PREDICTION OF HEAT CAPACITY FROM THERMAL CONDUCTIVITY FOR ORGANIC LIQUIDS

By

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PREDICTION OF HEAT CAPACITY FROM
THERMAL CONDUCTIVITY FOR
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PREFACE

A recently proposed equation relates the thermal conductivity of an organic liquid with its density and heat capacity. Because of the availability of good density and thermal conductivity measurements, the possibility of using this equation to predict the heat capacity for organic liquids was studied. An attempt was made to modify this equation in order to improve the accuracy of its prediction of heat capacity at different temperatures.

I am deeply indebted to my thesis adviser, Professor R. N. Maddox, for his valuable guidance and timely help in enabling me to complete my M.S. degree requirements. His great co-operation, encouragement and dedication to research have been a constant source of inspiration to me. I am very thankful to Dr. J. H. Erbar for his helpful suggestions.

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Finally, I express my deepest gratitude to my parents, my uncles and all the members of my family for their constant support and sacrifices in making my dreams come true.

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CHAPTER I

INTRODUCTION

Heat capacity values are frequently required in chemical engineering design calculations. In heat transfer calculations for example, they are needed to evaluate the Prandtl number, $C_p\mu/k$, and in performing heat balances. Accurate experimental data on liquid heat capacities are scarce. Even in the case of a familiar liquid like carbon tetrachloride, there are great variations in the heat capacity value as observed by different workers (1). Because of the difficulties involved in the experimental determination of heat capacity, several attempts have been made to predict this property. These have resulted in empirical or semi-empirical correlations involving known parameters.

A number of estimation techniques are available for predicting the heat capacity of gases (2). Although each technique has its limitations, the results are quite accurate. For liquids however, the available estimation techniques suffer from one or more defects. In the case of organic liquids, the available correlations are complex in nature and require knowledge of properties such as thermal conductivity, density, sonic velocity, intermolecular free length, latent heat of vaporization, critical temperature, molar volume etc. Apart from the fact these correlations require extensive data, they have such drawbacks as a high degree of inaccuracy and validity at one temperature only.

An equation for predicting the thermal conductivity of organic liquids at 293°K has been proposed (3). This equation is simple to use and involves knowledge of only the heat capacity and the density of the organic liquid. It also contains a temperature factor, which enables prediction of thermal conductivity for organic liquids at different temperatures.

The present study attempts to modify this equation to predict the heat capacity of organic liquids from a knowledge of their thermal conductivities and densities. Its objectives are:

1) To explore the possibility of using this equation, because of the simplicity of its form and nature, for predicting the heat capacity of organic liquids at different temperatures.

2) To modify the equation so as to improve the accuracy of its prediction at different temperatures.

CHAPTER II

LITERATURE REVIEW

The importance of heat capacity as a basic tool in all chemical engineering design cannot be overemphasized. The scarcity of accurate experimental data on heat capacities for liquids and the difficulties involved in their measurement have forced the engineer to resort to methods of estimating this property.

Thermodynamic routes for calculating the heat capacity for liquids are discussed by Gambill (4). When these routes fail, there are other methods for estimating this fundamental engineering property. Watson (5) presented a method for the general prediction of pressure correction to heat capacity at constant pressure based on a modified application of the theorem of corresponding states. Chow and Bright (6) proposed an equation for predicting the heat capacity for liquids at any condition from a single known value. Sakiadis and Coates (7) correlated data on the velocity of sound, infrared and Raman spectra to predict the heat capacity at constant pressure of organic liquids as a function of temperature. Johnson and Huang (8) suggested the addition of group heat capacities for estimating the heat capacities of organic liquids at 20°C. Watson's method for predicting the heat capacity of saturated liquids was modified by Ried and Sobel (9) for estimating saturated liquid heat capacities above the boiling point.

Several correlations between the heat capacity and the thermal conductivity of liquids have been proposed. Any of these could be used to predict the heat capacity from the thermal conductivity. The earliest correlation is due to Weber (10). According to the original empirical expression derived by him, the thermal conductivity of a liquid is proportional to its heat capacity and density. The equation is satisfactory for water, for which the agreement with observation is closer than 5 percent. However, it does not give accurate results for other liquids (11).

In 1923, Bridgeman (12) developed an equation for predicting the thermal conductivity of liquids. Using Bridgeman's apparatus for measuring thermal conductivity, Smith (11) presented a general equation for all non-metallic liquids at 20°C and atmospheric pressure. His equation shows the thermal conductivity as a function of the density, heat capacity, viscosity and molecular weight, but does not give the temperature co-efficient.

Sakiadis and Coates (13) proposed an equation relating the thermal conductivity with the density, heat capacity, sonic velocity and the intermolecular distance. Although their equation gives sufficiently accurate prediction of thermal conductivity and can be used to predict the heat capacity, knowing the thermal conductivity, the calculations involved are lengthy.

Denbeigh (14) related the Prandtl number of a liquid and its entropy of vaporization. His equation, which indirectly relates the thermal conductivity with the latent heat of vaporization at the normal boiling point, can be used to calculate the thermal conductivity or the heat capacity.

Palmer (15) modified the equations proposed by Smith and Weber and suggested a mechanism of heat conduction in associated liquids. Use of the equations proposed by Denbeigh and Palmer, require data on the latent heat of vaporization at the normal boiling point for the liquid.

From the several correlations mentioned so far, the thermal conductivity appears to be a function of several variables. Taking all the consistent variables in these correlations and using dimensional analysis, Pachaiappan et al (16) arrived at an equation for predicting the thermal conductivity of an organic liquid of known molecular weight at 20°C and 1 atm. pressure. This equation can also be used to predict the heat capacity, which is one of the parameters of the equation. A disadvantage of this equation is the need for data on the latent heat of vaporization at the boiling point, molar volume and the Lennard-Jones potential constant. Although the last two are fixed physical properties, they are often not known for many organic compounds. The equation was later modified by Pachaiyappan (17). He included the density as one of the parameters of the equation, instead of the molar volume and the molecular weight.

A simpler form of correlation between thermal conductivity and heat capacity was proposed by Narasimhan et al (3). Their equation is derived from the relationships proposed by Sakiadis and Coates (13), Weber (10) and Jacobson (18). It has two constants evaluated from experimental values of the thermal conductivity for 50 organic liquids at 293°K and a temperature factor for determing the thermal conductivity at temperatures varying from 273°K to 343°K.

Literature Summary

The literature reviewed above can be summarized as follows:

1) There are several ways of calculating the heat capacity for liquids with the help of thermodynamics. However, they are often not convinient for use owing to the lack of available data on various physical properties.

2) The correlations proposed by different workers (5,6,7,8,9) for predicting the heat capacity suffer from the same defects.

3) There are several equations which relate the thermal conductivity with the heat capacity. With the exception of the one proposed by Narasimhan et al (3), all the existing equations relating these two physical properties either require lengthy calculations and data on several other physical properties, or are valid at only one temperature.

4) Because of the availability of good density and thermal conductivity measurements, the equation proposed by Narasimhan et al (3), offers a very simple way of predicting the heat capacity for organic liquids.

5) It is possible to correlate the heat capacity, thermal conductivity and the density for organic liquids since they are functions of temperature. For most liquids, heat capacity increases with temperature, while the density and the thermal conductivity decrease with temperature (2).

CHAPTER III

THE EQUATION IN ORIGINAL FORM

The equation proposed by Sakiadis and Coates (13), is fairly complex, but predicts the thermal conductivity of liquids with high accuracy. The equation is:

$$k = C_p\rho U_s L \tag{1}$$

The equation derived by Jacobson (18) is:

$$U_s L\rho^{1/2} = \text{constant} \tag{2}$$

Eqn.(1) and Eqn.(2) can be combined to get:

$$k = yC_p\rho^{1/2} \tag{3}$$

Eqn.(3) shows that k is proportional to $C_p\rho^{1/2}$. However, according to Weber (11), k is proportional to $C_p\rho^{4/3}$. Thus, generalizing the correlation between k, C_p and ρ, Narasimhan et al (3) proposed the relationship:

$$k = yC_p\rho^x \tag{4}$$

By evaluating x and y from known experimental values of k at 293°K, for 50 organic liquids, they obtained the equation:

$$k = 0.877 \times 10^{-3}C_p\rho^{0.83} \tag{5}$$

They introduced a temperature factor into Eqn.(5) to give the general relation:

$$k = 0.877 \times 10^{-3}C_p\rho^{0.83}\left(\frac{293}{T}\right)^{0.38} \tag{6}$$

Eqn.(5) and Eqn.(6) can be used to predict the heat capacity of organic liquids, knowing only the thermal conductivity and the density. The validity of Eqn.(6) is tested for five organic liquids. Data reported by Vargaftik (19), are used for k, C_p and ρ at different temperatures for ethanol, propanol and aniline. C_p values for propanol are taken from the nomograph presented by Perry (20). For toluene and acetone, data reported by Gallant (21) are used. Most of the data obtained from these sources are essentially based on experimental results. In the absence of any evaluative commentary on the presentation of the data from these sources, the judgement of the authors in selection of the data is relied upon in the present study..

Figure 1 shows observed values of C_p and those calculated from Eqn.(6) for ethanol as a function of temperature. Similar curves are plotted in Figures 2, 3, 4 and 5 for propanol, aniline, toluene and acetone respectively. The results showing the percentage error, are tabulated in Tables I, II, III, IV and V. In the case of ethanol and propanol, the deviation from observed values is as high as 36% and 27 % respectively. For aniline and acetone, the deviation is higher at higher temperatures. Contrary to reported observed values, those calculated from Eqn.(6) for toluene show the heat capacity for the liquid decreasing with temperature. Although the predicted values for the other four liquids, show the heat capacity increasing with temperature, the increase is rather small. However, the fact that C_p does increase with temperature for these liquids, according to the predicted values, suggests that Eqn.(6) can be used to estimate C_p provided it is modified.

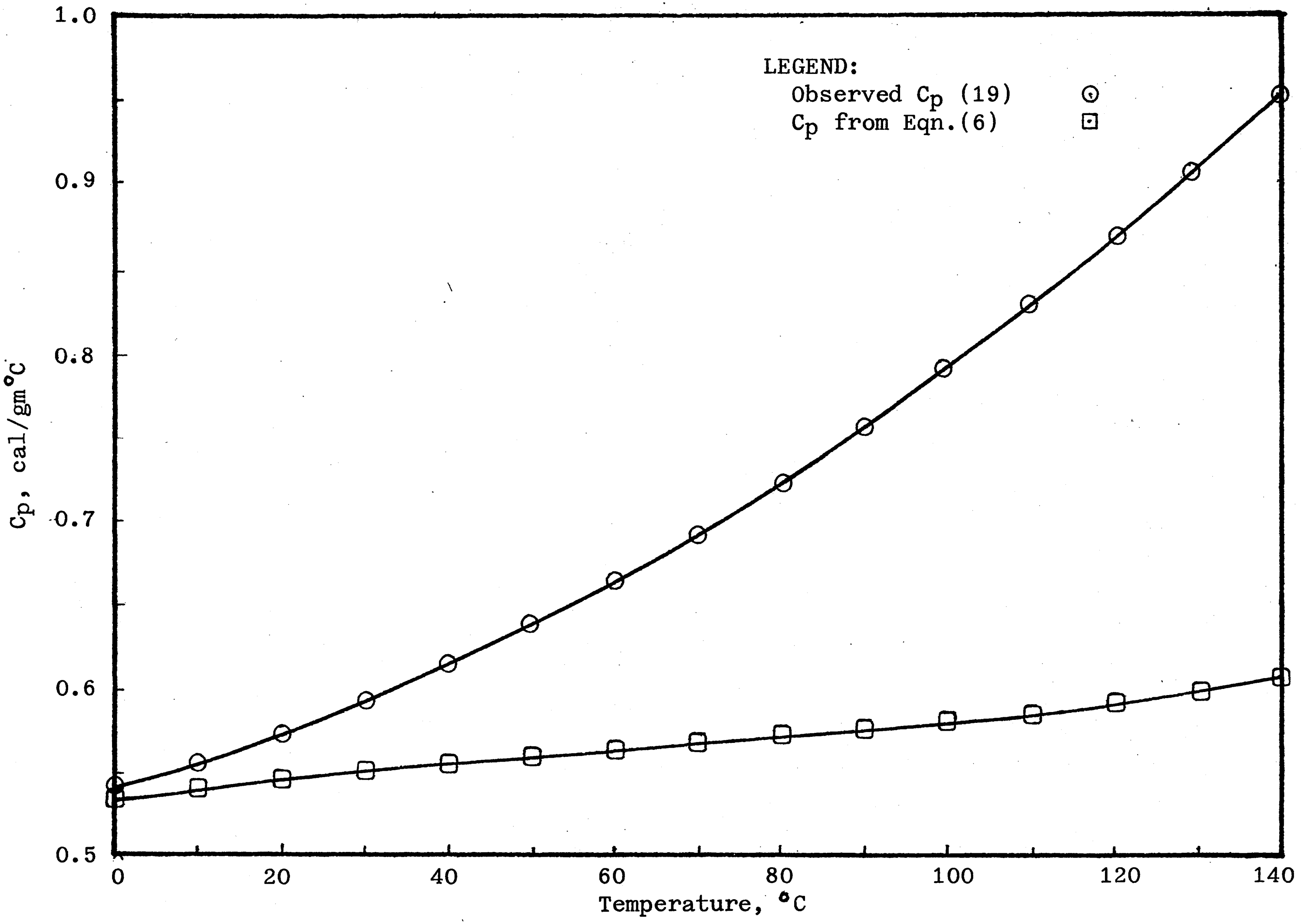

Figure 1. Cp for Ethanol

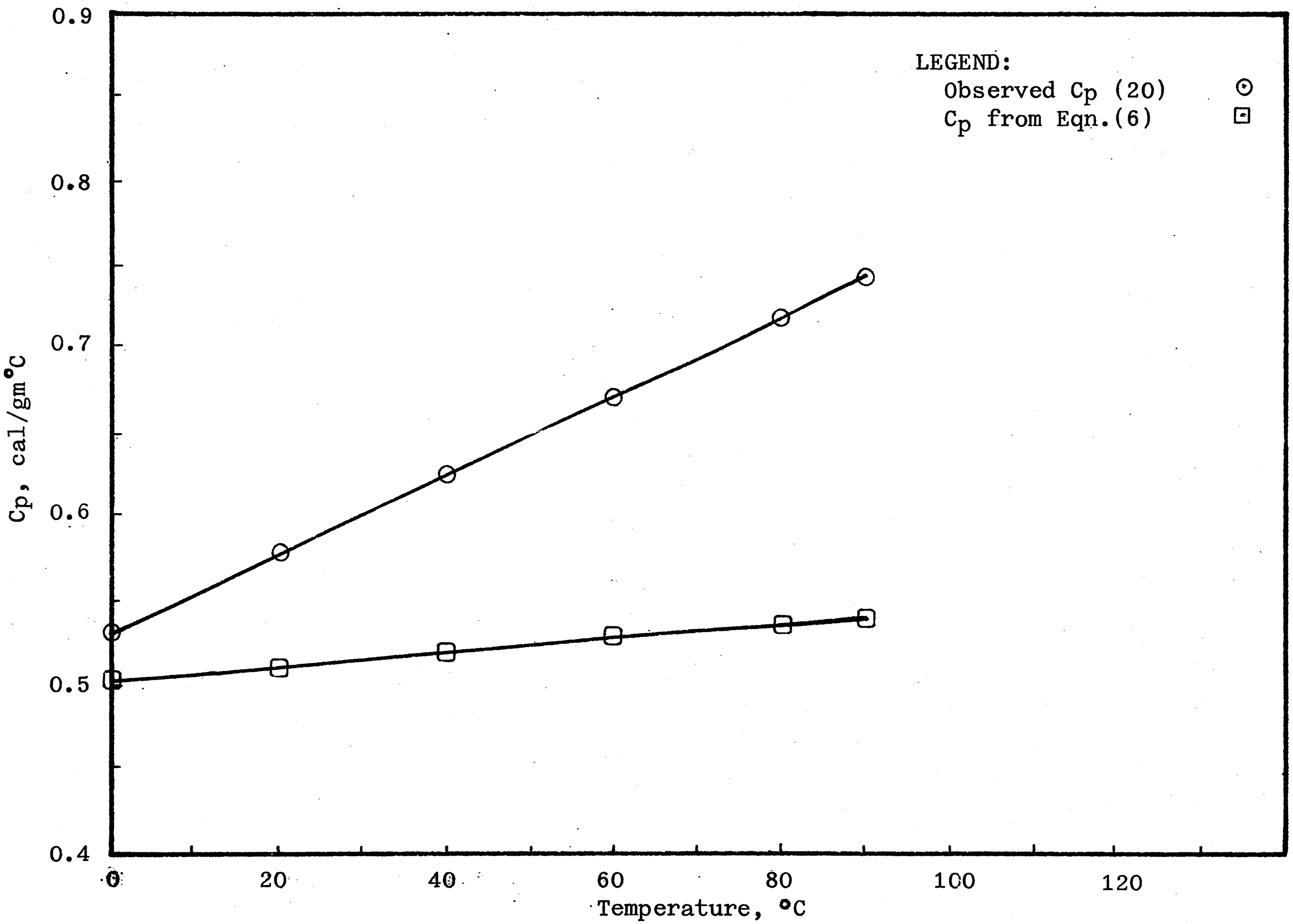

Figure 2. Cp for Propanol

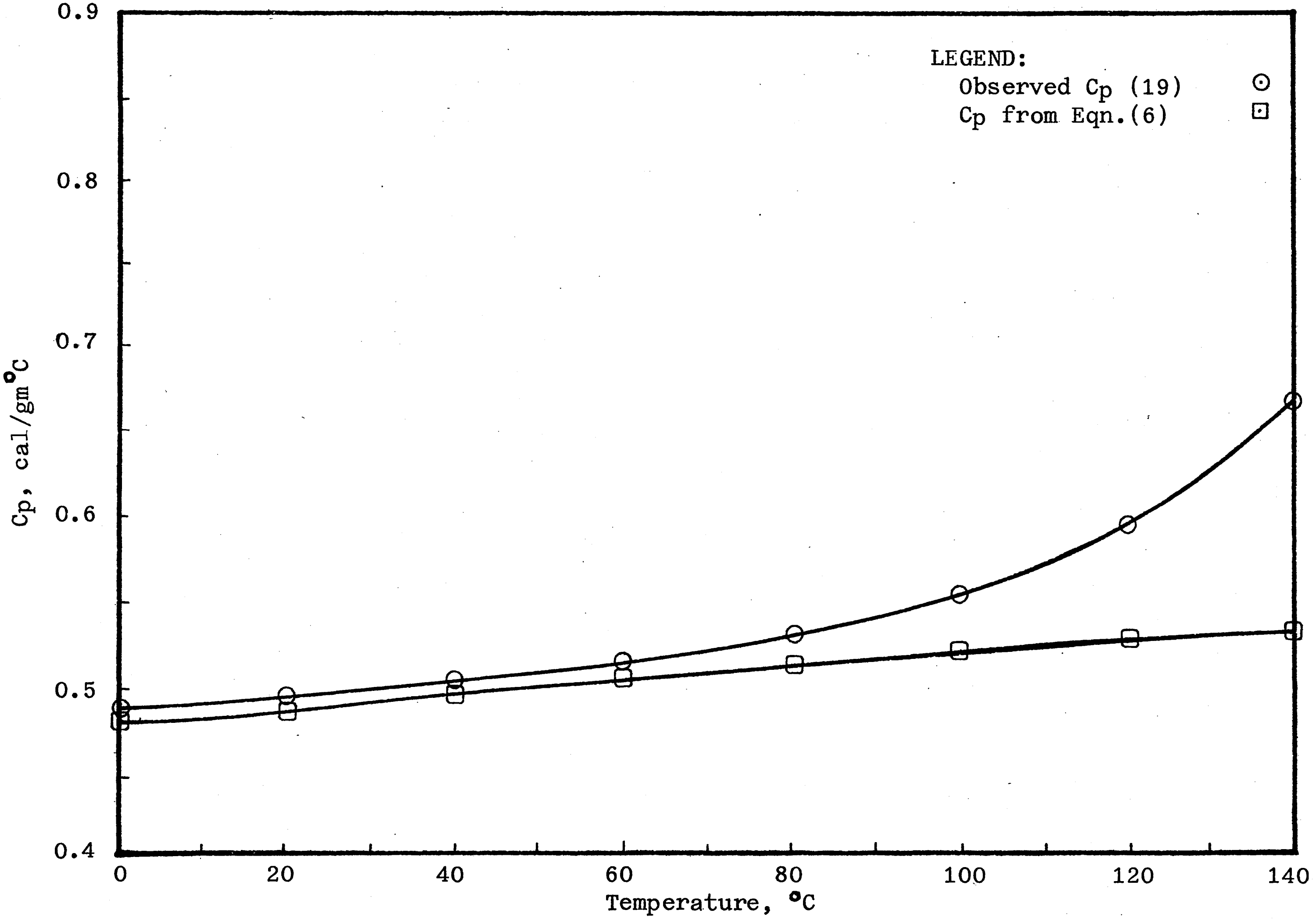

Figure 3. Cp for Aniline

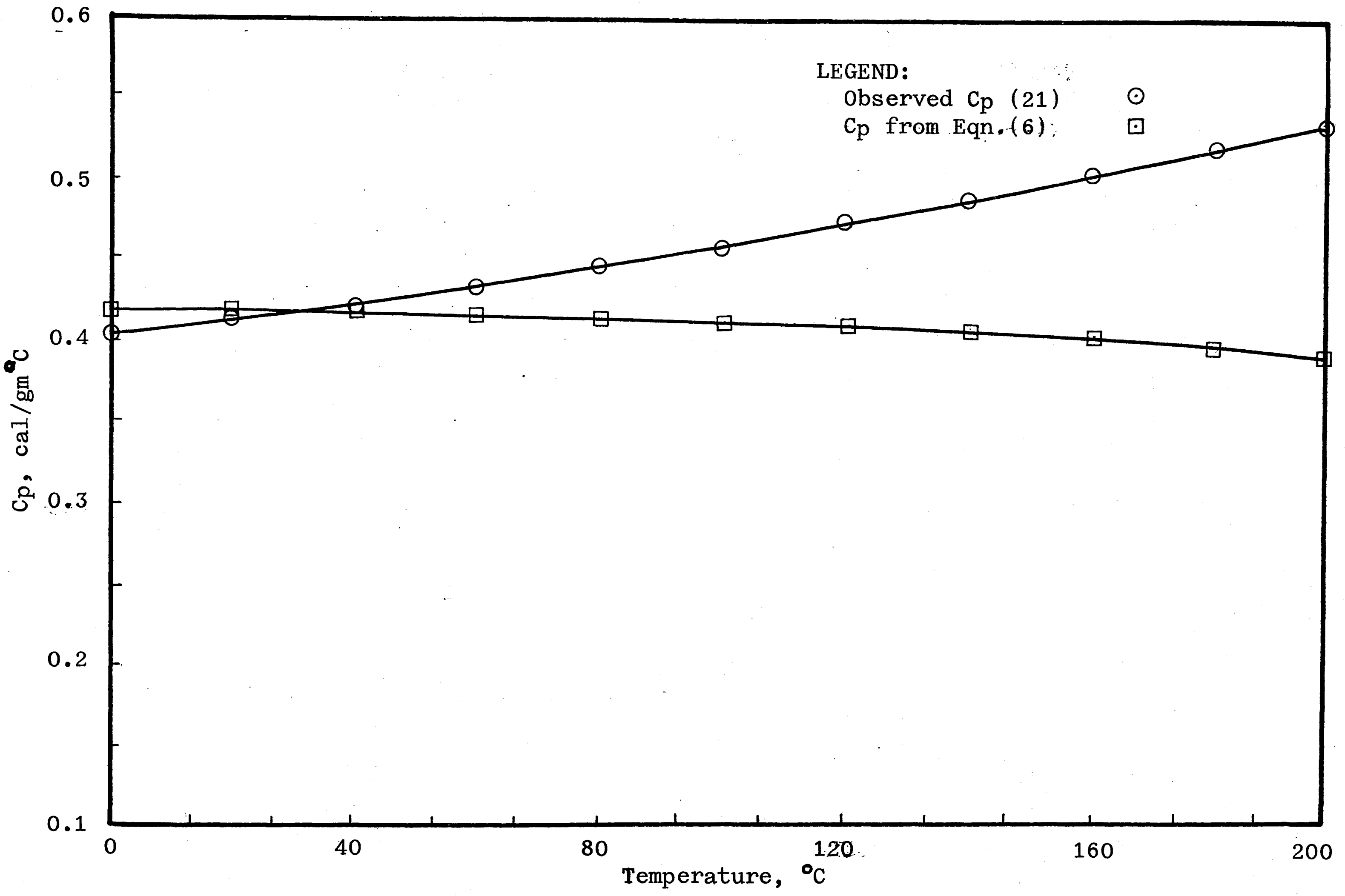

Figure 4. C_p for Toluene

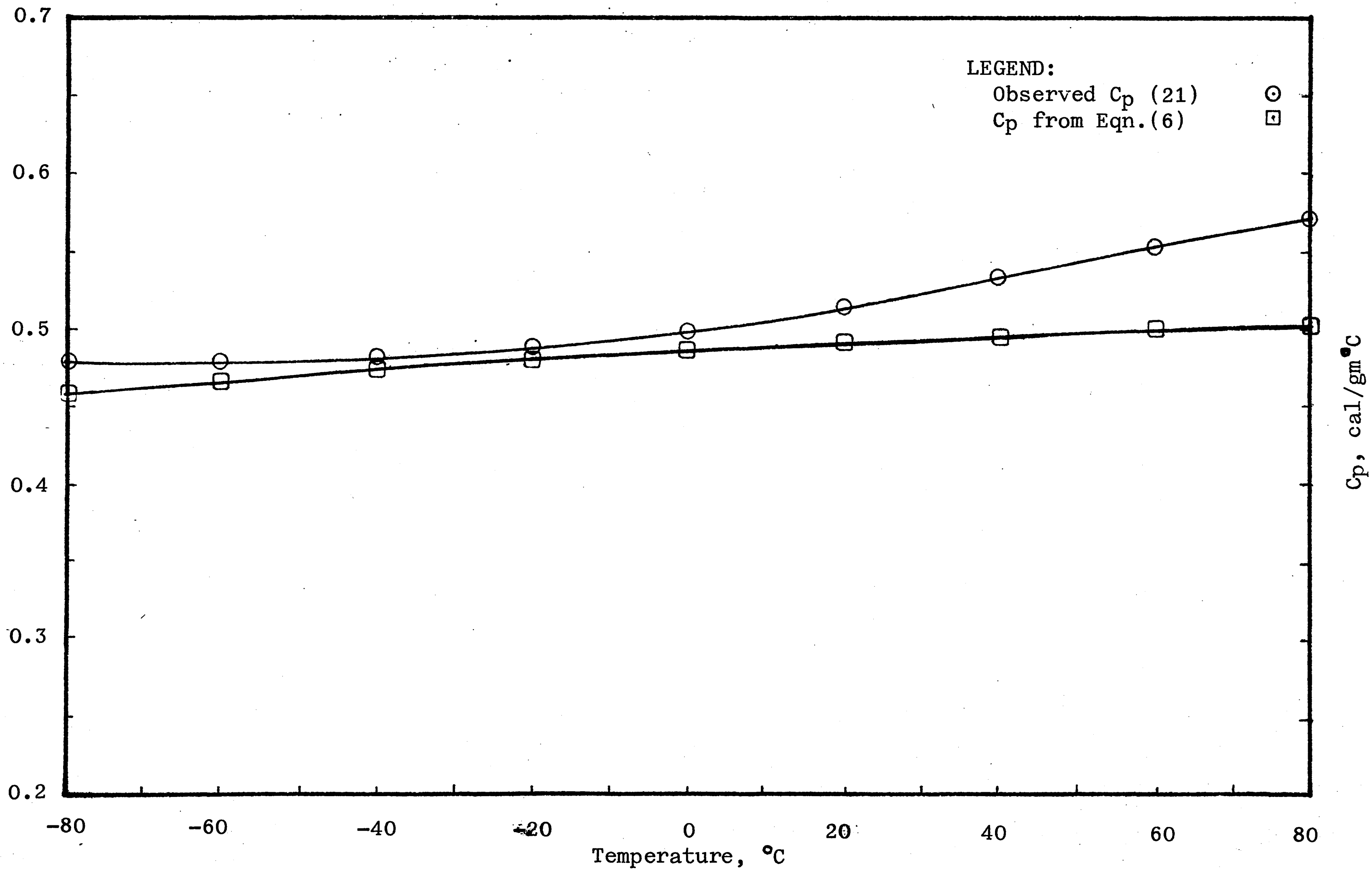

Figure 5. C_p for Acetone

TABLE I

OBSERVED AND CALCULATED HEAT CAPACITIES FOR ETHANOL

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^4$ cal/cm.sec.°C	C_p Observed cal/gm°C	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.8244	4.121	0.541	0.536	0.92
10	0.8163	4.061	0.557	0.540	3.05
20	0.8077	4.013	0.574	0.546	4.87
30	0.7993	3.953	0.593	0.549	7.41
40	0.7898	3.906	0.615	0.555	9.75
50	0.7812	3.846	0.639	0.558	12.67
60	0.7722	3.786	0.665	0.561	15.63
70	0.7633	3.738	0.693	0.566	18.32
80	0.7547	3.688	0.723	0.570	21.16
90	0.7446	3.633	0.755	0.574	23.97
100	0.7336	3.583	0.789	0.579	26.61
110	0.7215	3.528	0.825	0.584	29.21
120	0.7087	3.480	0.863	0.590	31.63
130	0.6954	3.428	0.903	0.596	33.99
140	0.6807	3.380	0.945	0.604	36.08

* $$\text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE II

OBSERVED AND CALCULATED HEAT CAPACITIES FOR PROPANOL

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^4$ cal/cm.sec.°C	C_p Observed cal/gm°C	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.8193	3.846	0.533	0.503	5.62
20	0.8035	3.750	0.580	0.512	11.72
40	0.7875	3.659	0.629	0.521	17.17
60	0.7700	3.564	0.672	0.530	21.13
80	0.7520	3.468	0.720	0.537	25.41
90	0.7425	3.421	0.745	0.541	27.38

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE III

OBSERVED AND CALCULATED HEAT CAPACITIES FOR ANILINE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^4 cal/cm.sec°C	C_p Observed cal/gm°C	Cp from Eqn.(6) cal/gm°C	Percent Error*
0	1.0373	4.445	0.485	0.478	1.44
20	1.0225	4.361	0.494	0.488	1.21
40	1.0070	4.278	0.506	0.497	1.77
60	0.9901	4.182	0.518	0.504	2.70
80	0.9718	4.063	0.532	0.509	4.32
100	0.9524	3.991	0.554	0.519	6.31
120	0.9328	3.919	0.599	0.529	11.68
140	0.9141	3.824	0.664	0.535	19.42

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE IV

OBSERVED AND CALCULATED HEAT CAPACITIES FOR TOLUENE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	C_p Observed cal/gm°C	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.885	34.4	0.406	0.422	3.79
20	0.870	33.0	0.415	0.422	1.68
40	0.850	31.6	0.424	0.422	0.47
60	0.833	30.2	0.434	0.419	3.45
80	0.815	28.8	0.446	0.417	6.50
100	0.793	27.5	0.462	0.416	9.95
120	0.770	26.1	0.477	0.412	13.62
140	0.745	24.8	0.492	0.411	16.46
160	0.720	23.4	0.507	0.405	20.11
180	0.697	22.0	0.522	0.398	23.75
200	0.670	20.6	0.536	0.392	26.86

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE V

OBSERVED AND CALCULATED HEAT CAPACITIES FOR ACETONE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec.°C	C_p Observed cal/gm°C	C_p from Eqn.(6) cal/gm°C	Percent Error*
-80	0.900	43.2	0.479	0.458	4.38
-60	0.875	41.7	0.482	0.470	2.48
-40	0.855	40.2	0.486	0.478	1.64
-20	0.835	38.7	0.492	0.484	1.62
0	0.810	37.2	0.504	0.488	3.17
20	0.790	35.8	0.518	0.496	4.24
40	0.765	34.3	0.534	0.500	6.36
60	0.740	32.8	0.552	0.503	8.87
80	0.715	31.4	0.572	0.506	11.53

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

CHAPTER IV

MODIFIED APPLICATION OF THE EQUATION

The small increase in the predicted value of C_p with temperature may be attributed to the temperature factor in Eqn.(6). In the case of toluene, even this does not help in obtaining an increase in the predicted values with temperature. If Eqn.(5) is used instead of Eqn.(6) for calculating C_p at different temperatures, the predicted values will decrease consistently with temperature for all compounds and the deviation from observed values will be greater. This is shown in Tables VI, VII, VIII, IX and X for all the five liquids considered.

The exponent x is an important factor in Eqn.(5). A better prediction could be obtained by considering x as a function of temperature instead of a constant in Eqn.(5). To determine how x varies with temperature, members of a homologous series are considered. Using Eqn.(5) with known observed values of k, C_p and ρ, x is calculated at different temperatures for each member of a series. Figure 6 shows the variation of x with temperature for ethyl, n-propyl and n-butyl alcohol. The results presented in Tables XI, XII and XIII indicate that x is of the same order of magnitude for all the three members. Hence, the points plotted in figure 6 lie within a relatively narrow band. A single curve, which will pass through a majority of these points can be obtained. This equation will represent the variation of x with temperature, for all the members of the series considered.

Assuming x to be a polynomial in T, several different orders of polynomials were tested, using the least squares method. The statistical package used with IBM 370/158 was the STATISTICAL ANALYSIS SYSTEM, originally developed at North Carolina State University by A. J. Barr and J. H. Goodnight. The best fit obtained was a polynomial of the second order. Thus, for the alcohols considered, x is given by the equation:

$$x = A + BT + CT^2 \tag{7}$$

where,

$A = -9.2655$

$B = 0.0547$

$C = -6.466 \times 10^{-5}$

$T =$ Temperature in °K.

Evaluating x from Eqn.(7) and using Eqn.(5), C_p is calculated for the three alcohols. The results are tabulated in Tables XIV, XV and XVI, and plotted in Figures 7, 8 and 9. The predicted values obtained from the modified application of Eqn.(5) are better than those calculated from Eqn.(6), the error involved being less than 5 percent.

To test the validity of Eqn.(7), its use is extended to other alcohols for which C_p is estimated by the same procedure. For n-heptyl alcohol, experimental values of k and ρ were obtained from Gallant (21). The results presented in Tables XVII, XVIII, XIX and

XX are plotted in Figures 10, 11, 12 and 13. They indicate in each case that the prediction of C_p is considerably improved by the combined use of Eqn(7) and Eqn.(5).

TABLE VI

OBSERVED AND CALCULATED HEAT CAPACITIES FOR ETHANOL

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^4$ cal/cm.sec°C	C_p Observed cal/gm°C	C_p from Eqn.(5) cal/gm°C	Percent Error*
0	0.8244	4.121	0.541	0.551	-1.94
10	0.8163	4.061	0.557	0.548	1.61
20	0.8077	4.013	0.574	0.546	4.87
30	0.7993	3.953	0.593	0.542	8.44
40	0.7898	3.906	0.615	0.541	11.90
50	0.7812	3.846	0.639	0.538	15.80
60	0.7722	3.786	0.665	0.535	19.50
70	0.7633	3.738	0.693	0.533	23.08
80	0.7547	3.688	0.723	0.531	26.55
90	0.7446	3.633	0.755	0.529	31.00
100	0.7336	3.583	0.789	0.528	33.07
110	0.7215	3.528	0.825	0.527	36.12
120	0.7087	3.480	0.863	0.528	38.80
130	0.6954	3.428	0.903	0.528	41.50
140	0.6807	3.380	0.945	0.530	43.90

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE VII

OBSERVED AND CALCULATED HEAT CAPACITIES FOR PROPANOL

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^4$ cal/cm.sec.°C	C_p Observed cal/gm°C	C_p from Eqn.(5) cal/gm°C	Percent Error*
0	0.8193	3.846	0.533	0.517	3.00
20	0.8035	3.750	0.580	0.512	11.70
40	0.7875	3.659	0.629	0.508	19.20
60	0.7700	3.564	0.672	0.504	25.00
80	0.7520	3.468	0.720	0.501	30.40
90	0.7425	3.421	0.745	0.499	33.00

* Percent Error = $\dfrac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$

TABLE VIII

OBSERVED AND CALCULATED HEAT CAPACITIES FOR ANILINE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^4$ cal/cm.sec°C	C_p Observed cal/gm°C	C_p from Eqn.(5) cal/gm°C	Percent Error*
0	1.0373	4.445	0.485	0.491	-1.34
20	1.0225	4.361	0.494	0.488	1.31
40	1.0070	4.278	0.506	0.484	4.28
60	0.9901	4.182	0.518	0.480	7.45
80	0.9718	4.063	0.532	0.474	10.98
100	0.9524	3.991	0.554	0.473	14.53
120	0.9328	3.919	0.599	0.473	21.07
140	0.9141	3.824	0.664	0.469	29.20

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE IX

OBSERVED AND CALCULATED HEAT CAPACITIES FOR TOLUENE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	Cp Observed cal/gm°C	Cp from Eqn.(5) cal/gm°C	Percent Error*
0	0.885	34.4	0.406	0.434	-6.89
20	0.870	33.0	0.415	0.422	-1.68
40	0.850	31.6	0.424	0.412	2.83
60	0.833	30.2	0.434	0.400	7.83
80	0.815	28.8	0.446	0.389	12.78
100	0.793	27.5	0.462	0.380	17.74
120	0.770	26.1	0.477	0.369	22.64
140	0.745	24.8	0.492	0.361	26.62
160	0.720	23.4	0.507	0.350	30.96
180	0.697	22.0	0.522	0.338	35.24
200	0.670	20.6	0.536	0.327	38.99

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE X

OBSERVED AND CALCULATED HEAT CAPACITIES FOR ACETONE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	C_p Observed cal/gm°C	C_p from Eqn.(5) cal/gm°C	Percent Error*
-80	0.900	43.2	0.479	0.537	-12.10
-60	0.875	41.7	0.482	0.531	-10.16
-40	0.855	40.2	0.486	0.522	-7.40
-20	0.835	38.7	0.492	0.512	-4.06
0	0.810	37.2	0.504	0.502	0.39
20	0.790	35.8	0.518	0.496	4.24
40	0.765	34.3	0.534	0.488	8.61
60	0.740	32.8	0.552	0.480	13.04
80	0.715	31.4	0.572	0.472	17.48

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

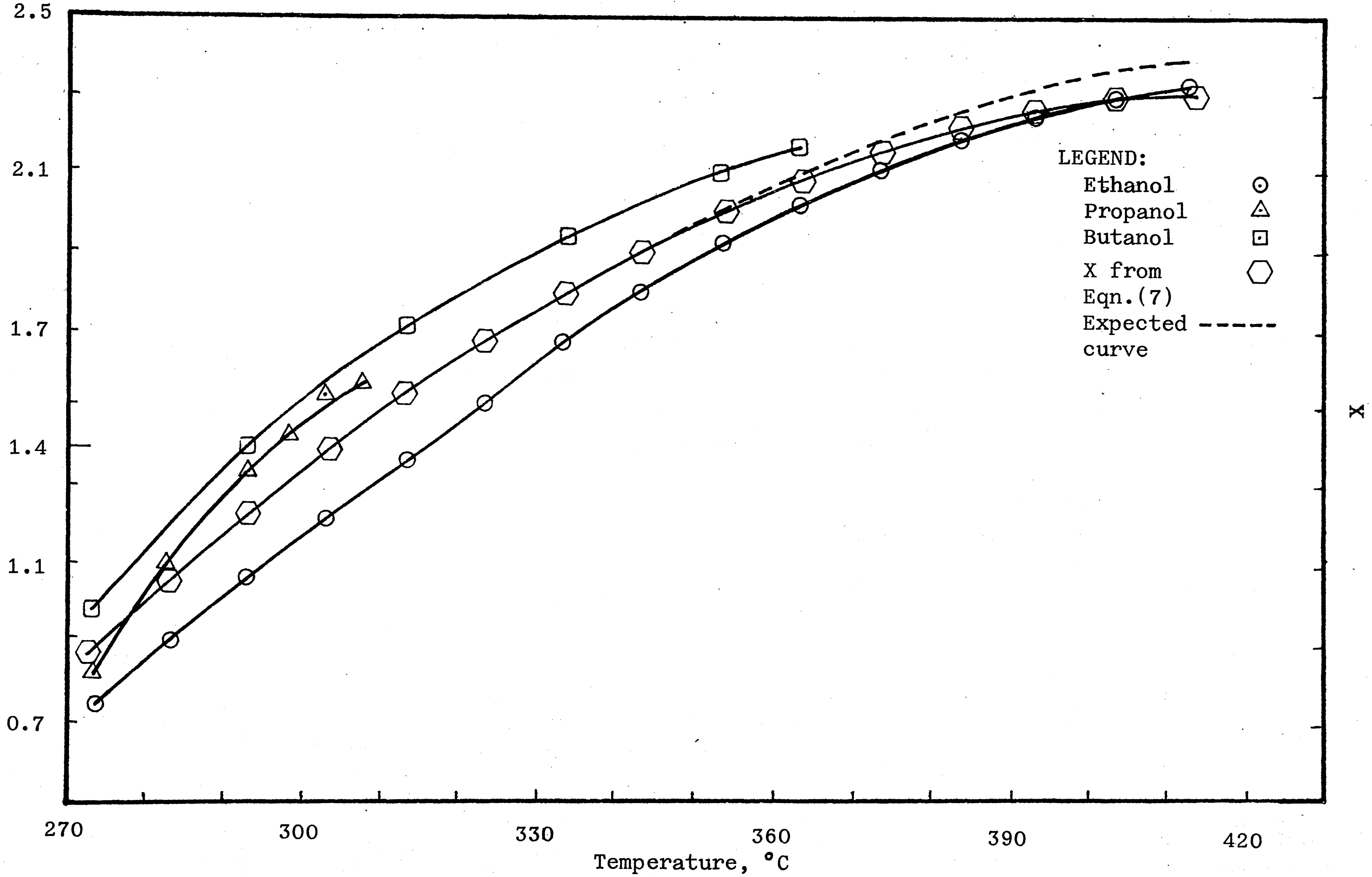

Figure 6. X as a function of temperature for Alcohols

TABLE XI

VARIATION OF X WITH TEMPERATURE FOR ETHANOL

Temperature °C	Thermal Conductivity $k \times 10^4$ cal/cm.sec.°C	C_p Observed cal/gm°C	$\frac{k}{yC_p}$	$\ln\frac{k}{yC_p}$	$\ln\rho$	x
0	4.121	0.541	0.8685	−0.1409	−0.1930	0.7300
10	4.061	0.557	0.8313	−0.1847	−0.2029	0.9103
20	4.013	0.574	0.7972	−0.2265	−0.2135	1.0608
30	3.953	0.593	0.7602	−0.2741	−0.2240	1.2236
40	3.906	0.615	0.7241	−0.3226	−0.2359	1.3675
50	3.846	0.639	0.6862	−0.3764	−0.2469	1.5245
60	3.786	0.665	0.6491	−0.4320	−0.2585	1.6711
70	3.738	0.693	0.6150	−0.4860	−0.2701	1.7993
80	3.688	0.723	0.5816	−0.5419	−0.2814	1.9257
90	3.633	0.755	0.5487	−0.6000	−0.2949	2,0345
100	3.583	0.789	0.5178	−0.6580	−0.3097	2.1246
110	3.528	0.825	0.4876	−0.7180	−0.3264	2.1997
120	3.480	0.863	0.4597	−0.7769	−0.3443	2.2564
130	3.428	0.903	0.4328	−0.8373	−0.3632	2.3053
140	3.380	0.945	0.4078	−0.8968	−0.3846	2.3310

TABLE XII

VARIATION OF X WITH TEMPERATURE FOR PROPANOL

Temperature °C	Thermal Conductivity $k \times 10^4$ cal/cm.sec.°C	C_p Observed cal/gm°C	$\frac{k}{yC_p}$	$\ln \frac{k}{yC_p}$	$\ln \rho$	x
0	3.846	0.533	0.8227	-0.1950	-0.1993	0.978
20	3.750	0.580	0.7373	-0.3046	-0.2187	1.392
40	3.659	0.629	0.6634	-0.4102	-0.2388	1.717
60	3.564	0.672	0.6047	-0.5028	-0.2613	1.924
80	3.469	0.720	0.5493	-0.5990	-0.2850	2.101
90	3.421	0.745	0.5235	-0.6470	-0.2977	2.173

TABLE XIII

VARIATION OF X WITH TEMPERATURE FOR BUTANOL

Temperature °C	Thermal Conductivity $k \times 10^3$ cal/cm.sec.°C	C_p Observed cal/gm°C	$\frac{k}{yC_p}$	$\ln \frac{k}{yC_p}$	$\ln \rho$	x
0	0.375	0.500	0.8551	-0.1564	-0.1928	0.811
10	0.372	0.529	0.8018	-0.2208	-0.2019	1.093
20	0.368	0.557	0.7531	-0.2835	-0.2112	1.342
25	0.366	0.570	0.7335	-0.3098	-0.2160	1.434
30	0.364	0.583	0.7125	-0.3389	-0.2206	1.536
35	0.363	0.590	0.7028	-0.3525	-0.2251	1.565

TABLE XIV

OBSERVED AND PREDICTED HEAT CAPACITIES FOR ETHANOL

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^4 cal/cm.sec.°C	x	Cp Observed cal/gm°C	Cp Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	Cp from Eqn.(6) cal/gm°C	Percent Error*
0	0.8244	4.121	0.858	0.541	0.554	-2.40	0.536	0.92
10	0.8163	4.061	1.046	0.557	0.572	-2.69	0.540	3.05
20	0.8077	4.013	1.221	0.574	0.593	-3.31	0.546	4.87
30	0.7993	3.953	1.383	0.593	0.614	-3.54	0.549	7.41
40	0.7898	3.953	1.532	0.615	0.639	-3.90	0.555	9.75
50	0.7812	3.846	1.668	0.639	0.662	-3.59	0.558	12.67
60	0.7722	3.786	1.791	0.665	0.685	-3.00	0.561	15.63
70	0.7633	3.738	1.901	0.693	0.712	-2.74	0.566	18.32
80	0.7547	3.688	1.999	0.723	0.738	-2.07	0.570	21.16
90	0.7446	3.633	2.083	0.755	0.765	-1.32	0.574	23.97
100	0.7336	3.583	2.154	0.789	0.796	-0.88	0.579	26.61
110	0.7215	3.528	2.213	0.825	0.828	-0.36	0.584	29.21
120	0.7087	3.480	2.258	0.863	0.863	0.00	0.590	31.63
130	0.6954	3.428	2.291	0.903	0.898	0.55	0.596	33.99
140	0.6807	3.380	2.311	0.945	0.937	0.84	0.604	36.08

* $$\text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XV

OBSERVED AND PREDICTED HEAT CAPACITIES FOR PROPANOL

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^4 cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.8193	3.846	0.858	0.533	0.520	2.40	0.503	5.62
20	0.8035	3.750	1.221	0.580	0.558	3.79	0.512	11.72
40	0.7875	3.659	1.532	0.629	0.601	4.45	0.521	17.17
60	0.7700	3.564	1.791	0.672	0.649	3.42	0.530	21.13
80	0.7520	3.468	1.999	0.720	0.699	2.91	0.537	25.41
90	0.7425	3.421	2.083	0.745	0.725	2.68	0.541	27.38

* $$\text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XVI

OBSERVED AND PREDICTED HEAT CAPACITIES FOR BUTANOL

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^3$ cal/cm.sec°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.8246	0.375	0.858	0.500	0.504	-0.8	0.488	2.40
10	0.8171	0.372	1.046	0.529	0.523	1.13	0.495	6.42
20	0.8096	0.368	1.221	0.557	0.542	2.69	0.499	10.41
25	0.8057	0.366	1.303	0.570	0.554	2.80	0.503	11.75
30	0.8020	0.364	1.383	0.583	0.563	3.43	0.505	13.37
35	0.7984	0.363	1.459	0.590	0.575	2.54	0.509	13.72

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

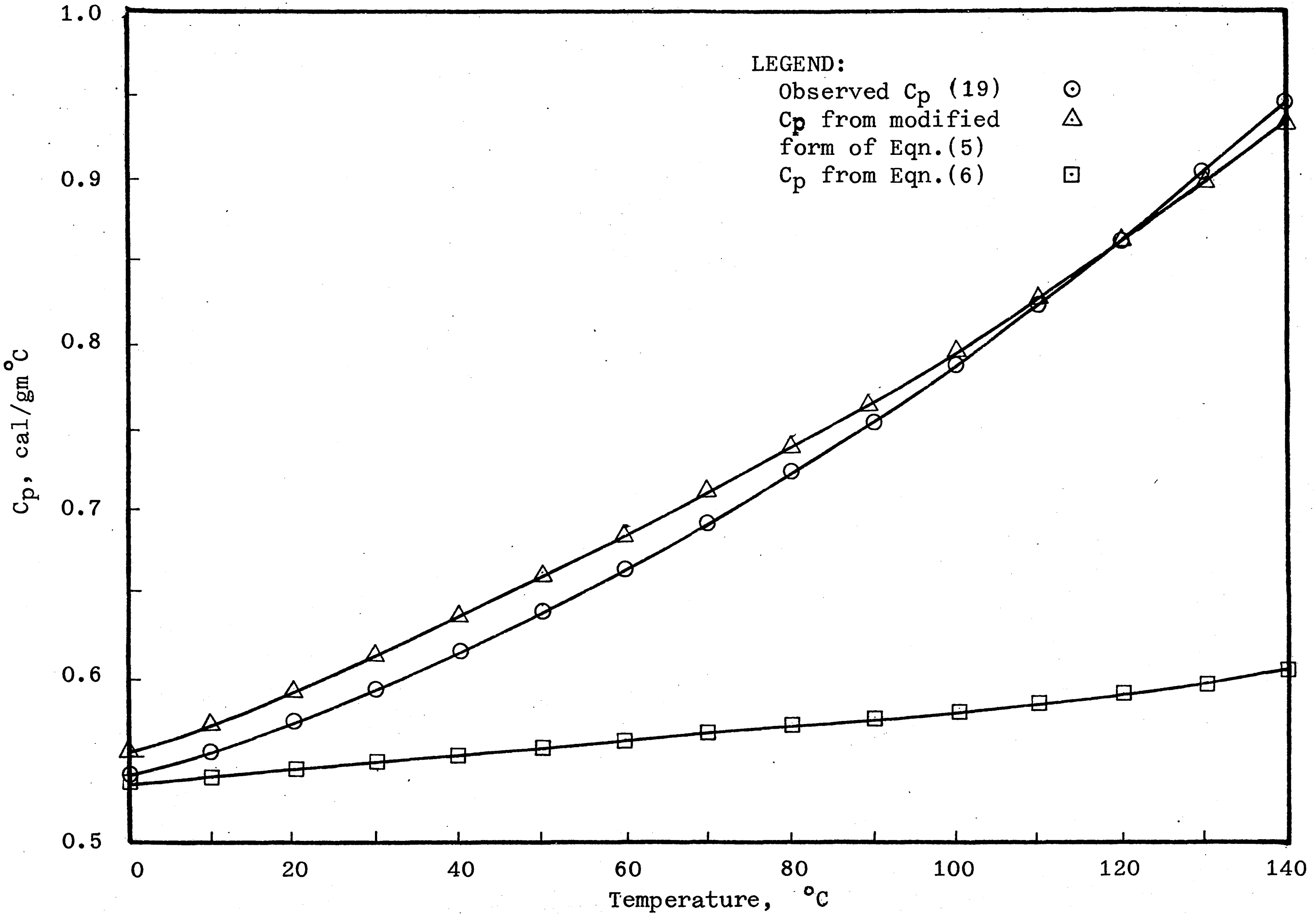

Figure 7. C_p for Ethanol

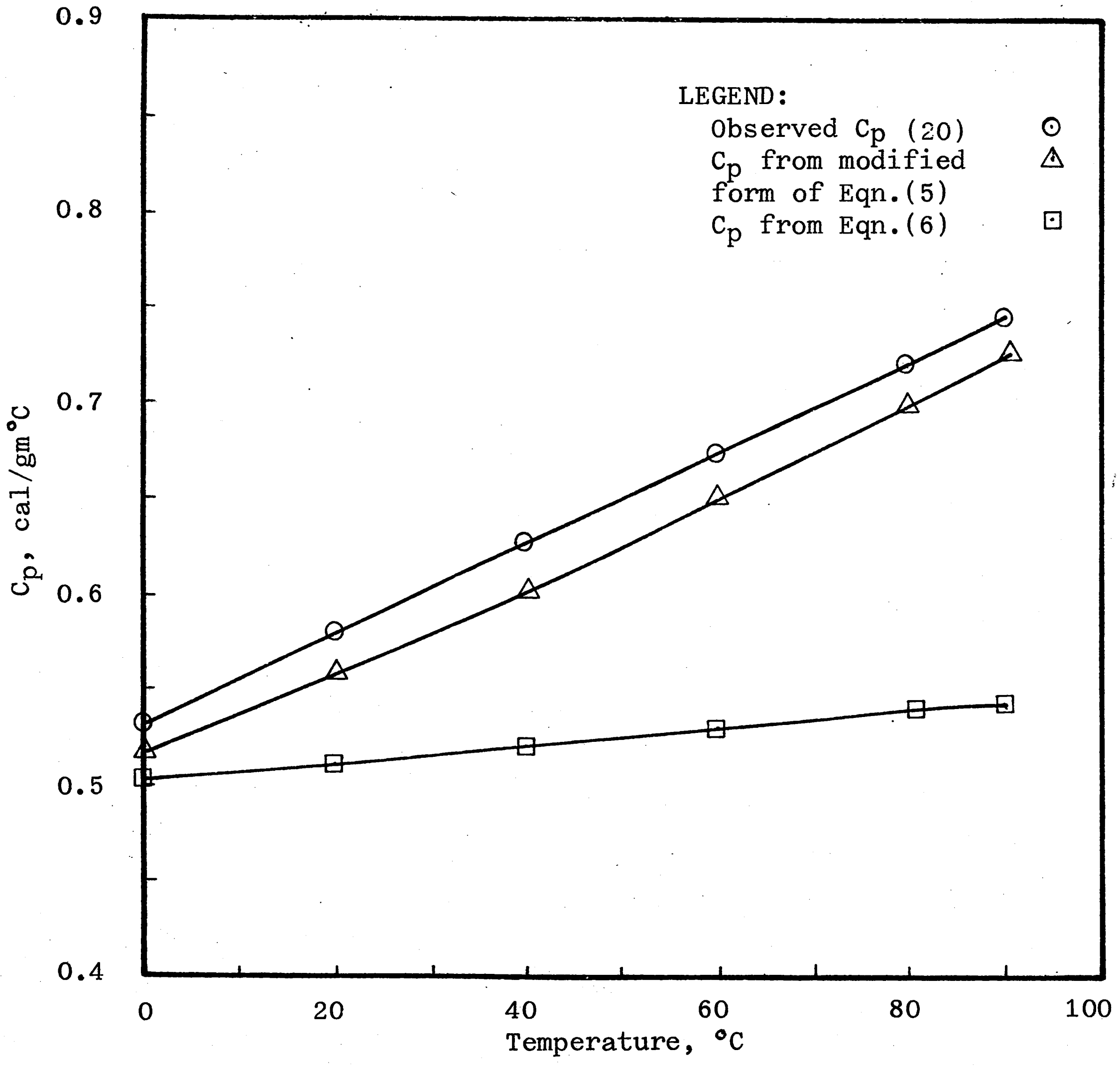

Figure 8. Cp for Propanol

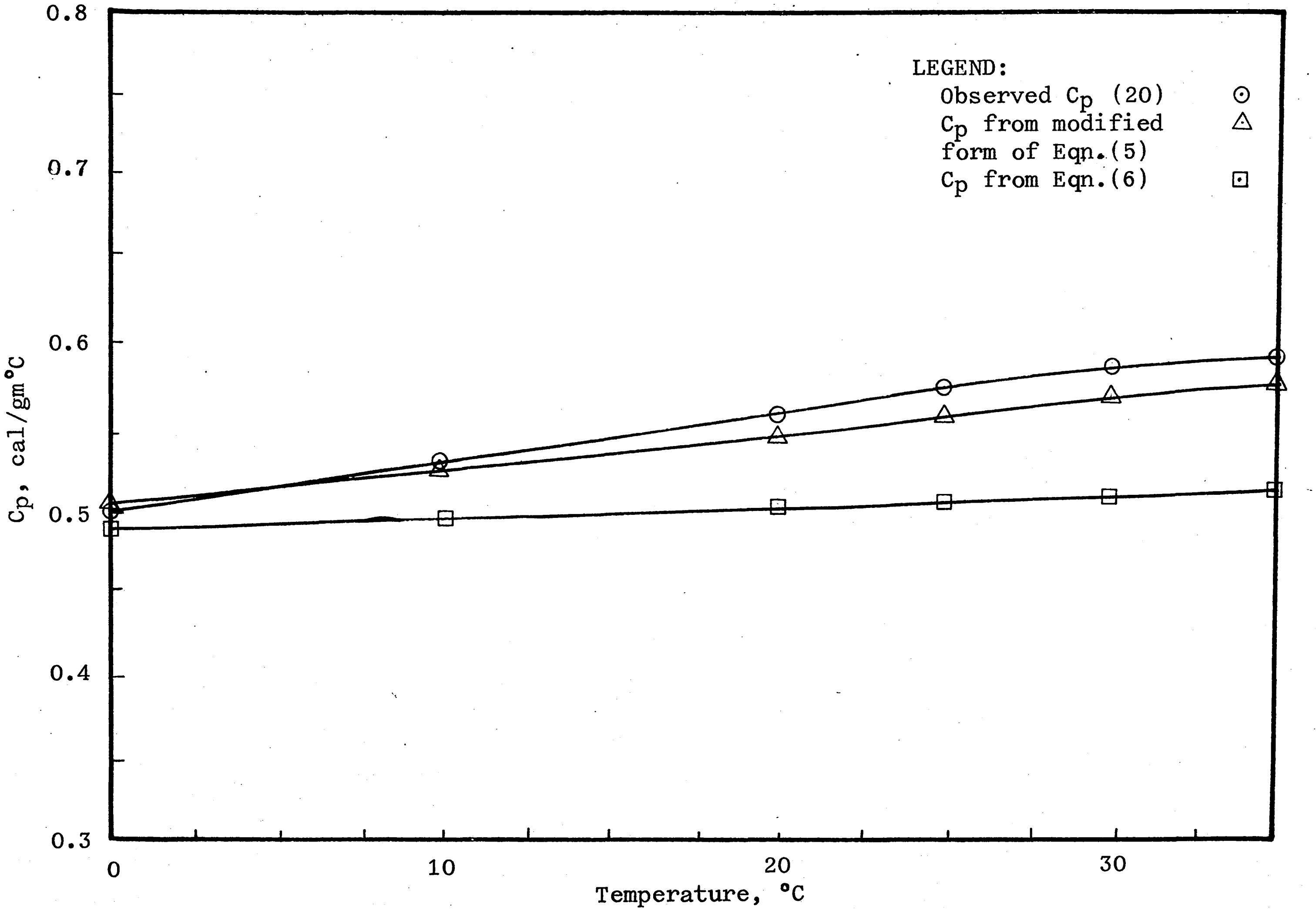

Figure 9. C_p for Butanol

TABLE XVII

OBSERVED AND PREDICTED HEAT CAPACITIES FOR n-HEPTYL ALCOHOL

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^3 cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
25	0.819	0.341	1.293	0.510	0.503	1.37	0.461	9.60
50	0.806	0.331	1.656	0.550	0.539	2.00	0.468	14.90
75	0.789	0.318	1.939	0.615	0.574	6.66	0.471	23.41
100	0.768	0.302	2.141	0.670	0.606	9.55	0.469	30.00
125	0.748	0.281	2.262	0.725	0.617	14.89	0.457	36.96
150	0.728	0.258	2.303	0.795	0.610	23.27	0.439	44.77
175	0.704	0.240	2.626	0.897	0.605	32.55	0.430	52.06
200	0.679	0.224	2.141	1.025	0.585	42.92	0.422	58.82

* Percent Error = $\dfrac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$

TABLE XVIII

OBSERVED AND PREDICTED HEAT CAPACITIES FOR HEXYL ALCOHOL

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.838	32.3	0.858	0.465	0.428	7.95	0.415	10.75
20	0.825	32.0	1.221	0.507	0.461	9.07	0.428	15.58
40	0.810	31.7	1.532	0.553	0.499	9.76	0.441	20.25
60	0.795	31.3	1.791	0.600	0.539	10.16	0.454	24.33
80	0.780	31.0	1.999	0.645	0.581	9.92	0.467	27.59
100	0.768	30.8	2.083	0.690	0.608	11.88	0.479	30.57
120	0.745	30.6	2.258	0.742	0.678	8.62	0.498	32.88
140	0.727	30.5	2.311	0.805	0.726	9.81	0.516	35.90

* $$\text{Percent Error} = \frac{(\text{Observed value}) - (\text{Calculated value})}{(\text{Observed value})}$$

TABLE XIX

OBSERVED AND PREDICTED HEAT CAPACITIES FOR ALLYL ALCOHOL

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn. (5) cal/gm°C	Percent Error	C_p from Eqn. (6) cal/gm°C	Percent Error*
0	0.870	40.40	0.858	0.450	0.519	-13.29	0.503	-11.77
20	0.855	39.53	1.221	0.490	0.545	-11.22	0.505	-3.06
40	0.835	38.92	1.532	0.530	0.584	-10.18	0.528	0.37
60	0.818	38.52	1.791	0.570	0.629	-10.35	0.544	4.56
80	0.796	38.30	1.991	0.625	0.689	-10.24	0.566	9.44
100	0.775	38.00	2.083	0.685	0.736	-6.92	0.586	14.45
120	0.750	37.89	2.258	0.755	0.827	-9.53	0.613	18.80
140	0.725	37.82	2.311	0.835	0.906	-7.83	0.641	23.23

* Percent Error = $\frac{(\text{Observed value}) - (\text{Calculated value})}{(\text{Observed value})}$

TABLE XX

OBSERVED AND PREDICTED HEAT CAPACITIES FOR AMYL ALCOHOL

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec.°C	x	C_p Observed cal/gm °C	C_p Calculated with modified form of Eqn.(5) cal/gm °C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.830	37.50	0.858	0.479	0.501	-4.39	0.485	-1.25
20	0.815	36.85	1.221	0.520	0.539	-3.65	0.497	4.42
40	0.800	36.40	1.532	0.564	0.584	-3.54	0.512	9.21
60	0.786	36.08	1.791	0.606	0.633	-4.45	0.527	13.03
80	0.771	35.72	1.991	0.656	0.684	-4.26	0.542	17.37
100	0.755	35.40	2.083	0.705	0.724	-2.69	0.558	20.85
120	0.738	35.00	2.258	0.755	0.792	-4.90	0.574	29.97
140	0.722	34.82	2.311	0.816	0.842	-3.08	0.592	27.45

* Percent Error = $\frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$

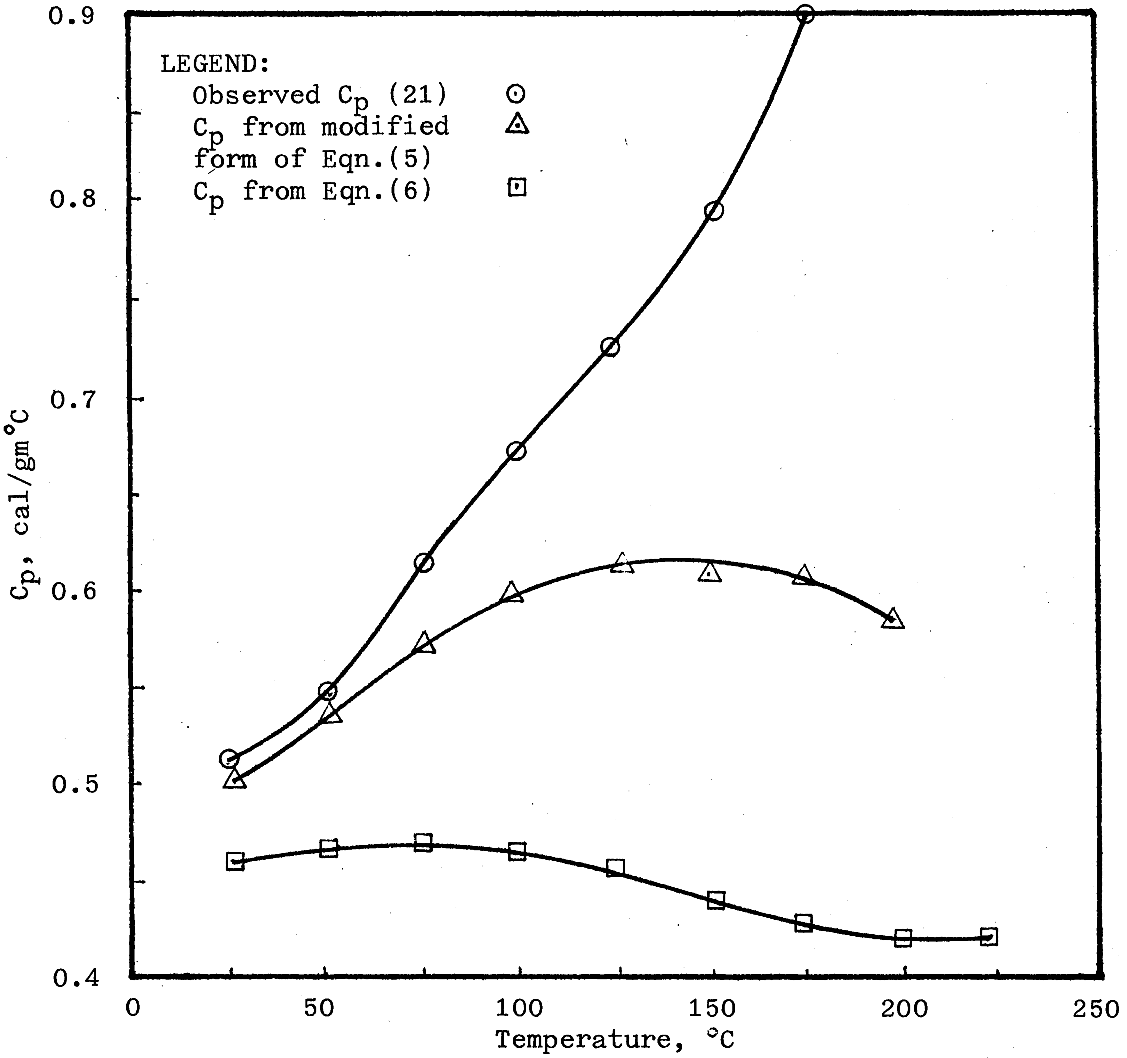

Figure 10. C_p for n-Heptyl Alcohol

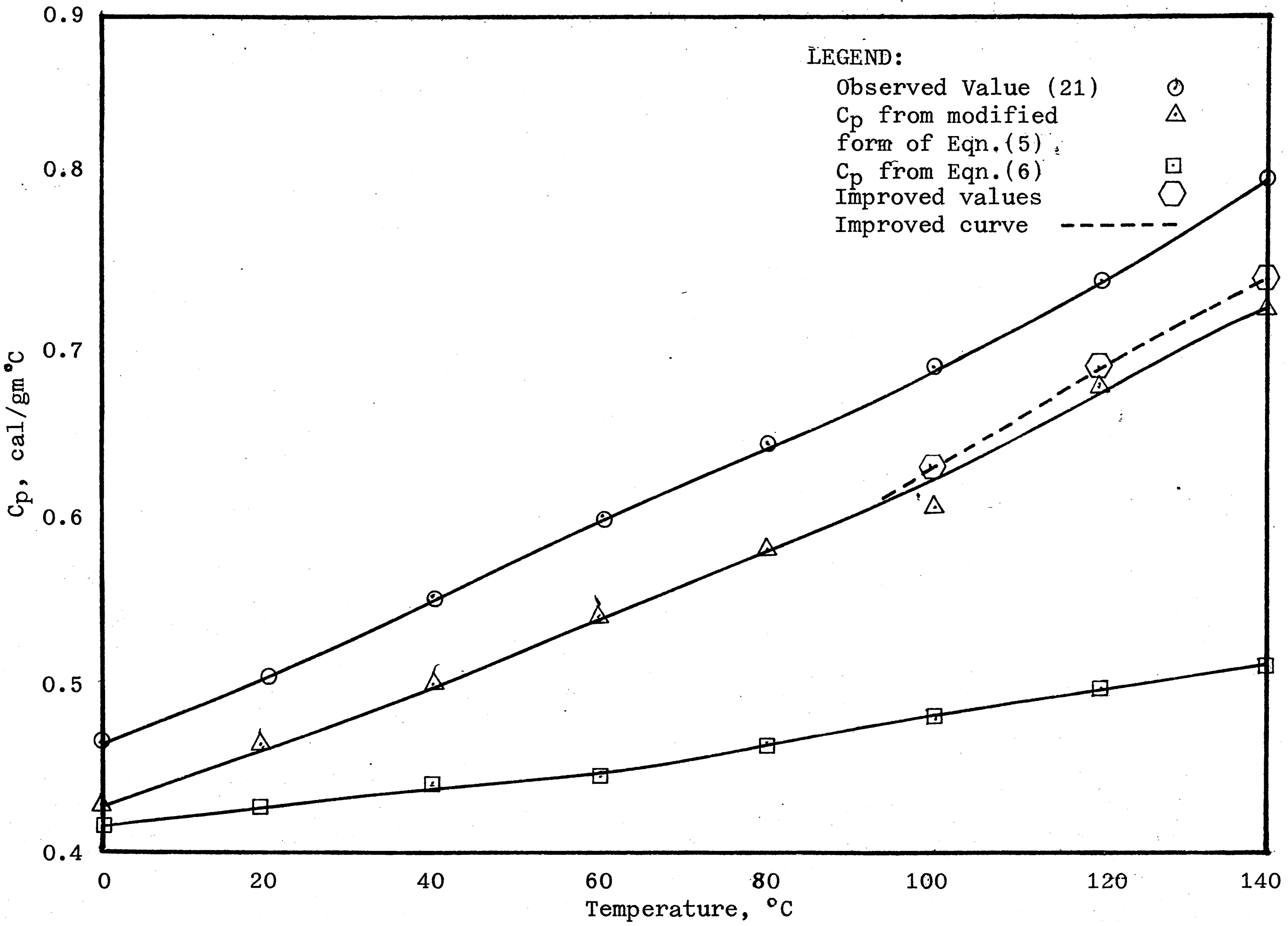

Figure 11. C_p for Hexyl alcohol

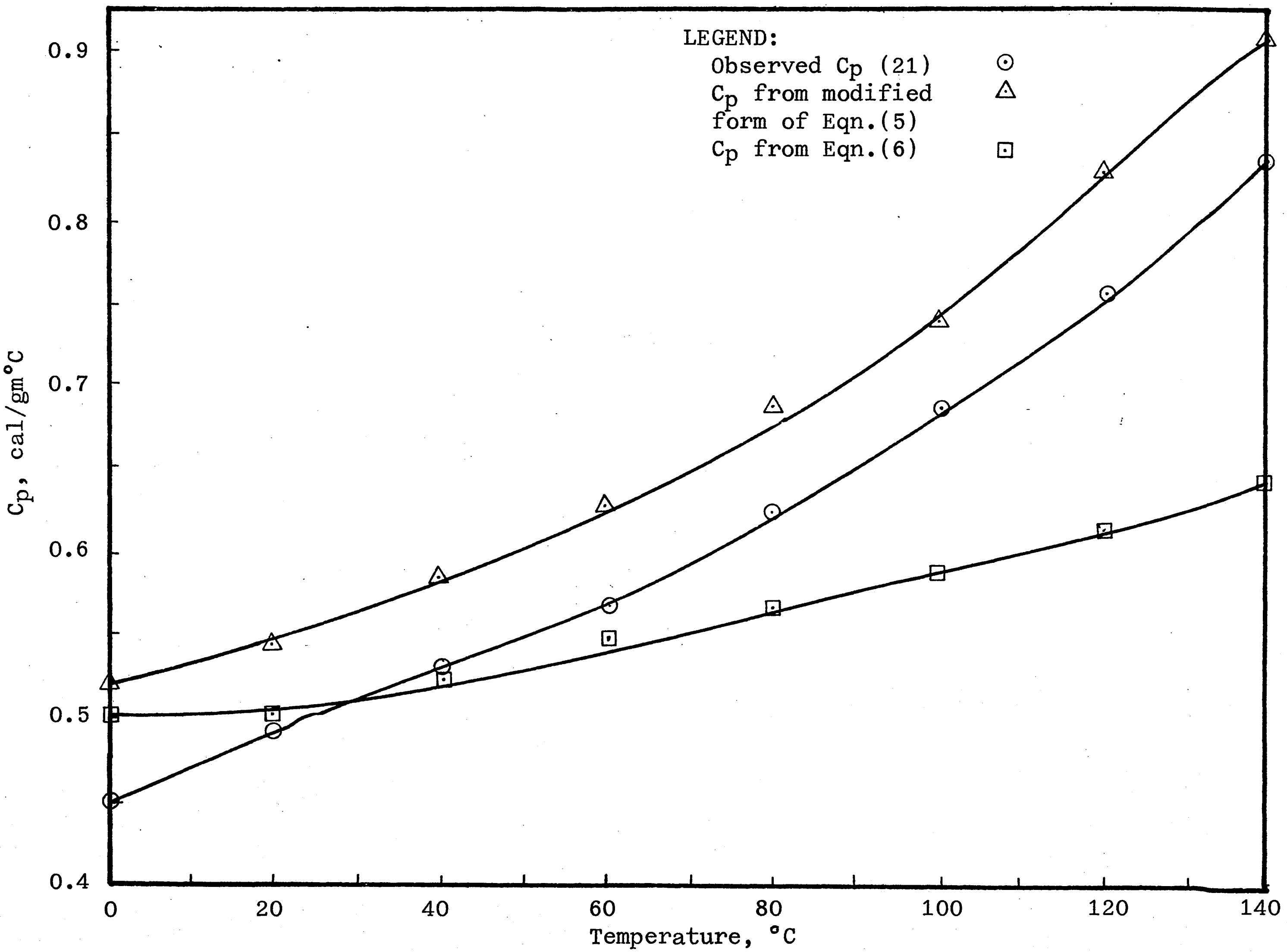

Figure 12. C_p for Allyl alcohol

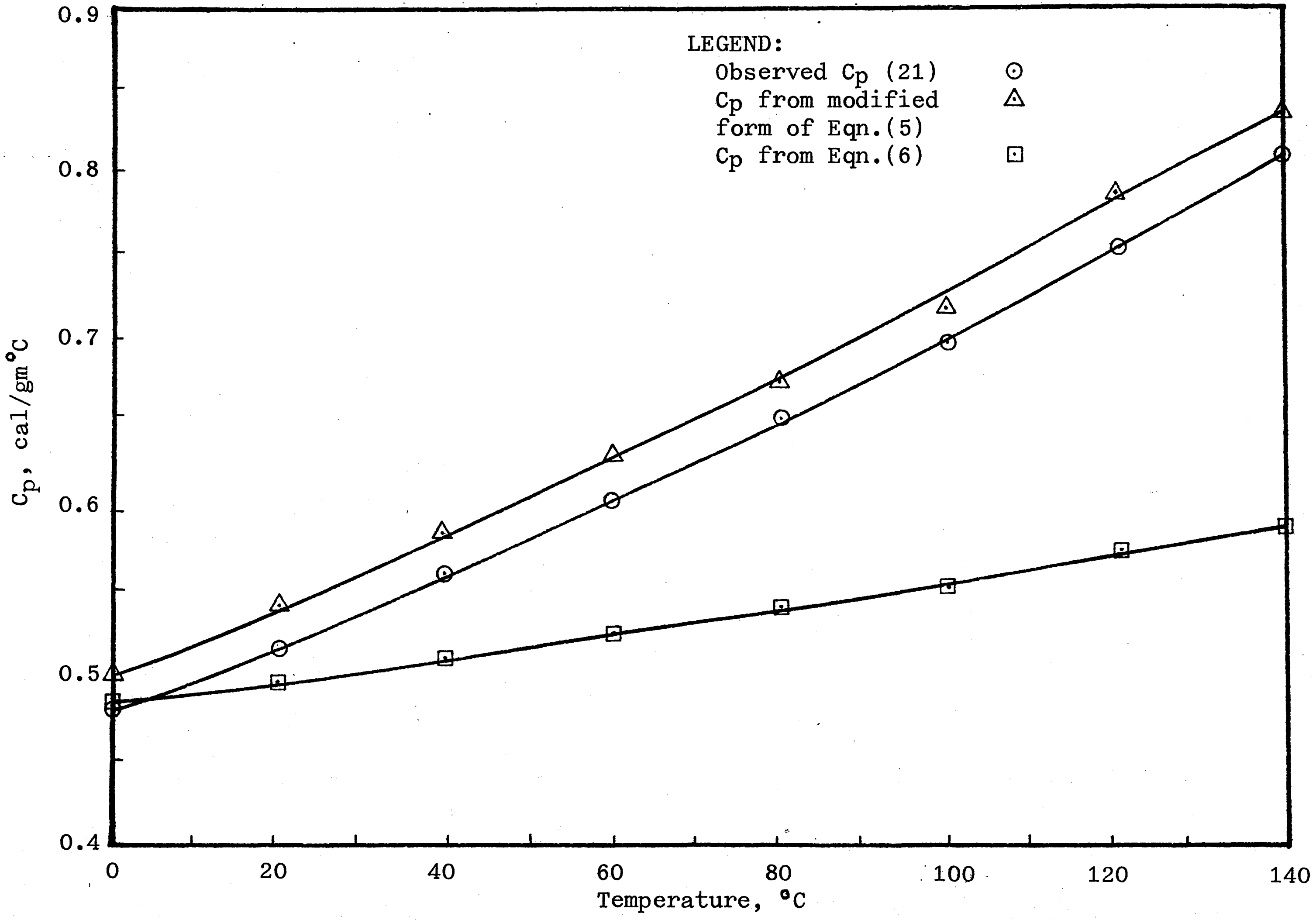

Figure 13. C_p for Amyl alcohol

CHAPTER V

PRESENTATION, ANALYSIS AND DISCUSSION OF THE RESULTS

Eqn.(7) is a general form of equation, applicable to other homologous series also. The value of the co-efficients A, B and C of the equation will be different for each series. The procedure followed for alcohols to calculate the value of the co-efficients is employed for ketones and aromatics. In each case, members belonging to a particular homologous series are considered. Using the computed values of the co-efficients, x is calculated at different temperatures and C_p is estimated from Eqn.(5). Data for k, C_p and are taken from Gallant (21). The results are presented in tables and figures as indicated below:

1) For Ketones

Compounds considered for determining the co-efficients:

Acetone, Methylethyl Ketone (MEK) and Diethyl Ketone (DEK).

Compounds for which C_p is predicted:

Acetone, MEK, DEK and MIBK.

Tables: XXI, XXII, XXIII, XXIV, XXV, XXVI and XXVII.

Figures: 14, 15, 16 and 17.

The Co-efficients:

$$A = -4.3107$$

$$B = 0.03188$$

$$C = -4.45 \times 10^{-5}$$

2) For Aromatic liquids

Compounds considered for determining the co-efficients:

Toluene, Ethylbenzene and Propylbenzene.

Compounds for which C_p is predicted:

Toluene, Ethylbenzene, Propylbenzene, Benzene, o, m, p-Xylene, Pyridine and Styrene.

Tables: XXVIII, XXIX, XXX, XXXI, XXXII, XXXIII, XXXIV, XXXV, XXXVI, XXXVII, XXXVIII and XXXIX.

Figures: 18, 19 20, 21, 22, 23, 24, 25, 26 and 27.

The Co-efficients:

$$A = -9.7134$$

$$B = 0.0522$$

$$C = 5.674 \times 10^{-5}$$

To determine the accuracy in the prediction of Cp for the miscellaneous alcohols, C_p values reported by Gallant (21) are used for comparison. Because data on liquid heat capacity for these compounds is almost non-existent, those reported by Gallant are values estimated at 20°C by the method of Johnson and Huang (8) and extrapolated over the range of temperature range by the method of Chow and Bright (5). The error is generally about 5-10 percent.

The predicted values from the modified application of Eqn.(5) for n-heptyl alcohol decrease with temperature above 140°C. This is to be expected. X is a second degree polynomial in T and the values of the co-efficients obtained for alcohols suggest that there is a point of inflection. The temperature corresponding to this point can be obtained by differentiating Eqn.(7) with respect to T and setting the derivative to zero. Thus,

$$\frac{dx}{dT} = B + 2CT = 0$$

$$T = -\frac{B}{2C}$$

$$= \frac{-0,0547}{-2 \times 6.466 \times 10^{-5}} \; {}^{\circ}K$$

$$= 423^{\circ}K$$

$$= 150^{\circ}C$$

For n-heptyl alcohol, x will decrease beyond 150°C. This will cause the predicted vakues to decrease with temperature beyond 150°C, as shown in Figure 10. Therefore, x should not be extrapolated beyond the range of temperature for which the co-efficients of Eqn.(7) are computed.

Figure 6. shows x obtained from Eqn.(7) as compared to the values used as input for fitting the curve. At higher temperatures, the values of x from Eqn.(7) are close to those for ethanol, because at these temperatures, reliable physical property data for only ethanol were available and used as input. If data for propanol and butanol were available over the same range of temperature, the values of x from Eqn.(7) at higher temperatures could be expected to be higher (see the broken line shown in Figure 6.). Reading the values of x from the expected curve for this region, the C_p values predicted for hexyl alcohol from Eqn.(5), are closer to the observed values (see the broken line shown in Figure 11.).

In computing the co-efficients of Eqn.(7) for alcohols and aromatics, methyl alcohol and benzene have not been considered in their respective series. The first member of a homologous series frequently does not fit a correlation of this nature. Table XXXIV shows that the modified application of Eqn.(5) for benzene, gives values which deviate substantially from the observed values. This is not so for acetone, the first of the ketones. In general however, the modified application of Eqn.(5) may be expected to work well for the higher members of a homologous series. Thus, the equation predicts values with an error of less than 10 percent for Methylisobutyl ketone (MIBK).

The general form of Eqn.(7) does not hold good for all series of compounds. Tables XL, XLI, XLII and XLIII show the variation of x with temperature for the aldehydes. Since x is not of the same order of magnitude for all the members of this series, a plot of x as a function of temperature will result in a large scatter of data points In such a case, a single curve, whose equation will represent the variation of x with temperature for all the members of the series considered cannot be fit to the data. Thus, this method cannot be used for estimating C_p for aldehydes.

In the case of aromatic compounds, the modified application of Eqn.(5) is also extended to compounds not belonging to the homologous series. Tables XXXV, XXXVI, XXXVII, XXXVIII and XXXIX indicate that the prediction of C_p is fairly accurate for o-xylene, p-xylene, m-xylene, pyridine and styrene. In each case, the prediction is better than that obtained from Eqn.(6).

Eqn.(5) can be used along with the general form of Eqn.(7) for predicting C_p for liquids at higher pressures also. The effect of pressure on the density and the thermal conductivity of liquids is usually neglected, except near the critical point (2). Hence, no significant error will be introduced by this estimation technique.

TABLE XXI

VARIATION OF X WITH TEMPERATURE FOR ACETONE

Temperature °C	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	C_p Observed cal/gm°C	$\frac{k}{\gamma C_p}$	$\ln \frac{k}{\gamma C_p}$	$\ln \rho$	x
-80	43.2	0.479	1.028	0.027	-0.105	-0.265
-60	41.7	0.482	0.986	-0.013	-0.133	0.102
-40	40.2	0.486	0.943	-0.058	-0.156	0.373
-20	38.7	0.492	0.896	-0.108	-0.180	0.603
0	37.2	0.504	0.841	-0.172	-0.210	0.818
20	35.8	0.518	0.788	-0.238	-0.235	1.010
40	34.3	0.534	0.732	-0.311	-0.267	1.162
60	32.8	0.552	0.677	-0.389	-0.301	1.292
80	31.4	0.572	0.625	-0.468	-0.335	1.396

TABLE XXII

VARIATION OF X WITH TEMPERATURE FOR METHYL ETHYL KETONE

Temperature °C	Thermal Conductivity $k \times 10^5$ cal/cm.sec°C	C_p Observed cal/gm°C	$\frac{k}{yC_p}$	$\ln \frac{k}{yC_p}$	$\ln \rho$	x
-80	40.8	0.495	0.939	-0.062	-0.105	0.588
-60	39.4	0.499	0.900	-0.105	-0.127	0.821
-40	38.2	0.503	0.865	-0.143	-0.150	0.954
-20	37.0	0.508	0.830	-0.185	-0.174	1.065
0	35.7	0.515	0.790	-0.235	-0.198	1.185
20	34.4	0.524	0.740	-0.289	-0.235	1.228
40	33.2	0.534	0.708	-0.344	-0.267	1.284
60	31.9	0.552	0.658	-0.417	-0.301	1.385
80	30.6	0.572	0.609	-0.494	-0.335	1.473

TABLE XXIII

VARIATION OF X WITH TEMPERATURE FOR DIETHYL KETONE

Temperature °C	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	C_p Observed cal/gm°C	$\frac{k}{yC_p}$	$\ln \frac{k}{yC_p}$	$\ln \rho$	x
-40	37.2	0.482	0.880	-0.127	-0.145	0.881
-20	36.1	0.490	0.840	-0.174	-0.162	1.072
0	35.0	0.500	0.798	-0.225	-0.186	1.209
20	34.0	0.513	0.755	-0.280	-0.204	1.369
40	32.9	0.526	0.713	-0.337	-0.229	1.473

TABLE XXIV

OBSERVED AND PREDICTED HEAT CAPACITIES FOR ACETONE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
-80	0.900	43.2	0.185	0.479	0.502	4.30	0.458	-4.38
-60	0.875	41.7	0.461	0.482	0.505	4.77	0.470	-2.48
-40	0.855	40.2	0.701	0.486	0.511	5.14	0.478	-1.64
-20	0.835	38.7	0.908	0.492	0.519	5.48	0.484	-1.62
0	0.810	37.2	1.070	0.504	0.531	5.35	0.488	-3.17
20	0.790	35.8	1.211	0.518	0.543	4.82	0.496	-4.24
40	0.765	34.3	1.310	0.534	0.555	3.93	0.500	-6.36
60	0.740	32.8	1.373	0.552	0.565	2.35	0.503	-8.87
80	0.715	31.4	1.400	0.572	0.572	0.00	0.506	-11.53

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XXV

OBSERVED AND PREDICTED HEAT CAPACITIES FOR METHYL ETHYL KETONE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
-80	0.900	40.8	0.185	0.495	0.474	4.04	0.432	12.72
-60	0.880	39.4	0.461	0.499	0.476	4.60	0.442	11.42
-40	0.860	38.2	0.701	0.503	0.484	3.25	0.451	10.33
-20	0.840	37.0	0.908	0.508	0.494	2.75	0.467	8.07
0	0.820	35.7	1.070	0.515	0.503	2.33	0.466	9.51
20	0.790	34.4	1.211	0.524	0.521	0.57	0.477	9.85
40	0.765	33.2	1.310	0.534	0.537	-0.56	0.483	9.55
60	0.740	31.9	1.373	0.552	0.549	0.54	0.490	11.23
80	0.715	30.6	1.400	0.572	0.558	2.44	0.493	13.81

* $$\text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XXVI

OBSERVED AND PREDICTED HEAT CAPACITIES FOR DIETHYL KETONE

Temperature °C	Density gm/ml	Thermal Conductivity $k \cdot x\ 10^5$ cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	Cp from Eqn.(6) cal/gm°C	Percent Error*
-40	0.865	37.2	0.701	0.482	0.469	2.69	0.438	7.92
-20	0.850	36.1	0.908	0.490	0.477	2.65	0.445	9.18
0	0.830	35.0	1.070	0.500	0.487	2.60	0.452	9.60
20	0.815	34.0	1.211	0.513	0.496	3.31	0.459	10.52
40	0.795	32.9	1.310	0.526	0.506	3.80	0.464	11.78

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XXVII

OBSERVED AND PREDICTED HEAT CAPACITIES FOR METHYL ISOBUTYL KETONE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	Cp from Eqn.(6) cal/gm°C	Percent Error*
-80	0.880	38.4	0.185	0.420	0.448	-6.66	0.414	1.42
-60	0.865	37.3	0.461	0.424	0.454	-7.07	0.424	0.00
-40	0.850	36.2	0.701	0.429	0.462	-7.69	0.432	-0.70
-20	0.835	35.2	0.908	0.436	0.472	-8.25	0.440	-0.92
0	0.815	34.2	1.070	0.445	0.485	-8.98	0.449	-0.89
20	0.800	33.1	1.211	0.454	0.494	-8.81	0.454	0.00
40	0.785	32.0	1.310	0.464	0.501	-7.97	0.457	1.52
60	0.765	31.0	1.373	0.477	0.510	-6.91	0.462	3.14
80	0.740	30.0	1.400	0.490	0.521	-6.32	0.471	3.87
100	0.725	28.8	1.391	0.506	0.513	-1.38	0.469	7.31
120	0.705	27.8	1.347	0.522	0.507	-1.50	0.472	9.57

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

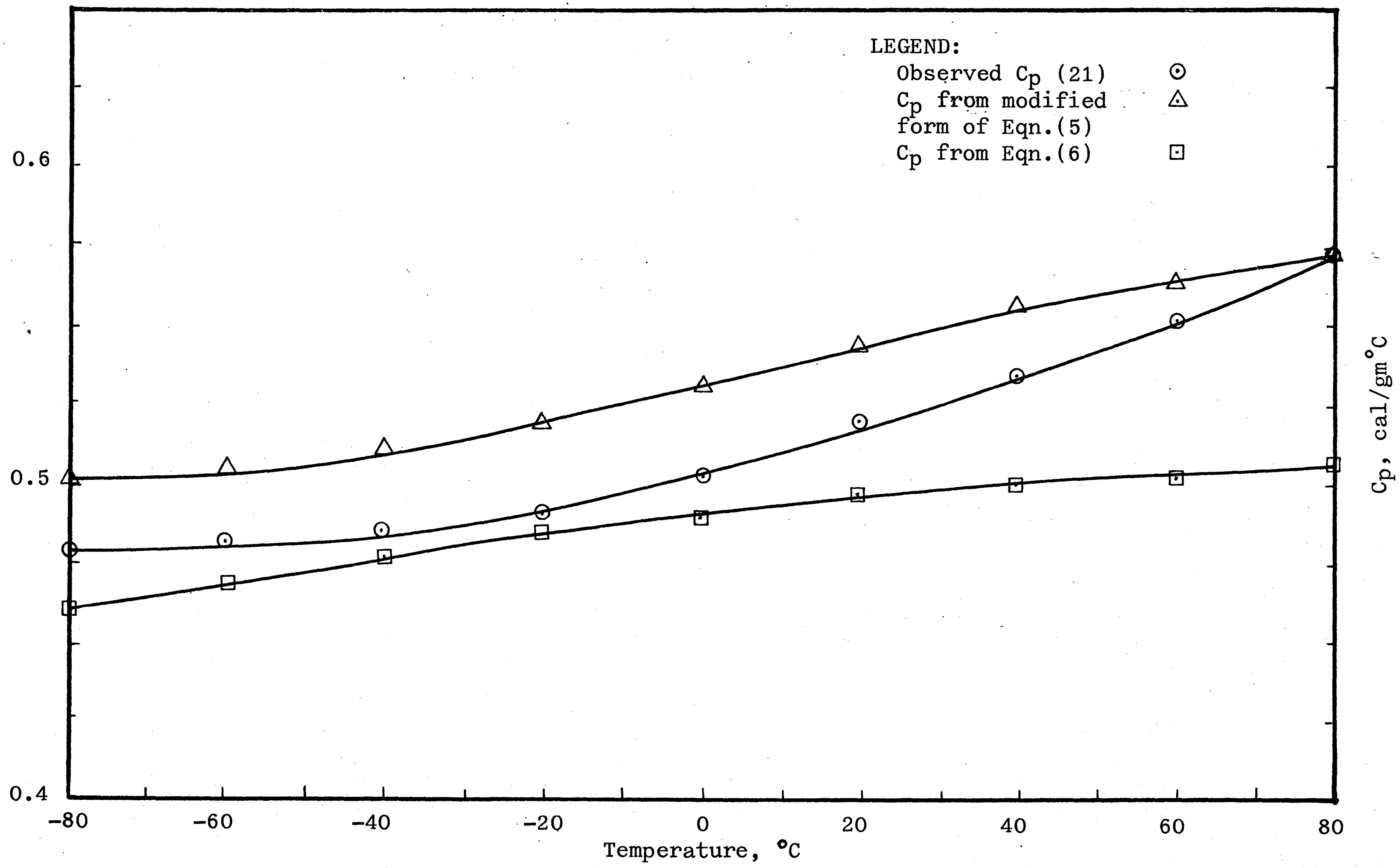

Figure 14. $\underline{C_p}$ for Acetone

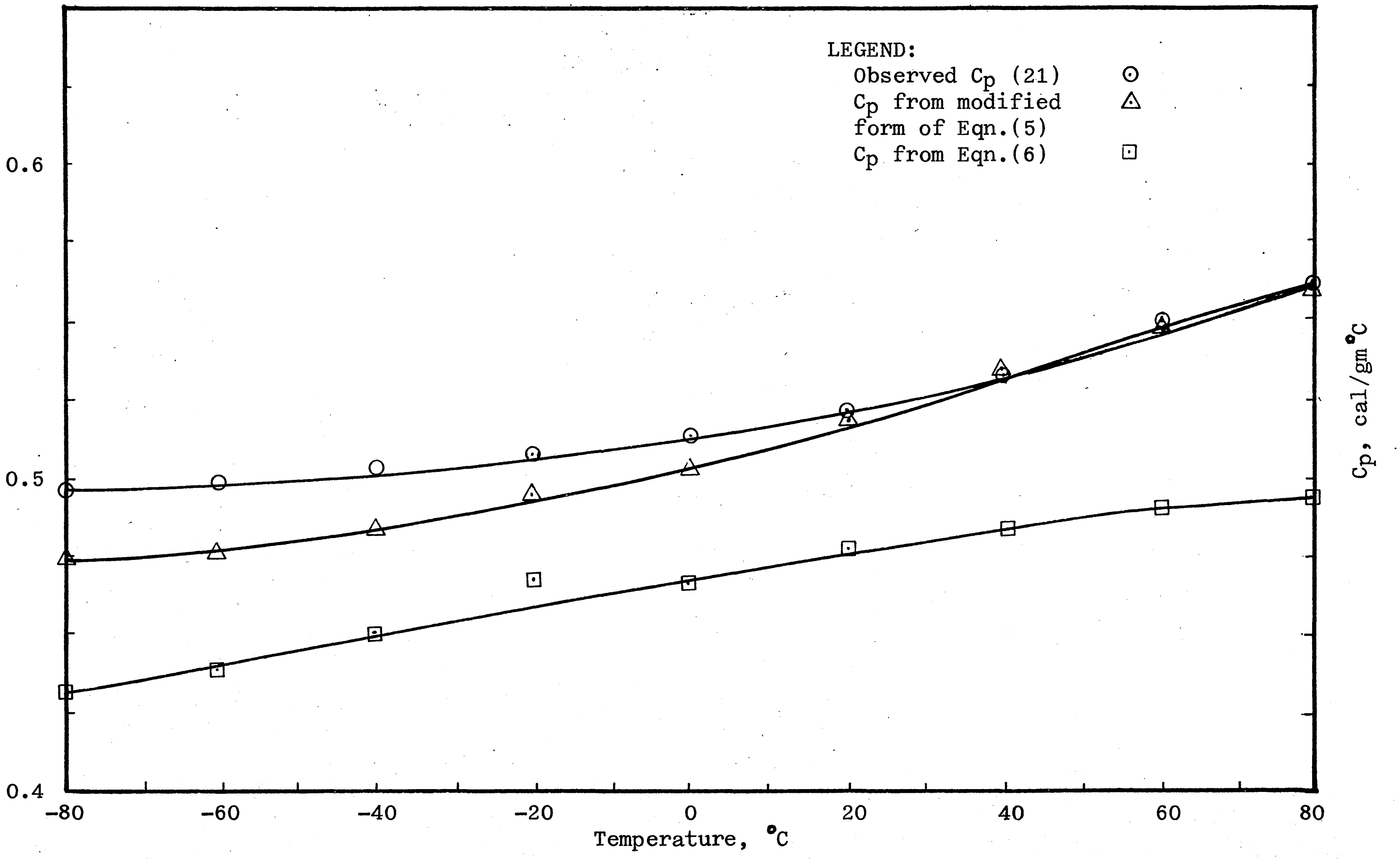

Figure 15. C_p for Methyl Ethyl Ketone (MEK)

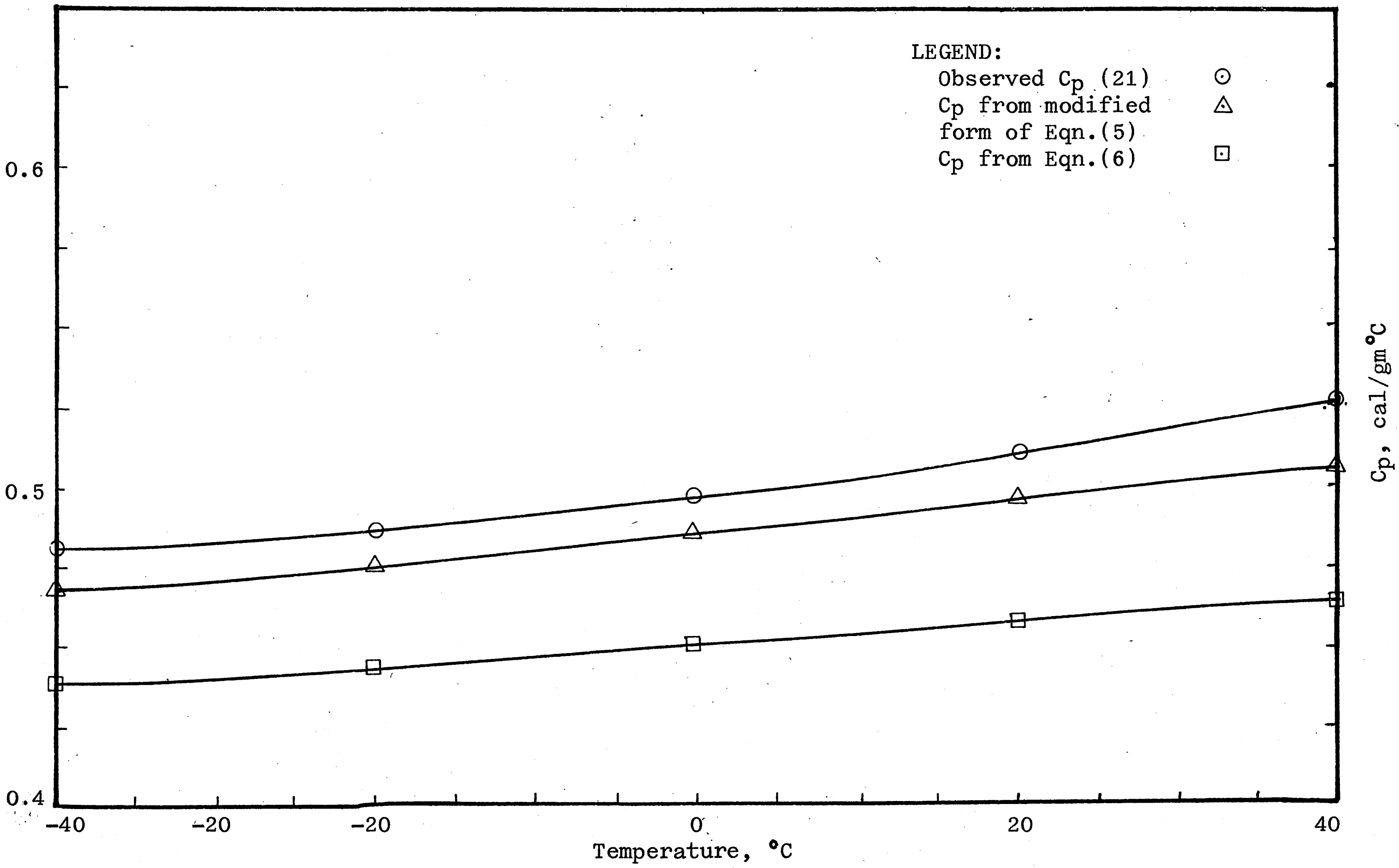

Figure 16. Cp for Diethyl Ketone (DEK)

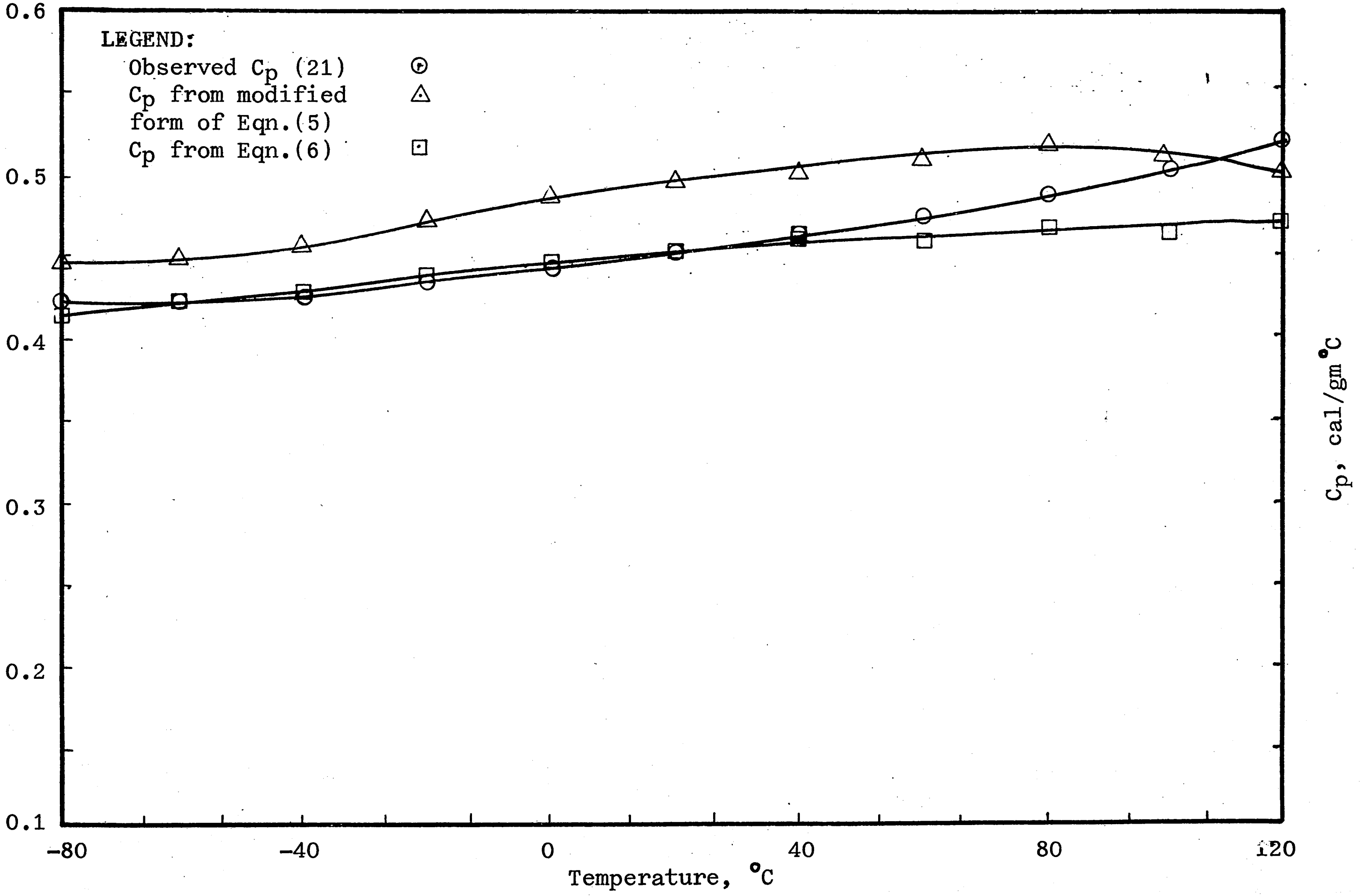

Figure 17. C_p for Methyl Isobutyl Ketone (MIBK)

TABLE XXVIII

VARIATION OF X WITH TEMPERATURE FOR TOLUENE

Temperature °C	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	C_p Observed cal/gm°C	$\frac{k}{yC_p}$	$\ln \frac{k}{yC_p}$	$\ln \rho$	x
0	34.4	0.406	0.966	-0.034	-0.122	0.282
20	33.0	0.415	0.906	-0.097	-0.139	0.703
40	31.6	0.424	0.849	-0.162	-0.162	1.000
60	30.2	0.434	0.793	-0.231	-0.182	1.266
80	28.8	0.446	0.736	-0.306	-0.204	1.496
100	27.5	0.462	0.678	-0.387	-0.231	1.670
120	26.1	0.477	0.623	-0.471	-0.261	1.804
140	24.8	0.492	0.574	-0.553	-0.294	1.881
160	23.4	0.507	0.526	-0.641	-0.328	1.954
180	22.0	0.522	0.480	-0.732	-0.360	2.030
200	20.6	0.536	0.438	-0.825	-0.400	2.060

TABLE XXIX

VARIATION OF X WITH TEMPERATURE FOR ETHYLBENZENE

Temperature °C	Thermal Conductivity k x 10^5 cal/cm.sec.°C	C_p Observed cal/gm°C	$\frac{k}{yC_p}$	$\ln\frac{k}{yC_p}$	$\ln\rho$	x
0	33.4	0.400	0.952	-0.049	-0.122	0.401
20	31.9	0.408	0.891	-0.114	-0.145	0.791
40	30.4	0.416	0.833	-0.182	-0.166	1.098
60	29.0	0.424	0.779	-0.248	-0.186	1.334
80	27.5	0.433	0.724	-0.322	-0.202	1.596
100	26.0	0.444	0.667	-0.403	-0.229	1.760
120	24.8	0.457	0.618	-0.480	-0.254	1.883
140	23.1	0.470	0.560	-0.579	-0.281	2.060
160	21.6	0.483	0.509	-0.673	-0.307	2.187
180	20.1	0.498	0.460	-0.776	-0.338	2.294
200	18.6	0.514	0.412	-0.885	-0.375	2.357

TABLE XXX

VARIATION OF X WITH TEMPERATURE FOR PROPYLBENZENE

Temperature °C	Thermal Conductivity $k \times 10^5$ cal/cm.sec°C	C_p Observed cal/gm °C	$\frac{k}{\gamma C_p}$	$\ln \frac{k}{\gamma C_p}$	$\ln \rho$	x
0	35.5	0.409	0.989	-0.010	-0.133	0.077
20	33.3	0.423	0.897	-0.107	-0.150	0.715
40	31.1	0.437	0.811	-0.208	-0.170	1.223
60	28.9	0.451	0.730	-0.313	-0.192	1.631
80	27.2	0.465	0.666	-0.404	-0.210	1.921
100	25.5	0.479	0.607	-0.499	-0.229	2.175
120	24.0	0.493	0.555	-0.588	-0.254	2.309
140	22.6	0.507	0.508	-0.676	-0.274	2.465
160	21.4	0.520	0.469	-0.756	-0.298	2.535
180	20.3	0.538	0.430	-0.843	-0.325	2.589
200	19.4	0.548	0.403	-0.907	-0.356	2.543

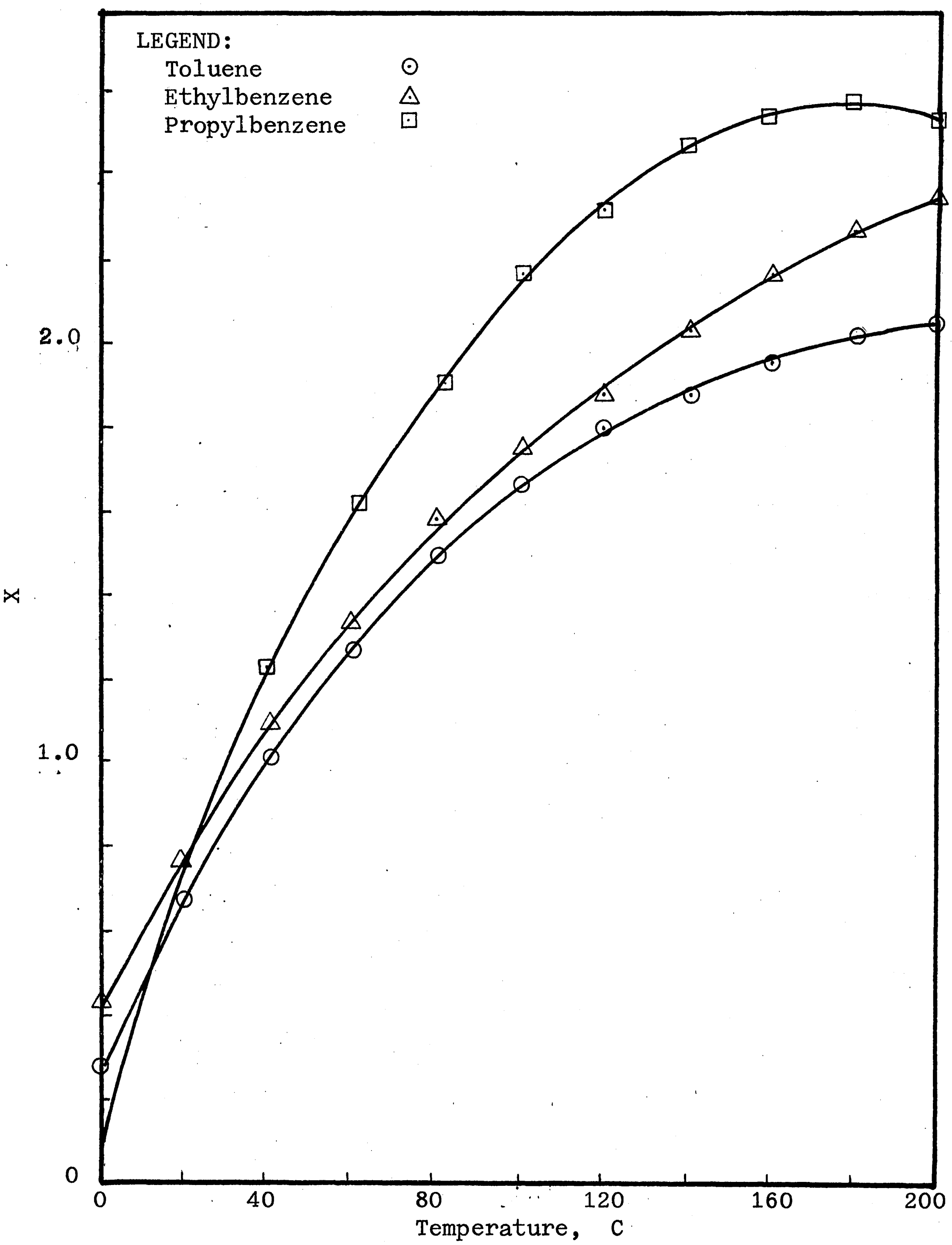

Figure 18. X as a function of temperature for Benzene compounds

TABLE XXXI

OBSERVED AND PREDICTED HEAT CAPACITIES FOR TOLUENE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.885	34.4	0.310	0.406	0.407	0.24	0.422	3.79
20	0.870	33.0	0.712	0.415	0.415	0.00	0.422	1.68
40	0.850	31.6	1.069	0.424	0.428	0.94	0.422	0.47
60	0.833	30.2	1.380	0.434	0.443	2.07	0.419	3.45
80	0.815	28.8	1.645	0.446	0.459	2.91	0.417	6.50
100	0.793	27.5	1.866	0.462	0.483	4.54	0.416	9.95
120	0.770	26.1	2.040	0.477	0.507	6.28	0.412	13.62
140	0.745	24.8	2.170	0.492	0.535	8.73	0.411	16.46
160	0.720	23.4	2.254	0.507	0.559	10.25	0.405	20.11
180	0.697	22.0	2.293	0.522	0.573	9.77	0.398	23.75
200	0.670	20.6	2.286	0.536	0.586	9.32	0.392	26.86

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XXXII

OBSERVED AND PREDICTED HEAT CAPACITIES FOR ETHYLBENZENE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm °C	Percent Error*
0	0.885	33.4	0.310	0.400	0.395	1.25	0.409	-2.25
20	0.865	31.9	0.712	0.408	0.403	1.22	0.410	-0.49
40	0.847	30.4	1.069	0.416	0.413	0.72	0.407	2.16
60	0.820	29.0	1.380	0.424	0.434	-2.35	0.408	3.77
80	0.817	27.5	1.645	0.433	0.437	-0.93	0.397	8.31
100	0.795	26.0	1.866	0.444	0.454	-2.25	0.392	11.71
120	0.775	24.8	2.040	0.457	0.475	-3.93	0.390	14.66
140	0.755	23.1	2.170	0.470	0.484	-2.97	0.378	19.57
160	0.735	21.6	2.254	0.483	0.492	-1.86	0.368	23.80
180	0.713	20.1	2.293	0.498	0.497	0.20	0.357	28.31
200	0.687	18.6	2.286	0.514	0.500	2.72	0.346	32.68

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XXXIII

OBSERVED AND PREDICTED HEAT CAPACITIES FOR PROPYLBENZENE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	Cp from Eqn.(6) cal/gm°C	Percent Error*
0	0.875	35.5	0.310	0.409	0.421	-2.93	0.440	-7.57
20	0.860	33.3	0.712	0.423	0.422	0.23	0.430	-1.65
40	0.843	31.1	1.069	0.437	0.425	2.74	0.418	4.34
60	0.829	28.9	1.380	0.451	0.429	6.12	0.405	10.19
80	0.810	27.2	1.645	0.465	0.438	5.80	0.396	14.83
100	0.795	25.5	1.866	0.479	0.446	6.88	0.384	19.83
120	0.775	24.0	2.040	0.493	0.460	6.69	0.377	23.52
140	0.760	22.6	2.170	0.507	0.467	7.88	0.365	27.41
160	0.742	21.6	2.254	0.520	0.478	8.07	0.361	30.57
180	0.722	20.3	2.293	0.538	0.488	9.29	0.357	33.64
200	0.700	19.4	2.286	0.548	0.499	8.94	0.356	35.05

* Percent Error = $\frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$

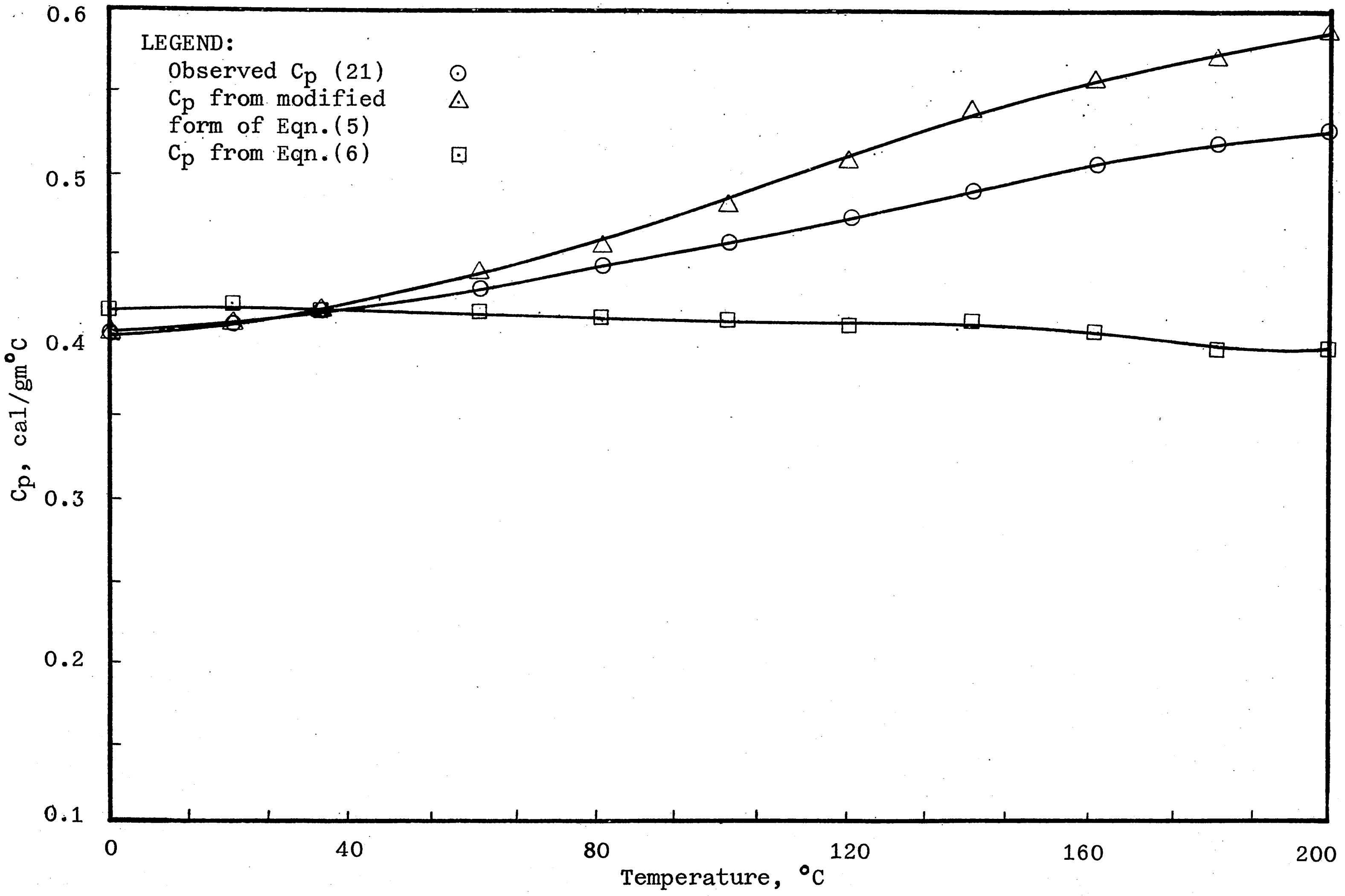

Figure 19. C_p for Toluene

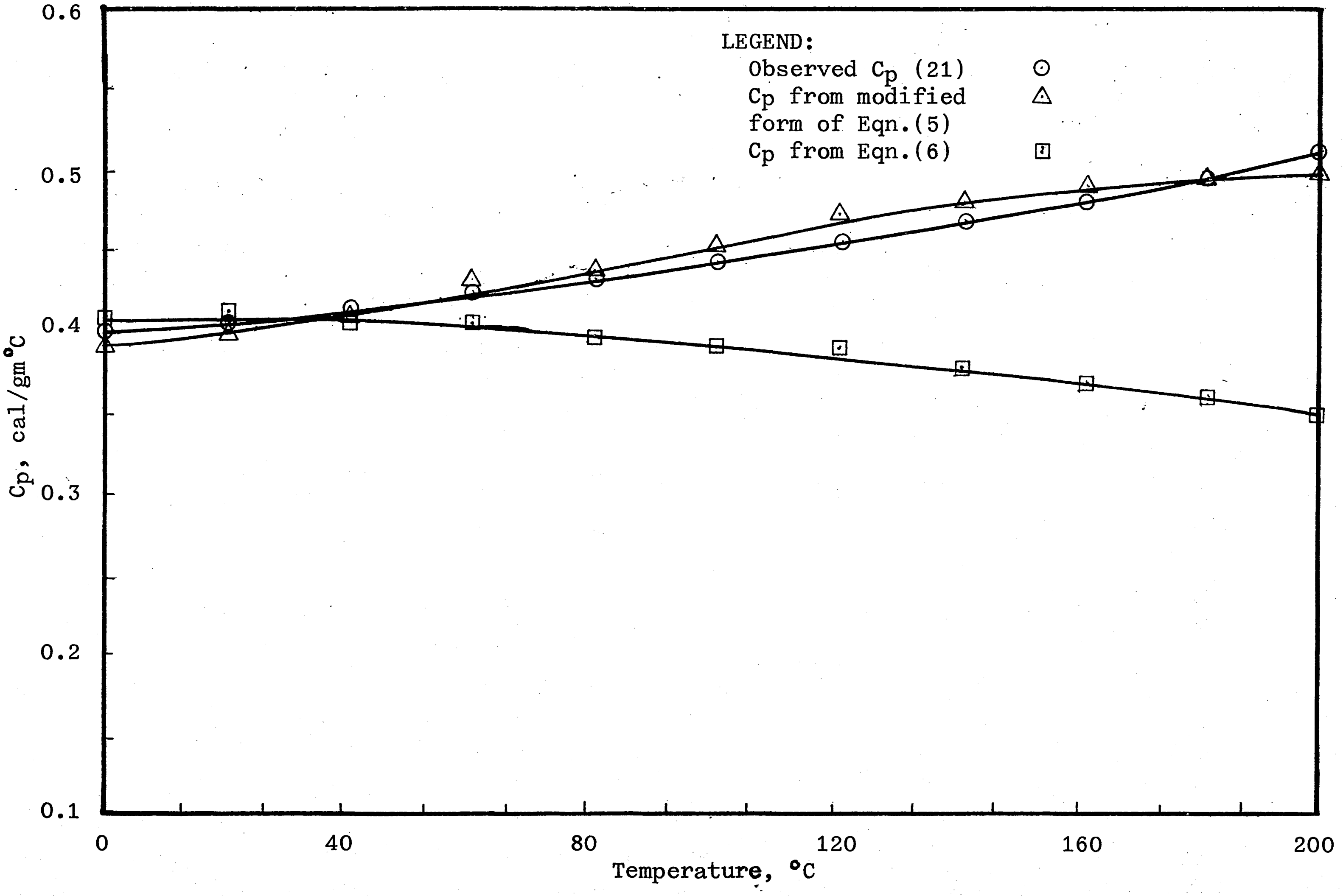

Figure 20. Cp for Ethylbenzene

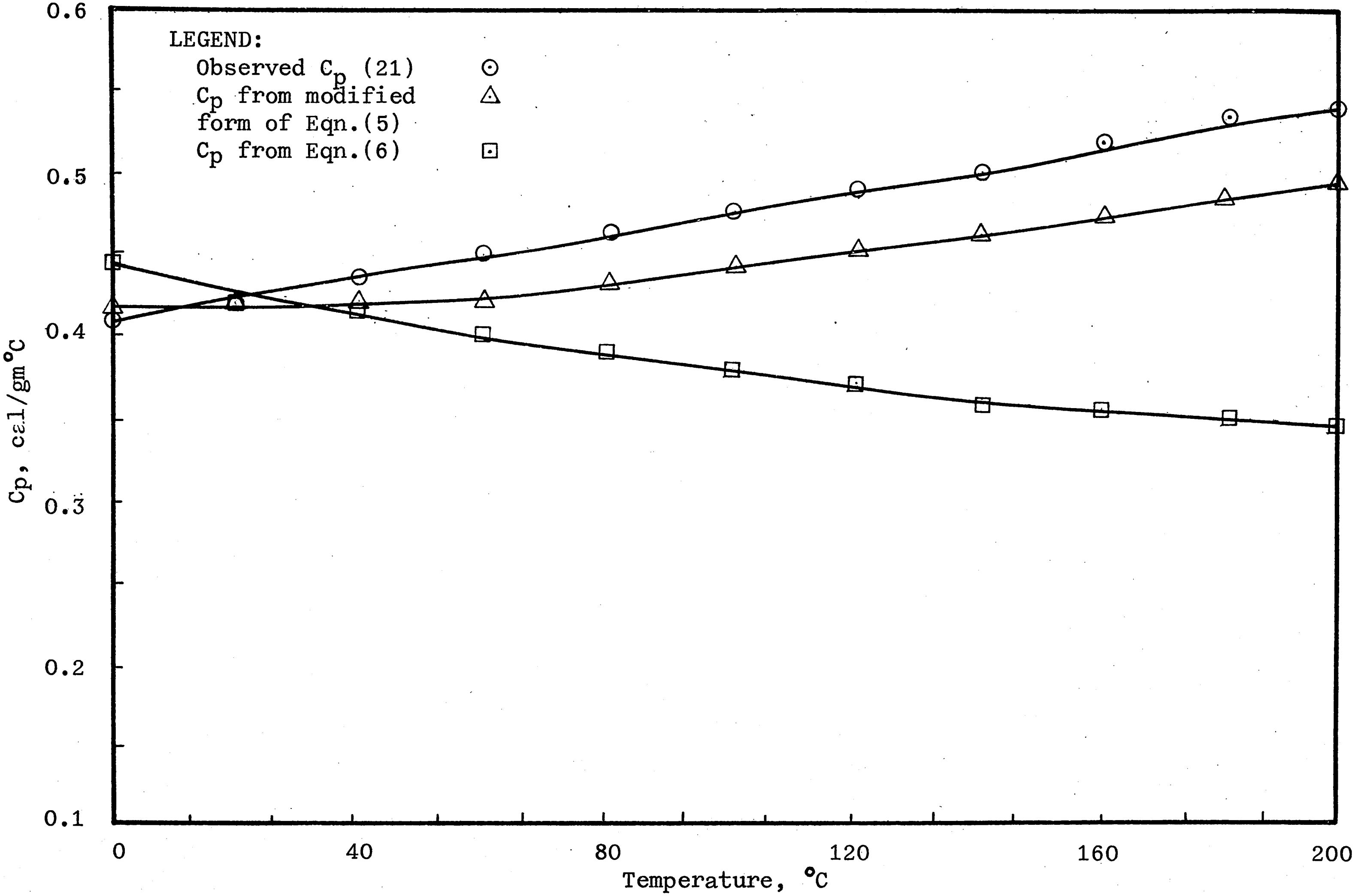

Figure 21. C_p for Propylbenzene

TABLE XXXIV

OBSERVED AND PREDICTED HEAT CAPACITIES FOR BENZENE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
20	0.878	35.3	0.712	0.416	0.441	-6.00	0.448	-7.69
40	0.860	33.6	1.069	0.430	0.450	-4.65	0.445	-3.68
60	0.839	32.1	1.380	0.444	0.466	-4.95	0.444	0.00
80	0.817	30.6	1.645	0.456	0.486	-6.57	0.442	3.07
100	0.795	29.1	1.866	0.470	0.509	-8.29	0.439	6.59
120	0.770	27.6	2.040	0.486	0.536	-10.28	0.436	10.28
140	0.745	26.1	2.170	0.502	0.563	-12.15	0.431	14.14
160	0.720	24.8	2.254	0.520	0.592	-13.84	0.430	17.30
180	0.690	23.6	2.293	0.538	0.630	-17.10	0.431	19.88
200	0.657	22.8	2.286	0.560	0.679	-21.25	0.441	21.25

$$* \quad \text{Percent Error} = \frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

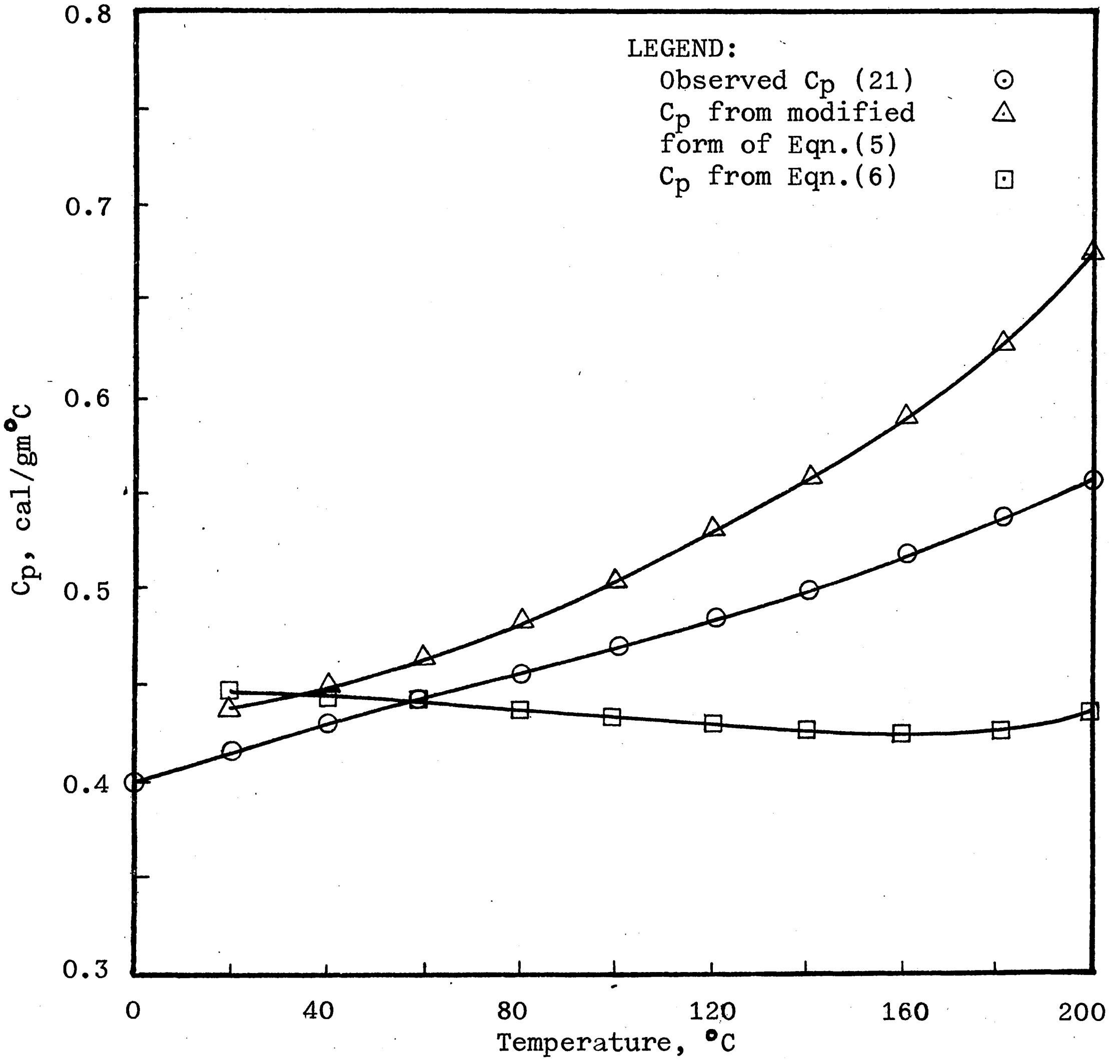

Figure 22. C_p for Benzene

TABLE XXXV

OBSERVED AND PREDICTED HEAT CAPACITIES FOR o-XYLENE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	x	Cp Observed cal/gm °C	Cp Calculated with modified form of Eqn.(5) cal/gm °C	Percent Error	Cp from Eqn.(6) cal/gm °C	Percent Error*
0	0.900	36.0	0.310	0.413	0.424	-2.66	0.460	-11.38
20	0.880	33.8	0.712	0.424	0.422	0.47	0.428	-0.94
40	0.863	31.9	1.069	0.432	0.425	1.62	0.421	2.54
60	0.845	30.0	1.380	0.440	0.431	2.04	0.412	6.35
80	0.830	28.4	1.645	0.449	0.439	2.22	0.404	10.02
100	0.812	26.8	1.866	0.459	0.450	1.96	0.397	13.50
120	0.794	25.4	2.040	0.470	0.463	1.48	0.391	16.80
140	0.775	24.1	2.170	0.492	0.477	3.04	0.386	21.54
160	0.754	22.7	2.254	0.507	0.489	3.55	0.379	25.24
180	0.732	21.4	2.293	0.511	0.498	2.54	0.372	27.20
200	0.707	20.0	2.286	0.528	0.503	4.73	0.364	31.06

$$* \quad \text{Percent Error} = \frac{(\text{Observed value}) - (\text{Calculated value})}{(\text{Observed value})}$$

TABLE XXXVI

OBSERVED AND PREDICTED HEAT CAPACITIES FOR p-XYLENE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec°C	x	C_p Observed cal/gm°C	C_p Calculated with modified form of Eqn.(5) cal/gm°C	Percent Error	Cp from Eqn.(6) cal/gm°C	Percent Error*
20	0.860	31.8	0.712	0.405	0.403	0.49	0.410	-1.23
40	0.840	29.9	1.069	0.420	0.410	2.38	0.404	3.80
60	0.823	28.4	1.380	0.435	0.423	2.75	0.398	8.50
80	0.805	27.0	1.645	0.451	0.439	2.66	0.394	12.63
100	0.785	25.8	1.866	0.468	0.462	1.28	0.393	16.02
120	0.767	24.6	2.040	0.486	0.481	1.02	0.390	19.75
140	0.748	23.4	2.170	0.504	0.501	0.59	0.386	23.41
160	0.727	22.0	2.254	0.522	0.514	1.63	0.378	27.58
180	0.705	20.8	2.293	0.540	0.528	2.22	0.374	30.74
200	0.682	19.6	2.286	0.559	0.536	4.11	0.368	34.16

* $$\text{Percent Error} = \frac{(\text{ Oberved value }) - (\text{ Calculated value })}{(\text{ Observed value })}$$

TABLE XXXVII

OBSERVED ANE PREDICTED HEAT CAPACITIES FOR m-XYLENE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated from modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
0	0.885	33.3	0.310	0.403	0.394	2.23	0.408	-1.24
20	0.870	30.9	0.712	0.410	0.389	5.12	0.395	3.65
40	0.850	29.9	1.069	0.416	0.424	2.64	0.399	4.08
60	0.833	28.4	1.380	0.424	0.416	1.88	0.394	7.07
80	0.815	25.9	1.645	0.434	0.413	4.83	0.374	13.82
100	0.793	24.5	1.866	0.446	0.430	3.58	0.370	17.04
120	0.772	23.1	2.040	0.460	0.446	3.04	0.364	20.87
140	0.750	21.9	2.170	0.476	0.466	2.10	0.361	24.16
160	0.726	20.7	2.254	0.490	0.485	1.02	0.356	27.34
180	0.704	19.5	2.293	0.505	0.497	1.58	0.350	30.67
200	0.680	18.2	2.286	0.520	0.501	3.65	0.341	34.42

* Percent Error = $\dfrac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$

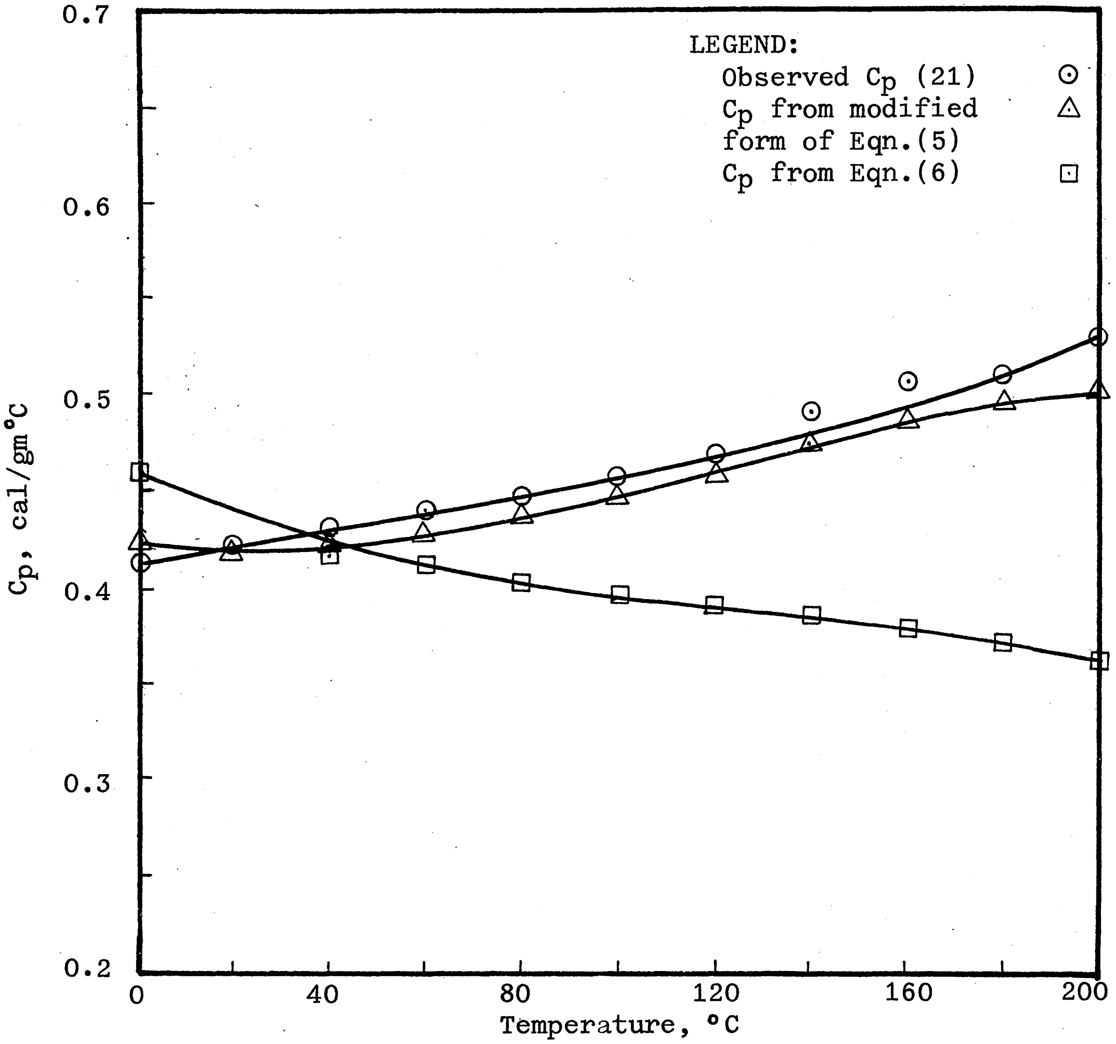

Figure 23. C_p for o-Xylene

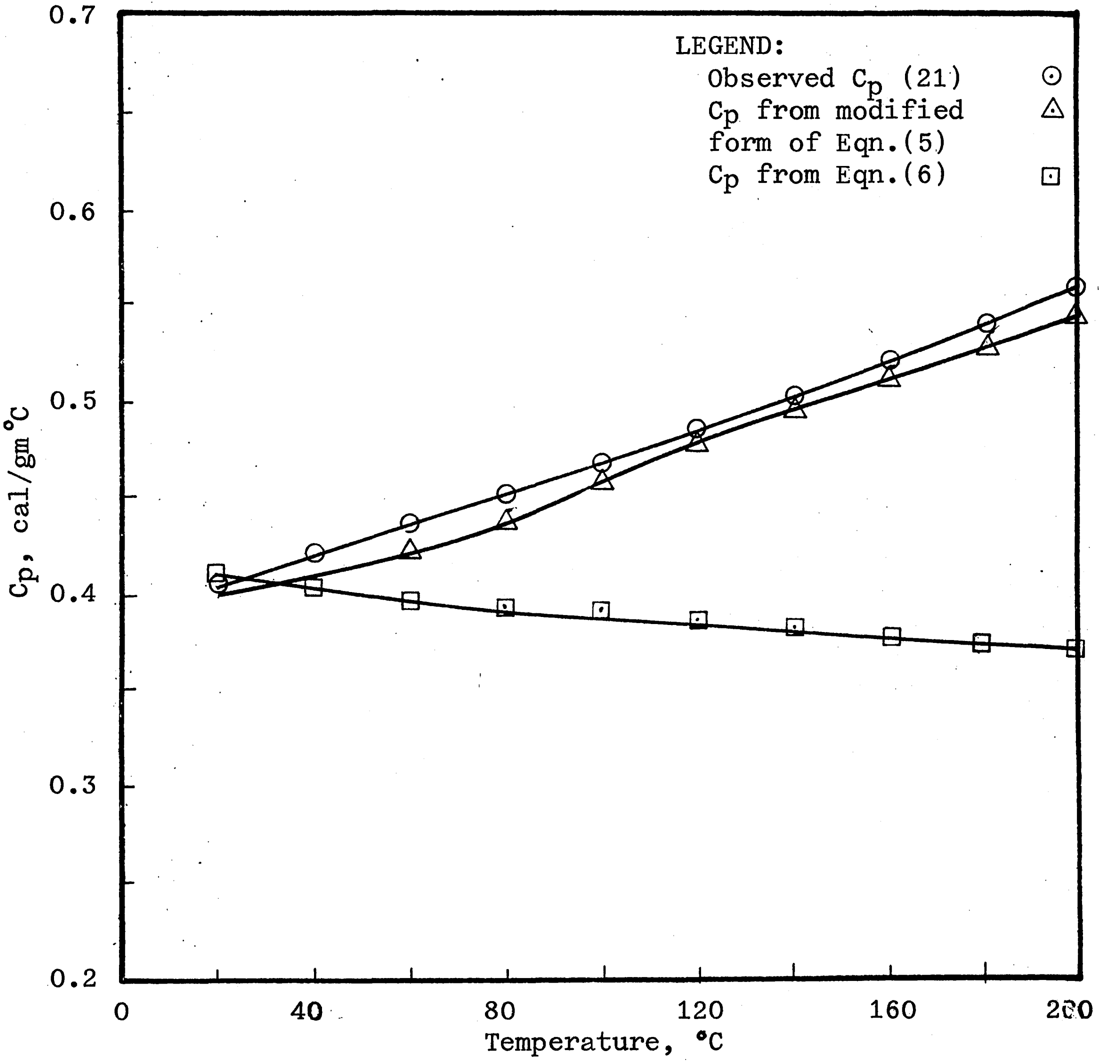

Figure 24. C_p for p-Xylene

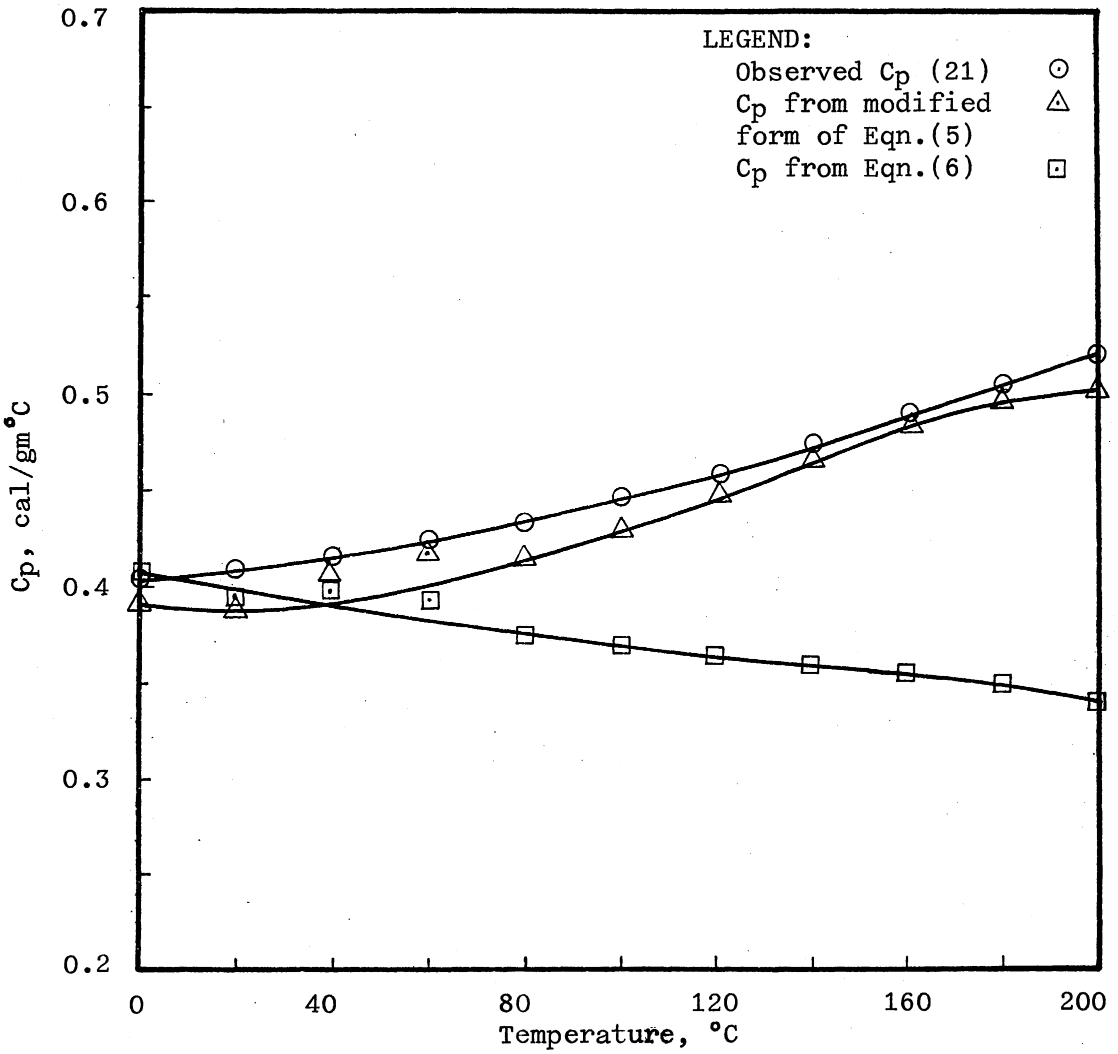

Figure 25. C_p for m-Xylene

TABLE XXXVIII

OBSERVED AND PREDICTED HEAT CAPACITIES FOR PYRIDINE

Temperature °C	Density gm/ml	Thermal Conductivity k x 10^5 cal/cm.sec.°C	x	C_p Observed cal/gm°C	Cp Calculated from modified form of Eqn.(5) cal/gm °C	Percent Error	Cp from Eqn.(6) cal/gm °C	Percent Error*
0	1.012	46.50	0.310	0.400	0.528	-32.00	0.510	-27.50
20	0.990	43.50	0.712	0.412	0.499	-21.11	0.500	-21.36
40	0.968	40.50	1.069	0.423	0.478	-13.00	0.486	-14.89
60	0.945	37.70	1.380	0.434	0.464	-6.91	0.472	-8.75
80	0.922	35.50	1.645	0.446	0.462	-3.58	0.464	-4.03
100	0.900	33.50	1.866	0.457	0.464	-1.50	0.456	0.22
120	0.880	31.50	2.040	0.468	0.466	0.42	0.446	4.70
140	0.860	30.00	2.170	0.480	0.474	1.25	0.441	8.12
160	0.835	28.50	2.254	0.494	0.487	1.41	0.437	11.54
180	0.800	26.70	2.293	0.508	0.507	0.19	0.432	14.96
200	0.782	25.00	2.286	0.525	0.500	4.76	0.418	20.38

$$* \quad \text{Percent Error} = \frac{(\text{Observed value}) - (\text{Calculated value})}{(\text{Observed value})}$$

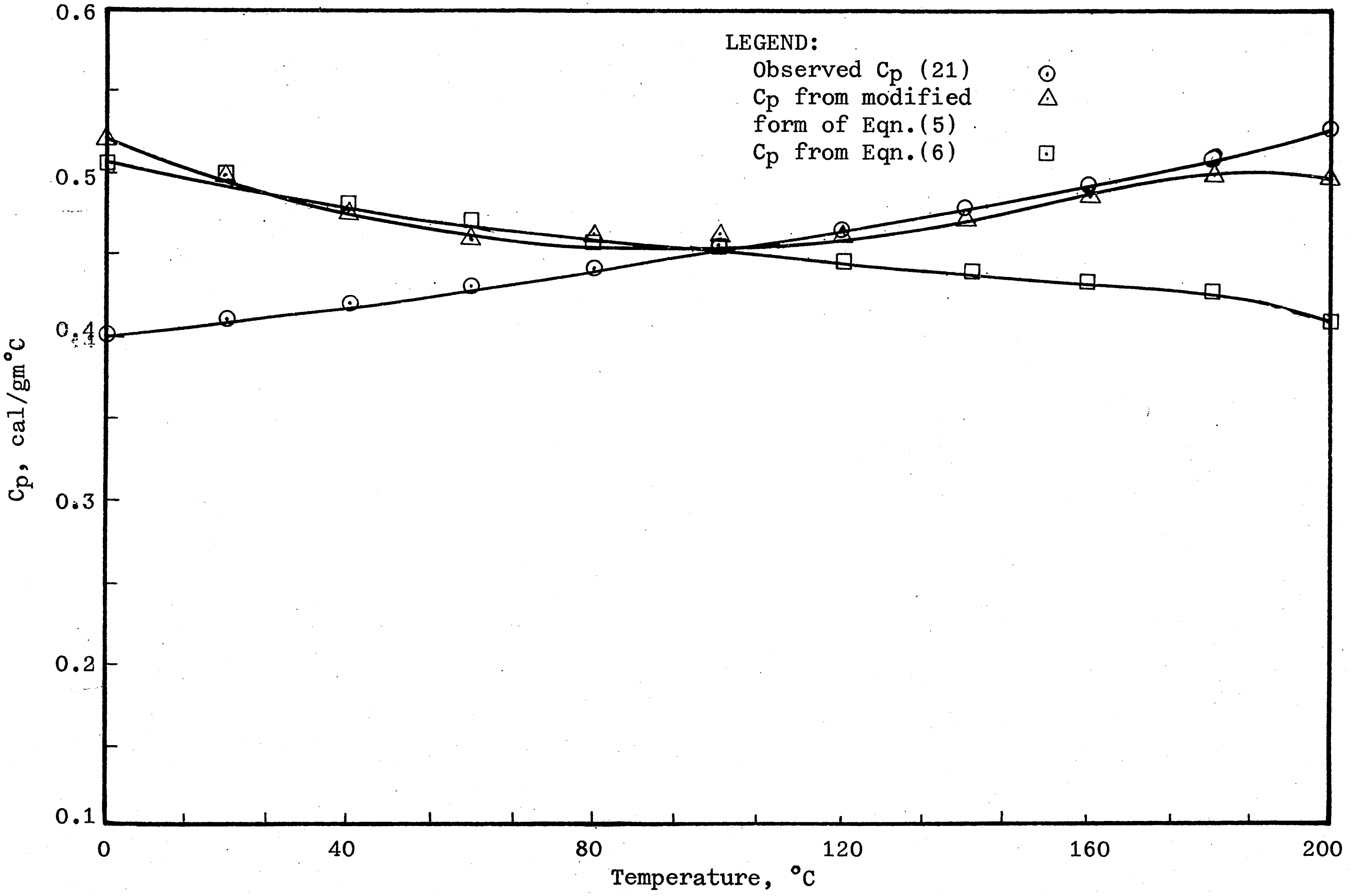

Figure 26. C_p for Pyridine

TABLE XXXIX

OBSERVED AND PREDICTED HEAT CAPACITIES FOR STYRENE

Temperature °C	Density gm/ml	Thermal Conductivity $k \times 10^5$ cal/cm.sec.°C	x	C_p Observed cal/gm°C	C_p Calculated from modified form of Eqn.(5) cal/gm°C	Percent Error	C_p from Eqn.(6) cal/gm°C	Percent Error*
20	0.900	34.9	0.712	0.400	0.429	-7.22	0.434	-8.57
40	0.883	33.2	1.069	0.417	0.432	-3.58	0.430	-3.06
60	0.865	31.6	1.380	0.435	0.440	-1.17	0.426	1.93
80	0.845	30.2	1.645	0.452	0.454	-0.37	0.425	6.07
100	0.825	29.1	1.866	0.475	0.475	0.00	0.426	10.31
120	0.805	28.2	2.040	0.502	0.500	0.40	0.430	14.37
140	0.787	27.5	2.170	0.532	0.527	0.97	0.435	18.16
160	0.768	27.0	2.254	0.572	0.572	0.00	0.444	22.36

* Percent Error = $\frac{(\text{ Observed value }) - (\text{ Calculated value })}{(\text{ Observed value })}$

TABLE XL

VARIATION OF X WITH TEMPERATURE FOR PROPIONALDEHYDE

Temperature °C	$\frac{k}{yC_p}$	$\ln\frac{k}{yC_p}$	Density gm/ml	$\ln\rho$	x
-40	1.094	0.090	0.855	-0.156	-0.577
-20	0.959	-0.041	0.825	-0.192	0.214
0	0.896	-0.109	0.815	-0.204	0.533
20	0.828	-0.188	0.790	-0.235	0.799
40	0.774	-0.256	0.770	-0.261	0.979
60	0.706	-0.347	0.745	-0.294	1.180

TABLE XLI

VARIATION OF X WITH TEMPERATURE FOR BUTRYLALDEHYDE

Temperature °C	$\frac{k}{yC_p}$	$\ln\frac{k}{yC_p}$	Density gm/ml	$\ln\rho$	x
-60	0.923	-0.079	0.885	-0.122	0.647
-40	0.884	-0.122	0.860	-0.150	0.815
-20	0.850	-0.162	0.840	-0.174	0.932
0	0.793	-0.231	0.819	-0.199	1.157
20	0.756	-0.279	0.795	-0.229	1.216
40	0.707	-0.345	0.775	-0.254	1.356
60	0.651	-0.428	0.755	-0.281	1.524

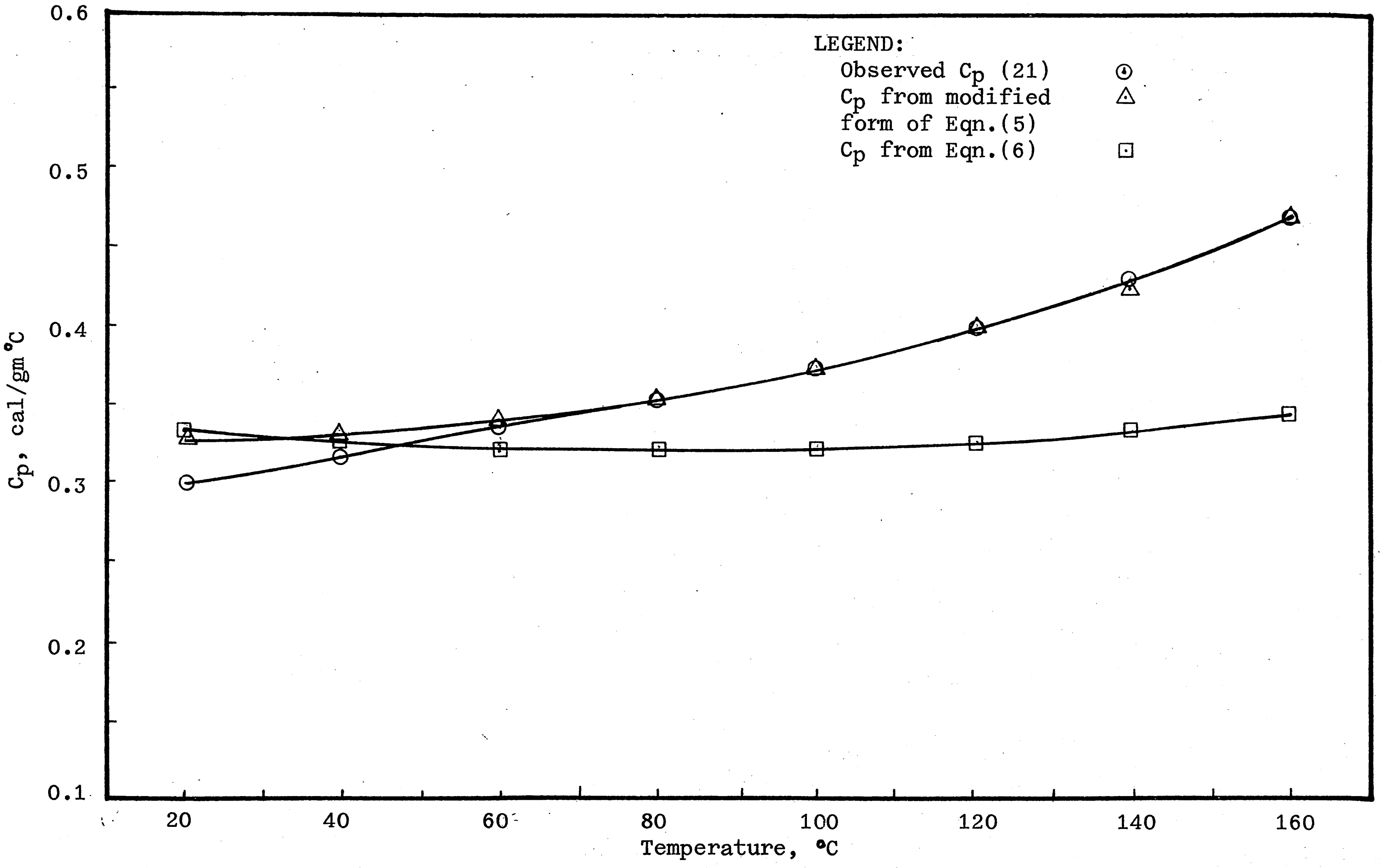

Figure 27. C_p for Styrene

TABLE XLII

VARIATION OF X WITH TEMPERATURE FOR FOMALDEHYDE

Temperature °C	$\frac{k}{yC_p}$	$\ln \frac{k}{yC_p}$	Density gm/ml	$\ln \rho$	x
-80	1.393	0.332	0.841	-0.173	-1.916
-60	1.237	0.213	0.820	-0.198	-1.075
-40	1.092	0.008	0.800	-0.223	-0.396
-20	0.961	-0.039	0.775	-0.254	0.154
0	0.851	-0.160	0.752	-0.284	0.565
20	0.753	-0.282	0.727	-0.318	0.889

TABLE XLIII

VARIATION OF X WITH TEMPERATURE FOR ACETALDEHYDE

Temperature °C	$\frac{k}{yC_p}$	$\ln \frac{k}{yC_p}$	Density gm/ml	$\ln \rho$	x
-60	1.957	0.671	0.875	-0.133	-5.029
-40	1.765	0.568	0.850	-0.162	-3.497
-20	1.683	0.520	0.825	-0.192	-2.706
0	1.567	0.449	0.800	-0.223	-2.015
20	1.433	0.360	0.775	-0.254	-1.414

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

Conclusions

1) Examination of the results presented shows that the heat capacity of organic liquids can be predicted from a knowledge of the thermal conductivity and the density, using a modified approach in the application of Eqn.(5).

2) The exponent x is not a constant, but a function of temperature. It exhibits a polynomial behaviour for alcohols, ketones and aromatic compounds.

3) The heat capacity values predicted from this technique yield better results than those obtained from Eqn.(6).

4) This technique can also be applied to predict the heat capacity of liquids at higher pressure.

5) This method of estimation is not applicable to aldehydes. It can be applied for any homologous series for which x is of the same order of magnitude for the members.

Recommendations

1) That the general form of Eqn.(7) be used only in the range for which the co-efficients of the equation have been computed. Any attempt to extrapolate x beyond this range of temperature may give

rise to large errors in the predicted values.

2) The general form of Eqn.(7) will work for the higher members of a homologous series. It may or may not do so for the first member. For aromatic coumpounds, Eqn.(7) can also be used for compounds not belonging to the series of benzene compounds. However, care must be exercised to choose only those compounds which have groups similar to those of the benzene compounds.

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APPENDIX A

NOMENCLATURE

A, B, C	Co-efficients of the plynomial in Eqn.(7)
C_p	Heat Capacity, cal/gm°C
k	Thermal Conductivity, cal/cm.sec.°C
L	Intermolecular free length, A
T	Temperature, °K
U_s	Sonic Velocity, cm/sec
x, y	Empirical Constants
ρ	Density, gm/ml

APPENDIX B

SAMPLE CALCULATIONS FOR EVALUATING C_p FOR ETHANOL USING EQN.(7)

Vargaftik (19) reports the specific volume, v for ethanol at different temperatures. At 0°C,

$$v \times 10^3 = 1.213 \text{ m}^3/\text{kg}$$

$$v = 1.213 \times 10^{-3} \text{ m}^3/\text{kg}$$

$$\rho = 1/v$$

$$= \frac{10^3}{1.213} \text{ kg/m}^3$$

$$= \frac{10^3}{1.213}\left(\frac{\text{kg}}{\text{m}^3}\right) 10^3 \left(\frac{\text{gm}}{\text{kg}}\right) \frac{1}{10^6}\left(\frac{\text{m}^3}{\text{cm}^3}\right)$$

$$= \frac{1}{1.213} \text{ gm/cm}^3$$

$$= 0.8244 \text{ gm/ml}$$

Figure 28 shows k as a function of temperature. A smooth curve was drawn through the points and the value of k at intermediate temperatures were obtained from the graph. At 0°C,

$$k \times 10^4 = 1725 \text{ W/m C}$$

$$= 1725\left(\frac{\text{W}}{\text{m C}}\right) \frac{1}{100}\left(\frac{\text{m}}{\text{cm}}\right)$$

$$= 17.25 \text{ W/cm}^\circ\text{C}$$

$$= (17.25)(0.2389) \text{ cal/cm.sec.}^\circ\text{C}$$

$$= 4.121 \text{ cal/cm.sec.}^\circ\text{C}$$

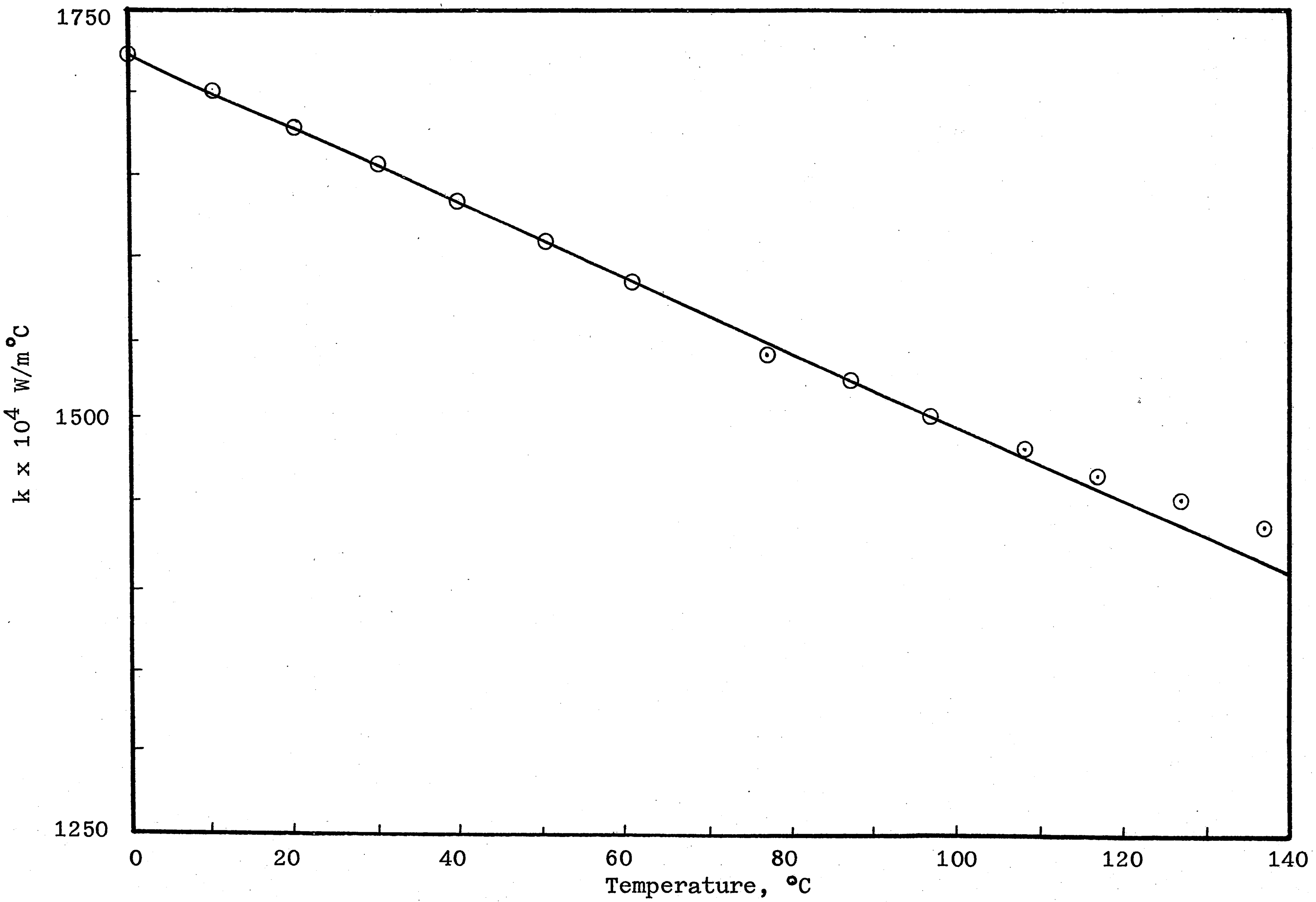

Figure 28. k as a function of temperature for Ethanol

$$k = 4.121 \times 10^{-4} \text{ cal/cm.sec.}^{\circ}\text{C}$$

$$y = 0.877 \times 10^{-3}$$

$$x = 0.83$$

Hence, from Eqn.(6),

$$4.121 \times 10^{-4} = 0.877 \times 10^{-3}\ C_p\ (0.8244)^{0.83} \left(\frac{293}{273}\right)^{0.38}$$

$$C_p = 0.536 \text{ cal/gm}^{\circ}\text{C}$$

APPENDIX C

SAMPLE CALCULATIONS FOR EVALUATING C_p FOR n-HEPTYL ALCOHOL USING EQN.(7) AND EQN.(5)

At 150°C,

$$k = 0.258 \times 10^{-3} \text{ cal/cm.sec.}^\circ\text{C}$$

$$= 0.7285 \text{ gm/ml}$$

$$150^\circ\text{C} = (150+273)^\circ\text{K} = 423^\circ\text{K}$$

From Eqn.(7),

$$x = -9.2655 + (0.0547)(423) + (-6.466 \times 10^{-5})(423)^2$$

$$= 2.303$$

From Eqn.(5),

$$0.258 \times 10^{-3} = 0.877 \times 10^{-3}\ C_p\ (0.7285)^{2.303}$$

$$C_p = 0.610 \text{ cal/gm}^\circ\text{C}$$

$$\text{Observed } C_p = 0.795 \text{ cal/gm}^\circ\text{C}$$

$$\text{Percent Error} = \frac{(0.795 - 0.610)}{(0.795)} \times 100$$

$$= 23.27$$

2

VITA

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