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Thermal Conductivity of Normal Pentane in the Temperature Range 306–360 K at Pressures up to 0.5 GPa

A. M. F. Palavra,[1] W. A. Wakeham,[2] and M. Zalaf[2]

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This paper reports the results of new, absolute measurements of the thermal conductivity of normal pentane in the temperature range 306 to 360 K at pressures up to 0.50 GPa. The experimental data have an estimated uncertainty of ±0.3%. The density dependence of the thermal conductivity along all of the isotherms cannot be represented by a common equation within its estimated uncertainty. Nevertheless, such a universal equation does provide a simple method of correlating the complete set of data with an error of no more than ±2.5%.

KEY WORDS: alkanes; hard-sphere theory; liquid; normal pentane; thermal conductivity.

1. INTRODUCTION

A recent qualitative study [1] has shown that the thermal conductivity and viscosity of a large number of normal alkanes in the dense liquid phase can be represented by means of a single consistent scheme based upon a hard-sphere model of the fluid. The thermodynamic conditions included in this study extended from 90 to 400 K for pressures up to 0.7 GPa and the fluids included ranged from ethane to undecane. Normal pentane was not included in the study because, at the time, no experimental thermal conductivity data of a high accuracy were available, although the viscosity has been determined along one isotherm up to 100 MPa by Cappi [2]. In

[1] Instituto Superior Tecnico, Complexo Interdisciplinar, Avenida Rovisco Pais, Lisbon, Portugal.

[2] Department of Chemical Engineering and Chemical Technology, Imperial College, Prince Consort Road, London SW7 2BY, United Kingdom.

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order to fill the gap in the available information before a complete and quantitative study of the same kind is repeated, we have performed new, absolute measurements of the thermal conductivity of normal pentane at pressures up to 0.5 GPa.

2. EXPERIMENTAL

The measurements have been carried out in the high-pressure transient hot-wire instrument described in detail elsewhere [3]. Apart from the replacement of the cell wires especially for these measurements, the operating procedure remained unchanged. The measurements have been carried out along four isotherms in the temperature range 306 to 360 K at pressures up to 0.5 GPa. The normal pentane sample was supplied by BDH Chemicals Ltd., with a stated purity better than 99%. Following distillation and degassing a chromatographic analysis demonstrated a purity in excess of 99.9%.

The density of normal pentane has been measured by a number of investigators [4–7] under the conditions of interest. For the purposes of applying small corrections in the analysis of the thermal conductivity data, we have consistently employed the results of Bridgman [5] together with the heat capacity data given by Vargaftik [8]. However, for the purposes of representing the thermal conductivity of normal pentane as a function of density, we prefer to employ the more accurate, although less extensive, data of Easteal and Woolf [4]. These new results cover the temperature range 278.15 to 338.15 K and pressures up to 280 MPa and have an estimated uncertainty of $\pm 0.2\%$. These densities are not entirely consistent with earlier data [5–7] in the overlapping range of states, the deviations exceeding 1% in some cases. Some doubt is therefore cast on the older results. Consequently, in our tabulation of results, we include densities only for those conditions which may be obtained by interpolation or a modest extrapolation of those covered by Easteal and Woolf. In other cases the uncertainty in the tabulated density would be larger than that in the corresponding thermal conductivity.

3. RESULTS

Tables I to IV list the experimental data for the thermal conductivity of normal pentane along the four isotherms at 305.8, 322.8, 342.5, and 359.5 K. In each table we provide the thermal conductivity adjusted to a nominal temperature by means of a linear correction, which never exceeded $\pm 0.2\%$, at both the experimental pressure, P, and the reference density, ρ

Table I. The Thermal Conductivity of *n*-Pentane at $T_{nom} = 305.8$ K

Pressure P (MPa)	Density ρ ($kg \cdot m^{-3}$)	Thermal conductivity ($mW \cdot m^{-1} \cdot K^{-1}$)	
		$\lambda(T_{nom}, \rho)$	$\lambda(T_{nom}, P)$
1.79	614.7	110.0	110.5
5.69	619.8	112.9	113.3
14.12	630.7	118.1	118.0
24.74	640.9	123.1	123.3
35.42	650.7	128.3	128.3
47.28	660.1	133.5	133.5
58.63	668.1	137.9	138.0
62.83	670.9	139.1	139.3
69.35	675.1	142.4	142.4
80.43	681.8	146.1	146.2
91.09	687.8	150.8	150.9
102.2	693.7	154.1	154.1
112.1	698.5	157.4	157.4
122.6	703.5	160.7	160.7
134.1	708.6	163.8	163.8
143.2	712.5	167.1	167.1
145.1	713.2	166.9	166.9
153.6	716.6	170.4	170.5
167.5	722.1	173.5	173.5
180.8	727.3	177.6	177.5
197.8	733.4	182.0	182.0
213.4	738.7	186.6	186.6
229.9	744.3	190.1	190.1
243.4	748.7	192.9	193.0
262.5	754.6	197.5	197.5
283.1	760.9	202.1	202.1
303.1	—	—	206.1
332.9	—	—	209.8
342.4	—	—	214.4
362.7	—	—	217.9
382.6	—	—	222.1
402.4	—	—	225.4
427.6	—	—	230.4
453.1	—	—	234.3
476.4	—	—	238.6
501.2	—	—	242.4

[3]. For the reasons set out above the density is not tabulated above 280 MPa for any isotherm and not at all for the highest isotherm.

For the purposes of interpolation we have represented the pressure dependence of the thermal conductivity along each isotherm by an equation of the form

$$\lambda = \lambda' \left\{ 1 + \sum_{i=1}^{4} a_i [(P - P')/P']^i \right\} \tag{1}$$

Table II. The Thermal Conductivity of *n*-Pentane at $T_{nom} = 322.8$ K

Pressure P (MPa)	Density ρ (kg · m^{-3})	Thermal conductivity (mW · m^{-1} · K^{-1})	
		$\lambda(T_{nom}, \rho)$	$\lambda(T_{nom}, P)$
3.69	601.0	106.0	106.2
4.85	602.9	106.9	107.0
14.86	615.9	112.9	113.1
24.85	627.5	118.1	118.2
37.93	640.3	124.5	124.5
52.35	652.3	130.7	130.6
65.38	661.8	136.0	135.9
70.27	664.9	137.4	137.4
81.04	671.9	142.0	142.0
94.44	679.7	146.7	146.7
112.2	689.0	151.4	151.3
124.4	695.0	115.2	155.1
142.3	703.1	161.5	161.5
155.8	708.8	165.5	165.5
173.2	715.9	170.2	170.2
173.4	716.0	170.3	170.3
187.4	721.4	173.1	173.1
203.4	727.4	177.3	177.3
217.4	732.5	181.1	181.1
236.9	739.4	185.5	185.5
257.6	746.4	190.0	190.0
277.9	753.0	194.7	194.7
300.3	—	—	199.7
322.1	—	—	203.6
342.3	—	—	207.8
368.1	—	—	212.6
394.3	—	—	217.3
417.0	—	—	221.0
441.5	—	—	225.5
465.4	—	—	228.9
497.8	—	—	234.1

The optimum coefficients are listed in Table V, while Fig. 1 illustrates the deviations of the experimental data from the correlation. In no case do the deviations exceed $\pm 1.0\%$, the standard deviation of the entire data set being $\pm 0.2\%$. Figure 1 also includes a comparison with earlier measurements of the thermal conductivity of *n*-pentane [9–11]. The earlier results generally deviate from the present correlation by more than the mutual uncertainty. The data of Carmichael et al. [9] and Bogatov et al. [11] are systematically lower than the current values, and those of

Table III. The Thermal Conductivity of *n*-Pentane at $T_{nom} = 342.5$ K

Pressure P (MPa)	Density ρ ($kg \cdot m^{-3}$)	Thermal conductivity ($mW \cdot m^{-1} \cdot K^{-1}$)	
		$\lambda(T_{nom}, \rho)$	$\lambda(T_{nom}, P)$
4.64	582.8	101.5	101.4
14.02	597.2	107.3	107.3
24.74	611.0	113.0	112.9
25.06	611.1	113.1	113.1
35.42	622.7	118.0	117.9
46.97	633.7	123.5	123.5
57.29	642.4	127.9	127.9
72.40	653.8	134.1	134.0
87.84	664.1	139.2	139.1
102.5	672.9	144.2	144.1
117.0	680.7	148.8	148.8
133.0	688.8	153.2	153.2
148.2	696.3	157.6	157.6
162.4	702.7	161.5	161.5
182.7	711.5	166.5	166.6
202.0	719.4	171.6	171.6
223.4	727.9	176.2	176.2
243.3	735.5	180.5	180.5
263.4	742.9	184.3	184.3
283.3	750.1	189.5	189.5
303.6	—	—	192.7
328.0	—	—	196.2
328.5	—	—	197.3
353.4	—	—	202.1
378.1	—	—	205.9
402.9	—	—	210.0
426.9	—	—	214.1
450.2	—	—	217.6
476.0	—	—	221.5
550.2	—	—	225.0

Table IV. The Thermal Conductivity of *n*-Pentane at $T_{nom} = 359.5$ K

Pressure P (MPa)	Thermal conductivity (mW · m^{-1} · K^{-1}), $\lambda(T_{nom}, P)$
4.01	98.30
4.22	97.92
14.44	104.1
25.27	109.5
35.42	114.5
46.97	119.5
57.50	123.5
67.22	127.4
82.16	133.1
97.98	138.0
112.7	142.9
127.5	147.3
142.5	151.8
158.4	156.0
174.2	159.9
188.9	163.9
205.5	166.3
205.7	166.4
209.2	168.6
224.5	173.5
253.4	178.5
273.6	182.8
292.9	186.5
314.6	190.8
337.9	195.0
362.7	199.7
363.3	199.5
363.5	199.7
383.0	203.0
407.4	207.6
427.6	210.4
447.0	213.6
466.5	216.7
486.0	219.5
505.5	222.4

Table V. Optimum Values for the Coefficients of the Correlation of the Thermal Conductivity of *n*-Pentane as a Function of Pressure

T (K)	λ' ($mW \cdot m^{-1} \cdot K^{-1}$)	P' (MPa)	$10a_1$	10^2a_2	10^2a_3	10^2a_4
305.8	194.36	250	2.892	−6.256	4.971	−3.026
322.8	188.38	250	2.927	−5.873	4.968	−4.183
342.5	181.79	250	2.821	−6.377	6.138	−4.409
359.5	177.39	250	2.963	−5.954	5.558	−4.486

Mukhamedzyanov and Usmanov [10] systematically higher. Owing to the higher precision of the present data, they are to be preferred to the earlier results.

4. THE DENSITY DEPENDENCE

Whereas the correlation of the pressure dependence of the thermal conductivity by means of Eq. (1) is suitable for interpolation, it has little or

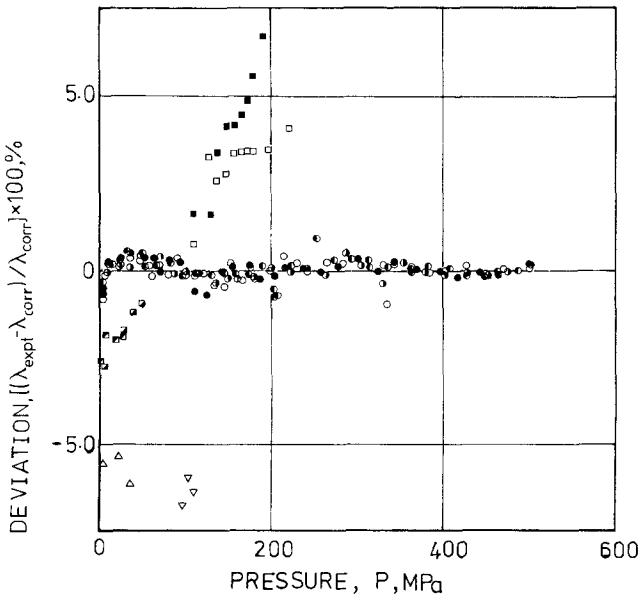

Fig. 1. Deviations of the experimental thermal conductivity from the correlation of Eq. (1). Present work: (○) 305.8 K; (●) 322.8 K; (◑) 342.5 K; (◐) 359.5 K. Ref. 9: (△) 305.8 K; (▽) 342.5 K. Ref. 10: (□) 305.8 K; (■) 342.5 K. Ref. 11: (◩) 305.8 K; (◪) 342.5 K.

no value for extrapolation and prediction. For such purposes it has been shown that a correlation in terms of the density or molar volume, V, is much more suitable. The hard-sphere model of the dense fluid state [12] suggests the form of such a correlation since it leads to the result that for a monatomic fluid the quantity, λ^*, defined by the equation

$$\lambda^* = 1.936 \times 10^7 \, \lambda V^{2/3} (RT/M)^{-1/2} = F_\lambda (V/V_0) \tag{2}$$

is a function of a reduced molar volume (V/V_0) only. Here V_0 is a characteristic molar volume of the fluid which is but weakly temperature dependent.

Recent studies [1, 13, 14] have shown that if the result of Eq. (2) is carried over to polyatomic fluids, the function F_λ is nearly universal among the large group of normal alkanes and, moreover, that the molar volume characteristic of thermal conductivity is consistent with that required for an analogous treatment of the viscosity [1]. At present there are insufficient viscosity data for *n*-pentane to warrant their inclusion in a complete analysis and the transport properties of the liquid normal alkanes are, in any event, scheduled to be included in a comprehensive correlation in the near-future. Consequently, here we confine our attention to the representation of the present experimental data by means of a correlation based upon Eq. (2). Accordingly, we have adopted the isotherm at 305.8 K as a reference and assigned to the characteristic molar volume, V_0, at that temperature the value

$$V_0(305.8 \text{ K}) = 6.256 \times 10^{-5} \text{ m}^3 \cdot \text{mol}^{-1} \tag{3}$$

chosen to be approximately consistent with those established for other normal alkanes [1]. Subsequently, we have determined the values of V_0 for the isotherms 322.8 and 342.5 K which secure the optimum degree of superposition of lines of λ^* against $\ln(V/V_0)$ for all three isotherms. In this way we have determined the values for V_0 listed in Table VI. The resulting single line has been represented by the equation

$$\lambda^* = 4.6022 - 2.0602 \, V^* \tag{4}$$

Table VI. Characteristic Volumes, V_0, and Coefficients of Eq. (6) for Normal Pentane

T (K)	$10^5 V_0$ ($m^3 \cdot mol^{-1}$)	A	B
305.8	6.256	4.6883	2.2138
322.8	6.213	4.6020	2.058
342.5	6.188	4.4731	1.847

where

$$V^* = V/V_0 \tag{5}$$

which provides a simple method of correlating the experimental data.

Figure 2 contains a plot of the deviations of the experimental data from this correlation. The maximum departure of any datum from the values generated by Eq. (4) is one of $\pm 3.8\%$, whereas the standard deviation is one of $+1.3\%$. These deviations exceed the estimated uncertainty of the experimental data and a closer examination of Fig. 2 reveals that the three individual isotherms display marked, different, and systematic deviations from a common correlation. This situation is similar to that observed for *n*-hexane [13]. Thus, whereas the temperature independence of the function F_λ of Eq. (1) suggested by the hard-sphere theory of a fluid is confirmed within limits suitable for correlations of a modest accuracy, there is distinct evidence of its failure under a more rigorous test.

Consequently, in order to provide a better representation of the density dependence of the present thermal conductivity data, we have represented it along each isotherm by means of an equation of the form

$$\ln \lambda^* = A - B \ln(V/V_0) \tag{6}$$

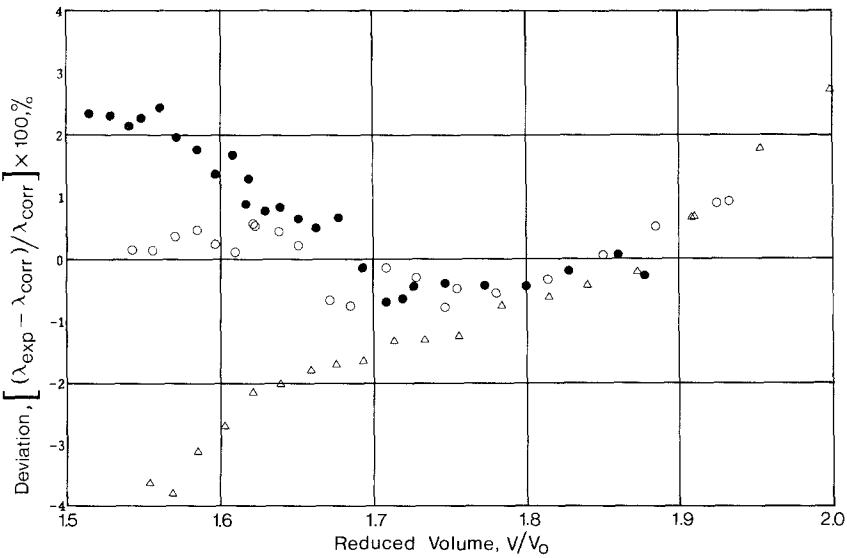

Fig. 2. Deviations of the experimental thermal conductivity data from the common correlation of Eq. (4) as a function of density. (○) 305.8 K; (●) 322.8 K; (△) 342.5 K.

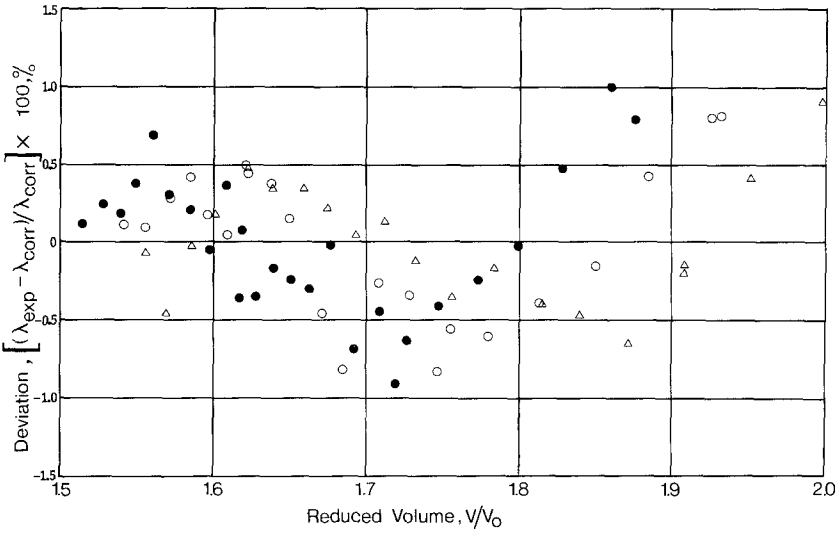

Fig. 3. Deviations of the experimental thermal conductivity data from individual correlations using Eq. (6). (○) 305.8 K; (●) 322.8 K; (△) 342.5 K.

in which A and B are allowed to be temperature dependent. The values of V_0 adopted in these representations are those given in Table VI, and the same table includes the optimum values of the coefficients A and B. Figure 3 contains the deviations of the thermal conductivity for the three isotherms from the correlations of Eq. (6). In this case the deviations amount to no more than $\pm 1.0\%$, whereas the standard deviation is one of $\pm 0.25\%$. These departures are much more nearly consistent with the combined uncertainty in the thermal conductivity and density.

5. CONCLUSION

The new results for the thermal conductivity of normal pentane presented in this paper are only moderately well represented by a single correlation based on a hard-sphere model of the fluid. Although the correlation may be adequate for some purposes, some refinement of the model is necessary to secure a representation of the data consistent with their estimated uncertainty.

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