PREDICTION OF LIQUID THERMAL CONDUCTIVITY

By

FAHAD MUHAMMED ALHABDAN

Bachelor of Science
University of Petroleum and Minerals
Dhahran, Sudi Arabia
1976

Master of Science
University of California
Davis, California
1979

Submitted to the Faculty of the Graduate College
of the Oklahoma State University
in partial fulfillment of the requirements
for the Degree of
DOCTOR OF PHILOSOPHY
December, 1983

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Thesis Approved:

R. N. Maddox
Thesis Adviser

Kenneth J. Bell

A. L. Hines

Norman N. Durham
Dean of Graduate College

PREFACE

A model for predicting liquid thermal conductivity over wide ranges of temperature and group lengths was developed. The Cox vapor pressure equation served as the base for this work. The model is capable of handling polar and nonpolar compounds with multiple groups.

The model was tested on 16 systems covering 22 groups. The model is promising and its extension to cover other groups and other physical properties is encouraged.

I wish to express my sincere gratitude to all the people who assisted me in this work and during my stay at Oklahoma State University. In particular, I am especially indebted to my major adviser, Dr. Robert N. Maddox, for his intelligent guidance, concern, and invaluable help.

I am also thankful to the other committee members, Dr. Kenneth J. Bell, Dr. Gilbert J. Mains, Dr. Anthony L. Hines, and the late Dr. John H. Erbar for their advisement in the course of this work.

I am thankful to the unforgettable friendship, encouragement, and company of Dr. Dulaihan Alharbi, Dr. Suleiman Diab, Dr. Daniel Chen, Dr. Fiasal Aljuwaihel, Dr. Muhammed Rahman, Dr. A. K. M. Uddin, Dr. Beleid Kuwairi, Khaled Gasem, and Abdullah Alazzaz.

Special thanks are due to King Saud University, and The Government of Saudi Arabia for providing the scholarship and financial support I received during the course of this work.

My family in Saudi Arabia, my wife, and my son Yasser, derserve my deepest appreciation for their constant support, moral encouragement, and understanding.

TABLE OF CONTENTS

LIST OF TABLES

NOMENCLATURE

A	constant in Equations (2.8), (2.26), (3.1), (3.4), (3.7)
a	constant in Equation (3.10)
a_{CH_2}	constant for methylene group in Equations (3.11), (3.14)
a_{CH_3}	constant for the methyl group in Equation (3.11)
a_i	constant for the i group in Equation (3.14)
a_o, a_1, a_2	parameters in Equations (3.2), (3.5), (3.9)
B	constant in Equations (2.13), (2.18), (2.26)
b	constant in Equation (3.10)
b_{CH_2}	constant for methylene group in Equations (3.10), (3.14)
b_{CH_3}	constant for methyl group in Equation (3.10)
C_p	constant pressure heat capacity
C_{p_o}	constant pressure heat capacity at T = 0 C
C_v	constant volume heat capacity
F	fitted value for one of the parameters in Equation (3.9)
F_n	dimensional factor in Equation (2.30)
FF_{CH_2}	decay ratio multiplier for methylene group
FF_i	decay ratio multiplier for the i group defined by Equation (3.16)
FF_i, FF_2	decay ratio multipliers defined by Equations (3.12), (3.13)
H	constant in Equation (2.15)
ΔH_{vb}	molal heat of vaporization at the normal boiling point temperature
K	liquid thermal conductivity

K_c	critical thermal conductivity
K_{L_o}	liquid thermal conductivity at T = 0 C
K_o	thermal conductivity for reference fluid
L	average distance between centers of molecules
M	molecular weight
N	constant in Equations (2.15), (2.19)
n_{CH_2}	number of methylene groups in Equation (3.15)
n_i	number of the i groups in Equation (3.16)
n_1, n_2	number of groups in Equations (3.12), (3.13)
p_c	critical pressure
Q_1, Q_2	constants in Equation (2.11)
R	gas constant
r	molecular radius in Equations (2.4), (2.10)
r	decay ratio in Equation (3.10)
r_{CH_2}	decay ratio for methylene group
r_i	decay ratio for the i group
r_1, r_2	decay ratio in Equations (3.12), (3.13)
ΔS	entropy change defined by Equation (2.16)
ΔS_v	entropy of vaporization
T	temperature, K
T_b	boiling point temperature, K
T_c	critical temperature, K
T_m	melting point temperature, K
T_r	reduced temperature defined as T/T_c
T_{rb}	reduced boiling point temperature defined as T_b/T_c
T_o	smoothed value for critical temperature

U	velocity of sound in the liquid
V_c	critical volume
V_m	melting volume
V_{mr}	reduced volume at the melting point temperature
V_r	reduced volume
w	constant in Equation (2.27)
Z	compressibility factor
∂	coefficient of expansion
β	constant in Equations (2.12), (2.13)
δ	mean distance of separation defined by Equation (2.3)
ρ	density
γ	frequency of vibration defined by Equation (2.6)
σ	Leonnard-Jones potential constant
ϕ	constant defined by Equation (2.28)
μ	liquid viscosity

CHAPTER I

INTRODUCTION

Engineers, whether designing and operating industrial plants, discovering new materials or transporting old ones are often dealing with liquids whose properties constitute important variables. The availability of reliable data on those properties and the availability of reliable techniques for predicting them are of great interest and concern for both industrialists and academicians.

The liquid state is intermediate between the solid and gaseous states. Liquid theory is in its primitive stages compared to both the gaseous and the solid theories. Thus, experimental data and reliable predictive techniques are not only welcomed, but a necessity in this field.

When energy is transferred from one body to the other by virtue of a temperature difference existing between them, it is said that heat is transferred. The flow of heat may occur in one or more of three essentially different ways. These three methods of heat transmission are conduction, radiation, and convection.

The process of conduction is dependent on the type of material. In general, the particles of matter (molecules, atoms, and electrons) in the high-temperature region, being at higher energy levels, will transmit some of their energy to the adjacent lower-temperature regions. In the case of conduction in gases the interchange of kinetic energy by molecular collision is probably the predominant mechanism. In nonmetallic liquids the process involves the propagation of lattic-vibration waves, similar to the propagation of sound, as well as molecular collision. In nonmetallic solids the primary mechanism is lattic-vibration-wave propagation, while in metallic solids the flow of free or nearly-free, electrons is primarily responsible for heat conduction. Heat may also be transferred by conduction from one body at higher temperature to another at lower temperature if the two bodies are in physical contact. In this process the heat flows by conduction through the boundaries of the two bodies.

The rate of heat transmission by conduction across an area A (square feet) of any homogeneous material is given by Fourier's law as:

$$q = -K\ A\ \frac{dT}{dl}\ \mathrm{Btu/Hr} \qquad (1.1)$$

Since the temperature gradient is measured in the direction of flow and since dT, the temperature change, is negative, i.e., the temperature decreases in passing through the positive distance dl, it is necessary to introduce negative sign in order that q, the quantity of heat flowing, may be positive.

Thermal conductivity K is defined as the time rate of transfer of heat by conduction through unit thickness across unit area, for unit difference of temperature. It is measured as Btu per hour per square foot for a thickness of one foot, and a difference of temperature of 1 degree F. Dimensions, $\mathrm{Btu/([hr\ ft^2 F]/ft)}$. In general, thermal conductivity is essential in proper design of industrial plants. It is essential in proper design of heat exchangers and cooling systems.

The objective of this study is to develop a liquid thermal conductivity prediction method applicable for a wide range of temperatures and a wide range of groups and chain lengths. This method should employ a group contribution type of technique so that it can be easily extended to predict thermal conductivity for arbitrary compounds. No other physical properties should be required in this method; only the structure of the particular compound should be needed. The proposed method should cover both polar and nonpolar compounds. More than twenty groups are investigated in the present work. The procedure of this study includes finding a good liquid thermal conductivity versus temperature correlation, choosing a suitable group contribution model, and using fitting programs to determine optimal group contribution values (predictive constants) in this predictive method. The resultant predictive constants are used to generate computed liquid thermal conductivity values which are then compared with experimental data either included or not included in the regression.

The Cox vapor pressure equation can be slightly modified to become an excellent correlation for liquid thermal conductivity. The Cox (6) equation for thermal conductivity is capable of correlating liquid thermal conductivity from the melting point to the critical point. The parameters in the Cox equation for thermal conductivity are generated by a new group contribution technique which involves the use of a geometric series, which enables this prediction method to cover a wide range of groups and chain lengths. In the proposed group contribution technique, each group contribution differs from the preceding one by a constant ratio r. The functional group contribution is not constant but is a fucntion of the number of groups in the homologous series. This new method can predict and correlate liquid thermal conductivity more accurately than any existing method for all compounds encountered in this work.

CHAPTER II

LITERATURE REVIEW

A fully satisfactory theory for the thermal conductivity of liquids is not available. None of the many empirical relationships that have been proposed appear to be entirely satisfactory. An approach to the problem of predicting the thermal conductivity of liquids that appeared more rewarding than the purely theoretical approach was the use of semi-empirical relations, in which what seemed to be reasonable qualitative theoretical equations were formulated and the constants adjusted to fit available experimental data.

In 1880, Weber (13), suggested that liquid thermal conductivity is proportional to the product $(\rho/M)^{4/3}$:

$$K = 0.359\, C_p \rho (\rho/M)^{1/3} \tag{2.1}$$

In 1923, Bridgman (3), proposed this relation:

$$K = 2\, R\, U\, \delta^{-2} \tag{2.2}$$

Where:

R = the gas constant;

δ = the mean distance of separation between centers of molecules and equated to

$$\delta = (M/\rho)^{1/3}; \text{ and} \tag{2.3}$$

U = the velocity of sound in the liquid.

The equation due to Kardos (10) in 1934, is:

$$K = \rho C_p \; UL/2r \tag{2.4}$$

where L is defined as the average distance between centers of molecules. When L was taken as 0.95×10^{-8} m for all liquids, this equation gave an average difference from the experimental values of 41 percent, but with L calculated for each liquid, differences of from 5.9 to 17.9 percent were obtained.

In 1936, Smith (26), proposed the same type of relation, slightly changing the constant from 0.359 to 0.43. Smith also proposed another relation that involved the viscosity, μ, in liquid thermal conductivity evaluation. The Smith equation is:

$$\begin{aligned} 10^6 K = 11 &+ [6450(C_p - 0.45)^3] + [1250(\rho/m)^{1/3}] \\ &+ [100(\mu/\rho)^{1/9}] \end{aligned} \tag{2.5}$$

Osida (14) in 1939, and Rao (18) in 1942, regarded the liquid state as approximating more closely that of the solid and assumed that the energy exchange occurs when two molecules approach each other while vibrating about a mean position with a frequency γ given by:

$$\gamma = f(T_m^{1/2}) \; (M^{-1/2}) \; (V_m^{-1/3}) \tag{2.6}$$

where f is a function of the density of each liquids rather than a numerical constant, T_m is melting point, V_m is the corresponding molecular volume. They both derived a final expression for the thermal conductivity of the form:

$$K = A \; C_p \; (M^{-1/3}) \; (\rho^{4/3}) \tag{2.8}$$

where the constant A is a function of temperature, but is approximated as equal to 3.58×10^{-3}. Equation (2.8) yielded values departing from experimental values by -18.5 to +18.5 percent at 30 C.

In 1948, Palmer (16), suggested another modification to the Weber (31) equation by the addition of the entropy of vaporization ΔS_r at the normal boiling point, cal/g-mole C. The Palmer equation is:

$$K = 9.47 \times 10^{-3} C_p \rho([\rho/M]^{1/3}) (\Delta S_r)^{-1} \tag{2.9}$$

In 1948, Borovik (2) introduced a similar relation:

$$K = A(C_r + 9R/4) \overline{U}/r^2 \tag{2.10}$$

with C_r the molar heat capacity at constant volume, r the molecular radius, and A a constant. The Borovik relation yielded deviations of -21 to +23 percent from experimental values.

In 1955-1957, Sakiadis and Coats (23), (24), introduced a corresponding states type equation:

$$K_{rb} = 2.26 Q_1 - 1.26 Q_2 - 2.10 (Q_1 - Q_2)T_r \tag{2.11}$$

where K_{rb} is the thermal conductivity at the reduced temperature ($T_r = T/T_c$), and Q_1 and Q_2 are constants, with values depending on the structure of the liquid and the homologous series to which it belongs.

Vargaftik (28, 29) in 1958-1959, introduced an additional coefficient β, to the equation proposed by Weber (31) in 1880.

$$K = (A/\beta) C_p (M^{-1/3}) (\rho^{4/3}) \tag{2.12}$$

Vargaftik found the product ($A C_p$) to be independent of temperature, and hence Vargaftik proposed the relations:

$$K = (B/\beta) (\rho^{4/3}) \tag{2.13}$$

where $B = A_o C_{p_o} (M^{-1/3})$ = constant. He recommended that the value for $(A_o C_{p_o})$ be taken at a temperature of $0.5T_c$ and that A have the value of 4.28×10^{-3}.

In 1961, Scheffy (25) proposed the equation:

$$K = 0.0466 (M^{0.3}) (T_m^{-0.216}) [1 - 1.26 \times 10^{-3}[T - T_m]) \qquad (2.14)$$

where T_m is the melting point temperature, Reid and Sherwood (19) compared and tabulated the results with 150 experimental points for 70 liquids and obtained a mean difference of 13 percent with extreme difference of -58 and +111 percent.

In a modification to the Weber (31) equation, Robbins and Kingrea (22) in 1962, proposed the following relation:

$$K = \frac{(88.0 - 4.94H)(0.001)}{\Delta S^k} \left(\frac{0.55}{T}\right)^N C_p \rho^{4/3} \qquad (2.15)$$

where ΔS^k is defined as:

$$\Delta S^k = \Delta H_{vb}/T_b + R \, Ln(273/T_b) \qquad (2.16)$$

and ΔH_{vb} is the molal heat of vaporization at the normal boiling point. The parameter H depends upon molecular structure and N upon the liquid density at 20°C. Robbins and Kingrea tested their equation with 70 organic liquids and 142 data points, where rarely the errors exceeded 10 percent.

Riedel (21) in 1962, on the basis of the principle of corresponding states, concluded that K/K_c, the ratio of the thermal conductivity at temperature T and critical temperature T_c, should be a universal function of T/T_c. The equation Riedel (21) suggested is:

$$K = K_c (1 + 6.7 [1 - T_r]^{2/3}) \qquad (2.17)$$

Horrocks and Mclaughlin (8), by regarding a liquid as a quasilattice structure, found that

$$\frac{1}{K}\left(\frac{dK}{dT}\right) = -\partial\left(\frac{1}{3} - B\right) \tag{2.18}$$

where ∂ is the coefficient of expansion, and B is a constant. this equation indicates that there should be a close connection between the expansion coefficient and the temperature coefficient of heat conduction.

In his book on thermal conductivity, Missenard (13) in 1965, suggested that

$$K_{L_o} = \frac{90 \times 10^{-6}\,(T_b\rho)^{1/2}\,C_{p_o}}{(M^{1/2})\,(N^{1/4})} \tag{2.19}$$

where K_{L_o} is liquid thermal conductivity at 0^o C, and C_{p_o} liquid constant pressure heat capacity at 0^o C, N number of atoms in the molecule. When this equation is combined with the Riedel (21) equation, one obtains

$$K = K_{L_o}\,\frac{3 + 20(1 - T_r)^{2/3}}{3 + 20(1 - 273/T_c)^{2/3}} \tag{2.20}$$

Another correlation for the thermal conductivity of organic liquids is based on dimensional analysis due to Pachiyappan, Ibrahim, and Kuloor (15) in 1966. From Experimental Data on 51 organic liquids Pachiyappan et al. (15) obtained:

$$K = \frac{5.6 \times 10^{-3}\,(M^{1.26})\,(C_p)\,(\Delta H_r^{1/2})\sigma}{V_m} \tag{2.21}$$

where σ is the Lennard-Jones potential constant. This equation gave an average departure of 11 percent with a standard deviation of 17 percent.

From a further consideration of an equation of the Bridgman (3) form, Viswanath (30) in 1967, obtained the equation:

$$K = \frac{3.6 \times 10^{-4}\ \Delta H_b}{C(V_m^{2/3})\ (M^{1/2})\ (T^{1/2})}\ \frac{(1 - T_r)}{(1 - T_{rb})}\ 0.38 \tag{2.22}$$

where ΔH_b is the latent heat of vaporization at the boiling point and T_{rb} is the reduced boiling point T_b/T_c. For sixteen organic substances considered by Reid and Sherwood (19) and 50 data points, Viswanath (30) finds this equation to give an average deviation of 9.5 percent.

In 1973, Sato (20) suggested that at the normal boiling point the thermal conductivity is:

$$K_{Lb} = 2.64 \times 10^{-3}/(M^{1/2}) \tag{2.23}$$

where K_{Lb} is the liquid thermal conductivity at the normal boiling point, and M is the molecular weight. To estimate thermal conductivity at other temperatures, this equation can be combined with Robbins and Kingrea (22) to get

$$K = ([2.64 \times 10^{-3}/M^{1/2}][C_p/C_{p_o}][\rho/\rho_o]^{4/3}[T_b/T]) \tag{2.24}$$

where the subscript b represents conditions at the normal boiling point. Also the Sato equation could be combined with that of Riedel (21) to give:

$$K = (2.64 \times 10^{-3})\ \frac{3 + 20(1 - T_r)^{2/3}}{3 + 20(1 - T_{rb})^{2/3}}\ (M^{-1/2}) \tag{2.25}$$

Poor results were found for low molecular weight hydrocarbons, and branched hydrocarbons (20). Generally the predicted value was larger than the experimental. The method is not applicable for highly polar liquids.

Only the molecular weight, the normal boiling point, and critical temperature need be known.

In 1978, Mathur, Singh, and Fitzerald (12) proposed the following relation

$$K = (T_r^{1/2})/([A - BZ]\ [V_r - 0.76\ V_{mr}]) \qquad (2.26)$$

where V_r is the reduced volume, V_{mr} is reduced volume at the melting point, and Z is the compressibility factor. A and B are constrants with the values $A = 5.23 \times 10^4$, $B = 11.454 \times 10^4$.

In 1980, Teja and Rice (27), developed an extension of the three parameter-corresponding states principle based on the properties of two non-spherical reference fluids to use for thermal conductivity evaluation. The following expression was proposed for thermal conductivity of fluids

$$(K\phi) = (K\phi)^{r1} + \frac{w + w^{r1}}{w^{r2} - w^{r1}} \quad (K\phi)^{r2} - (K\phi)^{r1} \qquad (2.27)$$

and ϕ is defined as

$$\phi = (M^{1/2})(V_c^{2/3})(T_c^{-1/2}) \qquad (2.28)$$

where the superscripts (r1) and (r2) refer to the properties of two non-spherical reference fluids. This equation states that the thermal conductivity of any fluid may be obtained from a knowledge of its parameters T_c, V_c, P_c, and w and the thermal conductivity of two similar reference fluids at the same reduced temperature and pressure. One of the major drawbacks of this method is the need for thermal conductivity data for two other reference fluids in order to determine liquid thermal conductivity.

In 1981, Baroncini, Filippo, Latini, and Pacetti (1), proposed a general correlation for organic liquid thermal conductivity of the following type

$$K = A([1 - T_r]^{0.38})/(T_r^{0.166}) \tag{2.29}$$

where T_r is the reduced temperature, and the factor A is temperature independent and characteristic of the particular compound. Values for 144 organic liquids were listed (1).

In 1981, Ely and Hanley (7) proposed a model for the prediction of the density, viscosity, and thermal conductivity. The model is based on an extended corresponding states model. The average percent deviation for thermal conductivity was reported as less than 10 percent. Their equation for thermal conductivity of pure fluids is given by

$$K = K_o(1 + \frac{K'}{K''})F \tag{2.30}$$

In this equation K denotes the thermal conductivity of the fluid, the subscript "o" denotes a reference fluid value, and the superscript "'" denotes the translational contribution, which is evaluated via a corresponding states principle. The superscript '"' denotes the contribution due to the internal degrees of freedom, and is calculated via a dilute gas type term (7). F_η is a dimensional factor.

The foregoing account has presented the data seeker with a considerable choice of possible equations, for which an independent assessment, based on well-substantiated experimental data, is still required. In due course this may become possible, as more recommended values become available, not only for thermal conductivities of liquids, but for the associated parameters of specific heat, density, etc.

In their book, Reid, Prausnitz, and Sherwood (20), concluded a critical survey of pure liquid thermal conductivity estimation techniques with the recommendation to use the Robbins and Kingrea (22) equation, Equation (2.15), for estimates between reduced temperatures of about 0.4 and 0.8. Liquid densities and heat capacities are required, as are the normal boiling point and latent heat of vaporization.

For quick estimates of liquid thermal conductivity, Reid, Prausnitz, and Sherwood (20), recommend the boiling point method, Equation (2.25), suggested by Sato (20).

CHAPTER III

PROPOSED MODEL

The Cox Vapor Pressure Equation

One of the objectives in this work is to develop a liquid thermal conductivity prediction method capable of covering a wide temperature range. To achieve this goal, a qualified liquid thermal conductivity as a function of temperature relation is a must. Based on the knowledge that a good function form for vapor pressure is usually equally good for thermal conductivity, and based upon Chen's (5) work in liquid viscosity prediction, the vaopr pressure equation developed by Cox, which can represent vapor pressure very well over the entire liquid range, is tested and proved to be, with a slight modification, an excellent correlation for liquid thermal conductivity.

Cox (6) found that the following equation is generally valid for vapor pressures of a variety of compounds:

$$\text{Log } (P) = A(1 - T_b/T) \tag{3.1}$$

in which

$$\text{Log } (A) = a_o + a_1 T_r + a_2 T_r^2 \tag{3.2}$$

and

$$T_r = T/T_c \tag{3.3}$$

where P is vapor pressure, atm, T temperature, K, T_b normal boiling point, T_c critical temperature, K, and a_o, a_1, a_2 are constants. If the reference point is changed from the normal boiling point to the critical point and natural logarithms are adopted, then the equation can be written as

$$\text{Log } (P/P_c) = A(1 - T_c/T) \qquad (3.4)$$

in which

$$L_nA = a_o + a_1T_r + a_2T_r^2 \qquad (3.5)$$

and

$$T_r = T/T_c \qquad (3.6)$$

The Cox Equation for Thermal Conductivity

Since thermal conductivity decreases with increase in temperature in almost straight line form, the natural logarithms can be dropped and the equation written:

$$K/K_o = A\ (T_c/T - 1) \qquad (3.7)$$

and

$$T_r = T/T_c \qquad (3.8)$$

This equation can be expressed in alternative form:

$$K/K_o = \exp(a_o + a_1T_r + a_2T_r^2)(1/T_r - 1) \qquad (3.9)$$

where:

$T_r = T/T_o$; and

T_o = smoothed value for T_c.

Equation (3.9), with five parameters a_o, a_1, a_2, K_o, and T_o, is the working equation in this study. T_o is chosen by fitting experimental critical temperature data (or estimations when experimental ones are not available) into a smoothed curve. Because T_o can be generated easily from an analytic equation, the reference temperature T_o, rather than T_c will be used in the prediction method.

Group Contribution Technique

The task remaining is to generate the parameters in Equation (3.9). The five parameters a_o, a_1, a_2, K_o, and T_o are considered to be group dependent. In an effort to obtain the group contribution values for these parameters, the work of Chen (5) was considered. In his work the contribution of each methylene group decreases in the alkane series at constant reduced temperature.

The model chosen for this work is a modified version of Chen (5) model. It is a geometric series in which each methylene group contribution differs from the preceding one by a constant ratio r so that the total n methylene group contributions amount to the partial sum of the first n terms of the geometric series. That is, a general form as follows is used to generate the parameters in Equation (3.9) for a homologous series

$$F = a + b(1 - r^n)/(1 - r) \qquad (3.10)$$

where F is the fitted value for one of the five parameters in Equation (3.9), n is the number of specific groups in that particular compound, and a, b, and r are adjustable constants. Since each methylene group contribution decreases with increasing number of carbon atoms in the compound, the constant r is called the decay ratio, with values restricted to be between zero and one.

Multi-Group Contribution

For a homologous series with more than one group available in the compound, Equation (3.10) has to be expanded to accommodate multi-group compounds. For an alkane type compound with only CH_2, and CH_3 groups available, Equation (3.10) is written as:

$$F = a_{CH_2} + b_{CH_2}FF_1 + a_{CH_3}FF_2 + (b_{CH_3}FF_1)FF_2 \qquad (3.11)$$

FF_1 and FF_2 are the decay ratio multipliers for the groups, and are defined in this form.

$$FF_1 = (1 - r_1^{n1})/(1 - r_1) \qquad (3.12)$$

$$FF_2 = (1 - r_2^{n2})/(1 - r_2) \qquad (3.13)$$

Where r_1 and r_2 are the decay ratios for the groups, and the subscripts refers to the CH_2 and CH_3 groups for a compound with only two groups. In a compound with M number of groups, Equation (3.11) could be written in this form.

$$F = a_{CH_2} + b_{CH_2}FF_{CH_2} + \sum_{i=2}^{m} (a_i + b_iFF_{CH_2})FF_i \qquad (3.14)$$

FF is defined as:

$$FF_{CH_2} = (1 - r_{CH_2}^{n_{CH_2}})/(1 - r_{CH_2}) \qquad (3.15)$$

The constants a_{CH_2}, b_{CH_2}, and r_{CH_2} are the constants for the methylene group, and n_{CH_2} is the number of the methylene groups in the compound.

The subscript i refers to other groups present in the compound structure. The FF_i is defined as:

$$FF_i = (1 - r_i^{ni})/(1 - r_i) \qquad (3.16)$$

All the work in this project is based upon Equation (3.14) as the working equation for group contribution evaluation for thermal conductivity.

CHAPTER IV

RESULTS AND COMPARISONS WITH OTHER METHODS

Regression Procedure

A nonlinear least-squares fitting routine MARQ written by Chandler (4) was used to find the optimal constants in this prediction method. First, the predictive constants related to T_o were obtained by fitting the experimental critical temperature data (or Lydersen's [11] estimation of critical temperature) with the porposed model represented by Equations (3.13), (3.14), and (3.15). Then with a_o, a_1, a_2, and K_o in terms of predictive constants, the remaining constants were obtained simultaneously by fitting experimental liquid thermal conductivity data for a homologous series. In the case of straight chain alkanes, for example, the first three constants representing the critical temperature were determined first, then the other 12 constants representing a_o, a_1, a_2, and K_o are fixed for the n-alkanes series.

After determining these constants for CH_2 and CH_3 groups, then the constants for any additional group (or groups) are fixed leaving the CH_2 and CH_3 group constants fixed.

Summary of Computed Results

The proposed method has been applied to alkanes, alcohols, alkanoic acids, esters, ketones, ethers, some nitro compounds, choloro, bromo, and iodo alkanes. Table I is a summary result for all compounds with their temperature ranges, maximum deviation, minimum deviation, temperature at maximum deviation, and their average percent deviations. Detailed results for each individual compound is given in Tables II, III, IV, and V. Detailed results for all compounds are tabulated in Appendix A. In Tables II, III, IV, V, the number of data points, temperature range, maximum percent error, minimum percent error, temperature where absolute maximum error occurs, and average absolute percent error are presented. Compounds which were not included in the regression are indicated by asterisks. The overall absolute percent error for 15 n-alkanes compounds is 1.018, with a maximum positive percent deviation of 4.65, and a maximum negative percent deviation of 4.70. For branched alkanes, Table IV, the overall absolute percent deviation for 26 branched alkanes compounds is 1.174, with a maximum negative percent deviation of 5.57. In the case of alkanes, the overall absolute percent deviation for 22 compounds and 220 points, is 0.732, with a maximum positive percent deviation of 5.89, and a maximum negative percent deviation of 3.65. For alcohols, 12 normal alcohols with 108 data points, were evaluated resulting in an overall absolute average percent deviation of 1.756, with maximum positive percent deviation of 5.05, and maximum negative percent deviation of 11.0. For n-alkyl esters, 131 compounds containing the (COO) group were evaluated in this work with an overall absolute average percent deviation of 0.865, and a maximum positive percent deviation of 6.30, and a maximum negative percent deviation of 5.13. Table I is a summary for all compound included in this work.

The percent deviation E is defined as:

$$E = ([\text{calc.} - \text{exp.}] / \text{exp.}) \times 100 \qquad (4.1)$$

TABLE I

SUMMARY FOR THERMAL CONDUCTIVITY RESULTS

Number of Systems = 16

Number of Groups = 12

System	NOS*	NPT*	Temp. Range Degre K	Max. Dev.	Max. Dev.	AAPD
Alkanes (Str)	15	260	93.15-669.15	4.65	-4.70	4.018
Alkanes (Bra)	27	270	113.15-470.15	6.56	-14.6	1.519
Alkenes	22	220	93.15-587.15	5.89	-3.65	0.732
Alcohols (OH)	17	211	199.00-508.15	5.05	-11.0	1.407
Acids	15	150	283.15-683.15	2.95	-6.06	0.931
Formates	14	140	193.15-667.15	8.86	-6.72	1.585
Esters	131	524	183.15-675.15	6.3	-5.13	0.865
Aldehydes	14	140	183.15-718.15	4.75	-2.06	0.722
Ketones	70	420	193.15-696.15	3.82	-2.78	1.100
Ethers	55	560	113.15-645.15	6.16	-3.20	2.821
Amines	4	040	243.15-680.15	1.22	-1.72	0.469
Nitro Compound	5	050	173.15-488.15	2.46	-1.20	0.620
Chloro Alkanes	19	190	153.15-548.15	11.2	-23.2	3.922
Bromo Alkanes	13	130	173.15-590.15	6.88	-13.2	3.358
Iodo Alkanes	16	160	213.15-678.15	8.74	-16.7	3.430
Crude Oil	16	160	283.33-477.15	13.8	-9.73	2.821
Total	453	3625				

Max. Pos. Dev. = 13.8

Max. Neg. Dev. = -16.7

Average Absolute Percent Deviation = 1.0526 (Overall)

*NOS is number of Sub-Systems

*NPT is number of Points

TABLE II

THERMAL CONDUCTIVITY FOR ALKANES

Number of Systems = 15

System	NPT	Temp. Range	Max. Dev.	Max. Dev.	Temp. at Max	AAPD
Propane	14	93.15-223.15	2.39	-0.69	123.15	0.902
N-Butane	14	143.15-273.15	0.58	-1.39	193.15	0.830
N-Pentane	16	153.15-303.15	0.71	-1.86	153.15	0.546
N-Hexane	13	183.15-303.15	2.31	-0.37	303.15	0.983
N-Heptane	16	183.15-333.15	2.52	-2.46	323.15	1.800
N-Octane*	15	223.15-373.15	2.38	-	323.15	1.890
N-Decane	8	303.15-415.15	-	-3.57	410.06	2.397
N-Undecane	31	307.75-637.45	4.65	-2.31	478.55	0.716
N-Dodecane	25	307.75-653.15	1.37	-3.15	478.55	0.845
N-Tridecane	35	307.75-669.35	1.13	-0.48	538.55	0.478
N-Tetradeca	19	307.80-509.80	1.08	-4.70	317.10	0.918
N-Hexadecan	12	313.15-533.15	1.29	-1.14	393.15	0.850
N-Heptadeca	13	313.15-553.15	2.44	-1.67	393.15	1.392
N-Octadecan*	14	313.15-573.15	2.92	-0.78	413.15	1.928
N-Nonadecan*	15	313.15-593.15	2.99	-0.49	413.15	2.003
Total	260					

Maximum Positive Deviation = 4.65

Maximum Negative deviation = -4.70

Ave. Abs. Perc. Dev. = 1.01881 (overall)

Ave. Abs. Perc. Dev. (Prediction) = 1.9406

Ave. Abs. Perc. Dev. (Regression) = 0.8159

*Not included in regression (predicted)

TABLE III

THERMAL CONDUCTIVITY FOR ALKENES

Number of Systems = 22

System	NPT	Temp. Range Degree K	Max. Dev.	Max. Dev.	Temp. at Max	AAPD
Ethylene	10	113.15-239.15	5.89	-3.09	113.15	1.951
Propylene	10	93.15-309.15	3.16	-0.50	117.15	1.297
But-1-ene	10	93.15-345.15	0.48	-3.31	93.15	0.598
But-2-3n3	10	153.15-351.15	2.79	-1.68	351.15	1.345
Isobutene	10	133.15-349.15	0.19	-0.15	157.15	0.103
Pent-1-ene	10	113.15-392.15	0.28	-3.63	113.15	0.606
Hex-1-ene	10	133.15-421.15	0.03	-3.65	133.15	0.642
Hex-2-ene	10	143.15-431.15	0.82	-0.90	175.15	0.609
Hex-3-ene*	10	153.15-432.15	0.69	-1.02	308.15	0.695
Hept-1-ene	10	163.15-451.15	0.13	-2.13	163.15	0.527
Hept-2-ene	10	173.15-461.15	0.81	-0.40	333.15	0.569
Hept-3-ene	10	143.15-458.15	0.64	-1.12	143.15	0.359
Oct-1-ene	10	173.15-479.15	0.88	-1.42	173.15	0.540
Oct-2-ene*	10	183.15-489.15	0.50	-0.52	183.15	0.400
Oct-3-ene	10	173.15-479.15	0.13	-1.13	173.15	0.212
Oct-4-ene	10	173.15-488.15	0.04	-1.19	173.15	0.322
Non-1-ene	10	193.15-499.15	0.32	-1.24	193.15	0.454
Dec-1-ene	10	213.15-519.15	1.21	-0.09	281.15	0.593
Undec-1-en	10	233.15-539.15	1.22	-0.05	267.15	0.607
Tridex-1-e*	10	253.15-568.15	1.68	-1.69	463.15	1.132
Tetradec-1-ene*	10	263.15-587.15	1.54	-3.24	479.15	1.714
Total	220					

Maximum Positive Deviation = 5.89

Maximum Negative deviation = -3.65

Ave. Abs. Perc. Dev. = 0.73257 (overall)

Ave. Abs. Perc. Dev. (prediction) = 1.42337

Ave. Abs. Perc. Dev. (Regression) = 0.66349

*Not included in regression (predicted)

TABLE IV

THERMAL CONDUCTIVITY FOR BRANCHED ALKANES

Number of Systems = 26

System	NPT	Temp. Range Degree K	Max. Dev.	Max. Dev.	at Max	AAPD
2,2DI-CI-C3	10	263.15-380.15	4.89	-2.68	380.15	2.149
2,2DI-CI-C4	10	173.15-416.15	5.46	-2.71	416.15	2.347
2,2DI-CI-C5	10	153.15-441.15	2.63	-2.32	441.15	1.280
2,3DI-CI-C5	10	153.15-450.15	6.56	-0.33	450.15	1.487
2,2DI-CI-C6	10	153.15-459.15	0.35	-1.61	425.15	0.943
3,3DI-CI-C6	10	153.15-459.15	0.92	-0.69	221.15	0.515
2-Methyl-C3	10	113.15-338.15	3.24	-2.05	113.15	1.406
2-Methyl-C4	10	113.15-383.15	3.78	-0.48	113.15	1.351
2-Methyl-C5	10	123.15-420.15	3.08	-1.44	123.15	1.234
3-Methyl-C5	10	123.15-420.15	2.55	-0.74	123.15	1.209
2,3DI-CI-C4	10	153.15-423.15	1.96	-1.78	363.15	1.053
2-Methyl-C6	10	163.15-442.15	1.90	-0.91	380.15	0.973
3-Methyl-C6	10	163.15-442.15	1.38	-1.30	380.15	0.850
2,3DI-CI-C5	10	153.15-450.15	2.88	-0.45	384.15	1.278
2,4DI-CI-C5	10	163.15-433.15	1.24	-2.20	433.15	0.799
2-Methyl-C7	10	173.15-461.15	1.82	-0.41	397.15	0.846
3-Methyl-C7	10	153.15-459.15	0.63	-1.84	255.15	0.906
4-Methyl-C7	10	153.15-459.15	–	-2.71	255.15	1.541
2,3DI-CI-C6	10	153.15-468.15	2.56	-0.45	398.15	1.084
2,4DI-CI-C6	10	153.15-468.15	1.20	-2.19	468.15	0.889
2,5DI-CI-C6	10	183.15-453.15	0.53	-1.37	273.15	0.728
3,4Di-CI-C6*	10	153.15-468.15	1.20	-2.19	468.15	0.889
2,3,4-tri-cl-c5	10	173.15-479.15	1.16	-2.64	479.15	1.154
2,2,3-tri-cl-c5	10	163.15-469.15	0.60	-5.57	163.15	1.775

TABLE IV (Continued)

Number of Systems = 26

System	NPT	Temp. Range Degree K	Max. Dev.	Max. Dev.	Temp. at Max	AAPD
2,3,3-tri-cl-c5*	10	173.15-470.15	1.69	-3.48	173.15	1.042
2,3,5-tri-cl-c6*	10	153.15-468.15	1.31	-1.24	398.15	0.803
Total	260					

Maximum Positive Deviation = 6.56

Maximum Negative Deviation = -5.57

Ave. Abs. Perc. Dev. = 1.1743 (overall)

Ave. Abs. Perc. Dev. (prediction) = 0.9113

Ave. Abs. Perc. Dev. (regression) = 1.2086

*Not included in regression (predicted)

TABLE V

THERMAL CONDUCTIVITY FOR (-OH) GROUP

System	NPT	Temp. Range Degree K	Max. Dev.	Max. Dev.	Temp. at Max	AAPD
Alcohols Number of Systems = 12						
Methanol	15	199.00-469.15	4.97	-2.75	391.15	1.459
Ethanol	13	233.15-471.15	4.24	-3.96	373.15	1.211
N-Propanol	17	200.00-479.15	4.14	-2.46	479.15	1.264
N-Butanol	13	203.40-373.15	2.85	-2.81	307.15	1.235
N-Pentanol	8	201.70-353.15	1.13	-3.16	253.15	1.956
N-Hexanol	9	243.50-423.15	5.05	-4.42	369.00	2.589
N-Heptanol*	15	246.80-436.25	2.65	-2.68	436.25	1.573
N-Octanol	3	293.15-485.15	2.32	-4.92	485.15	2.714
N-Nonanol	7	273.15-423.15	-	-4.38	423.15	1.450
N-Decanol	4	273.15-373.15	2.94	-	323.15	2.144
N-Tetradeca*	4	323.15-473.15	-	-11.0	473.15	5.785
N-Octadecan	3	337.15-373.15	0.86	-3.23	347.15	2.431
Polymethlene Glycols Number of Systems = 4						
Ethelene	20	223.15-508.15	2.35	-0.97	223.15	1.039
Trimethyle	20	223.15-508.15	-	-3.75	223.15	1.041
Tetramethy	20	223.15-508.15	1.58	-2.95	223.15	1.171
Pentamethy	20	223.15-508.15	2.24	-3.98	508.15	1.560
Glycerols Number of Systems = 1						
Glycerine	20	223.15-508.15	0.46	-1.15	223.15	0.290
Total	211					

Maximum Positive Deviation = 5.05

Maximum Negative Deviation = -11.0

Ave. Abs. Perc. Dev. = 1.40775 (overall)

Ave. Abs. Perc. Dev. (prediction) = 2.4557

Ave. Abs. Perc. Dev. (regression) = 1.1517

*Not included in regression (predicted)

where calc. is the calculated value, exp. is the experimental value. The average absolute percent deviation (AAPD) is defined as:

$$AAPD = ABS(E)/NPT \tag{4.2}$$

where ABS(E) is the absolute value of percent deviation, NPT is the number of data points for each compound. The maximum positive percent deviation is defined as the deviation with the largest positive value among NPT deviations. The maximum negative percent deviation is defined as the deviation with the largest negative value among NPT deviations. The overall average percent deviation is defined as:

$$AAPDO = AAPD/NC \tag{4.3}$$

where NC is the number of compounds within a certain group. The AAPDO is the average value of AAPD's.

Comparisons with Other Methods

Comparison of the proposed method with the method of Baroncini et al. (1), the boiling point method (Sato), and Robbins, and Kingrea (22) are presented in Tables VI, VII, VIII, IX, X. Table VI is a summary of all the comparisons made in this work, where the other tables are specific comparison for each group of compounds. Appendix B is a comprehensive list of all comparisons for all the compounds in this work.

As we can see from these tables, the proposed method performs significantly better than other liquid thermal conductivity methods. In addition, none of the other methods can cover a wide range of groups and temperatures. The Baroncini et al. (1) method requires a specific constant for each compound, also critical temperature is required. The boiling point method requires only boiling point, and molecular weight,

TABLE VI

SUMMARY FOR COMPARISON RESULTS

Number of Systems = 13

System	NPT	Temp. Range Degree K	Bar	Ave. Perc. Dev. Sato	Robn	Group
Alkanes (Str)	260	93.15-669.15	9.71	24.1	89.3	1.018
Alkanes (Bra)	270	113.15-470.15	8.40	17.3	13.3	1.519
Alkenes	220	93.15-587.15	8.27	12.6	59.9	0.732
Alcohols	111	199.00-508.15	6.82	13.6	50.8	1.407
Acids	150	283.15-683.15	8.90	10.3	58.5	0.931
Formates	140	193.15-667.15	13.2	13.8	75.1	1.585
Acetates	140	183.15-656.15	15.6	12.3	68.3	0.865
Aldehydes	140	183.15-718.15	7.78	12.7	63.3	0.722
Alkanone	140	193.15-603.15	7.92	12.9	56.3	1.100
Ethers	100	113.15-645.15	5.64	15.2	51.6	2.821
Chloro Alkan	190	193.15-615.15	5.42	21.2	45.8	3.923
Iodo Alkanes	160	173.15-680.15	11.7	82.9	62.1	3.431
Bromo Alkane	130	193.15-615.15	7.12	47.9	54.1	3.558
Overall Ave. Dev.			8.98	22.7	56.7	1.739
Total	2151					

Thermal Conductivity Methods:

Bar - Baroncini et al method	Eq. 2.29
Sato - Sato boiling point method	Eq. 2.25
Robn - Robin and Kingrea method	Eq. 2.15
Group - Proposed method	Eq. 3.9

TABLE VII

COMPARISON RESULTS FOR ALKANES

Number of Systems = 15

System	NPT	Temp. Range	Bar	Ave. Perc. Dev.		Group
		Degree K		Sato	Robn	
Propane	14	93.15-223.15	28.1	21.5	14.6	0.902
N-Butane	14	143.15-273.15	17.2	10.2	5.18	0.830
N-Pentane	16	153.15-303.15	10.3	3.52	5.52	0.546
N-Hexane	13	183.15-303.15	6.75	1.88	16.7	0.983
N-Heptane	16	183.15-333.15	3.55	5.74	18.7	1.800
N-Octane*	15	223.15-373.15	2.66	10.1	15.2	1.890
N-Decane	8	303.15-415.15	6.83	21.6	9.99	2.397
N-Undecane	31	307.75-637.45	12.8	17.5	73.9	0.716
N-Dodecane	25	307.75-653.15	14.6	20.7	10.8	0.845
N-Tridecane	35	307.75-669.35	14.9	20.5	79.3	0.478
N-Tetradeca	19	307.80-509.80	3.52	24.1	81.5	0.918
N-Hexadecan	12	313.15-533.15	1.48	25.7	85.8	0.850
N-Heptadeca	13	313.15-553.15	1.23	25.2	87.0	1.392
N-Octadecan*	14	313.15-573.15	3.30	24.2	88.3	1.928
N-Nonadecan*	15	313.15-593.15	4.38	24.1	89.3	2.003
Overall Ave.			9.71	24.1	49.3	1.018
Total	150					

Thermal Conductivity Methods:

Bar	Baroncini et al. method	Eq. 2.29
Sato	Sato boiling point method	Eq. 2.25
Robn	Robin and Kingrea method	Eq. 2.15
Group	Proposed method	Eq. 3.9

*Not included in regression (predicted)

TABLE VIII

COMPARISON RESULTS FOR ALKENES

Number of Systems = 22

System	NPT	Temp. Range Degree K	Bar	Ave. Perc. Dev.		
				Sato	Robn	Group
Ethylene	10	113.15-239.15	4.02	20.4	55.5	1.951
Propylene	10	93.15-309.15	7.92	26.7	24.0	1.297
But-1-ene	10	93.15-345.15	7.61	16.6	32.7	0.598
But-2-ene	10	153.15-351.15	10.8	15.1	44.0	1.345
Isobutene	10	133.15-349.15	15.5	9.72	33.4	0.103
Pent-1-ene	10	113.15-392.15	5.42	8.83	48.5	0.606
Hex-1-ene	10	133.15-421.15	3.95	3.39	52.4	0.642
Hex-2-ene	10	143.15-431.15	6.04	3.33	62.6	0.609
Hex-3-ene*	10	153.15-432.15	5.47	3.13	62.8	0.695
Hept-1-ene	10	163.15-451.15	2.52	4.56	59.6	0.527
Hept-2-ene	10	173.15-461.15	2.46	3.37	67.5	0.569
Hept-3-ene	10	143.15-458.15	2.57	3.60	66.4	0.359
Oct-1-ene	10	173.15-479.15	3.86	7.75	65.0	0.540
Oct-2-ene	10	183.15-489.15	2.54	7.05	73.1	0.400
Oct-3-ene	10	173.15-479.15	2.48	7.67	72.9	0.212
Oct-4-ene	10	173.15-488.15	2.63	7.59	73.1	0.322
Non-1-ene	10	193.15-499.15	6.63	12.2	68.8	0.454
Dec-1-ene	10	213.15-519.15	10.8	14.3	72.8	0.593
Undec-1-ene	10	233.15-539.15	14.5	17.0	76.0	0.607
Dodec-1-ene*	10	243.15-549.15	17.9	19.2	78.7	0.807
Tridec-1-ene*	10	253.15-568.15	21.5	20.9	80.9	1.132
Tetradec-1-ene*	10	263.15-587.15	24.6	22.8	82.7	1.714
Overall Ave.			8.27	12.6	59.9	0.733
Total	220					

*Not included in regression (predicted)

TABLE IX

COMPARISON RESULTS FOR BRANCHED ALKANES

Number of Systems = 26

System	NPT	Temp. Range Degree K	Bar	Ave. Perc. Dev. Bar	 Robn	Group
2,2DI-C1-C3	10	263.15-380.15	8.26	6.77	31.1	2.149
2,2DI-C1-C4	10	173.15-416.15	2.69	10.7	20.4	2.347
2,2DI-C1-C5	10	153.15-441.15	2.96	15.5	8.73	1.280
2,3DI-C1-C5	10	153.15-450.15	5.22	15.4	11.6	1.487
2,2DI-C1-C6	10	153.15-459.15	7.04	21.6	4.36	0.943
3,3DI-C1-C6	10	153.15-459.15	8.34	20.5	6.20	0.515
2-Methyl-C3	10	113.15-338.15	16.1	6.16	39.2	1.406
2-Methyl-C4	10	113.15-383.15	16.4	6.92	36.7	1.351
2-Methyl-C5	10	123.15-420.15	5.56	4.65	12.2	1.234
3-Methyl-C5	10	123.15-420.15	4.01	5.14	15.5	1.209
2,3DI-C1-C4	10	153.15-423.15	3.15	11.5	36.9	1.053
2-Methyl-C6	10	163.15-442.15	2.64	8.76	4.00	0.973
3-Methyl-C6	10	163.15-442.15	2.39	10.0	6.51	0.850
2,3DI-C1-C5	10	153.15-450.15	6.51	16.4	22.2	1.278
2,4DI-C1-C5	10	163.15-433.15	3.46	16.7	7.45	0.799
2-Methyl-C7	10	173.15-461.15	2.19	13.1	9.62	0.846
3-Methyl-C7	10	153.15-459.15	3.33	14.4	4.91	0.906
4-Methyl-C7	10	153.15-459.15	3.61	15.2	5.28	1.541
2,3DI-C1-C6	10	153.15-468.15	9.43	21.3	4.31	1.084
2,4DI-C1-C6	10	153.15-468.15	7.52	21.3	4.17	0.889
2,5DI-C1-C6	10	183.15-453.15	7.63	22.6	4.56	0.728
3,4DI-C1-C6*	10	153.15-468.15	10.3	24.3	3.88	0.889
2,3,4-tri-C1-C5	10	173.15-479.15	18.6	31.0	16.3	1.154
2,2,3-tri-C1-C5	10	163.15-469.15	17.5	30.5	18.4	1.775
2,3,3-tri-C1-C5*	10	173.15-470.15	19.2	30.2	9.76	1.042
2,3,5-tri-C1-C6*	10	153.15-468.15	16.7	32.5	11.6	0.803
Overall Ave.			8.40	17.3	13.3	1.174
Total	260					

*Not included in regression (predicted)

TABLE X

COMPARISON RESULTS FOR ALCOHOLS

Number of Systems = 11

System	NPT	Temp. Range Degree K	Bar	Ave. Perc. Dev. Sato	Ave. Perc. Dev. Robn	Group
Methanol	15	199.00-469.15	10.6	39.4	71.2	1.459
Ethanol	13	233.15-471.15	8.15	25.8	12.8	1.211
N-Propanol	17	200.00-479.15	5.05	15.8	71.7	1.264
N-Butanol	13	203.40-373.15	3.12	8.03	30.4	1.235
N-Pentanol	8	201.70-353.15	3.25	4.40	42.4	1.956
N-Hexanol	9	243.50-423.15	5.05	4.42	45.2	2.589
N-Heptanol*	15	246.80-436.25	5.59	3.31	61.9	1.573
N-Octanol	3	293.15-485.15	7.51	6.08	66.3	2.714
N-Nonanol	7	273.15-423.15	4.71	3.98	48.6	1.450
N-Decanol	4	273.15-373.15	9.22	1.68	73.5	1.144
N-Tetradeca*	4	323.15-473.15	14.8	7.31	3.59	5.785
N-Octadecan*	3	337.15-373.15	23.7	6.68	92.2	2.431
Overall Ave.			6.81	13.6	50.8	1.756
Total	111					

*Not included in regression (predicted)

but it fails with most compounds. The method of Robbins and Kingrea (22) requires other physical property data to predict thermal conductivity. Some of these data may not be readily available (e.g., liquid density, heat capacity, at desired temperatures) and have to be estimated. Also critical properties might be needed to evaluate some of these needed data. For very long chains the property prediction methods are not accurate, or not correct at all for some polar compounds.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

The following conclusions can be drawn from the results of this work:

The Cox equation, which is originally a vapor pressure correlation, becomes an excellent liquid thermal conductivity correlation with slight modification.

A prediction method, which is capable of covering a wide range of temperatures (from the melting point to the critical point) and a wide range groups and chain lengths, has been developed.

A new group contribution technique for predicting thermal conductivity employing the geometric series model is proposed, and is extended to multi-group compounds.

The methylene, and methyl groups are treated as two different groups in any given compound.

The proposed method is superior to any other currently existing method; it is applicable to and more accurate for a wide range of temperatures, and both short and long chain compounds.

The proposed method has been tested for both nonpolar (n-alkanes), and polar (n-alcohols) compounds. The same procedure is equally applicable to other homologous series.

Recommendations

The following recommendations are made for further investigation:

1. Apply the current method to other multi-functional group compound series.

2. Develop structural corrections for cyclic and aromatic compounds.

3. Apply the same approach to treat other pure compound physical properties.

4. Apply the same method to vapor and liquid thermal conductivities at the same time, which may result in critical thermal conductivity evaluation.

5. Apply the same method to as many groups as possible at the same time, which will result in better results, and more accurate prediction of compounds with different groups.

6. Apply the same geometric representation to evaluate constants for other established physical properties methods.

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APPENDIX A

SUMMARY OF COMPUTED RESULTS

TABLE XI

SUMMARY FOR THERMAL CONDUCTIVITY RESULTS

Number of Systems = 16
Number of Groups = 22

SYSTEM	NOS	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	AAPD
Alkanes(Str)	15	260	93.15-669.15	4.65	-4.70	1.018
Alkanes(Bra)	27	270	113.15-470.15	6.56	-14.6	1.519
Alkenes	22	220	93.15-587.15	5.89	-3.65	0.732
Alcohols(OH)	17	211	199.00-508.15	5.05	-11.0	1.407
Acids	15	150	283.15-683.15	2.95	-6.06	0.931
Formates	14	140	193.15-667.15	8.86	-6.72	1.585
Esters	131	524	183.15-675.15	6.30	-5.13	0.865
Aldehydes	14	140	183.15-718.15	4.75	-2.06	0.722
Ketones	70	420	193.15-696.15	3.82	-2.78	1.100
Ethers	55	560	113.15-645.15	6.16	-3.20	2.821
Amines	4	040	243.15-680.15	1.22	-1.72	0.469
Nitro Compound	5	050	173.15-488.15	2.46	-1.20	0.620
Chloro Alkanes	19	190	153.15-548.15	11.2	-23.2	3.922
Bromo Alkanes	13	130	173.15-590.15	6.88	-13.2	3.358
Iodo Alkanes	16	160	213.15-678.15	8.74	-16.7	3.430
Crude Oil	16	160	283.33-477.15	13.8	-9.73	2.821
Total	453	3625				

Max. Pos. Dev. = 13.8
Max. Neg. Dev. = -16.7
Average Absolute Percent Deviation = 1.0526 (Overall)

* NOS Number of Sub-Systems
* NOP Number of Points

TABLE XII

THERMAL CONDUCTIVITY FOR ALKANES

Number of Systems = 15

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Propane	14	93.15-223.15	2.39	-0.69	123.15	0.902
N-Butane	14	143.15-273.15	0.58	-1.39	193.15	0.830
N-Pentane	16	153.15-303.15	0.71	-1.86	153.15	0.546
N-Hexane	13	183.15-303.15	2.31	-0.37	303.15	0.983
N-Heptane	16	183.15-333.15	2.52	-2.46	323.15	1.800
*N-Octane	15	223.15-373.15	2.38	-----	323.15	1.890
N-Decane	8	303.15-415.15	----	-3.57	410.06	2.397
N-Undecane	31	307.75-637.45	4.65	-2.31	478.55	0.716
N-Dodecane	25	307.75-653.15	1.37	-3.15	478.55	0.845
N-Tridecane	35	307.75-669.35	1.13	-0.48	538.55	0.478
N-Tetradeca	19	307.80-509.80	1.08	-4.70	317.10	0.918
N-Hexadecan	12	313.15-533.15	1.29	-1.14	393.15	0.850
N-Heptadeca	13	313.15-553.15	2.44	-1.67	393.15	1.392
*N-Octadecan	14	313.15-573.15	2.92	-0.78	413.15	1.928
*N-Nonadecan	15	313.15-593.15	2.99	-0.49	413.15	2.003

Total 260
Maximum Positive Deviation = 4.65
Maximum Negative Deviation = -4.70
Ave. Abs. Perc. Dev. = 1.01881 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 1.9406
Ave. Abs. Perc. Dev. (Regression) = 0.8159

* Not Included in Regression (Predicted)

TABLE XIII

THERMAL CONDUCTIVITY FOR ALKENES

Number of Systems = 22

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Ethylene	10	113.15-239.15	5.89	-3.09	113.15	1.951
Propylene	10	93.15-309.15	3.16	-0.50	117.15	1.297
But-1-ene	10	93.15-345.15	0.48	-3.31	93.15	0.598
But-2-ene	10	153.15-351.15	2.79	-1.68	351.15	1.345
Isobutene	10	133.15-349.15	0.19	-0.15	157.15	0.103
Pent-1-ene	10	113.15-392.15	0.28	-3.63	113.15	0.606
Hex-1-ene	10	133.15-421.15	0.03	-3.65	133.15	0.642
Hex-2-ene	10	143.15-431.15	0.82	-0.90	175.15	0.609
*Hex-3-ene	10	153.15-432.15	0.69	-1.02	308.15	0.695
Hept-1-ene	10	163.15-451.15	0.13	-2.13	163.15	0.527
Hept-2-ene	10	173.15-461.15	0.81	-0.40	333.15	0.569
Hept-3-ene	10	143.15-458.15	0.64	-1.12	143.15	0.359
Oct-1-ene	10	173.15-479.15	0.88	-1.42	173.15	0.540
*Oct-2-ene	10	183.15-489.15	0.50	-0.52	183.15	0.400
Oct-3-ene	10	173.15-479.15	0.13	-1.13	173.15	0.212
Oct-4-ene	10	173.15-488.15	0.04	-1.19	173.15	0.322
Non-1-ene	10	193.15-499.15	0.32	-1.24	193.15	0.454
Dec-1-ene	10	213.15-519.15	1.21	-0.09	281.15	0.593
Undec-1-en	10	233.15-539.15	1.22	-0.05	267.15	0.607
*Tridec-1-e	10	253.15-568.15	1.68	-1.69	463.15	1.132
*Tetradec- -1-ene	10	263.15-587.15	1.54	-3.24	479.15	1.714

Total 220
Maximum Positive Deviation = 5.89
Maximum Negative Deviation = -3.65
Ave. Abs. Perc. Dev. = 0.73257 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 1.42337
Ave. Abs. Perc. Dev. (Regression) = 0.66349
* Not Included in Regression (Predicted)

TABLE XIV

THERMAL CONDUCTIVITY FOR BRANCHED ALKANES

Number of Systems = 26

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
2,2DI-Cl-C3	10	263.15-380.15	4.89	-2.68	380.15	2.149
2,2DI-Cl-C4	10	173.15-416.15	5.46	-2.71	416.15	2.347
2,2DI-Cl-C5	10	153.15-441.15	2.63	-2.32	441.15	1.280
2,3DI-Cl-C5	10	153.15-450.15	6.56	-0.33	450.15	1.487
2,2DI-Cl-C6	10	153.15-459.15	0.35	-1.61	425.15	0.943
3,3DI-Cl-C6	10	153.15-459.15	0.92	-0.69	221.15	0.515
2-Methyl-C3	10	113.15-338.15	3.24	-2.05	113.15	1.406
2-Methyl-C4	10	113.15-383.15	3.78	-0.48	113.15	1.351
2-Methyl-C5	10	123.15-420.15	3.08	-1.44	123.15	1.234
3-Methyl-C5	10	123.15-420.15	2.55	-0.74	123.15	1.209
2,3DI-Cl-C4	10	153.15-423.15	1.96	-1.78	363.15	1.053
2-Methyl-C6	10	163.15-442.15	1.90	-0.91	380.15	0.973
3-Methyl-C6	10	163.15-442.15	1.38	-1.30	380.15	0.850
2,3DI-Cl-C5	10	153.15-450.15	2.88	-0.45	384.15	1.278
2,4DI-Cl-C5	10	163.15-433.15	1.24	-2.20	433.15	0.799
2-Methyl-C7	10	173.15-461.15	1.82	-0.41	397.15	0.846
3-Methyl-C7	10	153.15-459.15	0.63	-1.84	255.15	0.906
4-Methyl-C7	10	153.15-459.15	----	-2.71	255.15	1.541
2,3DI-Cl-C6	10	153.15-468.15	2.56	-0.45	398.15	1.084
2,4DI-Cl-C6	10	153.15-468.15	1.20	-2.19	468.15	0.889
2,5DI-Cl-C6	10	183.15-453.15	0.53	-1.37	273.15	0.728

TABLE XIV (continue)

Number of Systems = 26

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
*3,4DI-Cl-C6	10	153.15-468.15	1.20	-2.19	468.15	0.889
2,3,4-tri-cl-c5	10	173.15-479.15	1.16	-2.64	479.15	1.154
2,2,3-tri-cl-c5	10	163.15-469.15	0.60	-5.57	163.15	1.775
*2,3,3-tri-cl-c5	10	173.15-470.15	1.69	-3.48	173.15	1.042
*2,3,5-tri-cl-c6	10	153.15-468.15	1.31	-1.24	398.15	0.803

Total 260
Maximum Positive Deviation = 6.56
Maximum Negative Deviation = -5.57
Ave. Abs. Perc. Dev. = 1.1743 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 0.9113
Ave. Abs. Perc. Dev. (Regression) = 1.2086

* Not Included in Regression (Predicted)

TABLE XV

THERMAL CONDUCTIVITY FOR (-OH) GROUP

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Alcohols			Number of Systems = 12			
Methanol	15	199.00-469.15	4.97	-2.75	391.15	1.459
Ethanol	13	233.15-471.15	4.24	-3.96	373.15	1.211
N-Propanol	17	200.00-479.15	4.14	-2.46	479.15	1.264
N-Butanol	13	203.40-373.15	2.85	-2.81	307.15	1.235
N-Pentanol	8	201.70-353.15	1.13	-3.16	253.15	1.956
N-Hexanol	9	243.50-423.15	5.05	-4.42	369.00	2.589
*N-Heptanol	15	246.80-436.25	2.65	-2.68	436.25	1.573
N-Octanol	3	293.15-485.15	2.32	-4.92	485.15	2.714
N-Nonanol	7	273.15-423.15	----	-4.38	423.15	1.450
N-Decanol	4	273.15-373.15	2.94	-----	323.15	2.144
*N-Tetradeca	4	323.15-473.15	----	-11.0	473.15	5.785
*N-Octadecan	3	337.15-373.15	0.86	-3.23	347.15	2.431
Polymethlene Glycols			Number of Systems = 4			
Ethelene	20	223.15-508.15	2.35	-0.97	223.15	1.039
Trimethyle	20	223.15-508.15	----	-3.75	223.15	1.041
Tetramethy	20	223.15-508.15	1.58	-2.95	223.15	1.171
Pentamethy	20	223.15-508.15	2.24	-3.98	508.15	1.560
Glycerols			Number of Systems = 1			
Glycerine	20	223.15-508.15	0.46	-1.15	223.15	0.290

Total 211
Maximum Positive Deviation = 5.05
Maximum Negative Deviation = -11.0
Ave. Abs. Perc. Dev. = 1.40775 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 2.4557
Ave. Abs. Perc. Dev. (Regression) = 1.1517
* Not Included in Regression (Predicted)

TABLE XVI

THERMAL CONDUCTIVITY FOR ALKANOIC ACIDS

Number of Systems = 15

SYSTEM (R - Acid)	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Acetic	10	283.15-508.15	2.95	-0.24	283.15	0.962
Propanoic	10	283.15-517.15	0.08	-1.84	413.15	1.218
Butanoic	10	273.15-534.15	0.46	-0.26	273.15	0.248
Pentanoic	10	273.15-552.15	0.41	-0.79	273.15	0.439
Hexanoic	10	273.15-561.15	1.23	-0.53	529.15	0.636
*Heptanoic	10	273.15-579.15	0.97	-0.72	511.15	0.564
Octanoic	10	293.15-599.15	0.95	-0.45	497.15	0.565
Nonanoic	10	303.15-609.15	----	-1.43	303.15	0.617
Decanoic	10	323.15-620.15	0.48	-1.03	620.15	0.379
Dodecanoic	10	333.15-639.15	0.34	-1.19	639.15	0.332
Tetradecan	10	343.15-667.15	0.47	-0.48	667.15	0.240
Hexadecano	10	353.15-686.15	1.11	-0.80	686.15	0.513
*Octadecano	10	363.15-656.15	0.49	-1.58	537.15	0.893
*Eicosanoic	10	363.15-675.15	----	-3.57	549.15	1.232
*Docosanoic	10	363.15-683.15	----	-6.06	555.15	2.006

Total 150
Maximum Positive Deviation = 2.95
Maximum Negative Deviation = -6.06
Ave. Abs. Perc. Dev. = 0.93151 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 1.9538
Ave. Abs. Perc. Dev. (Regression) = 0.5598
* Not Included in Regression (Predicted)

TABLE XVII

THERMAL CONDUCTIVITY FOR ALKYL FORMATES

Number of Systems = 14

SYSTEM (R - Formate)	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Methyl	10	193.15-373.15	4.59	-0.72	193.15	1.750
Ethyl	10	213.15-402.15	1.18	-1.17	402.15	0.710
Propyl	10	223.15-448.15	2.33	-3.49	223.15	1.991
Butyl	10	223.15-448.15	1.32	-3.30	223.15	1.122
Pentyl	10	243.15-477.15	0.98	-2.08	243.15	0.733
*Hexyl	10	243.15-495.15	0.53	-2.16	243.15	0.558
Heptyl	10	253.15-523.15	0.96	-1.27	523.15	0.691
Octyl	10	263.15-542.15	1.78	-1.37	356.15	1.056
Nonyl	10	273.15-552.15	1.94	-1.48	366.15	1.207
Decyl	10	283.15-580.15	1.97	-1.73	349.15	1.249
Dodecyl	10	293.15-599.15	0.94	-1.06	565.15	0.682
Tetradecyl	10	323.15-638.15	3.38	-2.22	638.15	1.622
*Hexadecyl	10	343.15-649.15	1.07	-4.07	488.15	3.149
*Octadecyl	10	343.15-667.15	8.86	-6.72	640.15	5.666

Total 140
Maximum Positive Deviation = 8.867
Maximum Negative Deviation = -6.72
Ave. Abs. Perc. Dev. = 1.58511 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 3.1250
Ave. Abs. Perc. Dev. (Regression) = 1.16514
* Not Included in Regression (Predicted)

TABLE XVIII

THERMAL CONDUCTIVITY FOR ALKYL ALDEHYDES

Number of Systems = 14

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Acetaldehy	10	183.15-372.15	1.04	-2.64	372.15	1.060
Propionald	10	213.15-411.15	1.32	-0.33	301.15	0.817
Butyraldeh	10	253.15-451.15	0.64	-0.03	451.15	0.335
Valeraldeh	10	273.15-471.15	0.53	-1.08	339.15	0.781
Hexanal	10	293.15-482.15	0.35	-1.01	377.15	0.685
*Heptanal	10	303.15-546.15	1.26	-0.37	546.15	0.458
Octanal	10	313.15-529.15	1.03	-0.23	313.15	0.340
Nonanal	10	333.15-453.15	1.22	-0.05	333.15	0.346
Decanal	10	353.15-569.15	0.87	-0.29	353.15	0.301
Dodecanal	10	363.15-588.15	1.08	-0.22	363.15	0.302
Tetradeca	10	363.15-606.15	0.05	-0.59	606.15	0.360
Hexaecan	10	373.15-643.15	0.91	-0.63	583.15	0.517
*Octadecan	10	383.15-689.15	2.23	-1.74	621.15	1.315
*Eicosanal	10	403.15-718.15	4.75	-2.06	648.15	2.491

Total 140
Maximum Positive Deviation = 4.75
Maximum Negative Deviation = -2.06
Ave. Abs. Perc. Dev. = 0.7225 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 1.4213
Ave. Abs. Perc. Dev. (Regression) = 0.53191

* Not Included in Regression (Predicted)

TABLE XIX

THERMAL CONDUCTIVITY FOR CHLORO ALKANES

Number of Systems = 19

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Chloro-c2	10	233.15-377.15	5.30	-3.04	233.15	2.396
1-Cl-c3	10	153.15-405.15	4.54	-3.54	291.15	2.894
1,2DI-CL-C3	10	233.15-476.15	2.34	-6.38	233.15	2.143
1,3DI-CL-C3	10	273.15-435.15	2.75	-5.01	435.15	3.091
1-Chloro-C4	10	173.15-452.15	5.02	-11.9	173.15	4.386
2-Chloro-C4	10	173.15-407.15	4.97	-12.2	407.15	4.755
1-CL-2-CL-c3	10	173.15-398.15	4.80	-9.85	398.15	4.199
1,4-DI-CL-c4	10	303.15-501.15	3.08	-9.97	501.15	3.347
1-Chloro-C5	10	263.15-470.15	6.43	-2.92	378.15	3.936
*2-Chloro-C5	10	153.15-459.15	3.53	-7.78	153.15	3.329
1,5DI-CL-C5	10	223.15-466.15	11.2	-3.09	223.15	4.952
1-Chloro-C6	10	263.15-479.15	6.38	-6.19	383.15	4.084
2-Chloro-C6	10	173.15-497.15	6.22	-14.0	173.15	5.078
1,6DI-CL-C6	10	323.15-503.15	5.88	-6.03	503.15	3.355
1-Chloro-C7	10	283.15-499.15	6.13	-7.24	283.15	4.079
1-Chloro-C8	10	283.15-499.15	5.73	-12.9	283.15	4.821
1,8DI-CL-C8	10	313.15-547.15	4.19	-11.7	547.15	3.935
1-Cl-C10	10	293.15-545.15	4.34	-23.2	293.15	6.478
*1,10-DI-Cl-C10	10	323.15-548.15	4.75	-6.82	548.15	3.265

Total 190
Maximum Positive Deviation = 11.2
Maximum Negative Deviation = -23.2
Ave. Abs. Perc. Dev. = 3.92287 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 3.2970
Ave. Abs. Perc. Dev. (Regression) = 3.9965

* Not Included in Regression (Predicted)

TABLE XX

THERMAL CONDUCTIVITY FOR IODO ALKANES

Number of Systems = 16

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
I-Methane	10	213.15-429.15	0.72	-6.63	429.15	3.166
I-Ethane	10	233.15-467.15	1.92	-4.36	467.15	1.606
1-I-Propane	10	233.15-467.15	3.83	-6.29	233.15	2.751
*1,3-DI-I-C3	10	273.15-678.15	----	-7.71	678.15	4.117
1-I-Butane	10	253.15-496.15	4.52	-7.96	253.15	3.341
2-I-Butane	10	263.15-497.15	8.74	-1.87	341.15	6.167
1,4-DI-I-C4	10	353.15-596.15	1.13	-0.59	515.15	0.875
1-I-Pentane	10	268.15-497.15	5.24	-9.11	268.15	3.892
1,5-DI-I-C5	10	293.15-599.15	3.62	-2.20	293.15	2.427
1-I-Hexane	10	273.15-543.15	6.04	-11.4	273.15	4.609
1,6-DI-I-C6	10	333.15-639.15	4.17	-8.04	639.15	3.698
1-I-Heptane	10	273.15-561.15	5.25	-16.7	273.15	5.316
1-I-Octane	10	323.15-584.15	4.74	-8.64	323.15	4.022
1,8-DI-I-C8	10	353.15-596.15	4.27	-5.94	596.15	2.964
1-I-Decane	10	353.15-596.15	1.93	-10.8	353.15	3.070
*1,10-DI-I--C10	10	393.15-591.15	3.92	-6.71	591.15	2.870

Total 160
Maximum Positive Deviation = 8.74
Maximum Negative Deviation = -16.7
Ave. Abs. Perc. Dev. = 3.43092 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 3.4935
Ave. Abs. Perc. Dev. (Regression) = 3.4219

* Not Included in Regression (Predicted)

TABLE XXI

THERMAL CONDUCTIVITY FOR BROMO ALKANES

Number of Systems = 13

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Br-Methane	10	193.15-373.15	6.82	-7.83	373.15	4.736
Br-Ethane	10	173.15-371.15	1.40	-10.0	173.15	2.449
1-Br-Propa	10	223.15-448.15	2.60	-6.85	223.15	2.390
1-Br-Butane	10	223.15-520.15	4.98	-13.1	520.15	5.056
1,4DI-Br-C4	10	293.15-590.15	----	-2.87	590.15	2.065
*1-Br-Pentan	10	253.15-496.15	6.88	-6.23	388.15	4.366
1,5DI-Br-C5	10	273.15-525.15	3.34	-1.49	273.15	1.401
1-Br-Hexane	10	273.15-525.15	6.22	-5.98	413.15	4.067
1,6DI-Br-C6	10	303.15-546.15	5.71	-2.66	303.15	3.084
1-Br-Heptan	10	273.15-525.15	5.52	-9.69	273.15	4.053
1-Br-Octane	10	293.15-527.15	4.02	-9.32	293.15	3.350
1,8DI-Br-C8	10	333.15-540.15	5.03	-7.85	540.15	3.458
*1-Br-Decane	10	323.15-548.15	0.57	-10.7	323.15	3.178

Total 130
Maximum Positive Deviation = 6.88
Maximum Negative Deviation = -13.2
Ave. Abs. Perc. Dev. = 3.35836 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 3.7720
Ave. Abs. Perc. Dev. (Regression) = 3.2835

* Not Included in Regression (Predicted)

TABLE XXII

THERMAL CONDUCTIVITY FOR ALPHATIC NITRO-COMPOUND

Alphatic Nitro-Compounds Number of Systems = 5

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Nitro-C2	10	183.15-507.15	2.46	-0.78	183.15	0.979
1-Nitro-C3	10	173.15-443.15	0.28	-1.20	293.15	0.648
1-Nitro-C4	10	193.15-526.15	0.39	-1.17	526.15	0.329
1-Nitro-C5	10	173.15-488.15	0.71	-1.19	173.15	0.712
1-Nitro-C6	10	173.15-488.15	1.14	-1.12	173.15	0.677

Total 50
Maximum Positive Deviation = 2.46
Maximum Negative Deviation = -1.20
Ave. Abs. Perc. Dev. = 0.62048

TABLE XXIII

THERMAL CONDUCTIVITY FOR ALPHATIC DIAMINES

Alphatic Di-Amines Number of Systems = 4

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Ethanol- -Amine	10	283.15-553.15	0.19	-0.16	283.15	0.121
DI-Ethanol- -Amine	10	301.15-635.15	1.22	-1.48	635.15	0.883
Tri-Ethanol - Amine	10	294.15-680.25	0.31	-0.29	637.35	0.202
Di-Ethylene -Tri-Amine	10	243.15-522.15	0.96	-1.72	243.15	0.671

Total 40
Maximum Positive Deviation = 1.22
Maximum Negative Deviation = -1.72
Ave. Abs. Perc. Dev. = 0.46946

TABLE XXIV

THERMAL CONDUCTIVITY FOR N-ALKYL ESTERS COMPOUNDS

Number of Systems = 131

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
R - Acetates		Number of Systems = 14				
Methyl	4	183.15-370.65	6.30	-0.31	370.65	3.113
Ethyl	4	193.15-388.15	2.75	-2.91	323.15	2.047
Propyl	4	203.15-413.15	0.57	-3.55	343.15	2.363
Butyl	4	213.15-445.65	----	-2.80	368.15	2.054
Pentyl	4	223.15-455.65	----	-2.31	455.15	1.604
Hexyl	4	233.15-473.15	----	-1.50	233.15	0.797
Heptyl	4	243.15-490.65	0.33	-0.75	490.65	0.371
Octyl	4	253.15-508.15	1.16	-0.17	423.15	0.691
*Nonyl	4	263.15-518.15	1.67	-----	433.15	0.991
Decyl	4	273.15-535.65	2.06	-0.50	448.15	1.229
Dodecyl	4	283.15-545.65	2.05	-----	458.15	1.125
Tetradecyl	4	303.15-580.65	1.79	-0.45	488.15	0.882
*Hexadcyl	4	313.15-598.15	1.43	-1.19	503.15	0.816
*Octadecyl	4	323.15-600.65	0.77	-2.10	323.15	0.818
R - Propionates		Number of Systems = 14				
Methyl	4	193.15-388.15	3.11	-1.99	193.15	1.864
Ethyl	4	203.15-398.15	1.01	-3.45	333.15	2.397
Propyl	4	213.15-408.15	0.65	-3.69	343.15	2.701
Butyl	4	223.15-448.15	----	-3.17	448.15	2.233
*Pentyl	4	223.15-470.65	----	-2.44	470.65	1.423
Hexyl	4	223.15-485.15	----	-1.36	485.65	0.533
Heptyl	4	233.15-488.15	0.62	-0.23	403.15	0.360
Octyl	4	243.15-505.65	1.13	-0.13	418.15	0.542
Nonyl	4	253.15-515.65	1.41	-0.24	428.15	0.757
Decyl	4	273.15-535.65	1.52	-0.20	448.15	0.757
Dodecyl	4	283.15-545.65	1.28	-0.96	458.15	0.815
Tetradecyl	4	303.15-580.65	0.93	-1.50	303.15	0.750
*Hexadcyl	4	313.15-598.15	0.49	-2.25	313.15	0.991
*Octadecyl	4	333.15-633.15	0.03	-2.80	333.15	1.426

TABLE XXIV (continue)

Number of Systems = 131 Continue

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
R - Butyrates		Number of Systems = 14				
Methyl	4	223.15-410.65	1.00	-1.52	348.15	1.036
Ethyl	4	233.15-420.65	----	-3.51	420.65	2.770
Propyl	4	243.15-430.65	----	-3.22	430.65	2.489
Butyl	4	248.15-435.65	----	-2.01	435.65	1.466
Pentyl	4	263.15-443.15	----	-0.73	443.15	0.444
Hexyl	4	268.15-448.15	0.18	-0.08	388.15	0.098
*Heptyl	4	283.15-500.65	0.69	-0.29	428.65	0.413
Octyl	4	273.15-453.15	0.93	-0.16	453.15	0.624
Nonyl	4	283.15-463.15	1.06	-0.32	463.15	0.704
Decyl	4	293.15-473.15	0.95	-0.57	473.15	0.664
Dodecyl	4	303.15-483.15	0.72	-1.31	303.15	0.681
Tetradecyl	4	313.15-493.15	0.35	-2.05	313.15	0.836
*Hexadcyl	4	313.15-538.15	0.04	-2.95	313.15	1.155
*Octadecyl	4	323.15-548.15	----	-3.75	323.15	1.801
R - Valerates		Number of Systems = 13				
Methyl	4	223.15-410.65	0.52	-1.62	348.15	1.121
Ethyl	4	233.15-420.65	----	-2.70	420.15	2.033
Propyl	4	243.15-430.65	----	-2.09	430.65	1.524
Butyl	4	253.15-440.65	----	-0.84	440.65	0.522
Pentyl	4	263.15-458.65	0.09	-0.29	458.15	0.143
Hexyl	4	273.15-468.15	0.37	-0.26	403.15	0.213
*Heptyl	4	283.15-478.15	0.63	-0.29	413.15	0.406
Octyl	4	293.15-488.65	0.73	-0.42	423.15	0.501
Nonyl	4	303.15-505.65	0.63	-0.67	303.15	0.449
Decyl	4	313.15-515.65	0.52	-0.91	313.15	0.423
Dodecyl	4	323.15-525.65	0.09	-1.64	323.15	0.575
*Tetradecyl	4	333.15-535.15	----	-2.31	333.15	0.993
*Hexadcyl	4	343.15-553.15	----	-2.88	343.15	1.377

TABLE XXIV (continue)

Number of Systems = 131

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
R - Hexanoates		Number of Systems = 13				
Methyl	4	233.15-413.15	----	-1.29	353.15	0.875
Ethyl	4	243.15-423.15	----	-1.63	423.15	1.168
Propyl	4	253.15-433.15	----	-0.75	433.15	0.498
Butyl	4	263.15-443.15	----	-0.23	443.15	0.123
Pentyl	4	273.15-460.65	0.27	-0.31	273.15	0.172
Hexyl	4	283.15-470.65	0.53	-0.34	408.15	0.363
Heptyl	4	293.15-488.15	0.64	-0.47	423.15	0.442
*Octyl	4	303.15-505.65	0.54	-0.72	303.15	0.389
Nonyl	4	313.15-523.15	0.45	-0.96	313.15	0.363
Decyl	4	323.15-540.65	0.29	-1.22	323.15	0.512
Dodecyl	4	333.15-550.65	----	-1.87	333.15	0.729
*Tetradecyl	4	343.15-560.65	----	-2.49	343.15	1.133
*Hexadecyl	4	363.15-595.15	----	-2.81	363.15	1.488
R - Heptanoates		Number of Systems = 12				
Methyl	4	273.15-430.65	----	-0.37	325.65	0.277
Ethyl	4	283.15-448.15	0.01	-0.41	448.15	0.155
Propyl	4	293.15-458.15	0.31	-0.05	403.15	0.214
Butyl	4	303.15-468.15	0.50	-----	413.15	0.303
Pentyl	4	313.15-478.15	0.55	-0.01	423.15	0.294
*Hexyl	4	323.15-488.15	0.66	-0.07	433.15	0.386
Heptyl	4	333.15-513.15	0.56	-0.28	453.15	0.298
Octyl	4	353.15-533.15	0.45	-0.36	473.15	0.326
Nonyl	4	363.15-543.15	0.29	-0.59	363.15	0.334
Decyl	4	373.15-560.65	0.18	-0.79	373.15	0.423
*Dodecyl	4	393.15-580.65	----	-1.22	393.15	0.694
*Tetradecyl	4	413.15-608.15	----	-1.53	413.15	1.029

TABLE XXIV (continue)

Number of Systems = 131

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
R - Octanoates		Number of Systems = 12				
Methyl	4	273.15-460.65	0.99	-----	398.15	0.851
Ethyl	4	283.15-470.65	0.74	-----	423.15	0.540
Propyl	4	293.15-488.15	0.82	-----	433.15	0.509
Butyl	4	303.15-498.15	0.78	-----	443.15	0.401
Pentyl	4	313.15-508.15	0.66	-0.19	273.15	0.327
Hexyl	4	323.15-518.15	0.56	-0.41	408.15	0.327
*Heptyl	4	333.15-528.15	0.46	-0.63	423.15	0.337
Octyl	4	343.15-545.15	0.30	-0.88	303.15	0.422
Nonyl	4	353.15-555.15	0.19	-1.09	313.15	0.505
Decyl	4	373.15-575.15	0.03	-1.15	323.15	0.603
*Dodecyl	4	393.15-595.15	----	-1.53	333.15	0.911
*Tetradecyl	4	413.15-608.15	----	-1.86	343.15	1.194
R - Decanoates		Number of Systems = 11				
Methyl	4	273.15-423.15	2.54	-----	423.15	2.063
Ethyl	4	293.15-443.15	1.64	-----	443.15	1.318
Propyl	4	313.15-463.15	1.18	-----	463.15	0.867
Butyl	4	323.15-473.15	0.74	-0.18	473.15	0.502
Pentyl	4	343.15-493.15	0.42	-0.49	343.15	0.338
Hexyl	4	353.15-508.15	0.25	-0.73	353.15	0.330
*Heptyl	4	373.15-523.15	0.16	-0.79	373.15	0.294
Octyl	4	393.15-543.15	0.03	-0.85	393.15	0.346
Nonyl	4	413.15-563.15	----	-0.93	413.15	0.502
Decyl	4	433.15-583.15	----	-0.94	433.15	0.628
*Dodecyl	4	453.15-618.15	----	-1.73	618.15	1.073

TABLE XXIV (continue)

Number of Systems = 131

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
R - Laurates			Number of Systems = 10			
Methyl	4	323.15-473.15	2.91	-----	473.15	2.513
Ethyl	4	343.15-493.15	1.73	-----	443.15	1.423
Propyl	4	363.15-513.15	1.01	-----	443.15	0.697
Butyl	4	383.15-533.15	0.52	-0.11	483.15	0.264
Pentyl	4	393.15-550.15	0.18	-0.52	393.15	0.280
Hexyl	4	413.15-570.65	0.00	-0.78	570.65	0.365
Heptyl	4	433.15-598.15	----	-1.56	598.15	0.682
Octyl	4	453.15-618.15	----	-2.11	618.15	0.900
Nonyl	4	473.15-638.15	----	-2.83	638.15	1.198
*Decyl	4	513.15-675.15	----	-5.13	675.15	2.071
R - Myristates			Number of Systems = 8			
Methyl	4	323.15-510.65	2.62	-----	448.15	2.096
Ethyl	4	333.15-520.65	1.43	-----	458.15	0.913
Propyl	4	353.15-540.65	0.72	-0.58	478.15	0.487
Butyl	4	373.15-560.65	0.26	-0.92	373.15	0.404
Pentyl	4	383.15-570.65	----	-1.37	383.15	0.694
Hexyl	4	393.15-580.65	----	-1.54	393.15	0.823
Heptyl	4	413.15-600.65	----	-1.53	413.15	0.973
*Octyl	4	433.15-628.15	----	-2.11	628.15	1.261

TABLE XXIV (continue)

Number of Systems = 131

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
R - Palmerates		Number of Systems = 6				
Methyl	4	323.15-510.65	2.33	-----	510.65	1.485
Ethyl	4	343.15-530.65	1.04	-0.66	530.65	0.764
Propyl	4	363.15-550.65	0.34	-1.20	363.15	0.498
Butyl	4	383.15-570.65	----	-1.48	383.15	0.623
Pentyl	4	393.15-588.15	----	-1.87	393.15	1.028
*Hexyl	4	413.15-615.65	----	-1.86	413.15	1.247
R - Stearates		Number of Systems = 4				
Methyl	4	373.15-538.15	1.75	-----	538.15	1.136
Ethyl	4	393.15-558.15	0.57	-0.74	393.15	0.459
Propyl	4	413.15-578.15	----	-1.24	413.15	0.550
Butyl	4	423.15-595.65	----	-1.69	423.15	1.067

Total 524
Maximum Positive Deviation = 6.30
Maximum Negative Deviation = -5.13
Ave. Abs. Perc. Dev. = 0.86581 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 1.00487
Ave. Abs. Perc. Dev. (Regression) = 0.86581

* Not Included in Regression (Predicted)

TABLE XXV

THERMAL CONDUCTIVITY FOR N-ALKYL KETONES

Number of Systems = 70

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Alkan-2-ones	Number of Systems = 14					
Acetone	6	193.15-359.82	1.79	-2.22	359.82	1.255
Butanone	6	213.15-379.15	----	-2.40	379.82	1.389
Pentan-2-one	6	223.15-389.82	0.66	-1.10	223.15	0.526
Hexan-2-one	6	233.15-399.82	1.64	-0.79	399.82	1.083
*Heptan-2-one	6	243.15-434.82	2.08	-0.65	434.82	1.221
Octan-2-one	6	263.15-446.48	1.42	-0.79	446.48	0.747
Nonan-2-one	6	273.15-464.82	2.75	-----	464.82	1.950
Decan-2-one	6	293.15-476.48	3.08	-----	476.48	2.498
Undecan-2-o	6	298.15-481.48	3.23	-----	481.48	2.754
Dodecan-2-o	6	303.15-503.15	3.37	-----	503.15	2.932
Tetradecan- -2-one	6	323.15-531.48	3.42	-----	531.48	2.765
Hexadecan- -2-one	6	333.15-549.82	3.59	-----	549.82	2.434
*Octadecan- -2-one	6	343.15-568.15	3.64	-----	568.15	1.878
*Eicosan-2-o	6	353.15-686.48	3.82	-0.52	586.48	1.762

TABLE XXV (continue)

Number of Systems = 70

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Alkan-3-ones		Number of Systems = 12				
Pentan-3-one	6	253.15-436.48	0.78	-0.31	326.48	0.454
Hexan-3-one	6	273.15-456.48	1.11	-----	383.15	0.930
Heptan-3-one	6	283.15-474.82	1.18	-0.15	474.82	0.689
Octan-3-one	6	293.15-493.15	0.13	-1.29	293.15	0.562
*Nonan-3-one	6	313.15-513.15	0.31	-0.86	313.15	0.388
Decan-3-one	6	323.15-489.48	0.69	-----	489.82	0.370
Undecan-3-o	6	338.15-516.48	0.95	-----	516.48	0.677
Dodecan-3-oN	6	353.15-536.48	1.23	-----	536.48	0.966
Tridecan-3-o	6	373.15-556.48	1.98	-----	556.48	1.627
Pentadecan -3-one	6	393.15-576.48	2.36	-----	578.48	1.710
*Heptadecan- -3-one	6	423.15-606.48	3.02	-----	606.48	1.888
*Nonadecan- -3-one	6	453.15-636.48	3.63	-----	636.48	2.280

TABLE XXV (continue)

Number of Systems = 70

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Alkan-4-ones		Number of Systems = 11				
Heptan-4-one	6	273.15-456.48	0.01	-0.88	273.15	0.229
Octan-4-one	6	313.15-513.15	----	-1.46	313.15	0.950
Nonan-4-one	6	303.15-494.82	----	-2.22	303.15	1.709
*Decan-4-one	6	323.15-489.82	----	-1.48	323.15	1.224
Undecan-4-o	6	333.15-516.48	----	-1.08	333.15	0.912
Dodecan-4-o	6	353.15-536.48	----	-0.46	353.15	0.342
Tridecan-4-one	6	373.15-556.48	0.26	-0.11	556.48	0.121
Tetradecan-4-one	6	393.15-576.48	0.48	-0.14	576.48	0.228
Hexadecan-4-one	6	423.15-606.48	1.71	-----	606.48	0.897
*Octadecan-4-one	6	453.15-636.48	2.45	-0.03	636.48	1.316
*Eicosan-4- -4-one	6	473.15-656.48	2.33	-0.16	656.48	1.421
Alkan-5-ones		Number of Systems = 9				
Nonan-5-one	6	303.15-494.82	----	-2.78	303.15	2.271
decan-5-one	6	323.15-489.48	----	-2.32	323.15	2.062
Undecan-5-o	6	333.15-516.48	----	-1.91	333.15	1.743
*Dodecan-5-o	6	353.15-536.48	----	-1.01	353.15	0.886
Tridecan-5-one	6	373.15-556.48	----	-0.91	373.15	0.738
Tetradecan-5-one	6	393.15-576.48	----	-0.68	393.15	0.368
Pentadecan-5-one	6	423.15-606.48	0.21	-0.71	423.15	0.328
Heptadecan-5-one	6	473.15-664.82	1.20	-0.40	626.48	0.668
*Nonadecan-5-one	6	493.15-676.48	----	-2.40	493.15	1.128

TABLE XXV (continue)

Number of Systems = 70

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Alkan-6-ones Number of Systems = 8						
Undecan-6-o	6	333.15-516.48	----	-2.19	333.15	2.024
Dodecan-6-o	6	353.15-536.48	----	-1.56	353.15	1.436
Tridecan- -6-one	6	373.15-556.48	----	-1.46	373.15	1.283
*Tetradecan- -6-one	6	393.15-576.48	----	-1.21	393.15	0.905
Pentadecan- -6-one	6	423.15-606.48	----	-1.24	423.15	0.735
Hexadecan- -6-one	6	473.15-664.82	0.19	-0.93	473.15	0.417
Octadecan- -6-one	6	473.15-664.82	1.20	-0.88	626.48	0.758
*Eicosan- -6-one	6	513.15-696.48	1.42	-0.24	623.15	0.799
Alkan-7-ones Number of Systems = 6						
Tridecan- -7-one	6	373.15-556.48	----	-1.46	373.15	1.283
Tetradecan- -7-one	6	393.15-576.48	----	-1.48	393.15	1.175
Pentadecan- -7-one	6	423.15-606.48	----	-1.51	423.15	1.003
Hexadecan- -7-one	6	473.15-664.82	----	-1.19	473.15	0.576
Heptadecan- -7-one	6	493.15-684.82	0.36	-0.95	493.15	0.473
*Nonadecan- -7-one	6	513.15-696.48	0.93	-0.72	623.15	0.542

TABLE XXV (continue)

Number of Systems = 70

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Alkan-8-ones Number of Systems = 5						
Pentadecan-8-one	6	423.15-606.48	----	-1.51	423.15	1.003
Hexadecan-8-one	6	473.15-664.82	----	-1.46	473.15	0.842
*Heptadecan-8-one	6	493.15-684.82	0.10	-1.22	493.15	0.559
Octadecan-8-one	6	493.15-684.82	0.69	-1.11	493.15	0.497
Eicosan-8-one	6	513.15-696.48	0.66	-1.01	513.15	0.556
Alkan-9-ones Number of Systems = 3						
Heptadecan-9-one	6	493.15-684.82	0.10	-1.22	493.15	0.559
*Octadecan-9-one	6	493.15-684.82	0.43	-1.37	493.15	0.558
Nonadecan-9-one	6	513.15-696.48	0.42	-1.24	513.15	0.545

TABLE XXV (continue)

Number of Systems = 70

SYSTEM	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Alkan-10-ones Number of Systems = 2						
Nonadecan- -10-one	6	493.15-684.82	0.47	-1.60	493.15	0.611
*Eicosan- -10-one	6	513.15-696.82	0.41	-1.27	513.15	0.558

Total 420

Maximum Positive Deviation = 3.82

Maximum Negative Deviation = -2.78

Ave. Abs. Perc. Dev. = 1.10001 (Overall)

Ave. Abs. Perc. Dev. (Prediction) = 1.13649

Ave. Abs. Perc. Dev. (Regression) = 1.08831

* Not Included in Regression (Predicted)

TABLE XXVI

THERMAL CONDUCTIVITY FOR N-ALKYL ETHERS

Number of Systems = 55

SYSTEM R - ETHER	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Methyl N-Alkyl Ethers Number of Systems = 10						
Dimethyl	10	210.15-334.40	5.52	-----	210.65	2.011
Methyl c2	10	113.15-365.15	2.31	-3.18	309.15	1.734
Methyl-N-c3	10	123.15-384.15	1.93	-1.42	384.15	0.876
Methyl-N-c4	10	163.15-424.15	4.18	-0.44	424.15	0.877
Methyl-N-c5	10	153.15-441.15	3.54	-1.01	441.15	0.909
*Methyl-N-c6	10	153.15-459.15	2.74	-1.20	459.15	0.999
Methyl-N-c7	10	153.15-477.15	2.16	-1.30	477.15	1.094
Methyl-N-c8	10	153.15-495.15	1.38	-1.06	457.15	1.021
Methyl-N-c9	10	153.15-513.15	1.41	-0.58	433.15	1.192
*Methyl-c10	10	153.15-531.15	1.46	-0.56	279.15	1.213
Ethyl N-Alkyl Ethers Number of Systems = 9						
Diethyl	10	163.15-383.15	0.15	-3.20	310.15	1.685
Ethyl -N-c3	10	163.15-406.15	0.25	-2.30	298.15	1.420
*Ethyl -N-c4	10	173.15-443.15	1.34	-1.33	443.15	0.954
Ethyl -N-c5	10	153.15-459.15	1.19	-1.59	153.15	0.555
Ethyl -N-c6	10	153.15-477.15	0.82	-1.62	153.15	0.421
Ethyl -N-c7	10	153.15-495.15	0.41	-1.35	153.15	0.340
Ethyl -N-c8	10	293.15-527.15	0.82	-0.65	293.15	0.514
Ethyl -N-c9	10	353.15-551.15	0.62	-1.27	551.15	0.510
*Ethyl -c10	10	353.15-551.15	1.01	-0.47	353.15	0.696

TABLE XXVI (continue)

Number of Systems = 55

SYSTEM R - ETHER	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Propyl N-Alkyl Ethers Number of Systems = 8						
DI-N-Propyl	10	173.15-443.15	1.26	-1.39	323.15	0.975
Propyl-N-c4	10	153.15-459.15	0.55	-1.75	153.15	0.683
Propyl-N-c5	10	153.15-477.15	0.19	-1.76	153.15	0.390
Propyl-N-c6	10	153.15-495.15	0.21	-1.47	153.15	0.343
Propyl-N-c7	10	163.15-514.15	0.76	-0.90	514.15	0.444
Propyl-N-c8	10	163.15-532.15	0.79	-1.22	532.15	0.505
Propyl-N-c9	10	163.15-541.15	1.16	-0.78	247.15	0.632
*Propyl-c10	10	163.15-550.15	0.83	-0.53	249.15	0.489
Butyl N-Alkyl Ethers Number of Systems = 7						
DI-N-Butyl	10	193.15-481.15	----	-0.81	481.15	0.624
Butyl-N-c5	10	183.15-498.15	0.08	-0.92	498.15	0.351
Butyl-N-c6	10	183.15-516.15	0.63	-1.22	516.15	0.424
Butyl -N-c7	10	183.15-525.15	0.66	-1.34	525.15	0.459
Butyl -N-c8	10	183.15-543.15	1.06	-1.07	543.15	0.639
Butyl -N-c9	10	183.15-552.15	0.72	-0.81	552.15	0.412
*Butyl -c10	10	183.15-570.15	0.58	-0.78	570.15	0.268
Pentyl N-Alkyl Ethers Number of Systems = 6						
DI-N-Pentyl	10	213.15-519.15	0.81	-0.84	519.15	0.486
Pentyl-N-c6	10	183.15-525.15	0.63	-1.43	525.15	0.467
Pentyl-N-c7	10	183.15-545.15	1.02	-1.19	543.15	0.615
Pentyl-N-c8	10	183.15-552.15	0.69	-0.90	552.15	0.396
Pentyl-N-c9	10	183.15-570.15	0.56	-0.85	570.15	0.266
*Pentyl-c10	10	183.15-570.15	0.59	-0.10	226.15	0.200

TABLE XXVI (continue)

Number of Systems = 55

S Y S T E M R - ETHER	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Hexyl N-Alkyl Ethers		Number of Systems = 5				
DI-N-Hexyl	10	243.15-549.15	1.05	-1.37	549.15	0.617
Hexyl -N-c7	10	233.15-557.15	0.72	-1.06	557.15	0.417
Hexyl -N-c8	10	233.15-575.15	0.57	-0.97	575.15	0.296
Hexyl -N-c9	10	233.15-575.15	0.59	-0.19	233.15	0.196
Hexyl -c10	10	233.15-593.15	0.22	-0.55	393.15	0.261
Heptyl N-Alkyl Ethers		Number of Systems = 4				
*DI-N-Heptyl	10	253.15-577.15	0.54	-1.06	577.15	0.296
*Heptyl-N-c8	10	263.15-578.15	0.52	-0.26	263.15	0.155
*Heptyl-N-c9	10	263.15-596.15	0.01	-0.67	374.15	0.346
*Heptyl-c10	10	263.15-596.15	0.41	-1.07	411.15	0.631

TABLE XXVI (continue)

Number of Systems = 55

SYSTEM R - ETHER	NPT	Temp. Range Degree K	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Octyl, Nonyl, Decyl N-Alkyl Ethers						
Number of Systems = 6						
DI-N-Octyl	10	273.15-597.15	0.01	-0.68	381.15	0.356
c8-N-Nonyl	10	283.15-598.15	0.42	-1.08	388.15	0.653
c8-N-Decyl	10	283.15-616.15	2.15	-1.17	616.15	0.994
DI-N-Nonyl	10	283.15-616.15	2.14	-1.18	616.15	0.995
*c9-N-Decyl	10	283.15-634.15	4.02	-1.21	634.15	1.422
*DI-N-Decyl	10	303.15-645.15	6.16	-1.34	645.15	1.974

Total 550
Maximum Positive Deviation = 6.16
Maximum Negative Deviation = -3.20
Ave. Abs. Perc. Dev. = 0.69611 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 0.78741
Ave. Abs. Perc. Dev. (Regression) = 0.67121

* Not Included in Regression (Predicted)

TABLE XXVII

THERMAL CONDUCTIVITY FOR CRUDE OIL CUTS

Number of Systems = 16

Crude Cut NAME	NPT	Boiling Range Degree F	Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Mid-Contint	10	200 - 400	----	-5.25	310.93	3.789
Mid-Contint	10	400 - 500	----	-3.63	310.93	2.348
Mid-Contint	10	500 - 600	----	-4.23	310.93	2.786
Mid-Contint	10	600 - 650	----	-2.88	310.93	1.521
Mid-Contint	10	650 - 755	1.91	-0.81	444.26	1.378
Mid-Contint	10	755 - 780	0.63	-1.75	310.93	0.554
Mid-Contint	10	780 - 850	0.71	-1.61	310.93	0.555
Ara-Light	10	200 - 400	3.76	-----	399.82	3.382
Ara-Light	10	400 - 500	4.48	-----	377.59	3.901
Ara-Light	10	500 - 600	2.28	-0.65	377.59	1.506
Ara-Light	10	600 - 700	1.94	-1.20	377.59	1.274
Ara-Light	10	700 - 850	1.41	-2.73	510.93	1.165
*North Sea	10	200 - 400	13.8	-----	510.93	9.635
*North Sea	10	400 - 500	4.64	-1.06	510.93	2.525
*North Sea	10	500 - 650	0.78	-3.85	310.93	1.226
*North Sea	10	650 - 850	----	-9.73	310.93	7.596

Total 160
Maximum Positive Deviation = 13.88
Maximum Negative Deviation = -9.73
Ave. Abs. Perc. Dev. = 2.82180 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 5.24580
Ave. Abs. Perc. Dev. (Regression) = 2.01380
Thermal Cond. = (NBP*SPG/100)

* Not Included in Regression (Predicted)

TABLE XXVIII

THERMAL CONDUCTIVITY FOR CRUDE OIL CUTS

Number of Systems = 16

Crude CUT NAME	NPT	BOilING Range Degree F			Max.+ Dev.	Max.- Dev.	Temp. at Max	AAPD
Mid-Contint	10	200	-	400	----	-7.57	451.67	7.004
Mid-Contint	10	400	-	500	----	-4.57	473.90	3.315
Mid-Contint	10	500	-	600	----	-2.90	473.90	2.111
Mid-Contint	10	600	-	650	0.07	-0.52	473.90	0.333
Mid-Contint	10	650	-	755	5.50	-----	473.90	4.848
Mid-Contint	10	755	-	780	2.40	-----	473.90	2.189
Mid-Contint	10	780	-	850	3.38	-----	473.90	2.159
Ara-Light	10	200	-	400	1.24	-----	388.71	0.704
Ara-Light	10	400	-	500	2.21	-0.56	366.49	0.866
Ara-Light	10	500	-	600	0.24	-2.84	473.90	1.614
Ara-Light	10	600	-	700	0.05	-2.54	466.49	1.638
Ara-Light	10	700	-	850	----	-7.30	429.45	6.290
*North Sea	10	200	-	400	9.62	-----	473.90	7.412
*North Sea	10	400	-	500	3.61	-----	366.49	3.219
*North Sea	10	500	-	650	5.03	-----	473.90	3.821
*North Sea	10	650	-	850	5.83	-2.09	407.23	1.854

Total 160
Maximum Positive Deviation = 5.83
Maximum Negative Deviation = -7.57
Ave. Abs. Perc. Dev. = 3.81029 (Overall)
Ave. Abs. Perc. Dev. (Prediction) = 4.07658
Ave. Abs. Perc. Dev. (Regression) = 3.08650
Thermal Cond. = (NBP/100)
Temperature Range = 366.49-473.90 K

* Not Included in Regression (Predicted)

APPENDIX B

COMPARISON TABLES

TABLE XXIX

SUMMARY FOR COMPARISON RESULTS

Number of Systems = 13

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	 Sato	 Robn	 Group
Alkanes(Str)	260	93.15-669.15	9.71	24.1	89.3	1.018
Alkanes(Bra)	270	113.15-470.15	8.40	17.3	13.3	1.519
Alkenes	220	93.15-587.15	8.27	12.6	59.9	0.732
Alcohols	111	199.00-508.15	6.82	13.6	50.8	1.407
Acids	150	283.15-683.15	8.90	10.3	58.5	0.931
Formates	140	193.15-667.15	13.2	13.8	75.1	1.585
Acetates	140	183.15-656.15	15.6	12.3	68.3	0.865
Aldehydes	140	183.15-718.15	7.78	12.7	63.3	0.722
Alkanone	140	193.15-603.15	7.92	12.9	56.3	1.100
Ethers	100	113.15-645.15	5.64	15.2	51.6	2.821
Chloro Alkan	190	193.15-615.15	5.42	21.2	45.8	3.923
Iodo Alkanes	160	173.15-680.15	11.7	82.9	62.1	3.431
Bromo Alkane	130	193.15-615.15	7.12	47.9	54.1	3.558
Overall Ave. Dev.			8.98	22.7	56.7	1.739
Total	2151					

Thermal Conductivity Methods :

Bar	:	Baroncini et. al. method	Eq. 2-29
Sato	:	Sato boiling point method	Eq. 2-25
Robn	:	Robin and Kingrea method	Eq. 2-15
Group	:	Proposed method	Eq. 3-7

TABLE XXX

COMPARISON RESULTS FOR ALKANES

Number of Systems = 15

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	Sato	Robn	Group
Propane	14	93.15-223.15	28.1	21.5	14.6	0.902
N-Butane	14	143.15-273.15	17.2	10.2	5.18	0.830
N-Pentane	16	153.15-303.15	10.3	3.52	5.52	0.546
N-Hexane	13	183.15-303.15	6.75	1.88	16.7	0.983
N-Heptane	16	183.15-333.15	3.55	5.74	18.7	1.800
*N-Octane	15	223.15-373.15	2.66	10.1	15.2	1.890
N-Decane	8	303.15-415.15	6.83	21.6	9.99	2.397
N-Undecane	31	307.75-637.45	12.8	17.5	73.9	0.716
N-Dodecane	25	307.75-653.15	14.6	20.7	10.8	0.845
N-Tridecane	35	307.75-669.35	14.9	20.5	79.3	0.478
N-Tetradeca	19	307.80-509.80	3.52	24.1	81.5	0.918
N-Hexadecan	12	313.15-533.15	1.48	25.7	85.8	0.850
N-Heptadeca	13	313.15-553.15	1.23	25.2	87.0	1.392
*N-Octadecan	14	313.15-573.15	3.30	24.2	88.3	1.928
*N-Nonadecan	15	313.15-593.15	4.38	24.1	89.3	2.003
Overall Ave.			9.71	24.1	49.3	1.018
Total	150					

* Not Included in Regression (Predicted)

TABLE XXXI

COMPARISON RESULTS FOR ALKENES

Number of Systems = 22

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev.			
			Bar	Sato	Robn	Group
Ethylene	10	113.15-239.15	4.02	20.4	55.5	1.951
Propylene	10	93.15-309.15	7.92	26.7	24.0	1.297
But-1-ene	10	93.15-345.15	7.61	16.6	32.7	0.598
But-2-ene	10	153.15-351.15	10.8	15.1	44.0	1.345
Isobutene	10	133.15-349.15	15.5	9.72	33.4	0.103
Pent-1-ene	10	113.15-392.15	5.42	8.83	48.5	0.606
Hex-1-ene	10	133.15-421.15	3.95	3.39	52.4	0.642
Hex-2-ene	10	143.15-431.15	6.04	3.33	62.6	0.609
*Hex-3-ene	10	153.15-432.15	5.47	3.13	62.8	0.695
Hept-1-ene	10	163.15-451.15	2.52	4.56	59.6	0.527
Hept-2-ene	10	173.15-461.15	2.46	3.37	67.5	0.569
Hept-3-ene	10	143.15-458.15	2.57	3.60	66.4	0.359
Oct-1-ene	10	173.15-479.15	3.86	7.75	65.0	0.540
*Oct-2-ene	10	183.15-489.15	2.54	7.05	73.1	0.400
Oct-3-ene	10	173.15-479.15	2.48	7.67	72.9	0.212
Oct-4-ene	10	173.15-488.15	2.63	7.59	73.1	0.322
Non-1-ene	10	193.15-499.15	6.63	12.2	68.8	0.454
Dec-1-ene	10	213.15-519.15	10.8	14.3	72.8	0.593
Undec-1-en	10	233.15-539.15	14.5	17.0	76.0	0.607
*Dodec-1-en	10	243.15-549.15	17.9	19.2	78.7	0.807
*Tridec-1-e	10	253.15-568.15	21.5	20.9	80.9	1.132
*Tetradec--1-ene	10	263.15-587.15	24.6	22.8	82.7	1.714
Overall Ave.			8.27	12.6	59.9	0.733
Total	220					

* Not Included in Regression (Predicted)

TABLE XXXII

COMPARISON RESULTS FOR BRANCHED ALKANES

Number of Systems = 26

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev.			
			Bar	Sato	Robn	Group
2,2DI-Cl-C3	10	263.15-380.15	8.26	6.77	31.1	2.149
2,2DI-Cl-C4	10	173.15-416.15	2.69	10.7	20.4	2.347
2,2DI-Cl-C5	10	153.15-441.15	2.96	15.5	8.73	1.280
2,3DI-Cl-C5	10	153.15-450.15	5.22	15.4	11.6	1.487
2,2DI-Cl-C6	10	153.15-459.15	7.04	21.6	4.36	0.943
3,3DI-Cl-C6	10	153.15-459.15	8.34	20.5	6.20	0.515
2-Methyl-C3	10	113.15-338.15	16.1	6.16	39.2	1.406
2-Methyl-C4	10	113.15-383.15	16.4	6.92	36.7	1.351
2-Methyl-C5	10	123.15-420.15	5.56	4.65	12.2	1.234
3-Methyl-C5	10	123.15-420.15	4.01	5.14	15.5	1.209
2,3DI-Cl-C4	10	153.15-423.15	3.15	11.5	36.9	1.053
2-Methyl-C6	10	163.15-442.15	2.64	8.76	4.00	0.973
3-Methyl-C6	10	163.15-442.15	2.39	10.0	6.51	0.850
2,3DI-Cl-C5	10	153.15-450.15	6.51	16.4	22.2	1.278
2,4DI-Cl-C5	10	163.15-433.15	3.46	16.7	7.45	0.799
2-Methyl-C7	10	173.15-461.15	2.19	13.1	9.62	0.846
3-Methyl-C7	10	153.15-459.15	3.33	14.4	4.91	0.906
4-Methyl-C7	10	153.15-459.15	3.61	15.2	5.28	1.541
2,3DI-Cl-C6	10	153.15-468.15	9.43	21.3	4.31	1.084
2,4DI-Cl-C6	10	153.15-468.15	7.52	21.3	4.17	0.889
2,5DI-Cl-C6	10	183.15-453.15	7.63	22.6	4.56	0.728
*3,4DI-Cl-C6	10	153.15-468.15	10.3	24.3	3.88	0.889
2,3,4-tri-cl-c5	10	173.15-479.15	18.6	31.0	16.3	1.154
2,2,3-tri-cl-c5	10	163.15-469.15	17.5	30.5	18.4	1.775
*2,3,3-tri-cl-c5	10	173.15-470.15	19.2	30.2	9.76	1.042
*2,3,5-tri-cl-c6	10	153.15-468.15	16.7	32.5	11.6	0.803
Total	260					
Overall Ave.			8.40	17.3	13.3	1.174

* Not Included in Regression (Predicted)

TABLE XXXIII

COMPARISON RESULTS FOR ALCOHOLS

Number of Systems = 11

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	Sato	Robn	Group
Methanol	15	199.00-469.15	10.6	39.4	71.2	1.459
Ethanol	13	233.15-471.15	8.15	25.8	12.8	1.211
N-Propanol	17	200.00-479.15	5.05	15.8	71.7	1.264
N-Butanol	13	203.40-373.15	3.12	8.03	30.4	1.235
N-Pentanol	8	201.70-353.15	3.25	4.40	42.4	1.956
N-Hexanol	9	243.50-423.15	5.05	4.42	45.2	2.589
*N-Heptanol	15	246.80-436.25	5.59	3.31	61.9	1.573
N-Octanol	3	293.15-485.15	7.51	6.08	66.3	2.714
N-Nonanol	7	273.15-423.15	4.71	3.98	48.6	1.450
N-Decanol	4	273.15-373.15	9.22	1.68	73.5	1.144
*N-Tetradeca	4	323.15-473.15	14.8	7.31	3.59	5.785
*N-Octadecan	3	337.15-373.15	23.7	6.68	92.2	2.431
Overall Ave.			6.81	13.6	50.8	1.756
Total	111					

* Not Included in Regression (Predicted)

TABLE XXXIV

COMPARISON RESULTS FOR GLYCOLS

Number of Systems = 4

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	Sato	Robn	Group
Ethelene	20	223.15-508.15	17.2	46.8	31.2	1.039
Trimethyle	20	223.15-508.15	16.8	34.6	34.6	1.041
Tetramethy	20	223.15-508.15	14.1	28.6	16.3	1.171
Pentamethy	20	223.15-508.15	14.2	25.5	9.55	1.560
Overall Ave. Dev.			15.6	33.9	9.55	1.203
Total	80					

TABLE XXXV

COMPARISON RESULTS FOR ALKANOIC ACIDS

Number of Systems = 15

SYSTEM (R - Acid)	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	Sato	Robn	Group
Acetic	10	283.15-508.15	9.04	23.4	33.4	0.962
Propanoic	10	283.15-517.15	5.99	13.6	11.2	1.218
Butanoic	10	273.15-534.15	5.24	8.34	28.9	0.248
Pentanoic	10	273.15-552.15	4.76	5.83	34.5	0.439
Hexanoic	10	273.15-561.15	4.14	5.30	41.3	0.636
*Heptanoic	10	273.15-579.15	3.95	5.97	47.9	0.564
Octanoic	10	293.15-599.15	3.89	6.42	54.2	0.565
Nonanoic	10	303.15-609.15	3.65	7.97	59.8	0.617
Decanoic	10	323.15-620.15	5.42	7.67	65.7	0.379
Dodecanoic	10	333.15-639.15	8.15	9.39	73.4	0.332
Tetradecan	10	343.15-667.15	11.0	10.1	78.8	0.240
Hexadecano	10	353.15-686.15	13.7	10.9	83.1	0.513
*Octadecano	10	363.15-656.15	16.3	12.3	86.4	0.893
*Eicosanoic	10	363.15-675.15	18.3	13.4	88.7	1.232
*Docosanoic	10	363.15-683.15	19.9	14.5	90.4	2.006
Overall Ave.			8.91	10.3	58.5	0.932
Total	150					

* Not Included in Regression (Predicted)

TABLE XXXVI

COMPARISON RESULTS FOR ALKYL FORMATES

Number of Systems = 14

S Y S T E M (R - Formate)	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	 Sato	 Robn	 Group
Methyl	10	193.15-373.15	2.36	38.3	35.4	1.750
Ethyl	10	213.15-402.15	2.06	25.6	47.0	0.710
Propyl	10	223.15-448.15	4.36	14.7	53.5	1.991
Butyl	10	223.15-448.15	3.54	6.80	65.3	1.122
Pentyl	10	243.15-477.15	2.06	2.93	71.3	0.733
*Hexyl	10	243.15-495.15	2.54	4.11	75.3	0.558
Heptyl	10	253.15-523.15	5.80	6.17	79.4	0.691
Octyl	10	263.15-542.15	10.1	7.48	82.6	1.056
Nonyl	10	273.15-552.15	13.7	9.22	85.0	1.207
Decyl	10	283.15-580.15	17.5	10.2	87.2	1.249
Dodecyl	10	293.15-599.15	23.5	12.9	89.9	0.682
Tetradecyl	10	323.15-638.15	28.9	14.9	92.0	1.622
*Hexadecyl	10	343.15-649.15	32.7	18.6	93.5	3.149
*Octadecyl	10	343.15-667.15	36.5	20.9	94.4	5.666
Overall Ave.			13.3	13.8	75.1	1.585
Total	140					

* Not Included in Regression (Predicted)

TABLE XXXVII

COMPARISON RESULTS FOR ALKYL ALDEHYDES

Number of Systems = 14

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	Sato	Robn	Group
Acetaldehy	10	183.15-372.15	24.7	40.4	12.3	1.060
Propionald	10	213.15-411.15	13.7	27.8	22.1	0.817
Butyraldeh	10	253.15-451.15	3.95	17.1	34.4	0.335
Valeraldeh	10	273.15-471.15	4.45	7.54	43.4	0.781
Hexanal	10	293.15-482.15	8.13	2.17	56.8	0.685
*Heptanal	10	303.15-546.15	8.56	2.99	61.9	0.458
Octanal	10	313.15-529.15	9.39	3.87	68.1	0.340
Nonanal	10	333.15-453.15	8.77	5.02	72.4	0.346
Decanal	10	353.15-569.15	8.19	6.43	76.5	0.301
Dodecanal	10	363.15-588.15	6.40	8.76	82.1	0.302
Tetradeca	10	363.15-606.15	5.56	11.8	85.7	0.360
Hexaecan	10	373.15-643.15	3.39	13.1	88.5	0.517
*Octadecan	10	383.15-689.15	2.11	14.7	90.6	1.315
*Eicosanal	10	403.15-718.15	1.54	16.4	91.9	2.491
Overall Ave.			7.78	12.7	63.3	0.773
Total	140					

* Not Included in Regression (Predicted)

TABLE XXXVIII

COMPARISON RESULTS FOR N-ALKYL ACETATES COMPOUNDS

Number of Systems = 14

SYSTEM (R-Acetate)	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	 Sato	 Robn	 Group
Methyl	10	183.15-370.65	3.73	24.0	24.2	3.113
Ethyl	10	193.15-388.15	3.58	13.3	35.2	2.047
Propyl	10	203.15-413.15	3.31	5.48	41.6	2.363
Butyl	10	213.15-445.65	2.63	3.63	55.8	2.054
Pentyl	10	223.15-455.65	3.49	6.56	68.7	1.604
Hexyl	10	233.15-473.15	6.99	6.56	68.7	0.797
Heptyl	10	243.15-490.65	10.9	8.10	73.2	0.371
Octyl	10	253.15-508.15	14.6	9.42	76.9	0.691
*Nonyl	10	263.15-518.15	17.9	11.0	79.9	0.991
Decyl	10	273.15-535.65	21.1	12.2	82.4	1.229
Dodecyl	10	283.15-545.65	26.2	15.4	85.8	1.125
Tetradecyl	10	303.15-580.65	31.0	17.2	88.4	0.882
*Hexadcyl	10	313.15-598.15	34.9	19.5	90.2	0.816
*Octadecyl	10	323.15-600.65	38.1	22.6	91.6	0.818
Overall Ave.			15.6	12.4	68.3	1.430
Total	140					

* Not Included in Regression (Predicted)

TABLE XXXIX

COMPARISON RESULTS FOR N-ALKYL ALKAN-2-ONES

Number of Systems = 14

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	sato	Robn	Group
Acetone	10	193.15-359.82	7.82	24.6	14.1	1.255
Butanone	10	213.15-379.15	1.33	14.0	21.7	1.389
Pentan-2-one	10	223.15-389.82	3.89	7.17	24.7	0.526
Hexan-2-one	10	233.15-399.82	7.95	1.82	36.0	1.083
*Heptan-2-one	10	243.15-434.82	11.0	3.95	51.4	1.221
Octan-2-one	10	263.15-446.48	13.4	8.62	51.4	0.747
Nonan-2-one	10	273.15-464.82	12.4	9.99	58.3	1.950
Decan-2-one	10	293.15-476.48	11.8	11.6	63.4	2.498
Undecan-2-o	10	298.15-481.48	11.2	13.3	67.5	2.754
Dodecan-2-o	10	303.15-503.15	9.69	13.8	72.0	2.932
Tetradecan--2-one	10	323.15-531.48	7.72	15.6	78.3	2.765
Hexadecan--2-one	10	333.15-549.82	5.88	17.3	82.8	2.434
*Octadecan--2-one	10	343.15-568.15	4.28	19.2	85.7	1.878
*Eicosan-2-o	10	353.15-686.48	2.39	20.6	87.9	1.762
Overall Ave. Dev.			7.92	12.9	56.3	1.799
Total	140					

* Not Included in Regression (Predicted)

TABLE XL

COMPARISON RESULTS FOR METHYL N-ALKYL ETHERS

Number of Systems = 10

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	sato	Robn	Group
Dimethyl	10	210.15-334.40	4.45	39.4	23.7	2.011
Methyl c2	10	113.15-365.15	1.64	25.1	23.6	1.734
Methyl-N-c3	10	123.15-384.15	3.06	15.7	23.5	0.876
Methyl-N-c4	10	163.15-424.15	1.28	8.38	47.6	0.877
Methyl-N-c5	10	153.15-441.15	1.58	2.04	54.0	0.909
*Methyl-N-c6	10	153.15-459.15	3.23	5.52	59.9	0.999
Methyl-N-c7	10	153.15-477.15	5.63	9.33	64.9	1.094
Methyl-N-c8	10	153.15-495.15	8.54	13.0	69.3	1.021
Methyl-N-c9	10	153.15-513.15	11.9	15.6	73.1	1.192
*Methyl-c10	10	153.15-531.15	15.0	17.6	75.9	1.213
Overall Ave. Dev.			5.64	15.2	51.6	1.192
Total	100					

* Not Included in Regression (Predicted)

TABLE XLI

COMPARISON RESULTS FOR CHLORO ALKANES

Number of Systems = 19

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	 sato	 Robn	 Group
Chloro-c2	10	233.15-377.15	0.93	13.7	3.33	2.396
1-Cl-c3	10	153.15-405.15	3.51	1.03	13.7	2.894
1,2DI-CL-C3	10	233.15-476.15	2.55	15.6	35.7	2.143
1,3DI-CL-C3	10	273.15-435.15	4.10	10.8	43.7	3.091
1-Chloro-C4	10	173.15-452.15	3.93	9.11	20.8	4.386
2-Chloro-C4	10	173.15-407.15	4.42	10.1	20.6	4.755
1-CL-2-C2- -C3	10	173.15-398.15	4.97	10.0	27.0	4.199
1,4-DI-CL- -C4	10	303.15-501.15	1.92	23.2	49.7	3.347
1-Chloro-C5	10	263.15-470.15	1.00	16.3	38.2	3.936
*2-Chloro-C5	10	153.15-459.15	1.38	16.3	38.2	3.329
1,5DI-CL-C5	10	223.15-466.15	3.96	30.2	57.2	4.952
1-Chloro-C6	10	263.15-479.15	3.24	19.4	51.8	4.084
2-Chloro-C6	10	173.15-497.15	2.35	20.6	49.5	5.078
1,6DI-CL-C6	10	323.15-503.15	5.23	37.1	64.1	3.355
1-Chloro-C7	10	283.15-499.15	7.50	22.9	60.5	4.079
1-Chloro-C8	10	283.15-499.15	11.5	25.4	66.9	4.821
1,8DI-CL-C8	10	313.15-547.15	7.46	45.6	70.3	3.935
1-Cl-C10	10	293.15-545.15	18.4	28.7	75.1	6.478
*1,10-DI- -Cl-C10	10	323.15-548.15	14.5	21.2	45.8	3.265
Overall Ave. Dev.			5.42	21.2	45.8	3.922
Total	190					

* Not Included in Regression (Predicted)

TABLE XLII

COMPARISON RESULTS FOR IODO ALKANES

Number of Systems = 16

SYSTEM	NPT	Temp. Range	Ave. Perc. Dev.			
		Degree K	Bar	sato	Robn	Group
I-Methane	10	213.15-429.15	5.24	26.3	14.1	3.166
I-Ethane	10	233.15-467.15	9.12	39.9	23.9	1.606
1-I-Propane	10	233.15-467.15	9.66	49.7	40.0	2.751
*1,3-DI-I-C3	10	273.15-678.15	22.5	112.	57.6	4.117
1-I-Butane	10	253.15-496.15	8.29	56.5	47.7	3.341
2-I-Butane	10	263.15-497.15	14.2	65.6	39.7	6.167
1,4-DI-I-C4	10	353.15-596.15	21.2	121.	70.2	0.875
1-I-Pentane	10	268.15-497.15	4.46	59.1	60.5	3.892
1,5-DI-I-C5	10	293.15-599.15	20.9	130.	75.4	2.427
1-I-Hexane	10	273.15-543.15	1.32	58.8	70.2	4.609
1,6-DI-I-C6	10	333.15-639.15	18.9	136.	77.4	3.698
1-I-Heptane	10	273.15-561.15	5.32	59.8	76.5	5.316
1-I-Octane	10	323.15-584.15	9.76	59.4	80.6	4.022
1,8-DI-I-C8	10	353.15-596.15	13.6	146.	84.3	2.964
1-I-Decane	10	353.15-596.15	17.2	59.7	85.4	3.070
*1,10-DI-I- -C10	10	393.15-591.15	5.26	145.	89.4	2.870
Overall Ave. Dev.			11.7	82.9	62.1	3.431
Total	160					

* Not Included in Regression (Predicted)

TABLE XLIII

COMPARISON RESULTS FOR BROMO ALKANES

Number of Systems = 13

SYSTEM	NPT	Temp. Range Degree K	Ave. Perc. Dev. Bar	sato	Robn	Group
Br-Methane	10	193.15-373.15	9.72	9.14	12.8	4.736
Br-Ethane	10	173.15-371.15	2.29	11.9	17.4	2.449
1-Br-Propa	10	223.15-448.15	5.89	24.8	27.4	2.390
1-Br-Butane	10	223.15-520.15	4.16	31.7	43.3	5.056
1,4DI-Br-C4	10	293.15-590.15	4.22	66.2	45.7	2.065
*1-Br-Pentan	10	253.15-496.15	1.32	35.2	58.0	4.366
1,5DI-Br-C5	10	273.15-525.15	8.40	80.9	59.4	1.401
1-Br-Hexane	10	273.15-525.15	3.58	38.9	67.6	4.067
1,6DI-Br-C6	10	303.15-546.15	9.33	89.1	63.8	3.084
1-Br-Heptan	10	273.15-525.15	7.45	41.1	73.2	4.053
1-Br-Octane	10	293.15-527.15	10.8	43.0	76.6	3.350
1,8DI-Br-C8	10	333.15-540.15	7.98	106.	76.1	3.458
*1-Br-Decane	10	323.15-548.15	17.4	45.4	81.4	3.178
Overall Ave. Dev.			7.12	47.9	54.1	3.358
Total	130					

* Not Included in Regression (Predicted)

2

VITA

Fahad Muhammed Alhabdan

Candidate for the Degree of

Doctor of Philosophy

Thesis: PREDICTION OF LIQUID THERMAL CONDUCTIVITY

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Quriah, Saudi Arabia, October 10, 1955, the son of Muhammed Ibrahim Alhabdan.

Education: Graduated from Alyammama High School, Riyadh, Saudi Arabia in June, 1971; received Bachelor of Science degree in Chemical Engineering from University of Petroleum and Minerals, Dhahran, Saudi Arabia, in June, 1976; received Master of Science in Chemical Engineering from the University of California, Davis, California, in December. 1979; completed requirements for the Doctor of Philosophy degree in Chemical Engineering at Oklahoma State University, Stillwater, Oklahoma, in December, 1983.

Professional Experience: Teaching Assistant, Department of Chemical Engineering, King Saud University, Riyadh, Saudi Arabia, 1976-1977; Teaching Assistant, School of Chemical Engineering, University of California, Davis, California, 1978-1979; Research Assistant, Fluid Properties Research, Inc., Oklahoma State University, Stillwater, Oklahoma, 1980-present.

Member in American Institute of Chemical Engineers; Omega Chi Epsilon Honor Society; National Society of Professional Engineers.