	1.4181	1.3979	0.8062
23	455.37	689.5	489.47	2.0278	2.5170	2.4613	1.4383	9.9257	12.3199	12.0472	7.0399	1.1939	1.4818	1.4490	0.8468
24	466.48	68.9	518.12	1.9741	1.9928	1.9902	1.1179	10.2283	10.3252	10.3118	5.7919	1.2303	1.2419	1.2403	0.6966
25	466.48	103.4	514.60	1.9844	2.0213	2.0171	1.1887	10.2118	10.4016	10.3800	6.1170	1.2283	1.2511	1.2485	0.7357
26	466.48	172.4	510.07	1.9895	2.0640	2.0564	1.2180	10.1476	10.5281	10.4889	6.2124	1.2205	1.2663	1.2616	0.7472
27	466.48	344.7	503.44	2.0025	2.1794	2.1613	1.2355	10.0817	10.9718	10.8810	6.2201	1.2126	1.3197	1.3088	0.7481
28	466.48	517.1	499.16	1.9934	2.2855	2.2538	1.2574	9.9501	11.4085	11.2503	6.2763	1.1968	1.3722	1.3532	0.7549
29	466.48	689.5	495.76	1.9709	2.3958	2.3453	1.3086	9.7708	11.8777	11.6270	6.4875	1.1752	1.4286	1.3985	0.7803
30	477.59	68.9	524.08	1.8979	1.9134	1.9109	1.0722	9.9466	10.0275	10.0145	5.6192	1.1964	1.2061	1.2045	0.6759
31	477.59	103.4	520.60	1.9020	1.9337	1.9297	1.1281	9.9016	10.0670	10.0460	5.8728	1.1910	1.2109	1.2083	0.7064
32	477.59	172.4	516.03	1.9200	1.9856	1.9782	1.1610	9.9077	10.2461	10.2082	5.9912	1.1917	1.2324	1.2278	0.7206
33	477.59	344.7	509.52	1.9229	2.0795	2.0623	1.1506	9.7977	10.5953	10.5081	5.8625	1.1785	1.2744	1.2639	0.7051
34	477.59	517.1	505.33	1.9166	2.1745	2.1448	1.1544	9.6853	10.9884	10.8384	5.8334	1.1649	1.3217	1.3036	0.7016
35	477.59	689.5	502.01	1.9040	2.2763	2.2299	1.1874	9.5584	11.4275	11.1945	5.9610	1.1497	1.3745	1.3465	0.7170
36	477.59	1034	496.39	1.8481	2.5122	2.4052	1.3624	9.1736	12.4705	11.9390	6.7630	1.1034	1.4999	1.4360	0.8134
37	488.71	68.9	530.04	1.8180	1.8305	1.8281	1.0240	9.6358	9.7026	9.6899	5.4277	1.1590	1.1670	1.1655	0.6528
38	488.71	103.4	526.56	1.8237	1.8510	1.8471	1.0733	9.6028	9.7467	9.7262	5.6518	1.1550	1.1723	1.1699	0.6798
39	488.71	172.4	522.03	1.8375	1.8952	1.8881	1.0937	9.5921	9.8935	9.8566	5.7093	1.1537	1.1900	1.1855	0.6867
40	488.71	344.7	515.57	1.8449	1.9840	1.9677	1.0724	9.5118	10.2289	10.1447	5.5291	1.1441	1.2303	1.2202	0.6650
41	488.71	517.1	511.45	1.8386	2.0673	2.0393	1.0588	9.4034	10.5731	10.4302	5.4155	1.1310	1.2717	1.2545	0.6514
42	488.71	689.5	508.22	1.8308	2.1593	2.1163	1.0744	9.3047	10.9739	10.7554	5.4605	1.1192	1.3199	1.2936	0.6568
43	488.71	1034	502.90	1.7890	2.3612	2.2685	1.1877	8.9967	11.8744	11.4082	5.9727	1.0821	1.4282	1.3722	0.7184
44	499.82	68.9	536.00	1.7344	1.7445	1.7422	0.9732	9.2961	9.3503	9.3379	5.2162	1.1181	1.1246	1.1232	0.6274
45	499.82	103.4	532.51	1.7415	1.7650	1.7612	1.0162	9.2739	9.3987	9.3787	5.4112	1.1155	1.1305	1.1281	0.6509
46	499.82	172.4	528.03	1.7506	1.8015	1.7947	1.0243	9.2437	9.5124	9.4765	5.4084	1.1118	1.1441	1.1398	0.6505
47	499.82	344.7	521.61	1.7608	1.8848	1.8692	0.9926	9.1845	9.8311	9.7497	5.1777	1.1047	1.1825	1.1727	0.6228
48	499.82	517.1	517.54	1.7603	1.9640	1.9375	0.9705	9.1100	10.1643	10.0274	5.0224	1.0957	1.2226	1.2061	0.6041
49	499.82	689.5	514.39	1.7538	2.0452	2.0051	0.9692	9.0213	10.5202	10.3138	4.9857	1.0851	1.2654	1.2405	0.5997
50	499.82	1034	509.31	1.7172	2.2165	2.1342	1.0311	8.7460	11.2890	10.8700	5.2514	1.0520	1.3578	1.3074	0.6316

51	499.82	1379	504.66	1.6557	2.4387	2.2604	1.2314	8.3559	12.3070	11.4074	6.2142	1.0050	1.4803	1.3721	0.7474
52	510.93	68.9	541.91	1.6552	1.6631	1.6609	0.9274	8.9697	9.0128	9.0006	5.0259	1.0789	1.0840	1.0826	0.6045
53	510.93	103.4	538.43	1.6636	1.6836	1.6799	0.9643	8.9571	9.0649	9.0453	5.1922	1.0774	1.0903	1.0880	0.6245
54	510.93	172.4	533.98	1.6677	1.7126	1.7060	0.9606	8.9051	9.1448	9.1097	5.1297	1.0711	1.0999	1.0957	0.6170
55	510.93	344.7	527.61	1.6793	1.7900	1.7751	0.9192	8.8599	9.4443	9.3654	4.8497	1.0657	1.1360	1.1265	0.5833
56	510.93	517.1	523.62	1.6744	1.8565	1.8314	0.8808	8.7674	9.7212	9.5895	4.6119	1.0545	1.1693	1.1534	0.5547
57	510.93	689.5	520.52	1.6746	1.9344	1.8967	0.8715	8.7163	10.0688	9.8726	4.5361	1.0484	1.2111	1.1875	0.5456
58	510.93	1034	515.61	1.6485	2.0884	2.0140	0.9001	8.4998	10.7677	10.3845	4.6410	1.0223	1.2951	1.2490	0.5582
59	510.93	1379	511.33	1.5966	2.2677	2.1222	1.0234	8.1638	11.5955	10.8515	5.2329	0.9819	1.3947	1.3052	0.6294
60	522.04	68.9	547.83	1.5725	1.5786	1.5764	0.8787	8.6147	8.6478	8.6359	4.8135	1.0362	1.0402	1.0387	0.5790
61	522.04	103.4	544.35	1.5819	1.5989	1.5954	0.9097	8.6108	8.7035	8.6843	4.9520	1.0357	1.0468	1.0445	0.5956
62	522.04	172.4	539.90	1.5886	1.6282	1.6219	0.9025	8.5768	8.7907	8.7564	4.8724	1.0316	1.0573	1.0532	0.5861
63	522.04	344.7	533.56	1.6005	1.6997	1.6853	0.8517	8.5394	9.0689	8.9922	4.5444	1.0271	1.0908	1.0816	0.5466
64	522.04	517.1	529.62	1.5979	1.7613	1.7374	0.8057	8.4628	9.3283	9.2014	4.2671	1.0179	1.1220	1.1067	0.5132
65	522.04	689.5	526.60	1.5944	1.8271	1.7915	0.7807	8.3960	9.6215	9.4341	4.1114	1.0099	1.1573	1.1347	0.4945
66	522.04	1034	521.86	1.5707	1.9611	1.8931	0.7774	8.1968	10.2341	9.8791	4.0570	0.9859	1.2310	1.1882	0.4880
67	522.04	1379	517.79	1.5379	2.1228	1.9982	0.8589	7.9632	10.9917	10.3466	4.4472	0.9578	1.3221	1.2445	0.5349
68	533.15	68.9	553.70	1.4941	1.4985	1.4964	0.8343	8.2730	8.2972	8.2855	4.6197	0.9951	0.9980	0.9966	0.5557
69	533.15	103.4	550.22	1.5043	1.5187	1.5153	0.8599	8.2770	8.3561	8.3373	4.7315	0.9955	1.0051	1.0028	0.5691
70	533.15	172.4	545.77	1.5133	1.5483	1.5421	0.8494	8.2593	8.4502	8.4166	4.6360	0.9934	1.0164	1.0123	0.5576
71	533.15	344.7	539.52	1.5166	1.6057	1.5919	0.7821	8.1825	8.6633	8.5885	4.2195	0.9842	1.0420	1.0330	0.5075
72	533.15	517.1	535.62	1.5150	1.6621	1.6392	0.7288	8.1148	8.9026	8.7797	3.9037	0.9760	1.0708	1.0560	0.4695
73	533.15	689.5	532.64	1.5142	1.7234	1.6897	0.6967	8.0653	9.1797	8.9999	3.7109	0.9701	1.1041	1.0825	0.4463
74	533.15	1034	528.03	1.4951	1.8437	1.7808	0.6706	7.8944	9.7354	9.4032	3.5407	0.9495	1.1710	1.1310	0.4259
75	533.15	1379	524.17	1.4670	1.9826	1.8727	0.7117	7.6895	10.3920	9.8162	3.7306	0.9249	1.2499	1.1807	0.4487
76	533.15	2068	516.57	1.3494	2.3722	1.8483	1.0967	6.9708	12.2541	9.5477	5.6651	0.8384	1.4739	1.1484	0.6814
77	544.26	68.9	559.53	1.4198	1.4227	1.4207	0.7941	7.9445	7.9606	7.9492	4.4431	0.9556	0.9575	0.9561	0.5344
78	544.26	103.4	556.05	1.4307	1.4428	1.4395	0.8146	7.9555	8.0226	8.0041	4.5295	0.9569	0.9649	0.9627	0.5448
79	544.26	172.4	551.65	1.4340	1.4649	1.4589	0.7935	7.9106	8.0809	8.0479	4.3772	0.9515	0.9720	0.9680	0.5265
80	544.26	344.7	545.39	1.4437	1.5239	1.5105	0.7257	7.8737	8.3112	8.2381	3.9577	0.9470	0.9997	0.9909	0.4760

81	544.26	517.1	541.53	1.4421	1.5748	1.5528	0.6657	7.8093	8.5283	8.4090	3.6047	0.9393	1.0258	1.0114	0.4336
82	544.26	689.5	538.60	1.4425	1.6313	1.5992	0.6268	7.7695	8.7863	8.6130	3.3757	0.9345	1.0568	1.0360	0.4060
83	544.26	1034	534.11	1.4236	1.7366	1.6779	0.5788	7.6033	9.2753	8.9618	3.0915	0.9145	1.1156	1.0779	0.3718
84	544.26	1379	530.38	1.4069	1.8654	1.7665	0.5970	7.4619	9.8935	9.3693	3.1665	0.8975	1.1900	1.1269	0.3809
85	544.26	2068	523.54	1.3194	2.1823	1.8642	0.8337	6.9073	11.4252	9.7596	4.3647	0.8308	1.3742	1.1739	0.5250
86	555.37	68.9	565.32	1.3495	1.3511	1.3491	0.7575	7.6291	7.6380	7.6267	4.2826	0.9176	0.9187	0.9173	0.5151
87	555.37	103.4	561.84	1.3610	1.3710	1.3677	0.7734	7.6466	7.7027	7.6845	4.3450	0.9197	0.9265	0.9243	0.5226
88	555.37	172.4	557.43	1.3661	1.3933	1.3875	0.7497	7.6151	7.7669	7.7344	4.1793	0.9159	0.9342	0.9303	0.5027
89	555.37	344.7	551.23	1.3737	1.4460	1.4330	0.6742	7.5721	7.9707	7.8993	3.7164	0.9108	0.9587	0.9501	0.4470
90	555.37	517.1	547.37	1.3790	1.4991	1.4779	0.6155	7.5479	8.2056	8.0896	3.3693	0.9079	0.9870	0.9730	0.4053
91	555.37	689.5	544.51	1.3718	1.5427	1.5119	0.5626	7.4697	8.4002	8.2327	3.0633	0.8984	1.0104	0.9902	0.3684
92	555.37	1034	540.11	1.3574	1.6398	1.5846	0.5015	7.3315	8.8564	8.5587	2.7085	0.8818	1.0652	1.0294	0.3258
93	555.37	1379	536.50	1.3455	1.7560	1.6657	0.4977	7.2185	9.4208	8.9366	2.6699	0.8682	1.1331	1.0749	0.3211
94	555.37	2068	530.17	1.2782	2.0256	1.7815	0.6387	6.7768	10.7389	9.4451	3.3861	0.8151	1.2917	1.1360	0.4073
95	566.48	68.9	571.03	1.2904	1.2908	1.2888	0.7317	7.3684	7.3708	7.3597	4.1785	0.8863	0.8866	0.8852	0.5026
96	566.48	103.4	567.59	1.2949	1.3031	1.2999	0.7359	7.3498	7.3961	7.3782	4.1768	0.8840	0.8896	0.8874	0.5024
97	566.48	172.4	563.18	1.3016	1.3256	1.3199	0.7101	7.3305	7.4656	7.4337	3.9990	0.8817	0.8980	0.8941	0.4810
98	566.48	344.7	556.97	1.3142	1.3796	1.3670	0.6350	7.3200	7.6838	7.6138	3.5366	0.8804	0.9242	0.9158	0.4254
99	566.48	517.1	553.20	1.3102	1.4192	1.3987	0.5626	7.2479	7.8509	7.7377	3.1125	0.8718	0.9443	0.9307	0.3744
100	566.48	689.5	550.34	1.3101	1.4652	1.4357	0.5114	7.2099	8.0637	7.9013	2.8143	0.8672	0.9699	0.9504	0.3385
101	566.48	1034	546.02	1.2975	1.5532	1.5011	0.4379	7.0849	8.4809	8.1965	2.3908	0.8522	1.0201	0.9859	0.2876
102	566.48	1379	542.54	1.2855	1.6551	1.5718	0.4129	6.9743	8.9798	8.5275	2.2402	0.8389	1.0801	1.0257	0.2694
103	566.48	2068	536.58	1.2312	1.8887	1.6863	0.4850	6.6063	10.1343	9.0482	2.6026	0.7946	1.2189	1.0883	0.3130
104	566.48	2758	530.42	1.1396	2.2432	1.5078	0.8276	6.0448	11.8982	7.9974	4.3898	0.7271	1.4311	0.9619	0.5280
105	577.59	68.9	576.69	1.2347	1.2341	1.2322	0.7088	7.1203	7.1168	7.1059	4.0877	0.8564	0.8560	0.8547	0.4917
106	577.59	103.4	573.25	1.2398	1.2463	1.2433	0.7092	7.1072	7.1446	7.1270	4.0657	0.8548	0.8593	0.8572	0.4890
107	577.59	172.4	568.85	1.2479	1.2690	1.2635	0.6816	7.0989	7.2189	7.1874	3.8772	0.8538	0.8683	0.8645	0.4663
108	577.59	344.7	562.68	1.2575	1.3166	1.3044	0.5999	7.0759	7.4084	7.3396	3.3753	0.8511	0.8911	0.8828	0.4060
109	577.59	517.1	558.90	1.2589	1.3580	1.3382	0.5295	7.0362	7.5901	7.4795	2.9595	0.8463	0.9129	0.8996	0.3560
110	577.59	689.5	556.09	1.2574	1.3986	1.3702	0.4726	6.9921	7.7774	7.6195	2.6281	0.8410	0.9355	0.9165	0.3161

111	577.59	1034	551.86	1.2445	1.4769	1.4274	0.3873	6.8678	8.1501	7.8771	2.1375	0.8261	0.9803	0.9475	0.2571
112	577.59	1379	548.46	1.2365	1.5710	1.4933	0.3497	6.7819	8.6165	8.1903	1.9181	0.8157	1.0364	0.9851	0.2307
113	577.59	2068	542.79	1.1918	1.7766	1.6015	0.3709	6.4688	9.6434	8.6929	2.0132	0.7781	1.1599	1.0456	0.2422
114	577.59	2758	537.34	1.1180	2.0593	1.6155	0.5786	6.0072	11.0652	8.6809	3.1092	0.7225	1.3309	1.0441	0.3740
115	577.59	3447	530.88	0.9880	2.5237	1.2984	1.1144	5.2453	13.3976	6.8929	5.9160	0.6309	1.6115	0.8291	0.7116
116	588.71	68.9	582.27	1.1896	1.1881	1.1862	0.6957	6.9266	6.9178	6.9070	4.0509	0.8331	0.8321	0.8308	0.4872
117	588.71	103.4	578.83	1.1952	1.2003	1.1973	0.6929	6.9185	6.9478	6.9304	4.0105	0.8321	0.8357	0.8336	0.4824
118	588.71	172.4	574.43	1.2047	1.2232	1.2178	0.6638	6.9202	7.0266	6.9956	3.8131	0.8324	0.8452	0.8414	0.4586
119	588.71	344.7	568.30	1.2110	1.2645	1.2526	0.5760	6.8821	7.1862	7.1186	3.2735	0.8278	0.8644	0.8562	0.3937
120	588.71	517.1	564.57	1.2097	1.3000	1.2808	0.5004	6.8297	7.3394	7.2310	2.8251	0.8215	0.8828	0.8697	0.3398
121	588.71	689.5	561.80	1.2061	1.3349	1.3075	0.4382	6.7756	7.4995	7.3455	2.4616	0.8150	0.9020	0.8835	0.2961
122	588.71	1034	557.60	1.1987	1.4106	1.3634	0.3493	6.6840	7.8653	7.6021	1.9474	0.8039	0.9460	0.9144	0.2342
123	588.71	1379	554.29	1.1920	1.4960	1.4230	0.2996	6.6073	8.2920	7.8875	1.6608	0.7947	0.9974	0.9487	0.1998
124	588.71	2068	548.88	1.1517	1.6762	1.5206	0.2793	6.3212	9.2004	8.3464	1.5329	0.7603	1.1066	1.0039	0.1844
125	588.71	2758	543.88	1.0931	1.9144	1.5771	0.4029	5.9450	10.4122	8.5778	2.1914	0.7151	1.2524	1.0317	0.2636
126	588.71	3447	538.51	1.0015	2.2614	1.4296	0.7294	5.3932	12.1779	7.6983	3.9278	0.6487	1.4648	0.9259	0.4724
127	599.82	103.4	584.37	1.1536	1.1574	1.1544	0.6790	6.7413	6.7633	6.7461	3.9679	0.8108	0.8135	0.8114	0.4773
128	599.82	172.4	579.96	1.1643	1.1805	1.1752	0.6489	6.7523	6.8463	6.8157	3.7634	0.8122	0.8235	0.8198	0.4527
129	599.82	344.7	573.88	1.1669	1.2154	1.2038	0.5555	6.6967	6.9752	6.9086	3.1880	0.8055	0.8390	0.8310	0.3834
130	599.82	517.1	570.15	1.1700	1.2524	1.2338	0.4824	6.6708	7.1406	7.0342	2.7504	0.8024	0.8589	0.8461	0.3308
131	599.82	689.5	567.42	1.1638	1.2816	1.2551	0.4152	6.6036	7.2723	7.1218	2.3557	0.7943	0.8747	0.8566	0.2833
132	599.82	1034	563.27	1.1604	1.3541	1.3089	0.3230	6.5361	7.6273	7.3726	1.8196	0.7862	0.9174	0.8868	0.2189
133	599.82	1379	560.04	1.1528	1.4300	1.3610	0.2619	6.4560	8.0085	7.6222	1.4670	0.7765	0.9633	0.9168	0.1764
134	599.82	2068	554.79	1.1231	1.5967	1.4559	0.2167	6.2311	8.8586	8.0771	1.2024	0.7495	1.0655	0.9715	0.1446
135	599.82	2758	550.14	1.0758	1.8030	1.5249	0.2820	5.9181	9.9189	8.3890	1.5514	0.7118	1.1930	1.0090	0.1866
136	599.82	3447	545.44	1.0030	2.0779	1.5038	0.4838	5.4705	11.3334	8.2022	2.6389	0.6580	1.3632	0.9866	0.3174
137	599.82	4137	540.49	0.8733	2.4330	1.5270	0.8223	4.7201	13.1503	8.2534	4.4445	0.5677	1.5817	0.9927	0.5346
138	610.93	103.4	589.82	1.1220	1.1246	1.1217	0.6746	6.6177	6.6330	6.6159	3.9790	0.7960	0.7978	0.7958	0.4786
139	610.93	172.4	585.46	1.1265	1.1406	1.1354	0.6366	6.5952	6.6779	6.6476	3.7272	0.7933	0.8032	0.7996	0.4483
140	610.93	344.7	579.38	1.1326	1.1766	1.1653	0.5454	6.5618	6.8170	6.7513	3.1598	0.7892	0.8199	0.8120	0.3801

141	610.93	517.1	575.64	1.1396	1.2149	1.1968	0.4750	6.5600	6.9937	6.8891	2.7341	0.7890	0.8412	0.8286	0.3289
142	610.93	689.5	572.92	1.1378	1.2458	1.2201	0.4104	6.5188	7.1375	6.9901	2.3511	0.7841	0.8585	0.8408	0.2828
143	610.93	1034	568.85	1.1297	1.3073	1.2639	0.3081	6.4263	7.4366	7.1894	1.7527	0.7730	0.8945	0.8647	0.2108
144	610.93	1379	565.70	1.1195	1.3731	1.3076	0.2361	6.3328	7.7677	7.3970	1.3356	0.7617	0.9343	0.8897	0.1606
145	610.93	2068	560.62	1.0937	1.5236	1.3943	0.1671	6.1318	8.5418	7.8168	0.9366	0.7375	1.0274	0.9402	0.1127
146	610.93	2758	556.22	1.0560	1.7065	1.4669	0.1910	5.8737	9.4920	8.1594	1.0622	0.7065	1.1417	0.9814	0.1278
147	610.93	3447	551.98	0.9940	1.9319	1.4896	0.3102	5.4866	10.6638	8.2220	1.7121	0.6599	1.2826	0.9889	0.2059
148	610.93	4137	547.62	0.9079	2.2252	1.4967	0.5389	4.9720	12.1855	8.1960	2.9512	0.5980	1.4657	0.9858	0.3550
149	610.93	4826	543.55	0.7424	2.5167	1.6682	0.7792	4.0353	13.6795	9.0677	4.2353	0.4854	1.6454	1.0907	0.5094
150	622.04	103.4	595.19	1.1000	1.1015	1.0987	0.6792	6.5471	6.5562	6.5393	4.0426	0.7875	0.7886	0.7865	0.4862
151	622.04	172.4	590.83	1.1056	1.1179	1.1128	0.6410	6.5324	6.6048	6.5748	3.7870	0.7857	0.7944	0.7908	0.4555
152	622.04	344.7	584.79	1.1077	1.1477	1.1366	0.5451	6.4775	6.7115	6.6466	3.1877	0.7791	0.8073	0.7994	0.3834
153	622.04	517.1	581.10	1.1109	1.1799	1.1622	0.4703	6.4557	6.8565	6.7535	2.7332	0.7765	0.8247	0.8123	0.3287
154	622.04	689.5	578.37	1.1131	1.2123	1.1873	0.4085	6.4380	7.0114	6.8668	2.3628	0.7744	0.8433	0.8259	0.2842
155	622.04	1034	574.34	1.1067	1.2700	1.2280	0.3039	6.3565	7.2939	7.0532	1.7457	0.7645	0.8773	0.8484	0.2100
156	622.04	1379	571.24	1.0999	1.3327	1.2701	0.2288	6.2830	7.6128	7.2554	1.3072	0.7557	0.9157	0.8727	0.1572
157	622.04	2068	566.33	1.0731	1.4651	1.3451	0.1370	6.0773	8.2972	7.6174	0.7761	0.7310	0.9980	0.9162	0.0934
158	622.04	2758	562.13	1.0413	1.6278	1.4155	0.1284	5.8534	9.1504	7.9572	0.7220	0.7040	1.1006	0.9571	0.0868
159	622.04	3447	558.19	0.9946	1.8254	1.4607	0.1978	5.5520	10.1890	8.1535	1.1043	0.6678	1.2255	0.9807	0.1328
160	622.04	4137	554.29	0.9266	2.0663	1.4821	0.3436	5.1359	11.4533	8.2149	1.9043	0.6177	1.3776	0.9881	0.2290
161	622.04	4826	550.60	0.8075	2.3170	1.5643	0.5140	4.4462	12.7572	8.6130	2.8302	0.5348	1.5344	1.0360	0.3404
162	622.04	5516	547.37	0.6414	2.5428	1.7477	0.6495	3.5111	13.9183	9.5664	3.5551	0.4223	1.6741	1.1506	0.4276
163	633.15	103.4	600.52	1.0803	1.0809	1.0781	0.6854	6.4874	6.4910	6.4742	4.1158	0.7803	0.7807	0.7787	0.4950
164	633.15	172.4	596.16	1.0870	1.0975	1.0925	0.6472	6.4800	6.5429	6.5132	3.8583	0.7794	0.7870	0.7834	0.4641
165	633.15	344.7	590.12	1.0920	1.1283	1.1174	0.5543	6.4438	6.6584	6.5942	3.2709	0.7751	0.8009	0.7931	0.3934
166	633.15	517.1	586.42	1.0985	1.1618	1.1444	0.4827	6.4419	6.8128	6.7113	2.8304	0.7748	0.8194	0.8072	0.3404
167	633.15	689.5	583.74	1.0970	1.1882	1.1639	0.4166	6.4038	6.9361	6.7939	2.4318	0.7702	0.8343	0.8172	0.2925
168	633.15	1034	579.75	1.0915	1.2418	1.2013	0.3100	6.3278	7.1993	6.9644	1.7973	0.7611	0.8659	0.8377	0.2162
169	633.15	1379	576.69	1.0868	1.3010	1.2410	0.2321	6.2675	7.5028	7.1568	1.3387	0.7538	0.9024	0.8608	0.1610
170	633.15	2068	571.91	1.0625	1.4213	1.3089	0.1258	6.0764	8.1287	7.4859	0.7196	0.7309	0.9777	0.9004	0.0866

171	633.15	2758	567.88	1.0362	1.5683	1.3765	0.0933	5.8842	8.9063	7.8171	0.5297	0.7078	1.0712	0.9402	0.0637
172	633.15	3447	564.19	0.9962	1.7399	1.4266	0.1219	5.6207	9.8164	8.0487	0.6880	0.6761	1.1807	0.9681	0.0827
173	633.15	4137	560.62	0.9406	1.9435	1.4600	0.2098	5.2733	10.8954	8.1849	1.1764	0.6343	1.3105	0.9845	0.1415
174	633.15	4826	557.23	0.8543	2.1631	1.5130	0.3284	4.7604	12.0531	8.4308	1.8297	0.5726	1.4497	1.0141	0.2201
175	633.15	5516	554.16	0.7315	2.3714	1.6341	0.4340	4.0537	13.1414	9.0557	2.4050	0.4876	1.5806	1.0892	0.2893
176	633.15	6205	551.56	0.5836	2.5493	1.7904	0.4945	3.2190	14.0612	9.8753	2.7273	0.3872	1.6913	1.1878	0.3280
177	644.26	103.4	605.77	1.0698	1.0695	1.0668	0.6998	6.4803	6.4787	6.4621	4.2394	0.7794	0.7793	0.7773	0.5099
178	644.26	172.4	601.40	1.0774	1.0864	1.0815	0.6621	6.4795	6.5338	6.5042	3.9816	0.7793	0.7859	0.7823	0.4789
179	644.26	344.7	595.36	1.0852	1.1182	1.1075	0.5724	6.4606	6.6574	6.5939	3.4080	0.7771	0.8008	0.7931	0.4099
180	644.26	517.1	591.71	1.0876	1.1456	1.1287	0.4970	6.4352	6.7787	6.6784	2.9409	0.7740	0.8153	0.8033	0.3537
181	644.26	689.5	589.03	1.0893	1.1733	1.1495	0.4340	6.4165	6.9112	6.7711	2.5566	0.7718	0.8313	0.8144	0.3075
182	644.26	1034	585.08	1.0839	1.2226	1.1833	0.3258	6.3415	7.1531	6.9232	1.9061	0.7628	0.8604	0.8327	0.2293
183	644.26	1379	582.06	1.0804	1.2779	1.2202	0.2455	6.2885	7.4384	7.1025	1.4287	0.7564	0.8947	0.8543	0.1718
184	644.26	2068	577.36	1.0627	1.3923	1.2863	0.1326	6.1357	8.0389	7.4268	0.7655	0.7380	0.9669	0.8933	0.0921
185	644.26	2758	573.50	1.0362	1.5215	1.3456	0.0770	5.9424	8.7257	7.7171	0.4417	0.7147	1.0495	0.9282	0.0531
186	644.26	3447	570.02	0.9997	1.6708	1.3941	0.0736	5.6984	9.5240	7.9464	0.4195	0.6854	1.1455	0.9558	0.0505
187	644.26	4137	566.71	0.9537	1.8470	1.4338	0.1203	5.4049	10.4669	8.1254	0.6819	0.6501	1.2589	0.9773	0.0820
188	644.26	4826	563.56	0.8871	2.0386	1.4778	0.1963	4.9993	11.4889	8.3282	1.1061	0.6013	1.3819	1.0017	0.1330
189	644.26	5516	560.67	0.7956	2.2291	1.5613	0.2735	4.4604	12.4977	8.7539	1.5333	0.5365	1.5032	1.0529	0.1844
190	644.26	6205	558.15	0.6778	2.3964	1.6777	0.3205	3.7830	13.3756	9.3639	1.7890	0.4550	1.6088	1.1263	0.2152
191	644.26	6895	556.05	0.5424	2.5312	1.7953	0.3232	3.0158	14.0746	9.9829	1.7969	0.3627	1.6929	1.2007	0.2161
∑				270.52	334.09	310.97	139.46	1450.83	1795.18	1668.90	741.22	174.50	215.92	200.73	89.15
Average (Overall)				**1.4163**	**1.7492**	**1.6281**	**0.7301**	**7.5960**	**9.3988**	**8.7377**	**3.8807**	**0.9136**	**1.1305**	**1.0510**	**0.4668**

Table C-14 Refrigerant (12) [17]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	263.15	25	104.35	0.5063	0.4680	0.4716	0.4649	0.5283	0.4883	0.4921	0.4851	0.0635	0.0587	0.0592	0.0584
2	273.15	25	106.94	0.5087	0.4813	0.4846	0.4837	0.5439	0.5147	0.5182	0.5173	0.0654	0.0619	0.0623	0.0622
3	283.15	25	109.49	0.5233	0.5046	0.5077	0.5118	0.5729	0.5525	0.5559	0.5603	0.0689	0.0665	0.0669	0.0674
4	293.15	25	111.99	0.5364	0.5248	0.5277	0.5359	0.6008	0.5878	0.5910	0.6001	0.0723	0.0707	0.0711	0.0722
5	303.15	25	114.44	0.5464	0.5404	0.5431	0.5548	0.6253	0.6185	0.6215	0.6350	0.0752	0.0744	0.0748	0.0764
6	313.15	25	116.86	0.5619	0.5606	0.5631	0.5778	0.6567	0.6551	0.6580	0.6752	0.0790	0.0788	0.0791	0.0812
7	323.15	25	119.23	0.5712	0.5737	0.5760	0.5933	0.6811	0.6840	0.6868	0.7074	0.0819	0.0823	0.0826	0.0851
8	333.15	25	121.57	0.5832	0.5887	0.5909	0.6104	0.7090	0.7157	0.7184	0.7420	0.0853	0.0861	0.0864	0.0892
9	343.15	25	123.86	0.5966	0.6047	0.6067	0.6280	0.7390	0.7490	0.7515	0.7779	0.0889	0.0901	0.0904	0.0936
10	353.15	25	126.11	0.6008	0.6109	0.6129	0.6357	0.7577	0.7704	0.7729	0.8017	0.0911	0.0927	0.0930	0.0964
11	363.15	25	128.34	0.6140	0.6258	0.6277	0.6518	0.7880	0.8031	0.8055	0.8364	0.0948	0.0966	0.0969	0.1006
12	373.15	25	130.53	0.6256	0.6389	0.6406	0.6658	0.8166	0.8339	0.8362	0.8690	0.0982	0.1003	0.1006	0.1045
13	263.15	50	98.41	0.5035	0.3831	0.3919	0.3545	0.4955	0.3770	0.3856	0.3489	0.0596	0.0453	0.0464	0.0420
14	273.15	50	101.03	0.5252	0.4295	0.4376	0.4130	0.5307	0.4339	0.4421	0.4173	0.0638	0.0522	0.0532	0.0502
15	283.15	50	103.60	0.5382	0.4623	0.4698	0.4560	0.5576	0.4789	0.4867	0.4724	0.0671	0.0576	0.0585	0.0568
16	293.15	50	106.11	0.5518	0.4918	0.4988	0.4941	0.5855	0.5218	0.5292	0.5243	0.0704	0.0628	0.0637	0.0631
17	303.15	50	108.59	0.5746	0.5275	0.5340	0.5372	0.6240	0.5729	0.5799	0.5833	0.0751	0.0689	0.0698	0.0702
18	313.15	50	111.01	0.5824	0.5459	0.5520	0.5618	0.6465	0.6060	0.6128	0.6236	0.0778	0.0729	0.0737	0.0750
19	323.15	50	113.39	0.5956	0.5678	0.5735	0.5890	0.6754	0.6438	0.6504	0.6679	0.0812	0.0774	0.0782	0.0803
20	333.15	50	115.74	0.6124	0.5917	0.5972	0.6174	0.7088	0.6848	0.6911	0.7146	0.0852	0.0824	0.0831	0.0860
21	343.15	50	118.04	0.6210	0.6063	0.6114	0.6358	0.7329	0.7156	0.7217	0.7505	0.0882	0.0861	0.0868	0.0903
22	353.15	50	120.30	0.6306	0.6209	0.6257	0.6537	0.7586	0.7469	0.7528	0.7863	0.0912	0.0898	0.0905	0.0946
23	363.15	50	122.52	0.6402	0.6346	0.6393	0.6702	0.7843	0.7775	0.7832	0.8211	0.0943	0.0935	0.0942	0.0988
24	373.15	50	124.71	0.6487	0.6466	0.6511	0.6845	0.8090	0.8064	0.8120	0.8536	0.0973	0.0970	0.0977	0.1027
25	283.15	100	97.58	0.5372	0.3346	0.3520	0.2874	0.5242	0.3265	0.3435	0.2804	0.0630	0.0393	0.0413	0.0337

26	293.15	100	100.13	0.5627	0.3960	0.4121	0.3679	0.5634	0.3965	0.4127	0.3684	0.0678	0.0477	0.0496	0.0443
27	303.15	100	102.63	0.5892	0.4517	0.4667	0.4399	0.6047	0.4635	0.4790	0.4515	0.0727	0.0558	0.0576	0.0543
28	313.15	100	105.09	0.6141	0.5003	0.5144	0.5023	0.6453	0.5257	0.5406	0.5279	0.0776	0.0632	0.0650	0.0635
29	323.15	100	107.48	0.6239	0.5296	0.5429	0.5434	0.6706	0.5692	0.5835	0.5841	0.0807	0.0685	0.0702	0.0703
30	333.15	100	109.84	0.6395	0.5614	0.5739	0.5852	0.7024	0.6166	0.6303	0.6428	0.0845	0.0742	0.0758	0.0773
31	343.15	100	112.16	0.6587	0.5941	0.6060	0.6266	0.7388	0.6663	0.6796	0.7028	0.0889	0.0801	0.0817	0.0845
32	353.15	100	114.43	0.6695	0.6161	0.6274	0.6559	0.7661	0.7050	0.7179	0.7506	0.0921	0.0848	0.0864	0.0903
33	363.15	100	116.67	0.6812	0.6373	0.6481	0.6834	0.7948	0.7436	0.7561	0.7973	0.0956	0.0894	0.0909	0.0959
34	373.15	100	118.87	0.6927	0.6568	0.6671	0.7082	0.8234	0.7808	0.7929	0.8418	0.0990	0.0939	0.0954	0.1013
35	303.15	200	96.46	0.5920	0.2527	0.2875	0.1726	0.5711	0.2437	0.2773	0.1665	0.0687	0.0293	0.0334	0.0200
36	313.15	200	98.96	0.6154	0.3301	0.3625	0.2816	0.6089	0.3266	0.3587	0.2787	0.0732	0.0393	0.0431	0.0335
37	323.15	200	101.41	0.6520	0.4110	0.4414	0.3893	0.6612	0.4168	0.4476	0.3948	0.0795	0.0501	0.0538	0.0475
38	333.15	200	103.80	0.6748	0.4703	0.4988	0.4714	0.7005	0.4882	0.5178	0.4893	0.0843	0.0587	0.0623	0.0589
39	343.15	200	106.15	0.6935	0.5193	0.5462	0.5398	0.7362	0.5512	0.5798	0.5730	0.0885	0.0663	0.0697	0.0689
40	353.15	200	108.45	0.7062	0.5572	0.5827	0.5944	0.7659	0.6043	0.6320	0.6446	0.0921	0.0727	0.0760	0.0775
41	363.15	200	110.71	0.7223	0.5946	0.6188	0.6460	0.7996	0.6582	0.6850	0.7151	0.0962	0.0792	0.0824	0.0860
42	373.15	200	112.92	0.7293	0.6195	0.6426	0.6830	0.8235	0.6996	0.7256	0.7713	0.0990	0.0841	0.0873	0.0928
43	393.15	200	117.24	0.7434	0.6620	0.6831	0.7447	0.8715	0.7761	0.8008	0.8730	0.1048	0.0933	0.0963	0.1050
44	413.15	200	121.42	0.7603	0.6997	0.7192	0.7961	0.9231	0.8496	0.8733	0.9666	0.1110	0.1022	0.1050	0.1163
45	303.15	300	92.66	0.5628	0.0011	0.0569	0.1733	0.5214	0.0010	0.0528	0.1606	0.0627	0.0001	0.0063	0.0193
46	313.15	300	95.22	0.6184	0.1440	0.1977	0.0245	0.5889	0.1371	0.1883	0.0233	0.0708	0.0165	0.0226	0.0028
47	323.15	300	97.71	0.6561	0.2543	0.3043	0.1791	0.6411	0.2485	0.2973	0.1750	0.0771	0.0299	0.0358	0.0211
48	333.15	300	100.14	0.6846	0.3423	0.3891	0.3048	0.6856	0.3428	0.3896	0.3052	0.0825	0.0412	0.0469	0.0367
49	343.15	300	102.52	0.7129	0.4197	0.4636	0.4141	0.7309	0.4303	0.4753	0.4246	0.0879	0.0518	0.0572	0.0511
50	353.15	300	104.84	0.7264	0.4741	0.5156	0.4958	0.7616	0.4971	0.5405	0.5198	0.0916	0.0598	0.0650	0.0625
51	363.15	300	107.13	0.7462	0.5282	0.5674	0.5731	0.7994	0.5658	0.6078	0.6139	0.0961	0.0681	0.0731	0.0738
52	373.15	300	109.37	0.7587	0.5696	0.6068	0.6344	0.8298	0.6229	0.6637	0.6938	0.0998	0.0749	0.0798	0.0834
53	393.15	300	113.72	0.7780	0.6343	0.6682	0.7305	0.8847	0.7213	0.7599	0.8307	0.1064	0.0868	0.0914	0.0999
54	413.15	300	117.91	0.7846	0.6743	0.7055	0.7932	0.9251	0.7951	0.8319	0.9353	0.1113	0.0956	0.1001	0.1125
55	313.15	400	92.44	0.6063	0.0739	0.0043	0.2819	0.5604	0.0683	0.0040	0.2606	0.0674	0.0082	0.0005	0.0313

56	323.15	400	94.98	0.6540	0.0786	0.1510	0.0646	0.6212	0.0747	0.1434	0.0613	0.0747	0.0090	0.0172	0.0074
57	333.15	400	97.46	0.6983	0.2082	0.2754	0.1195	0.6805	0.2029	0.2684	0.1165	0.0818	0.0244	0.0323	0.0140
58	343.15	400	99.86	0.7223	0.3022	0.3651	0.2597	0.7213	0.3018	0.3646	0.2594	0.0868	0.0363	0.0439	0.0312
59	353.15	400	102.22	0.7471	0.3850	0.4441	0.3817	0.7637	0.3936	0.4540	0.3902	0.0919	0.0473	0.0546	0.0469
60	363.15	400	104.53	0.7695	0.4558	0.5116	0.4859	0.8043	0.4765	0.5347	0.5079	0.0967	0.0573	0.0643	0.0611
61	373.15	400	106.78	0.7756	0.5027	0.5555	0.5612	0.8282	0.5368	0.5931	0.5992	0.0996	0.0646	0.0713	0.0721
62	393.15	400	111.17	0.7995	0.5904	0.6381	0.6938	0.8887	0.6563	0.7094	0.7713	0.1069	0.0789	0.0853	0.0928
63	413.15	400	115.40	0.8157	0.6534	0.6972	0.7894	0.9414	0.7540	0.8046	0.9110	0.1132	0.0907	0.0968	0.1096
64	323.15	500	92.76	0.6448	0.1170	0.0193	0.3421	0.5982	0.1085	0.0179	0.3173	0.0719	0.0131	0.0022	0.0382
65	333.15	500	95.29	0.7023	0.0546	0.1449	0.0966	0.6693	0.0520	0.1381	0.0920	0.0805	0.0063	0.0166	0.0111
66	343.15	500	97.73	0.7321	0.1774	0.2614	0.0884	0.7155	0.1733	0.2554	0.0864	0.0861	0.0208	0.0307	0.0104
67	353.15	500	100.13	0.7669	0.2889	0.3675	0.2525	0.7678	0.2893	0.3679	0.2528	0.0924	0.0348	0.0443	0.0304
68	363.15	500	102.45	0.7789	0.3647	0.4385	0.3728	0.7979	0.3736	0.4492	0.3819	0.0960	0.0449	0.0540	0.0459
69	373.15	500	104.73	0.8006	0.4399	0.5095	0.4859	0.8385	0.4607	0.5336	0.5089	0.1009	0.0554	0.0642	0.0612
70	393.15	500	109.16	0.8274	0.5501	0.6128	0.6559	0.9032	0.6005	0.6690	0.7160	0.1086	0.0722	0.0805	0.0861
71	413.15	500	113.40	0.8315	0.6150	0.6722	0.7641	0.9430	0.6975	0.7623	0.8665	0.1134	0.0839	0.0917	0.1042
72	433.15	500	117.50	0.8336	0.6625	0.7152	0.8425	0.9795	0.7784	0.8404	0.9899	0.1178	0.0936	0.1011	0.1191
73	453.15	500	121.47	0.8344	0.6977	0.7468	0.8992	1.0135	0.8475	0.9072	1.0923	0.1219	0.1019	0.1091	0.1314
74	323.15	750	88.44	0.6187	0.6712	0.4932	1.1644	0.5471	0.5936	0.4362	1.0297	0.0658	0.0714	0.0525	0.1239
75	333.15	750	91.08	0.6923	0.3952	0.2338	0.7530	0.6306	0.3600	0.2129	0.6859	0.0758	0.0433	0.0256	0.0825
76	343.15	750	93.65	0.7564	0.1691	0.0213	0.4152	0.7084	0.1584	0.0200	0.3888	0.0852	0.0190	0.0024	0.0468
77	353.15	750	96.11	0.7893	0.0050	0.1314	0.1580	0.7587	0.0048	0.1262	0.1518	0.0913	0.0006	0.0152	0.0183
78	363.15	750	98.52	0.8224	0.1358	0.2625	0.0609	0.8102	0.1338	0.2586	0.0600	0.0975	0.0161	0.0311	0.0072
79	373.15	750	100.87	0.8499	0.2527	0.3711	0.2436	0.8572	0.2549	0.3743	0.2457	0.1031	0.0307	0.0450	0.0295
80	393.15	750	105.38	0.8726	0.4133	0.5182	0.5067	0.9195	0.4355	0.5460	0.5340	0.1106	0.0524	0.0657	0.0642
81	413.15	750	109.69	0.8797	0.5198	0.6143	0.6872	0.9650	0.5702	0.6739	0.7538	0.1161	0.0686	0.0811	0.0907
82	433.15	750	113.85	0.8868	0.6005	0.6867	0.8206	1.0096	0.6836	0.7819	0.9343	0.1214	0.0822	0.0940	0.1124
83	453.15	750	117.85	0.8807	0.6500	0.7297	0.9074	1.0380	0.7660	0.8600	1.0695	0.1248	0.0921	0.1034	0.1286
84	323.15	1000	84.95	0.5818	1.3472	1.0534	2.2161	0.4943	1.1445	0.8949	1.8827	0.0595	0.1377	0.1076	0.2264
85	333.15	1000	87.77	0.6863	0.9178	0.6584	1.5635	0.6024	0.8056	0.5779	1.3723	0.0725	0.0969	0.0695	0.1651

86	343.15	1000	90.46	0.7603	0.5918	0.3594	1.0577	0.6877	0.5353	0.3251	0.9567	0.0827	0.0644	0.0391	0.1151
87	353.15	1000	93.04	0.8249	0.3271	0.1163	0.6461	0.7675	0.3044	0.1082	0.6011	0.0923	0.0366	0.0130	0.0723
88	363.15	1000	95.52	0.8547	0.1360	0.0571	0.3338	0.8164	0.1299	0.0546	0.3188	0.0982	0.0156	0.0066	0.0383
89	373.15	1000	97.94	0.8914	0.0330	0.2113	0.0640	0.8730	0.0324	0.2070	0.0627	0.1050	0.0039	0.0249	0.0075
90	393.15	1000	102.56	0.9216	0.2643	0.4194	0.3225	0.9451	0.2710	0.4301	0.3308	0.1137	0.0326	0.0517	0.0398
91	413.15	1000	106.95	0.9251	0.4108	0.5486	0.5793	0.9894	0.4393	0.5867	0.6196	0.1190	0.0528	0.0706	0.0745
92	433.15	1000	111.16	0.9226	0.5131	0.6376	0.7602	1.0255	0.5704	0.7087	0.8450	0.1233	0.0686	0.0852	0.1016
93	453.15	1000	115.21	0.9179	0.5871	0.7010	0.8897	1.0575	0.6764	0.8077	1.0250	0.1272	0.0814	0.0971	0.1233
94	353.15	1500	88.07	0.8712	1.1569	0.7134	1.9923	0.7673	1.0189	0.6283	1.7547	0.0923	0.1226	0.0756	0.2111
95	363.15	1500	90.78	0.9226	0.7915	0.4027	1.3741	0.8375	0.7185	0.3656	1.2474	0.1007	0.0864	0.0440	0.1500
96	373.15	1500	93.37	0.9619	0.5050	0.1581	0.8851	0.8981	0.4715	0.1476	0.8264	0.1080	0.0567	0.0178	0.0994
97	393.15	1500	98.25	1.0073	0.0978	0.1891	0.1782	0.9897	0.0961	0.1858	0.1751	0.1190	0.0116	0.0223	0.0211
98	413.15	1500	102.82	1.0120	0.1550	0.4011	0.2796	1.0406	0.1594	0.4125	0.2874	0.1252	0.0192	0.0496	0.0346
99	433.15	1500	107.17	1.0078	0.3285	0.5451	0.5959	1.0800	0.3520	0.5842	0.6386	0.1299	0.0423	0.0703	0.0768
100	453.15	1500	111.30	0.9855	0.4375	0.6320	0.8049	1.0969	0.4870	0.7035	0.8958	0.1319	0.0586	0.0846	0.1078
101	473.15	1500	115.28	0.9677	0.5193	0.6966	0.9557	1.1156	0.5986	0.8031	1.1017	0.1342	0.0720	0.0966	0.1325
102	493.15	1500	119.11	0.9490	0.5778	0.7416	1.0603	1.1304	0.6882	0.8833	1.2630	0.1360	0.0828	0.1062	0.1519
103	353.15	2000	83.60	0.9302	2.3320	1.3756	4.0728	0.7777	1.9496	1.1500	3.4048	0.0935	0.2345	0.1383	0.4095
104	363.15	2000	86.71	1.0054	1.6574	0.8994	2.8876	0.8718	1.4371	0.7798	2.5038	0.1049	0.1729	0.0938	0.3012
105	373.15	2000	89.57	1.0583	1.1706	0.5373	2.0202	0.9480	1.0486	0.4813	1.8095	0.1140	0.1261	0.0579	0.2176
106	393.15	2000	94.81	1.0976	0.5385	0.0557	0.8612	1.0406	0.5105	0.0528	0.8165	0.1252	0.0614	0.0064	0.0982
107	413.15	2000	99.61	1.1006	0.1499	0.2443	0.1328	1.0963	0.1493	0.2433	0.1323	0.1319	0.0180	0.0293	0.0159
108	433.15	2000	104.09	1.0792	0.0963	0.4321	0.3422	1.1234	0.1002	0.4497	0.3562	0.1351	0.0121	0.0541	0.0428
109	453.15	2000	108.35	1.0569	0.2680	0.5624	0.6708	1.1451	0.2904	0.6093	0.7269	0.1377	0.0349	0.0733	0.0874
110	473.15	2000	112.41	1.0316	0.3878	0.6515	0.8983	1.1596	0.4360	0.7323	1.0098	0.1395	0.0524	0.0881	0.1215
111	493.15	2000	116.31	1.0017	0.4693	0.7094	1.0521	1.1650	0.5458	0.8251	1.2237	0.1401	0.0657	0.0992	0.1472
112	393.15	4000	81.94	1.8608	4.0410	9.5945	7.7511	1.5248	3.3113	7.8620	6.3515	0.1834	0.3983	0.9456	0.7639
113	413.15	4000	89.38	1.6240	2.0743	0.2635	3.4312	1.4515	1.8540	0.2355	3.0668	0.1746	0.2230	0.0283	0.3689
114	433.15	4000	95.04	1.4921	1.1873	0.2019	1.5132	1.4181	1.1284	0.1918	1.4382	0.1706	0.1357	0.0231	0.1730
115	453.15	4000	99.98	1.3846	0.6708	0.3507	0.4097	1.3844	0.6707	0.3507	0.4096	0.1665	0.0807	0.0422	0.0493

116	473.15	4000	104.49	1.2819	0.3490	0.4720	0.2775	1.3395	0.3646	0.4933	0.2900	0.1611	0.0439	0.0593	0.0349
117	493.15	4000	108.73	1.2092	0.1149	0.5792	0.7463	1.3147	0.1249	0.6297	0.8115	0.1581	0.0150	0.0757	0.0976
∑				91.561	63.902	66.968	86.404	95.848	66.337	69.705	87.865	11.528	7.979	8.384	10.568
Average (Overall)				**0.7826**	**0.5462**	**0.5724**	**0.7385**	**0.8192**	**0.5670**	**0.5958**	**0.7510**	**0.0985**	**0.0682**	**0.0717**	**0.0903**

Table C-15 Isopentane [6]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	477.59	1013	391.76	0.0404	0.1629	0.1109	0.0182	0.1584	0.6380	0.4346	0.0714	0.0191	0.0767	0.0523	0.0086
2	477.59	2027	383.61	0.1352	0.3944	0.2233	0.2433	0.5187	1.5131	0.8565	0.9332	0.0624	0.1820	0.1030	0.1122
3	477.59	3040	376.75	0.3075	0.7356	0.0647	0.8296	1.1585	2.7712	0.2438	3.1254	0.1393	0.3333	0.0293	0.3759
4	477.59	4053	366.93	0.8832	1.5059	0.5063	2.5383	3.2406	5.5256	1.8579	9.3138	0.3898	0.6646	0.2235	1.1203
5	477.59	5066	356.84	1.6464	2.7246	1.7411	4.5832	5.8751	9.7225	6.2129	16.3548	0.7067	1.1694	0.7473	1.9671
6	477.59	6080	354.22	2.0495	2.9370	2.1292	4.6053	7.2598	10.4035	7.5418	16.3129	0.8732	1.2513	0.9071	1.9621
7	477.59	8106	351.59	2.3156	3.1245	2.3681	4.0811	8.1413	10.9855	8.3260	14.3486	0.9792	1.3213	1.0014	1.7258
8	477.59	10133	349.96	2.4393	3.2411	2.4489	3.4452	8.5366	11.3424	8.5702	12.0568	1.0268	1.3643	1.0308	1.4502
9	477.59	15199	347.33	2.6163	3.4316	2.4663	1.9061	9.0871	11.9189	8.5661	6.6205	1.0930	1.4336	1.0303	0.7963
10	477.59	20265	345.55	2.7297	3.5672	2.3899	0.5104	9.4325	12.3265	8.2582	1.7637	1.1345	1.4826	0.9933	0.2121
11	505.37	1013	402.19	0.0016	0.1531	0.1072	0.0606	0.0065	0.6157	0.4310	0.2439	0.0008	0.0741	0.0518	0.0293
12	505.37	2027	394.66	0.0871	0.3035	0.1703	0.0415	0.3437	1.1978	0.6719	0.1637	0.0413	0.1441	0.0808	0.0197
13	505.37	3040	389.05	0.2038	0.5091	0.1832	0.2978	0.7927	1.9807	0.7129	1.1585	0.0953	0.2382	0.0857	0.1393
14	505.37	4053	383.67	0.4044	0.7963	0.1363	0.7690	1.5515	3.0551	0.5230	2.9504	0.1866	0.3675	0.0629	0.3549
15	505.37	5066	377.84	0.7623	1.2211	0.2431	1.5293	2.8803	4.6139	0.9185	5.7782	0.3464	0.5550	0.1105	0.6950
16	505.37	6080	372.58	1.1305	1.7028	0.4979	2.2577	4.2121	6.3443	1.8549	8.4117	0.5066	0.7631	0.2231	1.0118
17	505.37	8106	367.63	1.8465	2.0731	1.1238	2.4131	6.7882	7.6212	4.1314	8.8714	0.8165	0.9167	0.4969	1.0670
18	505.37	10133	365.39	2.2196	2.1747	1.2661	1.9941	8.1103	7.9463	4.6263	7.2862	0.9755	0.9558	0.5564	0.8764
19	505.37	15199	362.40	2.6447	2.2736	1.2712	0.6912	9.5845	8.2395	4.6067	2.5051	1.1528	0.9910	0.5541	0.3013

20	505.37	20265	360.59	2.8734	2.3288	1.1587	0.5382	10.3612	8.3974	4.1782	1.9408	1.2462	1.0100	0.5026	0.2334
21	533.15	1013	412.67	0.0251	0.0893	0.0478	0.1434	0.1036	0.3684	0.1971	0.5916	0.0125	0.0443	0.0237	0.0712
22	533.15	2027	405.54	0.1041	0.1937	0.0824	0.1328	0.4220	0.7857	0.3342	0.5387	0.0508	0.0945	0.0402	0.0648
23	533.15	3040	400.55	0.2000	0.3276	0.0951	0.0346	0.8012	1.3124	0.3810	0.1387	0.0964	0.1579	0.0458	0.0167
24	533.15	4053	396.27	0.3329	0.4957	0.0363	0.1531	1.3193	1.9644	0.1439	0.6065	0.1587	0.2363	0.0173	0.0730
25	533.15	5066	392.22	0.5261	0.7070	0.1377	0.4318	2.0635	2.7730	0.5399	1.6935	0.2482	0.3335	0.0649	0.2037
26	533.15	6080	388.38	0.7688	0.9567	0.1516	0.7593	2.9857	3.7158	0.5886	2.9491	0.3591	0.4469	0.0708	0.3547
27	533.15	8106	382.73	1.3024	1.3366	0.2704	1.0940	4.9848	5.1156	1.0351	4.1869	0.5996	0.6153	0.1245	0.5036
28	533.15	10133	379.77	1.7980	1.4625	0.4614	0.8979	6.8282	5.5541	1.7523	3.4100	0.8213	0.6680	0.2108	0.4101
29	533.15	15199	376.33	2.4966	1.4883	0.4516	0.1859	9.3953	5.6009	1.6994	0.6995	1.1301	0.6737	0.2044	0.0841
30	533.15	20265	374.49	2.8551	1.4657	0.2978	1.2962	10.6919	5.4890	1.1151	4.8542	1.2860	0.6602	0.1341	0.5839
31	560.93	1013	422.85	0.0235	0.0636	0.0254	0.1780	0.0993	0.2690	0.1076	0.7527	0.0119	0.0324	0.0129	0.0905
32	560.93	2027	416.02	0.1008	0.1315	0.0344	0.2312	0.4192	0.5470	0.1431	0.9618	0.0504	0.0658	0.0172	0.1157
33	560.93	3040	411.43	0.1849	0.2216	0.0352	0.2223	0.7608	0.9119	0.1446	0.9148	0.0915	0.1097	0.0174	0.1100
34	560.93	4053	407.68	0.2899	0.3298	0.0061	0.1652	1.1818	1.3445	0.0250	0.6736	0.1421	0.1617	0.0030	0.0810
35	560.93	5066	404.36	0.4250	0.4568	0.0672	0.0673	1.7187	1.8473	0.2718	0.2723	0.2067	0.2222	0.0327	0.0327
36	560.93	6080	401.28	0.5803	0.6123	0.1441	0.0665	2.3288	2.4572	0.5783	0.2670	0.2801	0.2955	0.0696	0.0321
37	560.93	8106	396.27	0.9639	0.8835	0.1091	0.2388	3.8195	3.5012	0.4323	0.9461	0.4594	0.4211	0.0520	0.1138
38	560.93	10133	393.00	1.3795	1.0181	0.0027	0.1384	5.4215	4.0010	0.0108	0.5439	0.6521	0.4812	0.0013	0.0654
39	560.93	15199	389.14	2.2038	1.0056	0.0496	0.7622	8.5758	3.9132	0.1930	2.9659	1.0315	0.4707	0.0232	0.3567
40	560.93	20265	387.26	2.6834	0.9154	0.2489	1.7812	10.3918	3.5449	0.9640	6.8980	1.2499	0.4264	0.1159	0.8297
41	588.71	1013	432.76	0.0013	0.0678	0.0322	0.1754	0.0056	0.2935	0.1393	0.7589	0.0007	0.0353	0.0168	0.0913
42	588.71	2027	426.11	0.0639	0.1201	0.0329	0.2596	0.2725	0.5118	0.1403	1.1061	0.0328	0.0616	0.0169	0.1330
43	588.71	3040	421.79	0.1408	0.1804	0.0215	0.3058	0.5940	0.7610	0.0908	1.2898	0.0714	0.0915	0.0109	0.1551
44	588.71	4053	418.38	0.2299	0.2526	0.0051	0.3205	0.9617	1.0567	0.0214	1.3410	0.1157	0.1271	0.0026	0.1613
45	588.71	5066	415.42	0.3283	0.3432	0.0453	0.3041	1.3636	1.4257	0.1880	1.2632	0.1640	0.1715	0.0226	0.1519
46	588.71	6080	412.79	0.4476	0.4404	0.1043	0.2760	1.8476	1.8179	0.4305	1.1391	0.2222	0.2187	0.0518	0.1370
47	588.71	8106	408.38	0.7322	0.6303	0.1887	0.2429	2.9900	2.5739	0.7707	0.9921	0.3596	0.3096	0.0927	0.1193
48	588.71	10133	405.18	1.0563	0.7486	0.1948	0.3425	4.2798	3.0333	0.7894	1.3876	0.5148	0.3648	0.0949	0.1669
49	588.71	15199	401.01	1.8484	0.7318	0.3164	1.1076	7.4121	2.9346	1.2687	4.4414	0.8915	0.3530	0.1526	0.5342

50	588.71	20265	399.10	2.4111	0.5905	0.5629	2.0522	9.6228	2.3567	2.2464	8.1906	1.1574	0.2835	0.2702	0.9852
∑				53.841	53.628	24.865	47.720	201.702	198.941	90.266	176.985	24.260	23.928	10.857	21.288
Average (Overall)				**1.0768**	**1.0726**	**0.4973**	**0.9544**	**4.0340**	**3.9788**	**1.8053**	**3.5397**	**0.4852**	**0.4786**	**0.2171**	**0.4258**

Table C-16 Ammonia [22]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	243.15	50	106.16	0.9667	0.8899	0.8920	0.6975	1.0262	0.9447	0.9469	0.7405	0.1234	0.1136	0.1139	0.0891
2	253.15	50	107.61	0.9172	0.8252	0.8275	0.6272	0.9870	0.8880	0.8905	0.6749	0.1187	0.1068	0.1071	0.0812
3	263.15	50	109.01	0.8785	0.7746	0.7770	0.5720	0.9576	0.8444	0.8470	0.6236	0.1152	0.1016	0.1019	0.0750
4	273.15	50	110.35	0.8465	0.7333	0.7359	0.5272	0.9341	0.8092	0.8121	0.5818	0.1124	0.0973	0.0977	0.0700
5	283.15	50	111.65	0.8215	0.7010	0.7037	0.4922	0.9172	0.7827	0.7857	0.5496	0.1103	0.0941	0.0945	0.0661
6	293.15	50	112.90	0.8003	0.6740	0.6768	0.4635	0.9035	0.7610	0.7642	0.5233	0.1087	0.0915	0.0919	0.0629
7	303.15	50	114.12	0.7824	0.6516	0.6545	0.4400	0.8929	0.7436	0.7469	0.5021	0.1074	0.0894	0.0898	0.0604
8	313.15	50	115.31	0.7671	0.6328	0.6357	0.4207	0.8845	0.7296	0.7330	0.4851	0.1064	0.0878	0.0882	0.0584
9	323.15	50	116.46	0.7549	0.6177	0.6208	0.4061	0.8791	0.7194	0.7229	0.4729	0.1057	0.0865	0.0870	0.0569
10	333.15	50	117.58	0.7445	0.6053	0.6083	0.3945	0.8754	0.7117	0.7153	0.4639	0.1053	0.0856	0.0860	0.0558
11	343.15	50	118.68	0.7348	0.5939	0.5970	0.3847	0.8720	0.7048	0.7085	0.4566	0.1049	0.0848	0.0852	0.0549
12	353.15	50	119.75	0.7256	0.5835	0.5866	0.3764	0.8689	0.6987	0.7024	0.4507	0.1045	0.0840	0.0845	0.0542
13	373.15	50	121.83	0.7096	0.5659	0.5691	0.3647	0.8645	0.6894	0.6933	0.4443	0.1040	0.0829	0.0834	0.0534
14	393.15	50	123.83	0.6953	0.5510	0.5542	0.3575	0.8610	0.6823	0.6863	0.4427	0.1036	0.0821	0.0825	0.0532
15	413.15	50	125.76	0.6829	0.5385	0.5417	0.3544	0.8588	0.6772	0.6813	0.4457	0.1033	0.0815	0.0819	0.0536
16	433.15	50	127.63	0.6699	0.5258	0.5291	0.3525	0.8550	0.6711	0.6753	0.4499	0.1028	0.0807	0.0812	0.0541
17	453.15	50	129.45	0.6570	0.5137	0.5169	0.3522	0.8505	0.6649	0.6691	0.4559	0.1023	0.0800	0.0805	0.0548
18	473.15	50	131.22	0.6457	0.5032	0.5064	0.3544	0.8473	0.6603	0.6645	0.4650	0.1019	0.0794	0.0799	0.0559
19	243.15	100	100.03	1.2100	1.2452	1.2432	1.0504	1.2103	1.2456	1.2436	1.0507	0.1456	0.1498	0.1496	0.1264
20	253.15	100	101.55	1.1138	1.1134	1.1119	0.9059	1.1311	1.1307	1.1292	0.9199	0.1360	0.1360	0.1358	0.1106

21	263.15	100	103.00	1.0364	1.0080	1.0069	0.7899	1.0675	1.0382	1.0371	0.8136	0.1284	0.1249	0.1247	0.0979
22	273.15	100	104.38	0.9756	0.9248	0.9242	0.6980	1.0184	0.9654	0.9647	0.7287	0.1225	0.1161	0.1160	0.0876
23	283.15	100	105.72	0.9269	0.8583	0.8580	0.6244	0.9799	0.9074	0.9070	0.6601	0.1179	0.1091	0.1091	0.0794
24	293.15	100	107.00	0.8888	0.8059	0.8059	0.5663	0.9511	0.8623	0.8623	0.6060	0.1144	0.1037	0.1037	0.0729
25	303.15	100	108.24	0.8594	0.7649	0.7651	0.5209	0.9302	0.8279	0.8281	0.5638	0.1119	0.0996	0.0996	0.0678
26	313.15	100	109.44	0.8348	0.7309	0.7313	0.4836	0.9135	0.7999	0.8003	0.5292	0.1099	0.0962	0.0963	0.0637
27	323.15	100	110.60	0.8141	0.7025	0.7031	0.4530	0.9004	0.7770	0.7777	0.5011	0.1083	0.0935	0.0935	0.0603
28	333.15	100	111.74	0.7977	0.6800	0.6807	0.4292	0.8914	0.7598	0.7606	0.4796	0.1072	0.0914	0.0915	0.0577
29	343.15	100	112.84	0.7844	0.6616	0.6625	0.4105	0.8852	0.7466	0.7476	0.4632	0.1065	0.0898	0.0899	0.0557
30	353.15	100	113.92	0.7727	0.6457	0.6467	0.3950	0.8802	0.7356	0.7368	0.4501	0.1059	0.0885	0.0886	0.0541
31	373.15	100	116.02	0.7518	0.6188	0.6200	0.3713	0.8722	0.7178	0.7192	0.4308	0.1049	0.0863	0.0865	0.0518
32	393.15	100	118.02	0.7343	0.5973	0.5987	0.3558	0.8667	0.7050	0.7066	0.4200	0.1042	0.0848	0.0850	0.0505
33	413.15	100	119.96	0.7178	0.5783	0.5797	0.3452	0.8611	0.6937	0.6955	0.4141	0.1036	0.0834	0.0837	0.0498
34	433.15	100	121.84	0.7042	0.5632	0.5648	0.3405	0.8580	0.6862	0.6881	0.4149	0.1032	0.0825	0.0828	0.0499
35	453.15	100	123.66	0.6903	0.5484	0.5501	0.3379	0.8536	0.6782	0.6802	0.4179	0.1027	0.0816	0.0818	0.0503
36	473.15	100	125.43	0.6775	0.5354	0.5371	0.3383	0.8498	0.6715	0.6737	0.4244	0.1022	0.0808	0.0810	0.0510
37	253.15	150	97.87	1.3074	1.4099	1.4041	1.1984	1.2795	1.3798	1.3742	1.1729	0.1539	0.1660	0.1653	0.1411
38	263.15	150	99.37	1.1883	1.2447	1.2397	1.0164	1.1809	1.2369	1.2320	1.0101	0.1420	0.1488	0.1482	0.1215
39	273.15	150	100.80	1.0961	1.1160	1.1116	0.8735	1.1050	1.1249	1.1206	0.8806	0.1329	0.1353	0.1348	0.1059
40	283.15	150	102.17	1.0231	1.0136	1.0099	0.7595	1.0454	1.0357	1.0318	0.7760	0.1257	0.1246	0.1241	0.0933
41	293.15	150	103.48	0.9679	0.9347	0.9315	0.6709	1.0016	0.9673	0.9639	0.6943	0.1205	0.1163	0.1159	0.0835
42	303.15	150	104.74	0.9235	0.8711	0.8683	0.5995	0.9673	0.9125	0.9095	0.6279	0.1163	0.1097	0.1094	0.0755
43	313.15	150	105.96	0.8896	0.8215	0.8190	0.5436	0.9426	0.8704	0.8678	0.5760	0.1134	0.1047	0.1044	0.0693
44	323.15	150	107.14	0.8619	0.7810	0.7789	0.4984	0.9235	0.8368	0.8345	0.5340	0.1111	0.1006	0.1004	0.0642
45	333.15	150	108.29	0.8396	0.7481	0.7462	0.4621	0.9092	0.8101	0.8081	0.5004	0.1094	0.0974	0.0972	0.0602
46	343.15	150	109.40	0.8214	0.7210	0.7194	0.4328	0.8986	0.7888	0.7871	0.4735	0.1081	0.0949	0.0947	0.0570
47	353.15	150	110.49	0.8057	0.6981	0.6967	0.4088	0.8902	0.7714	0.7699	0.4517	0.1071	0.0928	0.0926	0.0543
48	373.15	150	112.60	0.7803	0.6617	0.6607	0.3733	0.8786	0.7451	0.7440	0.4204	0.1057	0.0896	0.0895	0.0506
49	393.15	150	114.61	0.7601	0.6339	0.6332	0.3500	0.8711	0.7265	0.7257	0.4011	0.1048	0.0874	0.0873	0.0482
50	413.15	150	116.56	0.7427	0.6113	0.6108	0.3349	0.8657	0.7125	0.7120	0.3904	0.1041	0.0857	0.0856	0.0470

51	433.15	150	118.44	0.7261	0.5911	0.5908	0.3251	0.8600	0.7001	0.6998	0.3850	0.1034	0.0842	0.0842	0.0463
52	453.15	150	120.26	0.7114	0.5740	0.5739	0.3206	0.8556	0.6904	0.6903	0.3855	0.1029	0.0830	0.0830	0.0464
53	473.15	150	122.04	0.6975	0.5586	0.5586	0.3195	0.8512	0.6817	0.6817	0.3899	0.1024	0.0820	0.0820	0.0469
54	493.15	150	123.76	0.6838	0.5441	0.5442	0.3207	0.8463	0.6734	0.6735	0.3969	0.1018	0.0810	0.0810	0.0477
55	263.15	200	96.72	1.3444	1.4922	1.4830	1.2595	1.3003	1.4433	1.4344	1.2182	0.1564	0.1736	0.1725	0.1465
56	273.15	200	98.20	1.2167	1.3125	1.3043	1.0600	1.1948	1.2889	1.2808	1.0409	0.1437	0.1550	0.1540	0.1252
57	283.15	200	99.60	1.1172	1.1713	1.1639	0.9022	1.1128	1.1667	1.1593	0.8986	0.1338	0.1403	0.1394	0.1081
58	293.15	200	100.94	1.0429	1.0634	1.0567	0.7804	1.0527	1.0734	1.0666	0.7877	0.1266	0.1291	0.1283	0.0947
59	303.15	200	102.23	0.9834	0.9765	0.9705	0.6822	1.0053	0.9983	0.9921	0.6974	0.1209	0.1201	0.1193	0.0839
60	313.15	200	103.47	0.9384	0.9092	0.9037	0.6056	0.9710	0.9407	0.9350	0.6266	0.1168	0.1131	0.1125	0.0754
61	323.15	200	104.66	0.9023	0.8547	0.8497	0.5437	0.9444	0.8945	0.8893	0.5691	0.1136	0.1076	0.1070	0.0684
62	333.15	200	105.82	0.8741	0.8112	0.8066	0.4946	0.9249	0.8584	0.8535	0.5234	0.1112	0.1032	0.1027	0.0630
63	343.15	200	106.94	0.8509	0.7753	0.7711	0.4547	0.9099	0.8292	0.8247	0.4862	0.1094	0.0997	0.0992	0.0585
64	353.15	200	108.04	0.8329	0.7469	0.7430	0.4235	0.8999	0.8069	0.8027	0.4576	0.1082	0.0971	0.0966	0.0550
65	373.15	200	110.15	0.8032	0.7010	0.6977	0.3761	0.8848	0.7722	0.7685	0.4143	0.1064	0.0929	0.0924	0.0498
66	393.15	200	112.18	0.7804	0.6667	0.6639	0.3447	0.8754	0.7479	0.7447	0.3867	0.1053	0.0900	0.0896	0.0465
67	413.15	200	114.13	0.7609	0.6391	0.6366	0.3239	0.8684	0.7295	0.7266	0.3697	0.1045	0.0877	0.0874	0.0445
68	433.15	200	116.02	0.7428	0.6154	0.6132	0.3102	0.8618	0.7139	0.7114	0.3599	0.1037	0.0859	0.0856	0.0433
69	453.15	200	117.85	0.7276	0.5961	0.5942	0.3038	0.8575	0.7025	0.7002	0.3580	0.1031	0.0845	0.0842	0.0431
70	473.15	200	119.62	0.7127	0.5783	0.5766	0.3011	0.8525	0.6918	0.6897	0.3602	0.1025	0.0832	0.0830	0.0433
71	493.15	200	121.35	0.6976	0.5614	0.5598	0.3011	0.8466	0.6813	0.6793	0.3655	0.1018	0.0819	0.0817	0.0440
72	283.15	300	95.87	1.3100	1.5018	1.4863	1.2146	1.2559	1.4397	1.4249	1.1644	0.1511	0.1732	0.1714	0.1401
73	293.15	300	97.27	1.1916	1.3280	1.3138	1.0182	1.1591	1.2917	1.2780	0.9904	0.1394	0.1554	0.1537	0.1191
74	303.15	300	98.60	1.1015	1.1930	1.1800	0.8642	1.0861	1.1763	1.1635	0.8521	0.1306	0.1415	0.1399	0.1025
75	313.15	300	99.88	1.0326	1.0874	1.0753	0.7429	1.0314	1.0861	1.0740	0.7420	0.1241	0.1306	0.1292	0.0892
76	323.15	300	101.10	0.9794	1.0039	0.9927	0.6465	0.9902	1.0150	1.0036	0.6537	0.1191	0.1221	0.1207	0.0786
77	333.15	300	102.29	0.9376	0.9370	0.9265	0.5693	0.9591	0.9585	0.9477	0.5823	0.1154	0.1153	0.1140	0.0700
78	343.15	300	103.43	0.9062	0.8848	0.8749	0.5089	0.9374	0.9151	0.9050	0.5264	0.1127	0.1101	0.1088	0.0633
79	353.15	300	104.54	0.8807	0.8417	0.8324	0.4598	0.9207	0.8799	0.8703	0.4807	0.1107	0.1058	0.1047	0.0578
80	373.15	300	106.69	0.8410	0.7749	0.7667	0.3863	0.8973	0.8267	0.8179	0.4121	0.1079	0.0994	0.0984	0.0496

81	393.15	300	108.73	0.8133	0.7277	0.7203	0.3386	0.8843	0.7913	0.7832	0.3682	0.1064	0.0952	0.0942	0.0443
82	413.15	300	110.69	0.7898	0.6901	0.6833	0.3058	0.8743	0.7639	0.7564	0.3385	0.1052	0.0919	0.0910	0.0407
83	433.15	300	112.59	0.7707	0.6607	0.6545	0.2857	0.8677	0.7439	0.7368	0.3217	0.1044	0.0895	0.0886	0.0387
84	453.15	300	114.43	0.7516	0.6341	0.6283	0.2722	0.8601	0.7256	0.7189	0.3115	0.1034	0.0873	0.0865	0.0375
85	473.15	300	116.21	0.7349	0.6118	0.6063	0.2662	0.8540	0.7110	0.7046	0.3093	0.1027	0.0855	0.0847	0.0372
86	493.15	300	117.95	0.7188	0.5916	0.5863	0.2648	0.8478	0.6977	0.6916	0.3123	0.1020	0.0839	0.0832	0.0376
87	513.15	300	119.64	0.7039	0.5737	0.5687	0.2677	0.8421	0.6864	0.6804	0.3203	0.1013	0.0826	0.0818	0.0385
88	533.15	300	121.29	0.6889	0.5565	0.5517	0.2728	0.8356	0.6750	0.6691	0.3308	0.1005	0.0812	0.0805	0.0398
89	293.15	400	94.56	1.3439	1.6056	1.5832	1.2803	1.2709	1.5183	1.4972	1.2107	0.1529	0.1826	0.1801	0.1456
90	303.15	400	95.95	1.2194	1.4169	1.3963	1.0645	1.1700	1.3596	1.3397	1.0213	0.1407	0.1635	0.1611	0.1228
91	313.15	400	97.27	1.1248	1.2699	1.2507	0.8948	1.0940	1.2352	1.2165	0.8703	0.1316	0.1486	0.1463	0.1047
92	323.15	400	98.52	1.0527	1.1548	1.1369	0.7608	1.0372	1.1378	1.1201	0.7496	0.1248	0.1369	0.1347	0.0902
93	333.15	400	99.73	0.9975	1.0639	1.0470	0.6545	0.9948	1.0610	1.0443	0.6528	0.1197	0.1276	0.1256	0.0785
94	343.15	400	100.90	0.9564	0.9931	0.9772	0.5713	0.9650	1.0020	0.9860	0.5765	0.1161	0.1205	0.1186	0.0693
95	353.15	400	102.03	0.9233	0.9351	0.9201	0.5036	0.9420	0.9540	0.9388	0.5138	0.1133	0.1148	0.1129	0.0618
96	373.15	400	104.19	0.8740	0.8470	0.8335	0.4032	0.9106	0.8825	0.8685	0.4201	0.1095	0.1062	0.1045	0.0505
97	393.15	400	106.26	0.8400	0.7851	0.7728	0.3370	0.8925	0.8342	0.8211	0.3581	0.1074	0.1003	0.0988	0.0431
98	413.15	400	108.24	0.8128	0.7375	0.7261	0.2918	0.8797	0.7982	0.7859	0.3159	0.1058	0.0960	0.0945	0.0380
99	433.15	400	110.14	0.7913	0.7009	0.6903	0.2635	0.8716	0.7720	0.7603	0.2902	0.1048	0.0929	0.0915	0.0349
100	453.15	400	111.99	0.7701	0.6685	0.6585	0.2441	0.8625	0.7486	0.7374	0.2733	0.1037	0.0900	0.0887	0.0329
101	473.15	400	113.78	0.7518	0.6416	0.6322	0.2343	0.8554	0.7300	0.7193	0.2666	0.1029	0.0878	0.0865	0.0321
102	493.15	400	115.52	0.7348	0.6182	0.6092	0.2313	0.8488	0.7141	0.7037	0.2672	0.1021	0.0859	0.0846	0.0321
103	513.15	400	117.22	0.7169	0.5955	0.5868	0.2315	0.8404	0.6980	0.6878	0.2714	0.1011	0.0840	0.0827	0.0326
104	533.15	400	118.87	0.7014	0.5763	0.5679	0.2371	0.8338	0.6850	0.6750	0.2819	0.1003	0.0824	0.0812	0.0339
105	553.15	400	120.49	0.6865	0.5586	0.5504	0.2454	0.8272	0.6730	0.6631	0.2957	0.0995	0.0810	0.0798	0.0356
106	303.15	500	93.82	1.3416	1.6517	1.6228	1.2837	1.2588	1.5497	1.5226	1.2045	0.1514	0.1864	0.1831	0.1449
107	313.15	500	95.18	1.2176	1.4585	1.4316	1.0603	1.1589	1.3882	1.3626	1.0092	0.1394	0.1670	0.1639	0.1214
108	323.15	500	96.48	1.1267	1.3109	1.2857	0.8875	1.0870	1.2647	1.2404	0.8563	0.1307	0.1521	0.1492	0.1030
109	333.15	500	97.71	1.0564	1.1935	1.1699	0.7494	1.0322	1.1662	1.1431	0.7323	0.1242	0.1403	0.1375	0.0881
110	343.15	500	98.90	1.0040	1.1021	1.0798	0.6410	0.9929	1.0900	1.0679	0.6339	0.1194	0.1311	0.1284	0.0763

111	353.15	500	100.05	0.9618	1.0271	1.0061	0.5525	0.9622	1.0276	1.0065	0.5528	0.1157	0.1236	0.1211	0.0665
112	373.15	500	102.24	0.9030	0.9175	0.8984	0.4245	0.9233	0.9380	0.9185	0.4340	0.1110	0.1128	0.1105	0.0522
113	393.15	500	104.32	0.8631	0.8407	0.8233	0.3393	0.9004	0.8770	0.8588	0.3540	0.1083	0.1055	0.1033	0.0426
114	413.15	500	106.31	0.8339	0.7845	0.7684	0.2830	0.8865	0.8340	0.8168	0.3009	0.1066	0.1003	0.0982	0.0362
115	433.15	500	108.23	0.8087	0.7392	0.7241	0.2445	0.8753	0.8000	0.7837	0.2647	0.1053	0.0962	0.0943	0.0318
116	453.15	500	110.08	0.7871	0.7024	0.6882	0.2205	0.8664	0.7733	0.7576	0.2427	0.1042	0.0930	0.0911	0.0292
117	473.15	500	111.88	0.7672	0.6711	0.6576	0.2067	0.8584	0.7508	0.7357	0.2313	0.1032	0.0903	0.0885	0.0278
118	493.15	500	113.63	0.7479	0.6429	0.6300	0.2002	0.8498	0.7305	0.7158	0.2274	0.1022	0.0879	0.0861	0.0274
119	513.15	500	115.33	0.7286	0.6169	0.6044	0.1989	0.8403	0.7114	0.6970	0.2294	0.1011	0.0856	0.0838	0.0276
120	533.15	500	116.99	0.7112	0.5942	0.5821	0.2033	0.8321	0.6952	0.6810	0.2379	0.1001	0.0836	0.0819	0.0286
121	553.15	500	118.61	0.6955	0.5744	0.5625	0.2123	0.8250	0.6813	0.6672	0.2518	0.0992	0.0819	0.0803	0.0303
122	303.15	600	92.03	1.4677	1.8966	1.8588	1.5199	1.3507	1.7454	1.7106	1.3988	0.1625	0.2099	0.2058	0.1682
123	313.15	600	93.44	1.3142	1.6558	1.6207	1.2409	1.2280	1.5471	1.5143	1.1594	0.1477	0.1861	0.1821	0.1395
124	323.15	600	94.76	1.2012	1.4714	1.4386	1.0245	1.1383	1.3943	1.3632	0.9709	0.1369	0.1677	0.1640	0.1168
125	333.15	600	96.03	1.1158	1.3271	1.2963	0.8537	1.0715	1.2743	1.2448	0.8198	0.1289	0.1533	0.1497	0.0986
126	343.15	600	97.24	1.0505	1.2128	1.1838	0.7176	1.0215	1.1793	1.1511	0.6978	0.1229	0.1418	0.1384	0.0839
127	353.15	600	98.40	1.0011	1.1224	1.0949	0.6095	0.9851	1.1045	1.0774	0.5998	0.1185	0.1328	0.1296	0.0721
128	373.15	600	100.62	0.9315	0.9891	0.9642	0.4515	0.9372	0.9952	0.9702	0.4543	0.1127	0.1197	0.1167	0.0546
129	393.15	600	102.72	0.8857	0.8973	0.8745	0.3469	0.9098	0.9217	0.8983	0.3563	0.1094	0.1109	0.1080	0.0429
130	413.15	600	104.73	0.8532	0.8309	0.8097	0.2775	0.8935	0.8701	0.8480	0.2906	0.1075	0.1047	0.1020	0.0350
131	433.15	600	106.65	0.8259	0.7783	0.7586	0.2302	0.8809	0.8301	0.8090	0.2455	0.1059	0.0998	0.0973	0.0295
132	453.15	600	108.52	0.8008	0.7341	0.7154	0.1981	0.8690	0.7966	0.7764	0.2150	0.1045	0.0958	0.0934	0.0259
133	473.15	600	110.32	0.7795	0.6982	0.6805	0.1801	0.8600	0.7703	0.7507	0.1987	0.1034	0.0926	0.0903	0.0239
134	493.15	600	112.07	0.7580	0.6654	0.6484	0.1699	0.8495	0.7457	0.7266	0.1904	0.1022	0.0897	0.0874	0.0229
135	513.15	600	113.78	0.7388	0.6374	0.6210	0.1684	0.8407	0.7253	0.7066	0.1916	0.1011	0.0872	0.0850	0.0230
136	533.15	600	115.45	0.7196	0.6113	0.5954	0.1715	0.8308	0.7057	0.6873	0.1979	0.0999	0.0849	0.0827	0.0238
137	553.15	600	117.07	0.7017	0.5879	0.5724	0.1793	0.8215	0.6883	0.6701	0.2099	0.0988	0.0828	0.0806	0.0252
138	303.15	800	89.05	1.7460	2.4310	2.3734	2.0542	1.5549	2.1648	2.1135	1.8293	0.1870	0.2604	0.2542	0.2200
139	313.15	800	90.56	1.5212	2.0783	2.0250	1.6454	1.3775	1.8820	1.8337	1.4900	0.1657	0.2264	0.2206	0.1792
140	323.15	800	91.96	1.3569	1.8103	1.7607	1.3306	1.2478	1.6648	1.6191	1.2236	0.1501	0.2002	0.1947	0.1472

141	333.15	800	93.29	1.2349	1.6033	1.5568	1.0845	1.1520	1.4956	1.4523	1.0117	0.1386	0.1799	0.1747	0.1217
142	343.15	800	94.54	1.1442	1.4423	1.3986	0.8912	1.0818	1.3636	1.3223	0.8425	0.1301	0.1640	0.1590	0.1013
143	353.15	800	95.75	1.0773	1.3168	1.2755	0.7390	1.0315	1.2608	1.2212	0.7076	0.1241	0.1516	0.1469	0.0851
144	373.15	800	98.02	0.9851	1.1337	1.0964	0.5174	0.9656	1.1112	1.0747	0.5072	0.1161	0.1337	0.1293	0.0610
145	393.15	800	100.16	0.9266	1.0097	0.9755	0.3710	0.9281	1.0113	0.9771	0.3716	0.1116	0.1216	0.1175	0.0447
146	413.15	800	102.20	0.8845	0.9193	0.8876	0.2713	0.9039	0.9395	0.9071	0.2773	0.1087	0.1130	0.1091	0.0334
147	433.15	800	104.14	0.8536	0.8523	0.8227	0.2058	0.8890	0.8876	0.8568	0.2144	0.1069	0.1068	0.1031	0.0258
148	453.15	800	106.02	0.8250	0.7962	0.7683	0.1603	0.8747	0.8442	0.8146	0.1699	0.1052	0.1015	0.0980	0.0204
149	473.15	800	107.84	0.7996	0.7497	0.7231	0.1317	0.8623	0.8085	0.7799	0.1421	0.1037	0.0972	0.0938	0.0171
150	493.15	800	109.61	0.7768	0.7105	0.6850	0.1167	0.8514	0.7787	0.7509	0.1279	0.1024	0.0937	0.0903	0.0154
151	513.15	800	111.33	0.7536	0.6743	0.6498	0.1096	0.8389	0.7507	0.7234	0.1220	0.1009	0.0903	0.0870	0.0147
152	533.15	800	113.00	0.7322	0.6427	0.6189	0.1109	0.8274	0.7262	0.6994	0.1253	0.0995	0.0874	0.0841	0.0151
153	553.15	800	114.64	0.7114	0.6136	0.5904	0.1175	0.8155	0.7034	0.6768	0.1347	0.0981	0.0846	0.0814	0.0162
154	573.15	800	116.23	0.6922	0.5878	0.5649	0.1290	0.8046	0.6832	0.6567	0.1500	0.0968	0.0822	0.0790	0.0180
155	313.15	1000	88.18	1.7480	2.5395	2.4656	2.1069	1.5415	2.2394	2.1743	1.8579	0.1854	0.2694	0.2615	0.2235
156	323.15	1000	89.68	1.5240	2.1751	2.1067	1.6787	1.3667	1.9505	1.8891	1.5053	0.1644	0.2346	0.2272	0.1811
157	333.15	1000	91.07	1.3608	1.8977	1.8339	1.3481	1.2392	1.7282	1.6700	1.2277	0.1491	0.2079	0.2009	0.1477
158	343.15	1000	92.38	1.2420	1.6850	1.6251	1.0912	1.1473	1.5565	1.5012	1.0080	0.1380	0.1872	0.1806	0.1212
159	353.15	1000	93.62	1.1529	1.5180	1.4616	0.8878	1.0794	1.4212	1.3684	0.8312	0.1298	0.1709	0.1646	0.1000
160	373.15	1000	95.96	1.0357	1.2807	1.2299	0.5967	0.9939	1.2289	1.1802	0.5725	0.1195	0.1478	0.1419	0.0689
161	393.15	1000	98.14	0.9638	1.1224	1.0760	0.4053	0.9459	1.1014	1.0560	0.3978	0.1138	0.1325	0.1270	0.0478
162	413.15	1000	100.20	0.9144	1.0094	0.9666	0.2760	0.9162	1.0115	0.9685	0.2766	0.1102	0.1217	0.1165	0.0333
163	433.15	1000	102.17	0.8770	0.9245	0.8845	0.1882	0.8960	0.9446	0.9037	0.1922	0.1078	0.1136	0.1087	0.0231
164	453.15	1000	104.07	0.8469	0.8582	0.8205	0.1302	0.8813	0.8931	0.8539	0.1355	0.1060	0.1074	0.1027	0.0163
165	473.15	1000	105.90	0.8175	0.8009	0.7651	0.0905	0.8658	0.8482	0.8103	0.0958	0.1041	0.1020	0.0975	0.0115
166	493.15	1000	107.68	0.7906	0.7522	0.7179	0.0669	0.8513	0.8099	0.7731	0.0720	0.1024	0.0974	0.0930	0.0087
167	513.15	1000	109.41	0.7650	0.7093	0.6763	0.0553	0.8369	0.7760	0.7400	0.0605	0.1007	0.0933	0.0890	0.0073
168	533.15	1000	111.09	0.7417	0.6722	0.6403	0.0543	0.8240	0.7468	0.7113	0.0603	0.0991	0.0898	0.0856	0.0073
169	553.15	1000	112.74	0.7181	0.6374	0.6063	0.0591	0.8095	0.7186	0.6835	0.0666	0.0974	0.0864	0.0822	0.0080
170	573.15	1000	114.34	0.6954	0.6057	0.5751	0.0693	0.7952	0.6926	0.6576	0.0792	0.0956	0.0833	0.0791	0.0095

171	593.15	1000	115.91	0.6746	0.5774	0.5472	0.0842	0.7820	0.6693	0.6343	0.0976	0.0941	0.0805	0.0763	0.0117
172	313.15	1200	86.12	2.0013	3.0473	2.9499	2.6316	1.7234	2.6242	2.5404	2.2662	0.2073	0.3156	0.3056	0.2726
173	323.15	1200	87.70	1.7073	2.5711	2.4814	2.0722	1.4974	2.2550	2.1763	1.8174	0.1801	0.2712	0.2618	0.2186
174	333.15	1200	89.17	1.4965	2.2134	2.1302	1.6455	1.3344	1.9737	1.8995	1.4673	0.1605	0.2374	0.2285	0.1765
175	343.15	1200	90.54	1.3451	1.9420	1.8644	1.3169	1.2178	1.7582	1.6879	1.1922	0.1465	0.2115	0.2030	0.1434
176	353.15	1200	91.82	1.2329	1.7309	1.6579	1.0583	1.1321	1.5894	1.5224	0.9718	0.1362	0.1912	0.1831	0.1169
177	373.15	1200	94.22	1.0868	1.4329	1.3676	0.6898	1.0240	1.3501	1.2886	0.6500	0.1232	0.1624	0.1550	0.0782
178	393.15	1200	96.45	0.9988	1.2363	1.1770	0.4487	0.9633	1.1924	1.1352	0.4327	0.1159	0.1434	0.1365	0.0520
179	413.15	1200	98.54	0.9428	1.1008	1.0461	0.2888	0.9290	1.0847	1.0308	0.2846	0.1117	0.1305	0.1240	0.0342
180	433.15	1200	100.54	0.9010	0.9994	0.9485	0.1796	0.9058	1.0048	0.9535	0.1806	0.1089	0.1209	0.1147	0.0217
181	453.15	1200	102.45	0.8647	0.9179	0.8700	0.1037	0.8859	0.9404	0.8913	0.1062	0.1066	0.1131	0.1072	0.0128
182	473.15	1200	104.30	0.8333	0.8515	0.8060	0.0539	0.8691	0.8881	0.8407	0.0563	0.1045	0.1068	0.1011	0.0068
183	493.15	1200	106.09	0.8040	0.7948	0.7514	0.0230	0.8529	0.8432	0.7971	0.0244	0.1026	0.1014	0.0959	0.0029
184	513.15	1200	107.83	0.7761	0.7451	0.7033	0.0064	0.8368	0.8034	0.7584	0.0069	0.1007	0.0966	0.0912	0.0008
185	533.15	1200	109.52	0.7478	0.6994	0.6590	0.0004	0.8190	0.7660	0.7217	0.0004	0.0985	0.0921	0.0868	0.0001
186	553.15	1200	111.18	0.7214	0.6589	0.6195	0.0022	0.8021	0.7325	0.6887	0.0025	0.0965	0.0881	0.0828	0.0003
187	573.15	1200	112.79	0.6969	0.6227	0.5841	0.0122	0.7860	0.7024	0.6588	0.0138	0.0945	0.0845	0.0792	0.0017
188	593.15	1200	114.36	0.6737	0.5899	0.5518	0.0272	0.7705	0.6746	0.6311	0.0311	0.0927	0.0811	0.0759	0.0037
189	333.15	1600	85.96	1.8013	2.9144	2.7858	2.3445	1.5484	2.5052	2.3947	2.0153	0.1862	0.3013	0.2880	0.2424
190	343.15	1600	87.46	1.5678	2.5001	2.3813	1.8420	1.3711	2.1865	2.0826	1.6109	0.1649	0.2630	0.2505	0.1938
191	353.15	1600	88.85	1.3997	2.1848	2.0742	1.4539	1.2436	1.9411	1.8428	1.2917	0.1496	0.2335	0.2217	0.1554
192	373.15	1600	91.39	1.1877	1.7502	1.6525	0.9105	1.0854	1.5995	1.5102	0.8320	0.1306	0.1924	0.1816	0.1001
193	393.15	1600	93.70	1.0691	1.4745	1.3864	0.5637	1.0018	1.3816	1.2991	0.5282	0.1205	0.1662	0.1563	0.0635
194	413.15	1600	95.86	0.9934	1.2844	1.2039	0.3315	0.9522	1.2312	1.1541	0.3178	0.1145	0.1481	0.1388	0.0382
195	433.15	1600	97.90	0.9409	1.1468	1.0722	0.1745	0.9211	1.1227	1.0498	0.1709	0.1108	0.1350	0.1263	0.0205
196	453.15	1600	99.85	0.8985	1.0397	0.9700	0.0664	0.8971	1.0382	0.9686	0.0663	0.1079	0.1249	0.1165	0.0080
197	473.15	1600	101.73	0.8603	0.9517	0.8857	0.0078	0.8752	0.9681	0.9011	0.0080	0.1053	0.1164	0.1084	0.0010
198	493.15	1600	103.55	0.8250	0.8773	0.8145	0.0562	0.8543	0.9084	0.8434	0.0582	0.1028	0.1093	0.1014	0.0070
199	513.15	1600	105.31	0.7913	0.8125	0.7522	0.0852	0.8333	0.8556	0.7922	0.0898	0.1002	0.1029	0.0953	0.0108
200	533.15	1600	107.02	0.7597	0.7557	0.6975	0.0984	0.8130	0.8088	0.7465	0.1053	0.0978	0.0973	0.0898	0.0127

201	553.15	1600	108.69	0.7280	0.7036	0.6471	0.1011	0.7912	0.7648	0.7033	0.1099	0.0952	0.0920	0.0846	0.0132
202	573.15	1600	110.32	0.6983	0.6571	0.6017	0.0941	0.7703	0.7249	0.6638	0.1038	0.0927	0.0872	0.0798	0.0125
203	593.15	1600	111.91	0.6687	0.6135	0.5591	0.0814	0.7484	0.6865	0.6256	0.0911	0.0900	0.0826	0.0753	0.0110
204	613.15	1600	113.47	0.6418	0.5746	0.5208	0.0627	0.7282	0.6520	0.5910	0.0712	0.0876	0.0784	0.0711	0.0086
205	633.15	1600	114.99	0.6163	0.5390	0.4856	0.0408	0.7087	0.6198	0.5584	0.0469	0.0852	0.0746	0.0672	0.0056
206	343.15	2000	84.85	1.8266	3.1345	2.9654	2.4812	1.5499	2.6596	2.5161	2.1053	0.1864	0.3199	0.3026	0.2532
207	353.15	2000	86.36	1.5873	2.6898	2.5341	1.9326	1.3708	2.3229	2.1884	1.6690	0.1649	0.2794	0.2632	0.2007
208	373.15	2000	89.06	1.2950	2.0925	1.9572	1.1805	1.1533	1.8636	1.7431	1.0514	0.1387	0.2242	0.2097	0.1265
209	393.15	2000	91.48	1.1362	1.7218	1.6013	0.7079	1.0394	1.5751	1.4649	0.6475	0.1250	0.1895	0.1762	0.0779
210	413.15	2000	93.71	1.0422	1.4752	1.3660	0.3983	0.9766	1.3824	1.2800	0.3733	0.1175	0.1663	0.1540	0.0449
211	433.15	2000	95.80	0.9777	1.2977	1.1973	0.1879	0.9366	1.2432	1.1470	0.1800	0.1127	0.1495	0.1380	0.0216
212	453.15	2000	97.79	0.9270	1.1617	1.0681	0.0425	0.9066	1.1360	1.0445	0.0416	0.1090	0.1366	0.1256	0.0050
213	473.15	2000	99.70	0.8849	1.0536	0.9656	0.0557	0.8822	1.0505	0.9627	0.0556	0.1061	0.1263	0.1158	0.0067
214	493.15	2000	101.54	0.8444	0.9615	0.8780	0.1227	0.8574	0.9764	0.8916	0.1246	0.1031	0.1174	0.1072	0.0150
215	513.15	2000	103.32	0.8053	0.8814	0.8015	0.1653	0.8320	0.9107	0.8282	0.1707	0.1001	0.1095	0.0996	0.0205
216	533.15	2000	105.06	0.7673	0.8103	0.7334	0.1890	0.8061	0.8513	0.7705	0.1985	0.0970	0.1024	0.0927	0.0239
217	553.15	2000	106.74	0.7305	0.7466	0.6719	0.1979	0.7798	0.7969	0.7172	0.2112	0.0938	0.0959	0.0863	0.0254
218	573.15	2000	108.39	0.6942	0.6879	0.6151	0.1963	0.7524	0.7456	0.6667	0.2127	0.0905	0.0897	0.0802	0.0256
219	593.15	2000	109.99	0.6615	0.6366	0.5651	0.1837	0.7276	0.7002	0.6215	0.2021	0.0875	0.0842	0.0748	0.0243
220	613.15	2000	111.56	0.6290	0.5882	0.5176	0.1664	0.7017	0.6562	0.5775	0.1856	0.0844	0.0789	0.0695	0.0223
221	633.15	2000	113.10	0.6002	0.5458	0.4758	0.1425	0.6788	0.6173	0.5381	0.1611	0.0816	0.0743	0.0647	0.0194
222	373.15	5000	80.03	1.6510	1.6096	0.8609	0.9850	1.3213	1.2882	0.6889	0.7883	0.1589	0.1549	0.0829	0.0948
223	393.15	5000	82.77	0.9899	1.3482	0.7921	0.1177	0.8193	1.1159	0.6556	0.0975	0.0986	0.1342	0.0789	0.0117
224	413.15	5000	85.86	1.3254	0.4179	0.0306	1.1642	1.1379	0.3588	0.0263	0.9995	0.1369	0.0432	0.0032	0.1202
225	433.15	5000	86.33	0.9988	2.3734	1.9825	0.5348	0.8623	2.0490	1.7115	0.4617	0.1037	0.2465	0.2059	0.0555
226	453.15	5000	88.51	1.0851	2.1661	1.8216	0.2013	0.9604	1.9171	1.6122	0.1782	0.1155	0.2306	0.1939	0.0214
227	473.15	5000	90.68	1.0011	1.8615	1.5511	0.1595	0.9078	1.6880	1.4066	0.1446	0.1092	0.2030	0.1692	0.0174
228	493.15	5000	92.73	0.9273	1.6189	1.3342	0.4092	0.8599	1.5013	1.2373	0.3795	0.1034	0.1806	0.1488	0.0456
229	513.15	5000	94.69	0.8558	1.4152	1.1502	0.5829	0.8104	1.3401	1.0892	0.5520	0.0975	0.1612	0.1310	0.0664
230	533.15	5000	96.57	0.7868	1.2407	0.9911	0.6990	0.7598	1.1981	0.9571	0.6750	0.0914	0.1441	0.1151	0.0812

231	553.15	5000	98.39	0.7163	1.0845	0.8470	0.7748	0.7048	1.0670	0.8334	0.7624	0.0848	0.1283	0.1002	0.0917
232	573.15	5000	100.15	0.6465	0.9441	0.7161	0.8188	0.6475	0.9455	0.7172	0.8200	0.0779	0.1137	0.0863	0.0986
233	593.15	5000	101.86	0.5792	0.8177	0.5970	0.8372	0.5899	0.8329	0.6082	0.8527	0.0710	0.1002	0.0731	0.1026
234	613.15	5000	103.52	0.5144	0.7029	0.4878	0.8363	0.5325	0.7277	0.5050	0.8657	0.0641	0.0875	0.0607	0.1041
235	633.15	5000	105.15	0.4532	0.5987	0.3876	0.8206	0.4765	0.6295	0.4076	0.8628	0.0573	0.0757	0.0490	0.1038
236	653.15	5000	106.73	0.3938	0.5020	0.2935	0.7960	0.4203	0.5358	0.3133	0.8496	0.0506	0.0644	0.0377	0.1022
237	673.15	5000	108.28	0.3390	0.4145	0.2073	0.7635	0.3671	0.4488	0.2244	0.8267	0.0442	0.0540	0.0270	0.0994
238	693.15	5000	109.79	0.2879	0.3341	0.1270	0.7269	0.3161	0.3668	0.1394	0.7980	0.0380	0.0441	0.0168	0.0960
239	713.15	5000	111.27	0.2391	0.2590	0.0508	0.6897	0.2661	0.2881	0.0566	0.7674	0.0320	0.0347	0.0068	0.0923
240	413.15	10000	75.19	3.5643	2.4940	2.6732	2.0629	2.6801	1.8753	2.0100	1.5511	0.3224	0.2256	0.2418	0.1866
241	433.15	10000	78.51	1.9482	2.2261	0.3277	0.2993	1.5296	1.7478	0.2573	0.2350	0.1840	0.2102	0.0309	0.0283
242	453.15	10000	82.09	2.1800	0.9235	0.3691	1.6854	1.7895	0.7581	0.3030	1.3835	0.2152	0.0912	0.0364	0.1664
243	473.15	10000	82.24	1.0343	3.5311	2.4854	0.4713	0.8506	2.9039	2.0440	0.3876	0.1023	0.3493	0.2458	0.0466
244	493.15	10000	84.76	0.9454	2.9413	2.0660	0.2908	0.8013	2.4930	1.7511	0.2465	0.0964	0.2999	0.2106	0.0296
245	513.15	10000	87.07	0.8581	2.4830	1.7196	0.8014	0.7471	2.1619	1.4972	0.6978	0.0899	0.2600	0.1801	0.0839
246	533.15	10000	89.23	0.7647	2.1047	1.4198	1.1503	0.6823	1.8780	1.2669	1.0264	0.0821	0.2259	0.1524	0.1235
247	553.15	10000	91.28	0.6632	1.7784	1.1510	1.3893	0.6054	1.6233	1.0506	1.2681	0.0728	0.1952	0.1264	0.1525
248	573.15	10000	93.24	0.5597	1.4935	0.9092	1.5456	0.5218	1.3925	0.8477	1.4410	0.0628	0.1675	0.1020	0.1733
249	593.15	10000	94.86	0.7279	1.5148	0.9619	1.3741	0.6905	1.4370	0.9125	1.3035	0.0831	0.1728	0.1098	0.1568
250	613.15	10000	96.57	0.7372	1.4000	0.8716	1.3135	0.7119	1.3519	0.8416	1.2684	0.0856	0.1626	0.1012	0.1526
251	633.15	10000	98.10	0.8605	1.4185	0.9079	1.1093	0.8441	1.3915	0.8906	1.0882	0.1015	0.1674	0.1071	0.1309
252	653.15	10000	100.41	0.1403	0.6040	0.1104	1.7110	0.1409	0.6065	0.1108	1.7181	0.0169	0.0730	0.0133	0.2067
253	673.15	10000	102.08	0.0428	0.4274	0.0567	1.6889	0.0437	0.4363	0.0579	1.7240	0.0053	0.0525	0.0070	0.2074
254	693.15	10000	103.70	0.0489	0.2658	0.2125	1.6542	0.0507	0.2756	0.2203	1.7154	0.0061	0.0331	0.0265	0.2063
255	713.15	10000	105.28	0.1348	0.1174	0.3583	1.6119	0.1419	0.1236	0.3772	1.6970	0.0171	0.0149	0.0454	0.2041
∑				232.97	262.77	241.84	148.29	237.24	261.93	242.55	146.54	28.54	31.50	29.17	17.63
Average (Overall)				**0.9136**	**1.0305**	**0.9484**	**0.5815**	**0.9304**	**1.0272**	**0.9512**	**0.5747**	**0.1119**	**0.1235**	**0.1144**	**0.0691**

Table C-17 Refrigerant (152a) [69]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	283.15	100	152.10	0.8912	0.9418	0.9351	0.5851	1.3556	1.4326	1.4222	0.8900	0.1630	0.1723	0.1711	0.1070
2	283.15	200	145.72	1.0178	1.2663	1.2466	0.8474	1.4831	1.8452	1.8165	1.2347	0.1784	0.2219	0.2185	0.1485
3	283.15	300	141.62	1.1854	1.6557	1.6207	1.2052	1.6788	2.3448	2.2952	1.7068	0.2019	0.2820	0.2761	0.2053
4	293.15	100	154.49	0.8685	0.8952	0.8890	0.5325	1.3418	1.3831	1.3735	0.8227	0.1614	0.1664	0.1652	0.0990
5	293.15	200	148.21	0.9648	1.1582	1.1401	0.7214	1.4299	1.7166	1.6896	1.0691	0.1720	0.2065	0.2032	0.1286
6	293.15	300	144.26	1.0730	1.4512	1.4190	0.9689	1.5478	2.0934	2.0469	1.3978	0.1862	0.2518	0.2462	0.1681
7	293.15	400	141.22	1.2032	1.7842	1.7357	1.2773	1.6993	2.5197	2.4512	1.8039	0.2044	0.3031	0.2948	0.2170
8	293.15	500	138.62	1.3892	2.1930	2.1253	1.6792	1.9258	3.0400	2.9462	2.3278	0.2316	0.3656	0.3544	0.2800
9	303.15	100	156.84	0.8541	0.8614	0.8557	0.4947	1.3395	1.3510	1.3421	0.7759	0.1611	0.1625	0.1614	0.0933
10	303.15	200	150.62	0.9328	1.0816	1.0648	0.6309	1.4050	1.6292	1.6038	0.9504	0.1690	0.1960	0.1929	0.1143
11	303.15	300	146.77	1.0079	1.3125	1.2827	0.8050	1.4794	1.9264	1.8827	1.1815	0.1779	0.2317	0.2264	0.1421
12	303.15	400	143.86	1.0945	1.5680	1.5234	1.0225	1.5745	2.2557	2.1916	1.4710	0.1894	0.2713	0.2636	0.1769
13	303.15	500	141.44	1.1977	1.8542	1.7926	1.2863	1.6939	2.6225	2.5354	1.8193	0.2037	0.3154	0.3050	0.2188
14	303.15	600	139.30	1.3220	2.1774	2.0961	1.6014	1.8415	3.0330	2.9197	2.2306	0.2215	0.3648	0.3512	0.2683
15	313.15	100	159.15	0.8410	0.8325	0.8273	0.4638	1.3384	1.3250	1.3166	0.7382	0.1610	0.1594	0.1584	0.0888
16	313.15	200	152.99	0.9108	1.0234	1.0076	0.5624	1.3934	1.5656	1.5415	0.8603	0.1676	0.1883	0.1854	0.1035
17	313.15	300	149.20	0.9706	1.2155	1.1878	0.6882	1.4481	1.8136	1.7722	1.0269	0.1742	0.2181	0.2132	0.1235
18	313.15	400	146.38	1.0307	1.4181	1.3769	0.8420	1.5087	2.0758	2.0154	1.2325	0.1815	0.2497	0.2424	0.1482
19	313.15	500	144.06	1.0966	1.6368	1.5802	1.0257	1.5797	2.3579	2.2764	1.4775	0.1900	0.2836	0.2738	0.1777
20	313.15	600	142.05	1.1685	1.8726	1.7985	1.2387	1.6598	2.6600	2.5548	1.7596	0.1996	0.3199	0.3073	0.2116
21	313.15	800	138.53	1.3665	2.4375	2.3203	1.7936	1.8931	3.3766	3.2142	2.4847	0.2277	0.4061	0.3866	0.2989
22	323.15	100	161.43	0.8308	0.8095	0.8046	0.4403	1.3412	1.3067	1.2988	0.7108	0.1613	0.1572	0.1562	0.0855
23	323.15	200	155.31	0.8924	0.9752	0.9604	0.5070	1.3860	1.5146	1.4917	0.7874	0.1667	0.1822	0.1794	0.0947
24	323.15	300	151.58	0.9414	1.1376	1.1117	0.5954	1.4270	1.7244	1.6851	0.9025	0.1716	0.2074	0.2027	0.1086
25	323.15	400	148.81	0.9884	1.3059	1.2675	0.7059	1.4708	1.9434	1.8862	1.0505	0.1769	0.2337	0.2269	0.1264

26	323.15	500	146.57	1.0344	1.4810	1.4286	0.8358	1.5160	2.1707	2.0939	1.2251	0.1823	0.2611	0.2518	0.1474
27	323.15	600	144.64	1.0846	1.6685	1.6004	0.9890	1.5688	2.4134	2.3148	1.4304	0.1887	0.2903	0.2784	0.1720
28	323.15	800	141.34	1.2034	2.0891	1.9832	1.3703	1.7009	2.9528	2.8032	1.9369	0.2046	0.3552	0.3372	0.2330
29	323.15	1000	138.45	1.3588	2.5906	2.4353	1.8726	1.8813	3.5866	3.3717	2.5927	0.2263	0.4314	0.4055	0.3118
30	333.15	100	163.67	0.8248	0.7928	0.7882	0.4248	1.3499	1.2976	1.2902	0.6953	0.1624	0.1561	0.1552	0.0836
31	333.15	200	157.60	0.8795	0.9377	0.9238	0.4651	1.3860	1.4778	1.4559	0.7330	0.1667	0.1777	0.1751	0.0882
32	333.15	300	153.91	0.9188	1.0749	1.0505	0.5218	1.4141	1.6543	1.6168	0.8032	0.1701	0.1990	0.1945	0.0966
33	333.15	400	151.19	0.9575	1.2177	1.1817	0.5997	1.4476	1.8411	1.7867	0.9067	0.1741	0.2214	0.2149	0.1091
34	333.15	500	149.00	0.9926	1.3631	1.3142	0.6916	1.4789	2.0310	1.9582	1.0305	0.1779	0.2443	0.2355	0.1239
35	333.15	600	147.13	1.0295	1.5164	1.4532	0.8011	1.5147	2.2311	2.1381	1.1787	0.1822	0.2684	0.2572	0.1418
36	333.15	800	143.98	1.1111	1.8506	1.7539	1.0732	1.5997	2.6645	2.5252	1.5452	0.1924	0.3205	0.3037	0.1859
37	333.15	1000	141.29	1.2016	2.2242	2.0851	1.4173	1.6977	3.1426	2.9461	2.0024	0.2042	0.3780	0.3543	0.2409
38	333.15	1200	138.83	1.3154	2.6595	2.4653	1.8577	1.8262	3.6923	3.4227	2.5791	0.2197	0.4441	0.4117	0.3102
39	333.15	1400	136.45	1.4706	3.1876	2.9185	2.4320	2.0068	4.3496	3.9825	3.3185	0.2414	0.5232	0.4790	0.3991
40	343.15	100	165.89	0.8197	0.7790	0.7748	0.4135	1.3599	1.2923	1.2853	0.6860	0.1636	0.1554	0.1546	0.0825
41	343.15	200	159.86	0.8652	0.9030	0.8899	0.4285	1.3831	1.4435	1.4225	0.6849	0.1664	0.1736	0.1711	0.0824
42	343.15	300	156.20	0.9048	1.0276	1.0046	0.4675	1.4133	1.6051	1.5691	0.7302	0.1700	0.1931	0.1887	0.0878
43	343.15	400	153.52	0.9365	1.1494	1.1155	0.5184	1.4376	1.7646	1.7125	0.7958	0.1729	0.2122	0.2060	0.0957
44	343.15	500	151.36	0.9659	1.2738	1.2280	0.5826	1.4621	1.9281	1.8587	0.8819	0.1759	0.2319	0.2236	0.1061
45	343.15	600	149.54	0.9943	1.4019	1.3430	0.6594	1.4869	2.0964	2.0083	0.9861	0.1788	0.2522	0.2416	0.1186
46	343.15	800	146.50	1.0508	1.6728	1.5835	0.8500	1.5395	2.4506	2.3198	1.2452	0.1852	0.2948	0.2790	0.1498
47	343.15	1000	143.95	1.1124	1.9707	1.8443	1.0949	1.6012	2.8367	2.6547	1.5761	0.1926	0.3412	0.3193	0.1896
48	343.15	1200	141.67	1.1789	2.2996	2.1267	1.3981	1.6701	3.2577	3.0129	1.9807	0.2009	0.3918	0.3624	0.2382
49	343.15	1400	139.53	1.2607	2.6763	2.4437	1.7793	1.7591	3.7343	3.4097	2.4827	0.2116	0.4492	0.4101	0.2986
50	343.15	1600	137.46	1.3612	3.1140	2.8012	2.2575	1.8710	4.2805	3.8505	3.1032	0.2250	0.5149	0.4631	0.3732
51	353.15	100	168.09	0.8166	0.7686	0.7646	0.4070	1.3726	1.2919	1.2853	0.6841	0.1651	0.1554	0.1546	0.0823
52	353.15	200	162.08	0.8593	0.8800	0.8675	0.4057	1.3927	1.4262	1.4060	0.6576	0.1675	0.1715	0.1691	0.0791
53	353.15	300	158.46	0.8885	0.9834	0.9616	0.4195	1.4079	1.5583	1.5238	0.6647	0.1693	0.1874	0.1833	0.0799
54	353.15	400	155.81	0.9148	1.0883	1.0562	0.4487	1.4253	1.6956	1.6457	0.6990	0.1714	0.2039	0.1979	0.0841
55	353.15	500	153.69	0.9399	1.1958	1.1526	0.4907	1.4445	1.8378	1.7714	0.7541	0.1737	0.2210	0.2131	0.0907

56	353.15	600	151.90	0.9651	1.3072	1.2519	0.5447	1.4660	1.9856	1.9016	0.8274	0.1763	0.2388	0.2287	0.0995
57	353.15	800	148.94	1.0107	1.5367	1.4537	0.6795	1.5053	2.2887	2.1651	1.0120	0.1811	0.2753	0.2604	0.1217
58	353.15	1000	146.48	1.0548	1.7811	1.6650	0.8527	1.5451	2.6089	2.4389	1.2490	0.1858	0.3138	0.2933	0.1502
59	353.15	1200	144.32	1.0995	2.0447	1.8885	1.0675	1.5869	2.9510	2.7255	1.5406	0.1909	0.3549	0.3278	0.1853
60	353.15	1400	142.34	1.1496	2.3358	2.1298	1.3328	1.6363	3.3247	3.0315	1.8971	0.1968	0.3999	0.3646	0.2282
61	353.15	1600	140.47	1.2001	2.6541	2.3849	1.6513	1.6857	3.7282	3.3500	2.3196	0.2028	0.4484	0.4029	0.2790
62	353.15	2000	136.80	1.3419	3.4457	2.9770	2.5429	1.8356	4.7137	4.0725	3.4786	0.2208	0.5670	0.4898	0.4184
63	363.15	100	170.26	0.8122	0.7582	0.7545	0.4016	1.3829	1.2909	1.2845	0.6837	0.1663	0.1553	0.1545	0.0822
64	363.15	200	164.28	0.8503	0.8567	0.8448	0.3847	1.3969	1.4073	1.3878	0.6320	0.1680	0.1693	0.1669	0.0760
65	363.15	300	160.68	0.8798	0.9514	0.9306	0.3865	1.4136	1.5286	1.4953	0.6209	0.1700	0.1839	0.1799	0.0747
66	363.15	400	158.05	0.9029	1.0434	1.0130	0.3991	1.4271	1.6491	1.6011	0.6307	0.1717	0.1984	0.1926	0.0759
67	363.15	500	155.97	0.9214	1.1339	1.0931	0.4198	1.4371	1.7685	1.7048	0.6547	0.1729	0.2127	0.2050	0.0788
68	363.15	600	154.21	0.9408	1.2283	1.1762	0.4520	1.4508	1.8942	1.8138	0.6971	0.1745	0.2278	0.2182	0.0838
69	363.15	800	151.32	0.9778	1.4245	1.3468	0.5421	1.4795	2.1555	2.0380	0.8203	0.1780	0.2593	0.2451	0.0987
70	363.15	1000	148.93	1.0138	1.6323	1.5248	0.6645	1.5099	2.4311	2.2709	0.9897	0.1816	0.2924	0.2731	0.1190
71	363.15	1200	146.86	1.0435	1.8476	1.7046	0.8132	1.5325	2.7134	2.5034	1.1943	0.1843	0.3264	0.3011	0.1436
72	363.15	1400	144.99	1.0778	2.0833	1.8977	1.0007	1.5626	3.0205	2.7514	1.4510	0.1880	0.3633	0.3309	0.1745
73	363.15	1600	143.24	1.1105	2.3357	2.0980	1.2246	1.5907	3.3458	3.0053	1.7542	0.1913	0.4024	0.3615	0.2110
74	363.15	2000	139.96	1.1810	2.9167	2.5296	1.8177	1.6529	4.0821	3.5403	2.5439	0.1988	0.4910	0.4258	0.3060
75	373.15	100	172.41	0.8111	0.7521	0.7486	0.4015	1.3984	1.2966	1.2906	0.6922	0.1682	0.1560	0.1552	0.0833
76	373.15	200	166.44	0.8474	0.8417	0.8304	0.3739	1.4104	1.4009	1.3821	0.6223	0.1696	0.1685	0.1662	0.0748
77	373.15	300	162.87	0.8715	0.9234	0.9036	0.3602	1.4194	1.5039	1.4717	0.5866	0.1707	0.1809	0.1770	0.0706
78	373.15	400	160.27	0.8898	1.0024	0.9734	0.3568	1.4261	1.6066	1.5601	0.5719	0.1715	0.1932	0.1877	0.0688
79	373.15	500	158.21	0.9083	1.0842	1.0453	0.3654	1.4369	1.7152	1.6537	0.5781	0.1728	0.2063	0.1989	0.0695
80	373.15	600	156.47	0.9240	1.1657	1.1163	0.3810	1.4459	1.8241	1.7467	0.5962	0.1739	0.2194	0.2101	0.0717
81	373.15	800	153.63	0.9560	1.3366	1.2635	0.4368	1.4687	2.0535	1.9412	0.6711	0.1767	0.2470	0.2335	0.0807
82	373.15	1000	151.32	0.9819	1.5113	1.4110	0.5150	1.4857	2.2869	2.1350	0.7793	0.1787	0.2751	0.2568	0.0937
83	373.15	1200	149.31	1.0060	1.6948	1.5627	0.6182	1.5020	2.5306	2.3333	0.9231	0.1807	0.3044	0.2806	0.1110
84	373.15	1400	147.52	1.0314	1.8914	1.7220	0.7498	1.5216	2.7902	2.5402	1.1061	0.1830	0.3356	0.3055	0.1330
85	373.15	1600	145.87	1.0538	2.0980	1.8843	0.9069	1.5371	3.0603	2.7485	1.3228	0.1849	0.3681	0.3306	0.1591

86	373.15	2000	142.83	1.0908	2.5517	2.2187	1.3122	1.5580	3.6445	3.1690	1.8742	0.1874	0.4384	0.3812	0.2254
87	383.15	100	174.54	0.8062	0.7430	0.7396	0.3994	1.4071	1.2968	1.2910	0.6972	0.1692	0.1560	0.1553	0.0839
88	383.15	200	168.60	0.8393	0.8233	0.8125	0.3613	1.4150	1.3881	1.3699	0.6092	0.1702	0.1670	0.1648	0.0733
89	383.15	300	165.04	0.8648	0.8999	0.8810	0.3407	1.4272	1.4852	1.4540	0.5623	0.1717	0.1786	0.1749	0.0676
90	383.15	400	162.46	0.8810	0.9699	0.9422	0.3261	1.4312	1.5757	1.5307	0.5298	0.1721	0.1895	0.1841	0.0637
91	383.15	500	160.41	0.8978	1.0427	1.0056	0.3232	1.4401	1.6725	1.6131	0.5184	0.1732	0.2012	0.1940	0.0624
92	383.15	600	158.70	0.9124	1.1154	1.0683	0.3270	1.4480	1.7701	1.6954	0.5189	0.1742	0.2129	0.2039	0.0624
93	383.15	800	155.91	0.9353	1.2603	1.1912	0.3499	1.4582	1.9650	1.8573	0.5455	0.1754	0.2363	0.2234	0.0656
94	383.15	1000	153.65	0.9547	1.4098	1.3156	0.3943	1.4669	2.1662	2.0213	0.6058	0.1764	0.2605	0.2431	0.0729
95	383.15	1200	151.70	0.9756	1.5691	1.4460	0.4626	1.4800	2.3803	2.1935	0.7018	0.1780	0.2863	0.2638	0.0844
96	383.15	1400	149.97	0.9931	1.7338	1.5775	0.5495	1.4893	2.6002	2.3657	0.8241	0.1791	0.3127	0.2845	0.0991
97	383.15	1600	148.39	1.0079	1.9057	1.7108	0.6562	1.4956	2.8279	2.5386	0.9737	0.1799	0.3401	0.3053	0.1171
98	383.15	2000	145.52	1.0373	2.2837	1.9897	0.9428	1.5094	3.3231	2.8953	1.3720	0.1816	0.3997	0.3482	0.1650
99	393.15	100	176.65	0.8055	0.7388	0.7357	0.4032	1.4229	1.3051	1.2995	0.7122	0.1711	0.1570	0.1563	0.0857
100	393.15	200	170.72	0.8347	0.8101	0.7997	0.3553	1.4249	1.3829	1.3652	0.6065	0.1714	0.1663	0.1642	0.0730
101	393.15	300	167.18	0.8564	0.8773	0.8592	0.3242	1.4318	1.4668	1.4364	0.5421	0.1722	0.1764	0.1728	0.0652
102	393.15	400	164.62	0.8734	0.9421	0.9156	0.3029	1.4377	1.5509	1.5072	0.4987	0.1729	0.1865	0.1813	0.0600
103	393.15	500	162.59	0.8871	1.0057	0.9702	0.2889	1.4424	1.6351	1.5775	0.4697	0.1735	0.1967	0.1897	0.0565
104	393.15	600	160.90	0.8992	1.0692	1.0243	0.2813	1.4468	1.7203	1.6481	0.4527	0.1740	0.2069	0.1982	0.0544
105	393.15	800	158.15	0.9182	1.1962	1.1306	0.2810	1.4522	1.8918	1.7880	0.4443	0.1747	0.2275	0.2151	0.0534
106	393.15	1000	155.93	0.9359	1.3283	1.2393	0.3013	1.4593	2.0712	1.9324	0.4698	0.1755	0.2491	0.2324	0.0565
107	393.15	1200	154.02	0.9531	1.4666	1.3512	0.3406	1.4680	2.2590	2.0811	0.5246	0.1766	0.2717	0.2503	0.0631
108	393.15	1400	152.35	0.9654	1.6070	1.4616	0.3934	1.4707	2.4482	2.2267	0.5993	0.1769	0.2945	0.2678	0.0721
109	393.15	1600	150.82	0.9785	1.7558	1.5761	0.4651	1.4758	2.6481	2.3771	0.7015	0.1775	0.3185	0.2859	0.0844
110	393.15	2000	148.09	0.9958	2.0700	1.8055	0.6567	1.4746	3.0654	2.6736	0.9725	0.1774	0.3687	0.3216	0.1170
111	403.15	100	178.74	0.8020	0.7324	0.7294	0.4055	1.4334	1.3091	1.3038	0.7248	0.1724	0.1575	0.1568	0.0872
112	403.15	200	172.83	0.8301	0.7981	0.7882	0.3520	1.4347	1.3794	1.3622	0.6083	0.1726	0.1659	0.1638	0.0732
113	403.15	300	169.30	0.8513	0.8600	0.8425	0.3149	1.4412	1.4560	1.4263	0.5331	0.1733	0.1751	0.1716	0.0641
114	403.15	400	166.76	0.8639	0.9154	0.8898	0.2833	1.4406	1.5264	1.4839	0.4724	0.1733	0.1836	0.1785	0.0568
115	403.15	500	164.74	0.8776	0.9735	0.9395	0.2626	1.4459	1.6039	1.5478	0.4326	0.1739	0.1929	0.1862	0.0520

116	403.15	600	163.07	0.8859	1.0278	0.9847	0.2441	1.4447	1.6760	1.6058	0.3981	0.1738	0.2016	0.1931	0.0479
117	403.15	800	160.35	0.9067	1.1446	1.0820	0.2296	1.4540	1.8354	1.7350	0.3682	0.1749	0.2208	0.2087	0.0443
118	403.15	1000	158.17	0.9195	1.2587	1.1742	0.2270	1.4543	1.9908	1.8572	0.3590	0.1749	0.2395	0.2234	0.0432
119	403.15	1200	156.30	0.9334	1.3795	1.2705	0.2426	1.4589	2.1561	1.9859	0.3792	0.1755	0.2593	0.2389	0.0456
120	403.15	1400	154.67	0.9446	1.5031	1.3668	0.2712	1.4610	2.3247	2.1139	0.4194	0.1757	0.2796	0.2543	0.0504
121	403.15	1600	153.19	0.9504	1.6272	1.4601	0.3095	1.4559	2.4927	2.2368	0.4741	0.1751	0.2998	0.2690	0.0570
122	403.15	2000	150.56	0.9667	1.8999	1.6585	0.4364	1.4554	2.8605	2.4970	0.6570	0.1751	0.3441	0.3003	0.0790
123	403.15	4000	139.66	0.8351	3.7128	2.2454	2.1544	1.1663	5.1855	3.1361	3.0090	0.1403	0.6237	0.3772	0.3619
124	413.15	100	180.81	0.7997	0.7278	0.7249	0.4103	1.4460	1.3159	1.3108	0.7419	0.1739	0.1583	0.1577	0.0892
125	413.15	200	174.92	0.8262	0.7879	0.7783	0.3516	1.4452	1.3782	1.3614	0.6149	0.1738	0.1658	0.1637	0.0740
126	413.15	300	171.40	0.8459	0.8441	0.8273	0.3088	1.4499	1.4469	1.4179	0.5293	0.1744	0.1740	0.1705	0.0637
127	413.15	400	168.87	0.8574	0.8940	0.8694	0.2712	1.4479	1.5097	1.4682	0.4579	0.1741	0.1816	0.1766	0.0551
128	413.15	500	166.87	0.8702	0.9467	0.9139	0.2442	1.4521	1.5797	1.5251	0.4075	0.1747	0.1900	0.1834	0.0490
129	413.15	600	165.21	0.8779	0.9955	0.9541	0.2193	1.4504	1.6446	1.5763	0.3624	0.1744	0.1978	0.1896	0.0436
130	413.15	800	162.53	0.8941	1.0975	1.0376	0.1874	1.4531	1.7837	1.6863	0.3045	0.1748	0.2145	0.2028	0.0366
131	413.15	1000	160.37	0.9076	1.2013	1.1208	0.1708	1.4555	1.9265	1.7974	0.2739	0.1751	0.2317	0.2162	0.0329
132	413.15	1200	158.54	0.9153	1.3039	1.2006	0.1637	1.4512	2.0672	1.9035	0.2596	0.1745	0.2486	0.2289	0.0312
133	413.15	1400	156.94	0.9261	1.4140	1.2855	0.1733	1.4533	2.2191	2.0174	0.2719	0.1748	0.2669	0.2427	0.0327
134	413.15	1600	155.50	0.9333	1.5254	1.3689	0.1922	1.4512	2.3720	2.1285	0.2989	0.1746	0.2853	0.2560	0.0359
135	413.15	2000	152.95	0.9417	1.7577	1.5349	0.2616	1.4404	2.6884	2.3477	0.4001	0.1732	0.3234	0.2824	0.0481
136	413.15	4000	142.89	0.8356	3.2371	2.1869	1.3862	1.1940	4.6256	3.1249	1.9808	0.1436	0.5564	0.3759	0.2382
137	423.15	400	170.97	0.8505	0.8743	0.8505	0.2627	1.4541	1.4948	1.4542	0.4492	0.1749	0.1798	0.1749	0.0540
138	423.15	500	168.98	0.8616	0.9213	0.8897	0.2298	1.4560	1.5568	1.5034	0.3883	0.1751	0.1872	0.1808	0.0467
139	423.15	600	167.33	0.8678	0.9645	0.9246	0.1988	1.4522	1.6139	1.5472	0.3327	0.1747	0.1941	0.1861	0.0400
140	423.15	800	164.67	0.8817	1.0554	0.9978	0.1540	1.4519	1.7379	1.6431	0.2536	0.1746	0.2090	0.1976	0.0305
141	423.15	1000	162.54	0.8938	1.1484	1.0714	0.1242	1.4528	1.8666	1.7414	0.2018	0.1747	0.2245	0.2095	0.0243
142	423.15	1200	160.74	0.9013	1.2405	1.1421	0.1035	1.4487	1.9940	1.8359	0.1663	0.1742	0.2398	0.2208	0.0200
143	423.15	1400	159.17	0.9087	1.3363	1.2145	0.0948	1.4463	2.1270	1.9332	0.1508	0.1740	0.2558	0.2325	0.0181
144	423.15	1600	157.76	0.9139	1.4340	1.2864	0.0951	1.4419	2.2623	2.0294	0.1500	0.1734	0.2721	0.2441	0.0180
145	423.15	2000	155.29	0.9190	1.6362	1.4287	0.1219	1.4271	2.5409	2.2187	0.1893	0.1717	0.3056	0.2669	0.0228

146	423.15	4000	145.83	0.8347	2.8840	2.0440	0.8463	1.2172	4.2056	2.9807	1.2341	0.1464	0.5058	0.3585	0.1484
147	433.15	400	173.04	0.8439	0.8566	0.8336	0.2580	1.4603	1.4822	1.4424	0.4464	0.1756	0.1783	0.1735	0.0537
148	433.15	500	171.07	0.8527	0.8978	0.8672	0.2194	1.4586	1.5357	1.4834	0.3753	0.1754	0.1847	0.1784	0.0451
149	433.15	600	169.43	0.8606	0.9391	0.9006	0.1865	1.4582	1.5911	1.5259	0.3159	0.1754	0.1914	0.1835	0.0380
150	433.15	800	166.79	0.8747	1.0226	0.9672	0.1335	1.4588	1.7055	1.6131	0.2226	0.1755	0.2051	0.1940	0.0268
151	433.15	1000	164.68	0.8836	1.1044	1.0304	0.0909	1.4552	1.8186	1.6969	0.1498	0.1750	0.2187	0.2041	0.0180
152	433.15	1200	162.91	0.8888	1.1855	1.0914	0.0572	1.4480	1.9313	1.7780	0.0931	0.1742	0.2323	0.2139	0.0112
153	433.15	1400	161.36	0.8948	1.2707	1.1547	0.0351	1.4439	2.0504	1.8632	0.0566	0.1737	0.2466	0.2241	0.0068
154	433.15	1600	159.98	0.8998	1.3580	1.2180	0.0217	1.4394	2.1725	1.9487	0.0346	0.1731	0.2613	0.2344	0.0042
155	433.15	2000	157.57	0.9035	1.5367	1.3421	0.0160	1.4236	2.4214	2.1148	0.0253	0.1712	0.2912	0.2544	0.0030
156	433.15	4000	148.57	0.8305	2.6053	1.8957	0.4473	1.2339	3.8707	2.8164	0.6645	0.1484	0.4656	0.3388	0.0799
∑				165.93	236.83	220.69	112.80	258.37	361.98	338.17	171.54	31.08	43.54	40.67	20.63
Average (Overall)				**1.0637**	**1.5181**	**1.4147**	**0.7231**	**1.6562**	**2.3204**	**2.1678**	**1.0996**	**0.1992**	**0.2791**	**0.2607**	**0.1323**

Table C-18 Refrigerant (134a) [76]

Pt. no.	T (K)	P (kPa)	$S_{(exp)}$ (J/mol.K)	AD%				AD (J/mol.K)				AD/R			
				L&K	P&R	Soave	This work	L&K	P&R	Soave	This work	L&K	P&R	Soave	This work
1	263.15	100	183.43	2.5779	2.7423	2.7328	1.4439	4.7288	5.0302	5.0129	2.6487	0.5688	0.6050	0.6030	0.3186
2	273.15	100	186.52	2.5415	2.6727	2.6640	1.3955	4.7406	4.9853	4.9690	2.6030	0.5702	0.5996	0.5977	0.3131
3	283.15	100	189.56	2.5106	2.6152	2.6071	1.3626	4.7590	4.9572	4.9418	2.5829	0.5724	0.5962	0.5944	0.3107
4	293.15	100	192.52	2.4873	2.5703	2.5628	1.3458	4.7886	4.9485	4.9339	2.5910	0.5760	0.5952	0.5934	0.3116
5	303.15	100	195.44	2.4679	2.5333	2.5262	1.3400	4.8233	4.9512	4.9373	2.6189	0.5801	0.5955	0.5939	0.3150
6	313.15	100	198.31	2.4538	2.5048	2.4981	1.3457	4.8661	4.9673	4.9540	2.6686	0.5853	0.5975	0.5959	0.3210
7	323.15	100	201.13	2.4462	2.4853	2.4789	1.3630	4.9199	4.9985	4.9857	2.7414	0.5918	0.6012	0.5997	0.3297
8	333.15	100	203.91	2.4356	2.4647	2.4587	1.3820	4.9664	5.0258	5.0135	2.8180	0.5974	0.6045	0.6030	0.3389
9	343.15	100	206.67	2.4230	2.4439	2.4381	1.4029	5.0076	5.0507	5.0388	2.8993	0.6023	0.6075	0.6061	0.3487
10	353.15	100	209.38	2.4145	2.4284	2.4229	1.4310	5.0555	5.0846	5.0730	2.9963	0.6081	0.6116	0.6102	0.3604

11	363.15	100	212.06	2.4056	2.4136	2.4083	1.4614	5.1013	5.1183	5.1070	3.0990	0.6136	0.6156	0.6143	0.3727
12	373.15	100	214.72	2.3968	2.3998	2.3947	1.4940	5.1463	5.1528	5.1419	3.2079	0.6190	0.6198	0.6185	0.3858
13	383.15	100	217.34	2.3887	2.3875	2.3826	1.5289	5.1917	5.1890	5.1783	3.3229	0.6244	0.6241	0.6228	0.3997
14	393.15	100	219.93	2.3818	2.3770	2.3722	1.5661	5.2384	5.2278	5.2172	3.4443	0.6301	0.6288	0.6275	0.4143
15	403.15	100	222.50	2.3717	2.3638	2.3591	1.6007	5.2771	5.2595	5.2491	3.5615	0.6347	0.6326	0.6314	0.4284
16	273.15	200	180.06	2.6888	3.0245	3.0037	1.6673	4.8414	5.4457	5.4083	3.0021	0.5823	0.6550	0.6505	0.3611
17	283.15	200	183.21	2.6280	2.9037	2.8844	1.5597	4.8147	5.3198	5.2846	2.8576	0.5791	0.6399	0.6356	0.3437
18	293.15	200	186.27	2.5858	2.8134	2.7955	1.4871	4.8166	5.2406	5.2072	2.7701	0.5793	0.6303	0.6263	0.3332
19	303.15	200	189.26	2.5539	2.7425	2.7257	1.4381	4.8335	5.1905	5.1587	2.7217	0.5814	0.6243	0.6205	0.3274
20	313.15	200	192.19	2.5290	2.6857	2.6699	1.4071	4.8604	5.1616	5.1312	2.7043	0.5846	0.6208	0.6172	0.3253
21	323.15	200	195.05	2.5130	2.6434	2.6284	1.3943	4.9016	5.1561	5.1269	2.7196	0.5896	0.6202	0.6167	0.3271
22	333.15	200	197.88	2.4966	2.6052	2.5910	1.3890	4.9404	5.1553	5.1272	2.7485	0.5942	0.6201	0.6167	0.3306
23	343.15	200	200.66	2.4867	2.5770	2.5635	1.3967	4.9897	5.1710	5.1439	2.8026	0.6002	0.6220	0.6187	0.3371
24	353.15	200	203.40	2.4738	2.5488	2.5359	1.4072	5.0318	5.1843	5.1580	2.8622	0.6052	0.6236	0.6204	0.3443
25	363.15	200	206.10	2.4642	2.5262	2.5138	1.4256	5.0788	5.2066	5.1810	2.9383	0.6109	0.6262	0.6232	0.3534
26	373.15	200	208.77	2.4585	2.5095	2.4975	1.4521	5.1325	5.2390	5.2140	3.0314	0.6173	0.6301	0.6271	0.3646
27	383.15	200	211.41	2.4475	2.4890	2.4775	1.4765	5.1742	5.2620	5.2376	3.1214	0.6223	0.6329	0.6300	0.3754
28	393.15	200	214.02	2.4368	2.4702	2.4591	1.5040	5.2152	5.2868	5.2630	3.2188	0.6273	0.6359	0.6330	0.3872
29	403.15	200	216.60	2.4270	2.4535	2.4427	1.5344	5.2569	5.3143	5.2909	3.3236	0.6323	0.6392	0.6364	0.3998
30	413.15	200	219.15	2.4185	2.4389	2.4284	1.5677	5.3002	5.3450	5.3220	3.4357	0.6375	0.6429	0.6401	0.4132
31	423.15	200	221.68	2.4069	2.4221	2.4119	1.5990	5.3358	5.3695	5.3469	3.5448	0.6418	0.6458	0.6431	0.4264
32	283.15	400	176.12	2.8271	3.4990	3.4511	1.9327	4.9790	6.1624	6.0780	3.4037	0.5989	0.7412	0.7311	0.4094
33	293.15	400	179.41	2.7324	3.2889	3.2451	1.7235	4.9023	5.9007	5.8221	3.0921	0.5896	0.7097	0.7003	0.3719
34	303.15	400	182.59	2.6630	3.1280	3.0875	1.5711	4.8623	5.7113	5.6374	2.8686	0.5848	0.6869	0.6781	0.3450
35	313.15	400	185.65	2.6186	3.0099	2.9723	1.4682	4.8613	5.5878	5.5180	2.7257	0.5847	0.6721	0.6637	0.3278
36	323.15	400	188.63	2.5860	2.9174	2.8822	1.3969	4.8778	5.5030	5.4365	2.6349	0.5867	0.6619	0.6539	0.3169
37	333.15	400	191.53	2.5629	2.8451	2.8119	1.3512	4.9088	5.4493	5.3857	2.5880	0.5904	0.6554	0.6478	0.3113
38	343.15	400	194.38	2.5463	2.7877	2.7563	1.3254	4.9496	5.4188	5.3578	2.5763	0.5953	0.6518	0.6444	0.3099
39	353.15	400	197.18	2.5331	2.7403	2.7105	1.3139	4.9947	5.4032	5.3444	2.5907	0.6008	0.6499	0.6428	0.3116
40	363.15	400	199.93	2.5196	2.6980	2.6695	1.3115	5.0374	5.3941	5.3373	2.6220	0.6059	0.6488	0.6420	0.3154

41	373.15	400	202.64	2.5124	2.6665	2.6392	1.3232	5.0910	5.4032	5.3480	2.6812	0.6123	0.6499	0.6433	0.3225
42	383.15	400	205.31	2.5024	2.6357	2.6095	1.3387	5.1376	5.4113	5.3575	2.7484	0.6179	0.6509	0.6444	0.3306
43	393.15	400	207.95	2.4907	2.6061	2.5809	1.3580	5.1794	5.4195	5.3671	2.8240	0.6230	0.6519	0.6455	0.3397
44	403.15	400	210.55	2.4832	2.5832	2.5589	1.3860	5.2284	5.4391	5.3878	2.9183	0.6289	0.6542	0.6480	0.3510
45	413.15	400	213.13	2.4706	2.5573	2.5337	1.4127	5.2656	5.4506	5.4003	3.0110	0.6333	0.6556	0.6495	0.3622
46	423.15	400	215.69	2.4586	2.5338	2.5108	1.4429	5.3028	5.4650	5.4155	3.1122	0.6378	0.6573	0.6514	0.3743
47	303.15	600	178.16	2.7712	3.5558	3.4841	1.7954	4.9370	6.3349	6.2071	3.1987	0.5938	0.7620	0.7466	0.3847
48	313.15	600	181.40	2.6919	3.3494	3.2838	1.5905	4.8831	6.0759	5.9570	2.8852	0.5873	0.7308	0.7165	0.3470
49	323.15	600	184.51	2.6408	3.1970	3.1364	1.4490	4.8727	5.8989	5.7872	2.6736	0.5861	0.7095	0.6961	0.3216
50	333.15	600	187.52	2.6069	3.0809	3.0246	1.3521	4.8887	5.7775	5.6719	2.5356	0.5880	0.6949	0.6822	0.3050
51	343.15	600	190.45	2.5836	2.9902	2.9374	1.2878	4.9205	5.6949	5.5944	2.4526	0.5918	0.6850	0.6729	0.2950
52	353.15	600	193.32	2.5633	2.9140	2.8643	1.2445	4.9553	5.6334	5.5373	2.4058	0.5960	0.6776	0.6660	0.2894
53	363.15	600	196.13	2.5490	2.8531	2.8060	1.2219	4.9992	5.5956	5.5033	2.3964	0.6013	0.6730	0.6619	0.2882
54	373.15	600	198.88	2.5375	2.8023	2.7575	1.2143	5.0467	5.5732	5.4841	2.4151	0.6070	0.6703	0.6596	0.2905
55	383.15	600	201.59	2.5255	2.7569	2.7141	1.2165	5.0914	5.5578	5.4715	2.4524	0.6124	0.6685	0.6581	0.2950
56	393.15	600	204.26	2.5197	2.7225	2.6815	1.2333	5.1466	5.5609	5.4771	2.5190	0.6190	0.6689	0.6588	0.3030
57	403.15	600	206.89	2.5108	2.6892	2.6497	1.2542	5.1947	5.5636	5.4819	2.5948	0.6248	0.6692	0.6594	0.3121
58	413.15	600	209.49	2.5002	2.6573	2.6192	1.2793	5.2378	5.5669	5.4870	2.6799	0.6300	0.6696	0.6600	0.3223
59	423.15	600	212.06	2.4888	2.6274	2.5905	1.3083	5.2778	5.5718	5.4936	2.7743	0.6348	0.6702	0.6608	0.3337
60	433.15	600	214.60	2.4772	2.5998	2.5640	1.3410	5.3162	5.5792	5.5024	2.8779	0.6394	0.6711	0.6618	0.3461
61	443.15	600	217.11	2.4662	2.5747	2.5398	1.3773	5.3545	5.5900	5.5143	2.9903	0.6440	0.6724	0.6633	0.3597
62	313.15	800	178.01	2.7755	3.7376	3.6353	1.8055	4.9405	6.6531	6.4710	3.2139	0.5942	0.8002	0.7783	0.3866
63	323.15	800	181.29	2.6967	3.5047	3.4121	1.5684	4.8889	6.3536	6.1857	2.8434	0.5880	0.7642	0.7440	0.3420
64	333.15	800	184.43	2.6444	3.3300	3.2451	1.4021	4.8771	6.1416	5.9851	2.5859	0.5866	0.7387	0.7199	0.3110
65	343.15	800	187.46	2.6096	3.1964	3.1179	1.2873	4.8921	5.9921	5.8449	2.4133	0.5884	0.7207	0.7030	0.2903
66	353.15	800	190.41	2.5816	3.0874	3.0142	1.2062	4.9156	5.8788	5.7394	2.2967	0.5912	0.7071	0.6903	0.2762
67	363.15	800	193.28	2.5648	3.0036	2.9348	1.1577	4.9572	5.8053	5.6724	2.2376	0.5962	0.6983	0.6823	0.2691
68	373.15	800	196.09	2.5517	2.9344	2.8695	1.1306	5.0035	5.7539	5.6266	2.2168	0.6018	0.6921	0.6768	0.2666
69	383.15	800	198.83	2.5450	2.8804	2.8187	1.1242	5.0602	5.7271	5.6045	2.2353	0.6086	0.6888	0.6741	0.2689
70	393.15	800	201.54	2.5311	2.8262	2.7674	1.1227	5.1013	5.6961	5.5776	2.2628	0.6136	0.6851	0.6709	0.2722

71	403.15	800	204.21	2.5223	2.7830	2.7266	1.1363	5.1508	5.6830	5.5680	2.3204	0.6195	0.6835	0.6697	0.2791
72	413.15	800	206.83	2.5149	2.7458	2.6916	1.1593	5.2015	5.6790	5.5671	2.3979	0.6256	0.6831	0.6696	0.2884
73	423.15	800	209.42	2.5049	2.7100	2.6578	1.1867	5.2457	5.6753	5.5660	2.4852	0.6309	0.6826	0.6695	0.2989
74	433.15	800	211.97	2.4983	2.6810	2.6305	1.2230	5.2958	5.6830	5.5760	2.5924	0.6370	0.6835	0.6707	0.3118
75	443.15	800	214.50	2.4863	2.6493	2.6003	1.2582	5.3331	5.6828	5.5777	2.6989	0.6415	0.6835	0.6709	0.3246
76	453.15	800	217.00	2.4744	2.6201	2.5724	1.2970	5.3695	5.6856	5.5821	2.8145	0.6458	0.6839	0.6714	0.3385
77	313.15	1000	174.96	2.8842	4.2025	4.0496	2.1418	5.0464	7.3528	7.0854	3.7474	0.6070	0.8844	0.8522	0.4507
78	323.15	1000	178.49	2.7582	3.8518	3.7172	1.7639	4.9232	6.8753	6.6350	3.1486	0.5922	0.8270	0.7981	0.3787
79	333.15	1000	181.80	2.6836	3.6044	3.4835	1.5087	4.8788	6.5527	6.3331	2.7428	0.5868	0.7882	0.7617	0.3299
80	343.15	1000	184.95	2.6350	3.4189	3.3089	1.3308	4.8735	6.3234	6.1200	2.4614	0.5862	0.7606	0.7361	0.2961
81	353.15	1000	187.99	2.5996	3.2733	3.1720	1.2053	4.8872	6.1535	5.9631	2.2659	0.5878	0.7401	0.7172	0.2725
82	363.15	1000	190.93	2.5792	3.1624	3.0683	1.1249	4.9245	6.0381	5.8584	2.1479	0.5923	0.7263	0.7046	0.2583
83	373.15	1000	193.80	2.5622	3.0705	2.9823	1.0723	4.9655	5.9505	5.7797	2.0781	0.5972	0.7157	0.6952	0.2499
84	383.15	1000	196.60	2.5526	2.9981	2.9150	1.0466	5.0183	5.8941	5.7308	2.0575	0.6036	0.7089	0.6893	0.2475
85	393.15	1000	199.34	2.5429	2.9352	2.8565	1.0368	5.0690	5.8511	5.6942	2.0667	0.6097	0.7038	0.6849	0.2486
86	403.15	1000	202.03	2.5355	2.8825	2.8075	1.0424	5.1225	5.8236	5.6721	2.1060	0.6161	0.7005	0.6822	0.2533
87	413.15	1000	204.69	2.5271	2.8352	2.7635	1.0580	5.1727	5.8033	5.6565	2.1656	0.6222	0.6980	0.6804	0.2605
88	423.15	1000	207.31	2.5144	2.7889	2.7200	1.0783	5.2126	5.7815	5.6387	2.2353	0.6270	0.6954	0.6782	0.2689
89	433.15	1000	209.88	2.5087	2.7540	2.6876	1.1128	5.2654	5.7800	5.6406	2.3355	0.6333	0.6952	0.6784	0.2809
90	443.15	1000	212.43	2.4962	2.7159	2.6516	1.1465	5.3027	5.7693	5.6329	2.4354	0.6378	0.6939	0.6775	0.2929
91	453.15	1000	214.95	2.4828	2.6800	2.6177	1.1839	5.3368	5.7606	5.6267	2.5449	0.6419	0.6929	0.6768	0.3061
92	323.15	1200	175.87	2.8448	4.2696	4.0774	2.0691	5.0033	7.5091	7.1709	3.6390	0.6018	0.9032	0.8625	0.4377
93	333.15	1200	179.41	2.7279	3.9130	3.7455	1.6804	4.8941	7.0205	6.7198	3.0149	0.5887	0.8444	0.8083	0.3626
94	343.15	1200	182.72	2.6608	3.6620	3.5127	1.4205	4.8617	6.6912	6.4183	2.5955	0.5848	0.8048	0.7720	0.3122
95	353.15	1200	185.87	2.6151	3.4709	3.3356	1.2383	4.8607	6.4513	6.1999	2.3016	0.5846	0.7760	0.7457	0.2768
96	363.15	1200	188.90	2.5853	3.3237	3.1996	1.1143	4.8838	6.2786	6.0442	2.1049	0.5874	0.7552	0.7270	0.2532
97	373.15	1200	191.83	2.5683	3.2104	3.0954	1.0356	4.9268	6.1585	5.9379	1.9865	0.5926	0.7407	0.7142	0.2389
98	383.15	1200	194.69	2.5533	3.1153	3.0078	0.9848	4.9710	6.0650	5.8558	1.9172	0.5979	0.7295	0.7043	0.2306
99	393.15	1200	197.47	2.5447	3.0393	2.9382	0.9611	5.0250	6.0018	5.8021	1.8979	0.6044	0.7219	0.6979	0.2283
100	403.15	1200	200.20	2.5402	2.9778	2.8820	0.9586	5.0854	5.9614	5.7697	1.9190	0.6117	0.7170	0.6940	0.2308

101	413.15	1200	202.88	2.5322	2.9209	2.8298	0.9664	5.1373	5.9260	5.7411	1.9606	0.6179	0.7128	0.6905	0.2358
102	423.15	1200	205.52	2.5227	2.8694	2.7822	0.9842	5.1848	5.8973	5.7181	2.0227	0.6236	0.7093	0.6878	0.2433
103	433.15	1200	208.12	2.5136	2.8238	2.7401	1.0116	5.2315	5.8770	5.7029	2.1054	0.6292	0.7069	0.6859	0.2532
104	443.15	1200	210.69	2.5062	2.7846	2.7039	1.0482	5.2802	5.8667	5.6967	2.2084	0.6351	0.7056	0.6852	0.2656
105	453.15	1200	213.23	2.4917	2.7421	2.6641	1.0839	5.3130	5.8469	5.6806	2.3112	0.6390	0.7033	0.6833	0.2780
106	333.15	1400	177.13	2.7864	4.2746	4.0435	1.9391	4.9354	7.5715	7.1621	3.4347	0.5936	0.9107	0.8614	0.4131
107	343.15	1400	180.64	2.6907	3.9340	3.7341	1.5651	4.8604	7.1062	6.7453	2.8272	0.5846	0.8547	0.8113	0.3400
108	353.15	1400	183.92	2.6345	3.6894	3.5123	1.3133	4.8454	6.7857	6.4598	2.4154	0.5828	0.8162	0.7770	0.2905
109	363.15	1400	187.06	2.5969	3.5027	3.3427	1.1389	4.8577	6.5519	6.2527	2.1304	0.5843	0.7881	0.7521	0.2562
110	373.15	1400	190.07	2.5736	3.3585	3.2121	1.0226	4.8916	6.3834	6.1051	1.9436	0.5884	0.7678	0.7343	0.2338
111	383.15	1400	192.98	2.5564	3.2418	3.1063	0.9461	4.9334	6.2561	5.9946	1.8258	0.5934	0.7525	0.7210	0.2196
112	393.15	1400	195.82	2.5458	3.1482	3.0217	0.9029	4.9851	6.1648	5.9172	1.7681	0.5996	0.7415	0.7117	0.2127
113	403.15	1400	198.58	2.5408	3.0733	2.9544	0.8867	5.0457	6.1031	5.8670	1.7608	0.6069	0.7341	0.7057	0.2118
114	413.15	1400	201.31	2.5293	3.0021	2.8896	0.8813	5.0916	6.0436	5.8170	1.7741	0.6124	0.7269	0.6997	0.2134
115	423.15	1400	203.97	2.5242	2.9460	2.8389	0.8964	5.1487	6.0090	5.7906	1.8284	0.6193	0.7228	0.6965	0.2199
116	433.15	1400	206.59	2.5175	2.8951	2.7927	0.9214	5.2009	5.9810	5.7695	1.9035	0.6256	0.7194	0.6939	0.2290
117	443.15	1400	209.19	2.5058	2.8449	2.7466	0.9508	5.2418	5.9512	5.7455	1.9890	0.6305	0.7158	0.6911	0.2392
118	453.15	1400	211.74	2.4957	2.8012	2.7064	0.9893	5.2843	5.9311	5.7304	2.0948	0.6356	0.7134	0.6892	0.2520
119	333.15	1600	174.83	2.8661	4.7120	4.3880	2.3152	5.0109	8.2380	7.6716	4.0477	0.6027	0.9909	0.9227	0.4868
120	343.15	1600	178.63	2.7254	4.2427	3.9751	1.7755	4.8684	7.5786	7.1006	3.1716	0.5856	0.9115	0.8541	0.3815
121	353.15	1600	182.10	2.6463	3.9210	3.6907	1.4233	4.8189	7.1399	6.7206	2.5917	0.5796	0.8588	0.8083	0.3117
122	363.15	1600	185.35	2.5995	3.6866	3.4830	1.1863	4.8182	6.8332	6.4558	2.1987	0.5795	0.8219	0.7765	0.2645
123	373.15	1600	188.44	2.5761	3.5140	3.3305	1.0316	4.8544	6.6219	6.2760	1.9439	0.5839	0.7965	0.7549	0.2338
124	383.15	1600	191.43	2.5552	3.3716	3.2038	0.9235	4.8915	6.4544	6.1332	1.7678	0.5883	0.7763	0.7377	0.2126
125	393.15	1600	194.32	2.5455	3.2615	3.1064	0.8603	4.9464	6.3378	6.0363	1.6718	0.5949	0.7623	0.7260	0.2011
126	403.15	1600	197.14	2.5367	3.1687	3.0239	0.8249	5.0008	6.2467	5.9612	1.6261	0.6015	0.7513	0.7170	0.1956
127	413.15	1600	199.89	2.5283	3.0891	2.9529	0.8111	5.0538	6.1748	5.9026	1.6212	0.6079	0.7427	0.7100	0.1950
128	423.15	1600	202.58	2.5236	3.0235	2.8946	0.8182	5.1124	6.1252	5.8641	1.6575	0.6149	0.7367	0.7053	0.1994
129	433.15	1600	205.24	2.5150	2.9625	2.8398	0.8354	5.1617	6.0802	5.8284	1.7146	0.6208	0.7313	0.7010	0.2062
130	443.15	1600	207.84	2.5098	2.9118	2.7945	0.8673	5.2163	6.0519	5.8080	1.8026	0.6274	0.7279	0.6986	0.2168

131	453.15	1600	210.41	2.4996	2.8619	2.7492	0.9034	5.2594	6.0218	5.7846	1.9009	0.6326	0.7243	0.6958	0.2286
132	343.15	1800	176.61	2.7722	4.6066	4.2424	2.0764	4.8959	8.1356	7.4924	3.6671	0.5889	0.9785	0.9012	0.4411
133	353.15	1800	180.31	2.6661	4.1862	3.8862	1.5911	4.8073	7.5482	7.0072	2.8689	0.5782	0.9079	0.8428	0.3451
134	363.15	1800	183.72	2.6062	3.8916	3.6336	1.2726	4.7881	7.1496	6.6757	2.3379	0.5759	0.8599	0.8029	0.2812
135	373.15	1800	186.92	2.5739	3.6765	3.4484	1.0619	4.8111	6.8721	6.4459	1.9850	0.5787	0.8266	0.7753	0.2388
136	383.15	1800	189.98	2.5544	3.5105	3.3049	0.9216	4.8530	6.6693	6.2788	1.7509	0.5837	0.8022	0.7552	0.2106
137	393.15	1800	192.94	2.5381	3.3742	3.1862	0.8274	4.8971	6.5103	6.1476	1.5964	0.5890	0.7831	0.7394	0.1920
138	403.15	1800	195.80	2.5333	3.2698	3.0959	0.7776	4.9601	6.4022	6.0617	1.5225	0.5966	0.7701	0.7291	0.1831
139	413.15	1800	198.60	2.5244	3.1770	3.0146	0.7499	5.0133	6.3094	5.9869	1.4893	0.6030	0.7589	0.7201	0.1791
140	423.15	1800	201.32	2.5213	3.1026	2.9498	0.7488	5.0758	6.2461	5.9384	1.5075	0.6105	0.7513	0.7143	0.1813
141	433.15	1800	204.00	2.5117	3.0318	2.8870	0.7580	5.1239	6.1849	5.8896	1.5464	0.6163	0.7439	0.7084	0.1860
142	443.15	1800	206.63	2.5086	2.9758	2.8379	0.7872	5.1835	6.1487	5.8638	1.6266	0.6235	0.7396	0.7053	0.1956
143	453.15	1800	209.22	2.4990	2.9200	2.7880	0.8208	5.2283	6.1091	5.8330	1.7172	0.6289	0.7348	0.7016	0.2065
144	343.15	2000	174.48	2.8393	5.0546	4.5369	2.5079	4.9542	8.8194	7.9162	4.3759	0.5959	1.0608	0.9522	0.5263
145	353.15	2000	178.53	2.6898	4.4888	4.0922	1.8251	4.8019	8.0136	7.3055	3.2582	0.5776	0.9639	0.8787	0.3919
146	363.15	2000	182.13	2.6134	4.1175	3.7898	1.3996	4.7596	7.4990	6.9023	2.5490	0.5725	0.9020	0.8302	0.3066
147	373.15	2000	185.46	2.5714	3.8523	3.5699	1.1204	4.7690	7.1446	6.6209	2.0779	0.5736	0.8593	0.7964	0.2499
148	383.15	2000	188.63	2.5432	3.6484	3.3983	0.9307	4.7971	6.8818	6.4102	1.7555	0.5770	0.8277	0.7710	0.2112
149	393.15	2000	191.65	2.5299	3.4932	3.2674	0.8103	4.8485	6.6945	6.2619	1.5530	0.5832	0.8052	0.7532	0.1868
150	403.15	2000	194.56	2.5210	3.3674	3.1606	0.7353	4.9049	6.5517	6.1494	1.4307	0.5900	0.7880	0.7396	0.1721
151	413.15	2000	197.39	2.5189	3.2676	3.0761	0.6989	4.9722	6.4500	6.0720	1.3795	0.5980	0.7758	0.7303	0.1659
152	423.15	2000	200.16	2.5136	3.1796	3.0005	0.6841	5.0311	6.3642	6.0058	1.3692	0.6051	0.7655	0.7224	0.1647
153	433.15	2000	202.86	2.5092	3.1046	2.9359	0.6902	5.0902	6.2980	5.9558	1.4002	0.6122	0.7575	0.7164	0.1684
154	443.15	2000	205.51	2.5040	3.0385	2.8785	0.7115	5.1460	6.2445	5.9157	1.4621	0.6190	0.7511	0.7115	0.1759
155	453.15	2000	208.12	2.4954	2.9770	2.8245	0.7422	5.1936	6.1959	5.8784	1.5448	0.6247	0.7452	0.7070	0.1858
156	363.15	2500	178.12	2.6226	4.8033	4.1590	1.9501	4.6713	8.5556	7.4079	3.4735	0.5619	1.0291	0.8910	0.4178
157	373.15	2500	181.93	2.5543	4.3592	3.8674	1.4078	4.6472	7.9309	7.0360	2.5612	0.5590	0.9539	0.8463	0.3081
158	383.15	2500	185.40	2.5182	4.0483	3.6422	1.0618	4.6688	7.5056	6.7527	1.9686	0.5616	0.9028	0.8122	0.2368
159	393.15	2500	188.65	2.4985	3.8163	3.4663	0.8352	4.7133	7.1993	6.5390	1.5755	0.5669	0.8659	0.7865	0.1895
160	403.15	2500	191.72	2.4949	3.6431	3.3330	0.6952	4.7832	6.9845	6.3899	1.3328	0.5753	0.8401	0.7686	0.1603

161	413.15	2500	194.68	2.4910	3.5005	3.2203	0.6064	4.8494	6.8147	6.2691	1.1806	0.5833	0.8197	0.7540	0.1420
162	423.15	2500	197.54	2.4872	3.3812	3.1242	0.5565	4.9132	6.6793	6.1717	1.0994	0.5910	0.8034	0.7423	0.1322
163	433.15	2500	200.33	2.4856	3.2822	3.0438	0.5388	4.9794	6.5751	6.0977	1.0794	0.5989	0.7909	0.7334	0.1298
164	443.15	2500	203.04	2.4864	3.1999	2.9767	0.5470	5.0486	6.4971	6.0440	1.1107	0.6072	0.7815	0.7270	0.1336
165	453.15	2500	205.71	2.4835	3.1253	2.9147	0.5701	5.1088	6.4289	5.9958	1.1728	0.6145	0.7733	0.7212	0.1411
166	373.15	3000	178.27	2.5105	5.0170	4.0175	1.9927	4.4755	8.9438	7.1619	3.5523	0.5383	1.0758	0.8614	0.4273
167	383.15	3000	182.25	2.4705	4.5292	3.8392	1.3649	4.5025	8.2545	6.9970	2.4875	0.5416	0.9928	0.8416	0.2992
168	393.15	3000	185.81	2.4521	4.1923	3.6468	0.9760	4.5563	7.7897	6.7761	1.8135	0.5480	0.9369	0.8150	0.2181
169	403.15	3000	189.12	2.4427	3.9402	3.4815	0.7243	4.6196	7.4516	6.5840	1.3698	0.5556	0.8963	0.7919	0.1648
170	413.15	3000	192.23	2.4466	3.7518	3.3516	0.5706	4.7030	7.2120	6.4428	1.0968	0.5657	0.8674	0.7749	0.1319
171	423.15	3000	195.22	2.4469	3.5954	3.2379	0.4735	4.7768	7.0189	6.3209	0.9245	0.5745	0.8442	0.7603	0.1112
172	433.15	3000	198.10	2.4520	3.4705	3.1452	0.4257	4.8573	6.8749	6.2306	0.8433	0.5842	0.8269	0.7494	0.1014
173	443.15	3000	200.89	2.4551	3.3639	3.0641	0.4097	4.9320	6.7579	6.1555	0.8231	0.5932	0.8128	0.7404	0.0990
174	453.15	3000	203.62	2.4575	3.2728	2.9934	0.4193	5.0037	6.6639	6.0950	0.8538	0.6018	0.8015	0.7331	0.1027
175	373.15	3500	173.85	2.3894	6.0006	1.9393	3.1972	4.1540	10.4322	3.3715	5.5583	0.4996	1.2548	0.4055	0.6685
176	383.15	3500	178.91	2.3776	5.1396	3.7050	1.9295	4.2538	9.1954	6.6287	3.4521	0.5116	1.1060	0.7973	0.4152
177	393.15	3500	182.99	2.3674	4.6287	3.7308	1.2541	4.3323	8.4703	6.8272	2.2949	0.5211	1.0188	0.8212	0.2760
178	403.15	3500	186.60	2.3750	4.2853	3.5982	0.8521	4.4316	7.9961	6.7142	1.5900	0.5330	0.9618	0.8076	0.1912
179	413.15	3500	189.92	2.3843	4.0291	3.4612	0.5980	4.5283	7.6521	6.5735	1.1357	0.5447	0.9204	0.7907	0.1366
180	423.15	3500	193.06	2.3911	3.8261	3.3361	0.4361	4.6164	7.3869	6.4408	0.8419	0.5553	0.8885	0.7747	0.1013
181	433.15	3500	196.05	2.4042	3.6688	3.2340	0.3464	4.7135	7.1928	6.3404	0.6792	0.5669	0.8651	0.7626	0.0817
182	443.15	3500	198.94	2.4122	3.5354	3.1420	0.3002	4.7989	7.0334	6.2507	0.5972	0.5772	0.8460	0.7518	0.0718
183	453.15	3500	201.74	2.4205	3.4244	3.0631	0.2905	4.8830	6.9083	6.1794	0.5860	0.5873	0.8309	0.7432	0.0705
184	383.15	4000	174.96	2.1744	6.0002	0.1189	2.9844	3.8044	10.4983	0.2080	5.2217	0.4576	1.2627	0.0250	0.6281
185	393.15	4000	180.00	2.2364	5.1762	3.4089	1.7467	4.0255	9.3174	6.1362	3.1441	0.4842	1.1207	0.7381	0.3782
186	403.15	4000	184.07	2.2752	4.6871	3.6118	1.0952	4.1879	8.6274	6.6480	2.0160	0.5037	1.0377	0.7996	0.2425
187	413.15	4000	187.68	2.2994	4.3406	3.5270	0.6979	4.3154	8.1463	6.6194	1.3098	0.5191	0.9798	0.7962	0.1575
188	423.15	4000	191.00	2.3224	4.0832	3.4150	0.4526	4.4359	7.7991	6.5227	0.8645	0.5335	0.9381	0.7845	0.1040
189	433.15	4000	194.14	2.3429	3.8822	3.3079	0.3038	4.5485	7.5367	6.4218	0.5897	0.5471	0.9065	0.7724	0.0709
190	443.15	4000	197.13	2.3607	3.7197	3.2116	0.2210	4.6536	7.3325	6.3309	0.4356	0.5597	0.8819	0.7615	0.0524

191	453.15	4000	200.01	2.3711	3.5803	3.1214	0.1809	4.7424	7.1610	6.2433	0.3618	0.5704	0.8613	0.7509	0.0435
192	383.15	5000	166.21	3.6429	6.4969	3.5901	6.0351	6.0549	10.7984	5.9670	10.0309	0.7283	1.2988	0.7177	1.2065
193	393.15	5000	176.01	0.4780	4.7936	0.5524	1.8641	0.8412	8.4370	0.9723	3.2810	0.1012	1.0148	0.1170	0.3946
194	403.15	5000	181.11	0.4743	4.2886	1.2090	0.6557	0.8591	7.7669	2.1897	1.1876	0.1033	0.9342	0.2634	0.1428
195	413.15	5000	183.11	2.0417	5.1250	3.3429	1.1815	3.7385	9.3842	6.1211	2.1635	0.4497	1.1287	0.7362	0.2602
196	423.15	5000	186.99	2.1178	4.6868	3.4380	0.6539	3.9602	8.7641	6.4288	1.2228	0.4763	1.0541	0.7732	0.1471
197	433.15	5000	190.49	2.1764	4.3719	3.3903	0.3377	4.1459	8.3281	6.4582	0.6434	0.4987	1.0017	0.7768	0.0774
198	443.15	5000	193.76	2.2154	4.1230	3.3030	0.1413	4.2925	7.9887	6.3999	0.2738	0.5163	0.9609	0.7698	0.0329
199	453.15	5000	196.84	2.2495	3.9271	3.2158	0.0326	4.4279	7.7301	6.3300	0.0642	0.5326	0.9298	0.7614	0.0077
200	383.15	6000	160.09	5.3556	8.6060	6.6901	7.8665	8.5737	13.7772	10.7101	12.5933	1.0312	1.6571	1.2882	1.5147
201	393.15	6000	168.35	2.6836	6.5894	3.8395	4.4330	4.5179	11.0934	6.4640	7.4630	0.5434	1.3343	0.7775	0.8976
202	403.15	6000	175.50	0.7536	5.3699	2.1175	1.9427	1.3225	9.4239	3.7162	3.4093	0.1591	1.1335	0.4470	0.4101
203	413.15	6000	180.29	0.4220	4.9736	2.1122	0.9225	0.7608	8.9670	3.8081	1.6631	0.0915	1.0785	0.4580	0.2000
204	423.15	6000	182.90	1.8230	5.4805	3.3425	1.1296	3.3343	10.0239	6.1134	2.0661	0.4011	1.2057	0.7353	0.2485
205	433.15	6000	186.94	1.9425	4.9735	3.3826	0.5402	3.6314	9.2976	6.3236	1.0098	0.4368	1.1183	0.7606	0.1215
206	443.15	6000	190.56	2.0294	4.6089	3.3484	0.1858	3.8671	8.7826	6.3805	0.3540	0.4651	1.0564	0.7674	0.0426
207	453.15	6000	193.90	2.0888	4.3236	3.2731	0.0324	4.0502	8.3835	6.3465	0.0628	0.4872	1.0084	0.7634	0.0076
∑				515.67	703.90	627.36	256.61	1003.58	1354.00	1213.96	491.66	120.71	162.86	146.01	59.14
Average (Overall)				**2.4911**	**3.4005**	**3.0307**	**1.2397**	**4.8482**	**6.5411**	**5.8645**	**2.3752**	**0.5831**	**0.7868**	**0.7054**	**0.2857**

هذه العلاقة الجديدة المعدلة قللت الإنحرافات في نتائج معادلـة Soave عنـد مقارنتهـا بالنتـائج المختبرية حيث ان المعدل المطلق للانحراف لعشرين مركب نقي ككل مع 2791 نقطة مختبريـة قبل التعديل هو 4.3084 جول\مول.كلڤن بينما اصبح 2.4621 جول\مول.كلڤن لقيمـة الإنتروپـي المتبقي مع التعديل. بذلك تعطي معادلة SRK بعد هذا التعديل نتائج أكثـر دقـة لحسـاب قيمـة الإنتروپي المتبقي للأبخرة المحمصة للمركبات النقية من باقي المعادلات المذكورة.

الخلاصة

ان التنبؤ بالقيمة الصحيحة لمقدار الإنتروبي (entropy) أساسي في عمليات تصميم المعدات، حيث أنها تسهم في تحديد متطلبات الحرارة و الشغل للعملية الصناعية وتمثل معرفة قيمة الإنتروبي المتبقي خطوة مهمة جداً في حساب قيمة الإنتروبي للغازات. بما أن القيم المختبرية لدالة العشوائية للأبخرة المحمصة محدود ولبعض المركبات والغازات الشائعة فقط مع مدى محدود لدرجات الحرارة والضغط، لذلك قد توجه الاهتمام الى حسابها باستخدام معادلات الحالة.

في هذه الدراسة تم إستخدام معادلات مهمة لإحتساب قيمة الإنتروبي المتبقي للأبخرة المحمصة النقية منها معادلات Lee-Kesler، Virial المقطوعة لحدين مرة ولثلاثة حدود مرة. بالاضافة الى استخدام المعادلات التكعيبية للحالة المتمثلة بمعادلتي: Soave-Redlich-Kwong و Peng-Robinson. جربت هذه المعادلات على 2791 نقطة مختبرية للبخار المحمص لعشرين مركب نقي(14 مركب نقي غير قطبي و6 مركب نقي قطبي). كان المعدل المطلق للانحراف للعشرين مركب ككل مع 2791 نقطة مختبرية لتلك المعادلات هو، 4.0591 ، 4.5849 ، 4.9686 ، 5.0350 ، و 4.3084 جول\مول.كلفن لمقدار الإنتروبي المتبقي على التوالي.

قد وجد من تلك النتائج ان معادلة Lee-Kesler هي الاقل انحراف عن النتائج المختبرية عند مقارنتها ببقية المعادلات لكنها غير مفضلة الاستخدام في أحيان كثيرة لحاجتها الى وقت أكثر من غيرها بالإضافة إلى كونها ليست سهلة في التطبيق كما هو الحال في المعادلات التكعيبية للحالة. بعد ملاحظة إن معادلة SRK كانت هي الأقرب في دقتها لمعادلة Lee-Kesler في حساب مقدار الإنتروبي المتبقي للأبخرة المحمصة، لكنها طورت اساسا للحسابات المتعلقة بالتوازن بين حالتي البخار والسائل لذلك وللتغلب على هذه المسألة، بذلت المحاولات بإتجاه إمكانية تعديلها لزيادة دقتها في حساب مقدار الإنتروبي المتبقي للأبخرة المحمصة قدر الإمكان.

تم تعديل معادلة SRK بإعادة تعريف المتغير α في المعادلة ليكون دالة للضغط المنقوص وكذلك عامل القطبية للمركبات القطبية بالإضافة لكونه اساساً دالة لدرجة الحرارة المنقوصة وعامل اللامركزية المضمن في المتغير n لهذه المعادلة بإستخدام الطرق الإحصائية كما يلي:

$$\alpha = [1 + n(\gamma)]^2$$

$$\gamma = -0.920338 \ P_r^{-0.34091} + 0.064049 \ T_r^4 \omega - 0.370002 \ \omega - P_r^{0.996932} \ Tr^{-4} \chi$$

شكر و تقدير

الحمد لله رب العالمين الذي ساعدني و أعانني على إكمال هذا البحث و أرجو أن أنال في انجازه حسن القبول.

يشرفني أن أتقدم بجزيل الشكر و الامتنان الى استاذي الفاضل المشرف الاستاذ الدكتور **محمود عمرعبد الله** المحترم الذي أثرى هذا البحث برأيه السديد و علمه الوفير وبما بذله من جهد في توجيهي و متابعتي. وجزيل الشكر و الامتنان الى استاذي الفاضل المشرف الثاني الدكتور**سرمد طالب نجم** المحترم لما قدمه لي من مجهود في أرشادي و متابعتي مما كان له الاثر الكبير في انجاز هذا البحث.

ويسعدني أن أتقدم بخالص شكري الى السيد رئيس قسم الهندسة الكيمياوية الاستاذ الدكتور **قاسم جبار سليمان** المحترم لتشجيعه لي ومساعدتي دوما.

والشكر الجزيل الى السيد عميد كلية الهندسة في جامعة النهرين لما قدمه من دعم و مساندة.

وشكري وتقديري موصول الى كافة منتسبي القسم وزملائي طلبة الدراسات العليا جميعا والى كل من مد لي يد العون وساعدني.

وشكرا شكرا الى من كانوا خير سند لي في ازاحة العقبات، وتسهيل الصعوبات أغلى من في الوجود أمي و أبي وجميع أفراد عائلتي.

شهد زهير

تنبؤ وعلاقات عامة
لقيمة الإنتروپي المتبقي للبخار
المحمص للمركبات النقية

رسالة

مقدمة إلى كلية الهندسة في جامعة النهرين

وهي جزء من متطلبات نيل درجة ماجستير علوم

في الهندسة الكيمياوية

من قبل

شهد زهير النجار

(بكالوريوس علوم في الهندسة الكيمياوية 2005)

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