Reference Correlation of the Thermal Conductivity of n-Hexane from the Triple Point to 600 K and up to 500 MPa

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Reference Correlation of the Thermal Conductivity of *n*-Hexane from the Triple Point to 600 K and up to 500 MPa

M. J. Assael[a] **S. K. Mylona, and Ch. A. Tsiglifisi**

Laboratory of Thermophysical Properties and Environmental Processes, Chemical Engineering Department, Aristotle University, Thessaloniki 54124, Greece

M. L. Huber and R. A. Perkins

Applied Chemicals and Materials Division, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305, USA

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This paper contains new, representative reference equations for the thermal conductivity of *n*-hexane. The equations are based in part upon a body of experimental data that has been critically assessed for internal consistency and for agreement with theory whenever possible. In the case of the dilute-gas thermal conductivity, a theoretically based correlation was adopted in order to extend the temperature range of the experimental data. Moreover, in the critical region, the experimentally observed enhancement of the thermal conductivity is well represented by theoretically based equations containing just one adjustable parameter. The correlations are applicable for the temperature range from the triple point to 600 K and pressures up to 500 MPa. The overall uncertainty (considered to be estimates of a combined expanded uncertainty with a coverage factor of 2) of the proposed correlation is estimated, for pressures less than 500 MPa and temperatures less than 600 K, to be less than 6%. © *2013 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.* [http://dx.doi.org/10.1063/1.4793335]

Key words: critical phenomena; *n*-hexane; thermal conductivity; transport properties.

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[a] Author to whom correspondence should be addressed. Electronic mail: assael@auth.gr.

1. Introduction

In a series of recent papers, new reference correlations for the thermal conductivity of normal and parahydrogen,[1] toluene,[2] SF_6,[3] and benzene,[4] covering a wide range of conditions of temperature and pressure, were reported. In this paper, the work is extended to the thermal conductivity of *n*-hexane.

The goal of this work is to critically assess the available literature data, and provide a wide-ranging correlation for the thermal conductivity of *n*-hexane that is valid over gas, liquid, and supercritical states, and that incorporates densities provided by the recent equation of state of Span and Wagner.[5] It should further be noted that although there are some alternative approaches today for such correlations (e.g., neural networks), we preferred to follow a procedure based upon kinetic theory and our previous work, as will be discussed in Secs. 2 and 3.

2. Methodology

The thermal conductivity λ is expressed as the sum of three independent contributions, as

$$\lambda(\rho, T) = \lambda_o(T) + \Delta\lambda(\rho, T) + \Delta\lambda_c(\rho, T), \qquad (1)$$

where ρ is the density, T is the temperature, and the first term, $\lambda_o(T) = \lambda(0, T)$, is the contribution to the thermal conductivity in the dilute-gas limit, where only two-body molecular interactions occur. The final term, $\Delta\lambda_c(\rho, T)$, the critical enhancement, arises from the long-range density fluctuations that occur in a fluid near its critical point, which contribute to divergence of the thermal conductivity at that point. Finally, the term $\Delta\lambda(\rho, T)$, the residual property, represents the contribution of all other effects to the thermal conductivity of the fluid at elevated densities including many-body collisions, molecular-velocity correlations, and collisional transfer.

The identification of these three separate contributions to the thermal conductivity and to transport properties in general is useful because it is possible to some extent to treat both $\lambda_o(T)$ and $\Delta\lambda_c(\rho, T)$ theoretically. In addition, it is possible to derive information about $\lambda_o(T)$ from experiment. In contrast, there is almost no theoretical guidance concerning the residual contribution, $\Delta\lambda(\rho, T)$, so that its evaluation is based entirely on experimentally obtained data.

The analysis described above should be applied to the best available experimental data for the thermal conductivity. Thus, a prerequisite to the analysis is a critical assessment of the experimental data. For this purpose, two categories of experimental data are defined: primary data employed in the development of the correlation, and secondary data used simply for comparison purposes. According to the recommendation adopted by the Subcommittee of Transport Properties (now known as The International Association for Transport Properties) of the International Union of Pure and Applied Chemistry, the primary data are identified by a well-established set of criteria.[6] These criteria have been successfully employed to establish standard reference values for the viscosity and thermal conductivity of fluids over wide ranges of conditions, with uncertainties in the range of 1%. However, in many cases, such a narrow definition unacceptably limits the range of the data representation. Consequently, within the primary data set, it is also necessary to include results that extend over a wide range of conditions, albeit with a poorer accuracy, provided they are consistent with other more accurate data or with theory. In all cases, the accuracy claimed for the final recommended data must reflect the estimated uncertainty in the primary information.

3. The Correlation

Table 1 summarizes, to the best of our knowledge, the experimental measurements[7–36] of the thermal conductivity of *n*-hexane reported in the literature. Thirty sets are included in the table. From these sets, eight were considered as primary data.

The data of Watanabe and Seong,[7] Assael *et al.*,[9] and Li *et al.*[10] were measured in an absolute transient hot-wire instrument with an uncertainty of less than 0.5%, and these three sets were considered as primary data. Also in the primary data set, the measurements of Tanaka *et al.*,[8] performed in an absolute transient hot-wire instrument with an uncertainty of 1%, were included. Two more transient hot-wire sets were considered as primary data: the absolute measurements of Mukhamedzyanov and Usmanov[13] and the relative measurements of Kashiwagi *et al.*,[11] both with an uncertainty of 2%. Finally, the measurements of Naziev *et al.*[12] and Golubev and Naziev,[14] both performed in concentric-cylinder instruments, were also included in the primary data set, as they extend to both low[12] and higher[14] temperatures.

Figure 1 shows the temperature and pressure range of the primary measurements outlined in Table 1. Temperatures for all data were converted to the ITS-90 temperature scale. The development of the correlation requires densities; Span and Wagner[5] in 2003 reviewed the thermodynamic properties of *n*-hexane and developed an accurate, wide-ranging equation of state up to 600 K and 100 MPa, with an uncertainty of 0.2%. Dymond *et al.*[37] measured the density of *n*-hexane from 298 to 373 K and up to 500 MPa, with an uncertainty of better than

TABLE 1. Thermal conductivity measurements of *n*-hexane

1st author	Year publ.	Technique employed[a]	Purity (%)	Uncertainty (%)	No. of data	Temperature range (K)	Pressure range (MPa)
Primary data							
Watanabe[7]	2002	THW (Abs)	98.00	0.48	22	298–337	0.02–101
Tanaka[8]	1988	THW (Abs)	99.00	1.0	45	283–373	0.1–250
Assael[9]	1987	THW (Abs)	99.50	0.5	12	297–325	0.1
Li[10]	1984	THW (Abs)	99.90	0.3	77	307–360	1.8–643
Kashiwagi[11]	1982	THW (Rel)	99.00	2.0	4	298–333	0.1
Naziev[12]	1981	CC (Abs)	na	1.5	78	196–473	0.1–50
Mukhamedzyanov[13]	1971	THW (Abs)	99.69	2.0	70	298–448	0.1–220
Golubev[14,b]	1962	CC (Abs)	na	na	153	293–633	0.1–49
Secondary Data							
Jicheng[15]	1989	HW (Rel)	na	2.0	5	423–523	25
Rowley[16]	1988	THW	na	2.0	1	303	0.1
Naziev[17,b]	1984	CC (Abs)	na	na	14	423–623	0.1–2
El-Sharkawy[18]	1983	AC HW	98.90	2.0	9	273–293	0.01–0.24
Shashkov[19,b]	1983	HF (Abs)	na	1.5	5	332–370	0.003
Filippov[20]	1980	AC HW	na	1.5	11	282–475	0.01–1.85
Bulanov[21]	1974	CC (Rel)	na	3.0	7	303–370	0.02–0.23
Mallan[22]	1972	THW (Rel)	na	2.5	18	296–366	0.02–0.2
Brykov[23]	1970	HF (Abs)	na	2.0	13	183–204	0.1
Gray[24,b]	1970	SSHW	na	1.2	2	323–373	0.05–0.25
Bogatov[25]	1969	SSHW	na	1.5	53	293–473	0.1–49
Jobst[26]	1964	THW	na	2.0	12	183–333	0.1
Mukhamedzyanov[27]	1963	THW (Rel)	na	1.0	6	303–320	0.02–0.05
Vilim[28]	1960	THW	na	2.0	3	293–341	0.016–0.1
Lambert[29]	1955	THW	na	na	1	339	0.1
Sakiadis[30]	1955	PP	99.0	1.5	10	303–330	0.1
Filippov[31]	1954	CC	na	3.0	6	289–333	0.01–0.076
Vines[32,b]	1954	HW (Rel)	na	na	5	348–434	0.1
Lambert[33,b]	1950	THW	na	na	12	339–358	0.01–0.04
Mann[34,b]	1931	SSHW	na	na	1	273	0.006
Smith[35]	1930	CC (Rel)	na	na	2	303–333	0.1
Hernqvist[36]	1913	na	na	na	6	276–277	0.1

[a] Abs, absolute; ACHW, AC hot wire; CC, coaxial cylinder; HF, hot filament; HW, hot wire; na, not available; PP, parallel plate; Rel, relative; SSHW, steady-state hot wire; THW, transient hot wire.

[b] Includes vapor data employed to derive the dilute-gas thermal-conductivity correlation.

0.04% at high pressures. To test the pressure extrapolation behavior of the equation of Span and Wagner[5] up to 500 MPa, we compared the densities computed from the EOS with the density measurements of Dymond *et al.*,[37] and found that the EOS can be used at pressures up to 500 MPa with uncertainty rising up to 1% only at the highest temperature and pressures. Hence the Span and Wagner[5] equation was employed up to 600 K and 500 MPa – limits that hence also restrict the present thermal conductivity correlation. Finally, the ideal-gas isobaric heat capacity employed by Span and Wagner was obtained from Jaeschke and Schley[38] with an uncertainty of 0.05% for the range 200–1000 K. Deviations in the critical region are higher for the above properties. We also adopt the values for the critical point and triple point from their equation of state; the critical temperature, T_c, and the critical density, ρ_c, were taken to be equal to 507.82 K and 233.182 kg m^{-3}, respectively. The triple-point temperature is 177.83 K.[5]

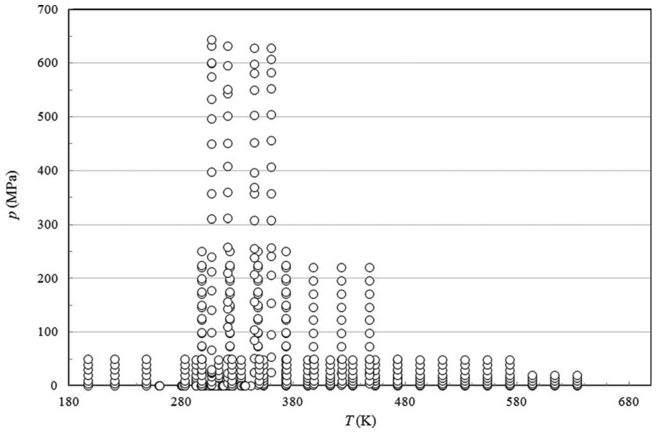

FIG. 1. Temperature and pressure ranges of the primary experimental thermal conductivity data for *n*-hexane.

3.1. The dilute-gas limit

From the primary measurements shown in Table 1, only one investigator[14] performed measurements near the dilute-gas limit. To increase the number of data sets, six more investigators that performed thermal-conductivity measurements near the dilute-gas limit,[17,19,24,32–34] from the secondary data, were also included. As only two of the six sets extend over

600 K,[14,17] a theoretically based scheme was preferred in order to correlate the dilute-gas limit thermal conductivity, $\lambda_o(T)$, over a wide temperature range. The same scheme was successfully adopted in the case of the dilute-gas limit thermal conductivity correlation of normal and parahydrogen,[1] toluene,[2] SF_6,[3] and benzene.[4]

A reasonable estimate of the thermal conductivity, $\lambda_o(T)$, of a pure dilute gas may be obtained from the viscosity, $\eta_o(T)$, and ideal-gas heat capacity at constant volume, C_{vo}, through the modified Eucken correlation,[39]

$$f_{\mathrm{Eu}} = \frac{\lambda_o(T)\, M}{\eta_o(T)\, C_{vo}} = 1.32 + 1.77\left(\frac{R}{C_{vo}}\right). \qquad (2)$$

In the above equation, M represents the molar mass of n-hexane[5] (86.17536 g/mol), and R the universal gas constant[40] (8.3144721 $\mathrm{J\,mol^{-1}\,K^{-1}}$). To employ the above equation, the dilute-gas viscosity and the ideal-gas heat capacity at constant volume are required. The dilute-gas viscosity, η_o (μPa s), can be written[39] as a function of the reduced collision integral $\Omega^*(T^*)$, as

$$\eta_o(T) = \frac{5}{16}\left[\frac{MRT}{\pi}\right]^{1/2}\frac{1}{\sigma^2\Omega^*(T^*)} = 0.0266957\,\frac{\sqrt{MT}}{\sigma^2\Omega^*(T^*)}, \qquad (3)$$

where T (K) is the absolute temperature, and σ (nm) is the Lennard-Jones length parameter. The reduced collision integral can be calculated[41] as a function of the reduced temperature, $T^* = T\,(k_B/\varepsilon)$, for the range $0.3 < T^* < 100$, as

$$\Omega^*(T^*) = 1.16145(T^*)^{-0.14874} + 0.52487\,e^{-0.7732T^*} + 2.16178\,e^{-2.43787T*} - 6.435\times10^{-4}(T^*)^{0.14874} \times \sin[18.0323(T^*)^{-0.7683} - 7.27371], \qquad (4)$$

where ε (J) is the Lennard-Jones depth parameter, and k_B is the Boltzmann constant (1.3806503×10^{-23} $\mathrm{J\,K^{-1}}$). The ideal-gas heat capacity at constant volume, C_{vo}, can be obtained from the heat capacity at constant pressure, C_{po} ($\mathrm{J\,mol^{-1}\,K^{-1}}$), as ($C_{po} - C_{vo} = R$), as this is given by[38]

$$\frac{C_{po}}{R} = 4.0 + 11.6977\left(\frac{182.326/T}{\sinh(182.326/T)}\right)^2 + 26.8142\left(\frac{859.207/T}{\cosh(859.207/T)}\right)^2 + 38.6164\left(\frac{1826.59/T}{\sinh(1826.59/T)}\right)^2. \qquad (5)$$

Equations (2)–(5) form a consistent scheme for the calculation of the dilute-limit thermal conductivity. It should be noted that the above equations assume that n-hexane behaves like a Lennard-Jones gas. Furthermore, the fixed numerical values employed in the modified Eucken correlation, Eq. (2), were preferred to the various more theoretically complex versions of that equation, employing quantities such as the rotational collision number and the diffusion of the internal energy in the gas; quantities not easily accessible and beyond the scope of this work. The approximation in Eq. (2) is simpler and at the same time produced very good results. In the above scheme, the only unknowns are the Lennard-Jones parameters, σ and ε/k_B. The seven sets of thermal conductivity measurements in the dilute-gas limit[14,17,19,24,32–34] were used to optimize these two parameters. The values thus obtained were $\sigma = 0.550$ nm and $\varepsilon/k_B = 590$ K. These values also predict the viscosity values of Vogel and Strehlow[42] within 2.5%.

For ease of use, the values of the dilute-gas limit thermal conductivity, $\lambda_o(T)$ ($\mathrm{mW\,m^{-1}\,K^{-1}}$), obtained by the scheme of Eqs. (2)–(5), were fitted, as

$$\lambda_o(T) = 6.6742 - 23.7619(T/T_c) + 72.0155(T/T_c)^2 - 18.3714(T/T_c)^3. \qquad (6)$$

Values calculated by Eq. (6) do not deviate from the values calculated by the scheme of Eqs. (2)–(5) by more than 0.1% over the temperature range from 180 K to 1000 K, and hence Eq. (6) was used for the dilute-gas limit thermal conductivity for the work described in all of Secs. 3.2–3.4.

The experimental dilute-limit thermal-conductivity values, as well as the values calculated by Eq. (6), are shown in Fig. 2, while Fig. 3 presents the percentage deviations of the dilute-gas experimental data from the values calculated by Eq. (6). In both figures, it can be seen that there is a distinct difference between the data of Golubev and Naziev[14] and Naziev *et al.*,[17] even though these data originate from the same laboratory. Since no explanation was given, and we have no other dataset to include in this region, both sets were used in deriving the correlation.

Based upon the aforementioned discussion, Eqs. (2)–(5) or Eq. (6) represent the dilute-gas limit thermal conductivity to within 7% at the 95% confidence level.

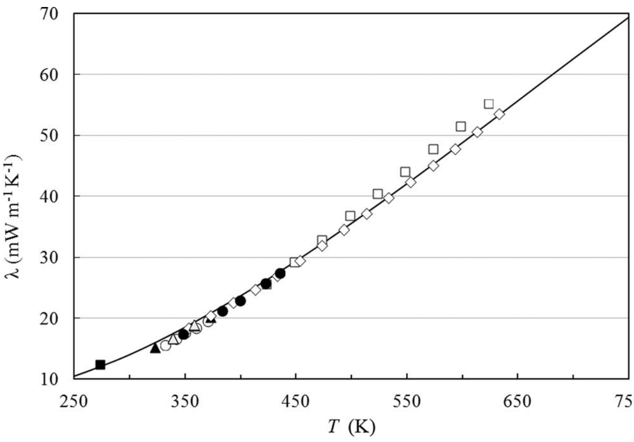

FIG. 2. Dilute-gas limit thermal conductivity as a function of temperature. Golubev and Naziev[14] (◊); Naziev *et al.*[17] (□); Shashkov *et al.*[19] (○); Gray *et al.*[24] (▲); Vines and Bennett[32] (●); Lambert *et al.*[33] (Δ); Mann and Dickins[34] (■); Eq. (6) (—).

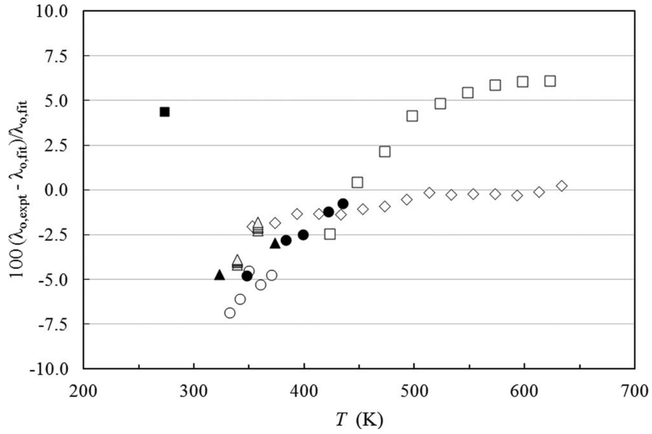

FIG. 3. Percentage deviations of primary experimental data for dilute-gas *n*-hexane from the values calculated by Eq. (6). Golubev and Naziev[14] (◊); Naziev *et al.*[17] (□); Shashkov *et al.*[19] (○); Gray *et al.*[24] (▲); Vines and Bennett[32] (●); Lambert *et al.*[33] (Δ); Mann and Dickins[34] (■).

3.2. The residual thermal conductivity

The thermal conductivities of pure fluids exhibit an enhancement over a large range of densities and temperatures around the critical point and become infinite at the critical point. This behavior can be described by models that produce a smooth crossover from the singular behavior of the thermal conductivity asymptotically close to the critical point to the residual values far away from the critical point.[43–45] The density-dependent terms for thermal conductivity can be grouped according to Eq. (1) as $[\Delta\lambda(\rho, T) + \Delta\lambda_c(\rho, T)]$. To assess the critical enhancement either theoretically or empirically, we need to evaluate, in addition to the dilute-gas thermal conductivity, the residual thermal-conductivity contribution. The procedure adopted during this analysis used ODRPACK (Ref. 46) to fit all the primary data simultaneously to the residual thermal conductivity and the critical enhancement, while maintaining the parameters in Eq. (6) already obtained from the fit of the dilute-gas thermal-conductivity data. The density values employed were obtained by the equation of state of Span and Wagner.[5]

The residual thermal conductivity was represented with a polynomial in temperature and density,

$$\Delta\lambda(\rho, T) = \sum_{i=1}^{5} (B_{1,i} + B_{2,i}(T/T_c))(\rho/\rho_c)^i. \qquad (7)$$

The coefficients $B_{1,i}$ and $B_{2,i}$ are shown in Table 2.

TABLE 2. Coefficients of Eq. (7) for the residual thermal conductivity of *n*-hexane

i	$B_{1,i}$ (W m^{-1} K^{-1})	$B_{2,i}$ (W m^{-1} K^{-1})
1	$-3.014\,08 \times 10^{-2}$	$2.182\,08 \times 10^{-2}$
2	$1.679\,75 \times 10^{-1}$	$-1.008\,33 \times 10^{-1}$
3	$-1.297\,39 \times 10^{-1}$	$7.741\,80 \times 10^{-2}$
4	$3.828\,33 \times 10^{-2}$	$-2.159\,45 \times 10^{-2}$
5	$-3.702\,94 \times 10^{-3}$	$2.124\,87 \times 10^{-3}$

3.3. The critical enhancement

3.3.1. Simplified crossover model

The theoretically based crossover model proposed by Olchowy and co-workers[43–45] is complex and requires solution of a quartic system of equations in terms of complex variables. A simplified crossover model has also been proposed by Olchowy and Sengers.[47] The critical enhancement of the thermal conductivity from this simplified model is given by

$$\Delta\lambda_c = \frac{\rho C_p R_D k_B T}{6\pi\bar{\eta}\xi}(\bar{\Omega} - \bar{\Omega}_0), \qquad (8)$$

with

$$\bar{\Omega} = \frac{2}{\pi}\left[\left(\frac{C_p - C_v}{C_p}\right)\arctan(\bar{q}_D\xi) + \frac{C_v}{C_p}\bar{q}_D\xi\right], \qquad (9)$$

and

$$\bar{\Omega}_0 = \frac{2}{\pi}\left[1 - \exp\left(-\frac{1}{(\bar{q}_D\xi)^{-1} + (\bar{q}_D\xi\rho_c/\rho)^2/3}\right)\right]. \qquad (10)$$

In Eqs. (8)–(10), k_B is Boltzmann's constant, $\bar{\eta}$ is the viscosity, and C_p and C_v are the isobaric and isochoric specific heat obtained from Span and Wagner.[5] To estimate the viscosity, an unpublished correlation[48] implemented in the REFPROP (Ref. 49) program was employed. The correlation length ξ is given by

$$\xi = \xi_0\left(\frac{p_c\rho}{\Gamma\rho_c^2}\right)^{\nu/\gamma}\left[\left.\frac{\partial\rho(T,\rho)}{\partial p}\right|_T - \left(\frac{T_{\mathrm{ref}}}{T}\right)\left.\frac{\partial\rho(T_{\mathrm{ref}},\rho)}{\partial p}\right|_T\right]^{\nu/\gamma}. \qquad (11)$$

As already mentioned, the coefficients $B_{1,i}$ and $B_{2,i}$ in Eq. (7) and $\bar{q}_D$ in Eqs. (9) and (10) were fitted with ODRPACK (Ref. 46) to the primary data for the thermal conductivity of *n*-hexane. This crossover model requires the universal constants[47] $R_D = 1.02$, $\nu = 0.63$, and $\gamma = 1.239$, and system-dependent amplitudes Γ and ξ_0. For this work we adopted the values $\Gamma = 0.05803$ and estimated $\xi_0 = 2.364 \times 10^{-10}$ m, using the method presented by Perkins *et al.*[50] The effective cutoff wavelength $\bar{q}_D^{-1}$ was found equal to 7.37×10^{-10} m. The reference temperature T_{ref}, far above the critical temperature where the critical enhancement is negligible, was calculated by $T_{\mathrm{ref}} = (^3/_2)\,T_c$,[51] which for *n*-hexane is 761.7 K.

Table 3 summarizes comparisons of the primary data with the correlation. We have defined the percent deviation as

TABLE 3. Evaluation of the *n*-hexane thermal-conductivity correlation for the primary data

1st Author	Year publ.	AAD (%)	BIAS (%)
Watanabe[7]	2002	3.31	−3.31
Tanaka[8]	1988	4.02	−4.02
Assael[9]	1987	0.30	0.30
Li[10]	1984	0.56	−0.12
Kashiwagi[11]	1982	0.81	0.09
Naziev[12]	1981	1.88	−1.59
Mukhamedzyanov[13]	1971	2.07	0.42
Golubev[14]	1962	3.52	2.93
Entire data set		2.46	−0.21

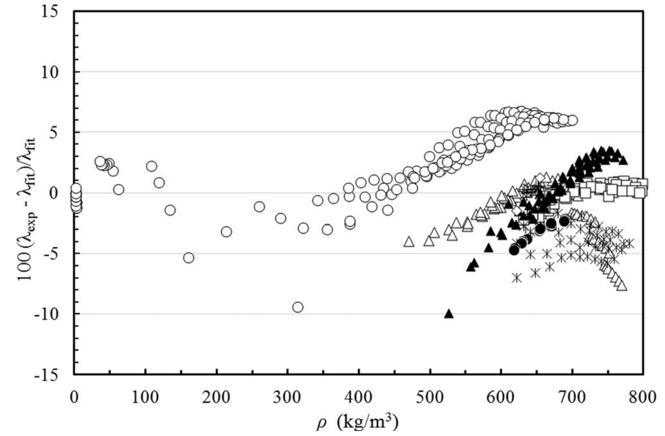

FIG. 4. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the present model as a function of density. Watanabe and Seong[7] (●); Tanaka *et al.*[8] (⚹); Assael *et al.*[9] (+); Li *et al.*[10] (□); Kashiwagi *et al.*[11] (◊); Naziev *et al.*[12] (Δ); Mukhamedzyanov and Usmanov[13] (▲); Golubev and Naziev[14] (◯).

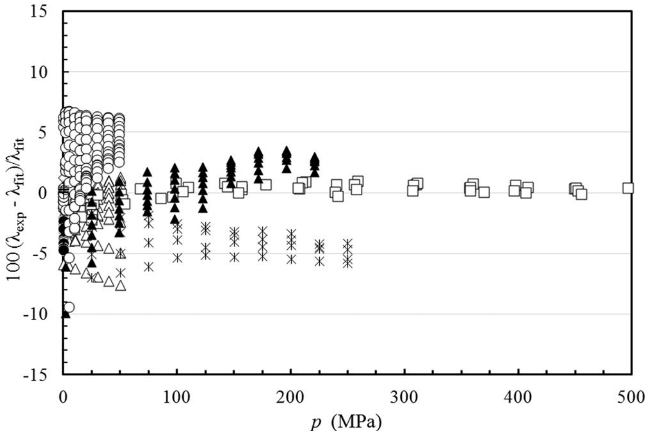

FIG. 6. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the present model as a function of pressure. Watanabe and Seong[7] (●); Tanaka *et al.*[8] (⚹); Assael *et al.*[9] (+); Li *et al.*[10] (□); Kashiwagi *et al.*[11] (◊); Naziev *et al.*[12] (Δ); Mukhamedzyanov and Usmanov[13] (▲); Golubev and Naziev[14] (◯).

PCTDEV = $100*(\lambda_{\mathrm{exp}} - \lambda_{\mathrm{fit}})/\lambda_{\mathrm{fit}}$, where λ_{exp} is the experimental value of the thermal conductivity and λ_{fit} is the value calculated from the correlation. Thus, the average absolute percent deviation (AAD) is found with the expression AAD = $(\sum|\mathrm{PCTDEV}|)/n$, where the summation is over all n points, and the bias percent is found with the expression BIAS = $(\sum \mathrm{PCTDEV})/n$. The standard deviation of the overall fit is 3.2%.

Figure 4 shows the percentage deviations of all primary thermal-conductivity data from the values calculated by Eqs. (1) and (6)–(11), as a function of the density, while Figs. 5 and 6 show the same deviations but as a function of the temperature and pressure. The primary data for *n*-hexane listed in Table 1 cover a wide range of conditions and extend to 643 MPa. As mentioned earlier, although the EOS of Span and Wagner[5] used here for density is recommended only to 100 MPa, comparisons with the data of Dymond *et al.*[37] indicate that it may extrapolated to 500 MPa. Based on comparisons with the primary data, we calculate the uncertainty (considered to be estimates of a combined expanded uncertainty with a coverage factor of 2) for pressures less than 500 MPa and temperatures less than 600 K to be less than 6%. Uncertainties in the critical region are much larger, since the thermal conductivity approaches infinity at the critical point and is very sensitive to small changes in density.

Figure 7 shows the percentage deviations of the secondary data from the values calculated by the proposed scheme. The majority of the deviations, except some very old sets, are within 5% of the present correlation.

Finally, Fig. 8 shows a plot of the thermal conductivity of *n*-hexane as a function of the temperature for different pressures.

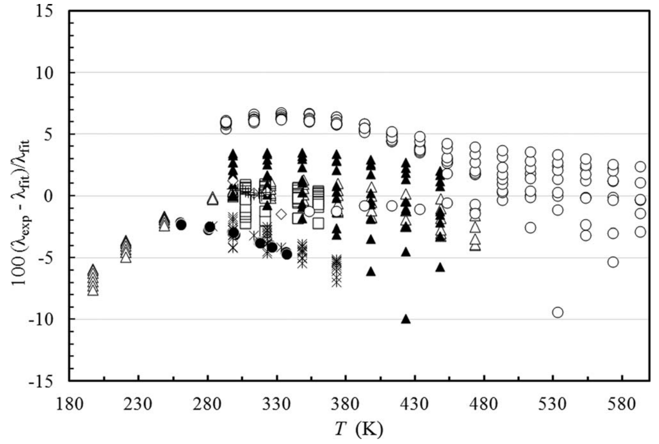

FIG. 5. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by the present model as a function of temperature. Watanabe and Seong[7] (●); Tanaka *et al.*[8] (⚹); Assael *et al.*[9] (+); Li *et al.*[10] (□); Kashiwagi *et al.*[11] (◊); Naziev *et al.*[12] (Δ); Mukhamedzyanov and Usmanov[13] (▲); Golubev and Naziev[14] (◯).

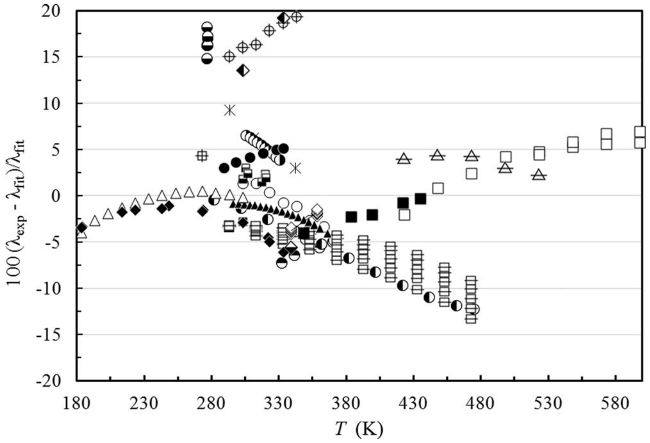

FIG. 7. Percentage deviations of secondary experimental data of *n*-hexane from the values calculated by the present model as a function of temperature. Jicheng *et al.*[15] (⍙); Rowley *et al.*[16] (◨); Naziev *et al.*[17] (□); El-Sharkawy *et al.*[18] (⊕); Shashkov *et al.*[19] (◒); Filippov *et al.*[20] (◐); Bulanov *et al.*[21] (◯); Mallan *et al.*[22] (▲); Brykov *et al.*[23] (Δ); Gray *et al.*[24] (⦶); Bogatov[25] (⊟); Jobst[26] (♦); Mukhamedzyanov *et al.*[27] (⬓); Vilim[28] (⚹); Lambert *et al.*[29] (⬙); Sakiadis and Coates[30] (◑); Filippov[31] (●); Vines and Bennett[32] (■); Lambert *et al.*[33] (◊); Mann and Dickins[34] (⊞); Smith[35] (⬖); Hernqvist[36] (◒).

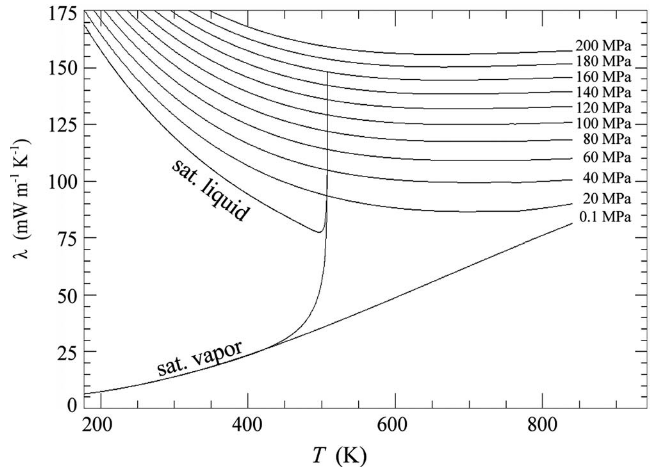

FIG. 8. Thermal conductivity of *n*-hexane as a function of temperature for different pressures.

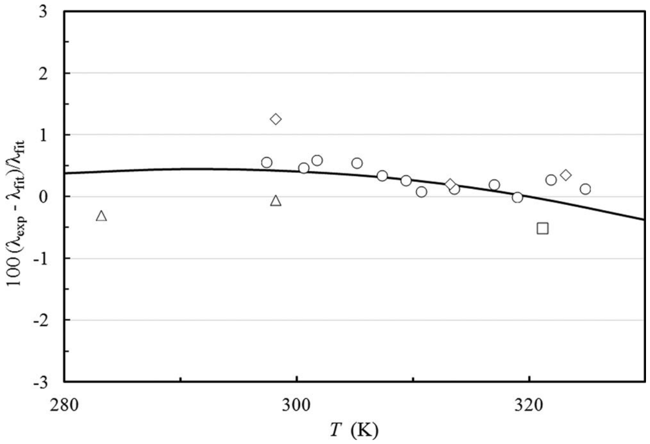

FIG. 10. Percentage deviations of selected primary experimental data of *n*-hexane at 0.101325 MPa from the values calculated by Eqs. (1) and (6)–(11). Assael *et al.*[9] (◯); Li *et al.*[10] (□); Kashiwagi *et al.*[11] (◊); Naziev *et al.*[12] (Δ); values calculated by Eq. (13) (——).

3.3.2. Empirical critical enhancement

For applications at state points that are relatively distant from the critical point (at least 10–15 K from the critical temperature), the critical enhancement is adequately represented by the following empirical expression:

$$\Delta\lambda_c(\rho,T) = \frac{C_1}{C_2 + |\Delta T_c|}\exp[-(C_3\Delta\rho_c)^2], \qquad (12)$$

where $\Delta T_c = (T/T_c) - 1$ and $\Delta\rho_c = (\rho/\rho_c) - 1$. This equation does not require accurate information on the compressibility, specific heat, and viscosity of *n*-hexane in the critical region, as does the theory of Olchowy and Sengers.[47] The coefficients of Eqs. (6) and (7) were fixed, while the coefficients of Eq. (12) were fitted to the primary data. The values obtained were $C_1 = 0.6 \times 10^{-3}$ W m^{-1} K^{-1}, $C_2 = 7.0 \times 10^{-2}$, and $C_3 = 1.8$. Figure 9 shows the percentage deviations between the primary data and the values calculated by Eqs. (1), (6), (7), and (12), as a function of the temperature. By comparing Figs. 5 and 9, it can be seen that employing Eq. (12) results in very little deterioration in the representation of the data.

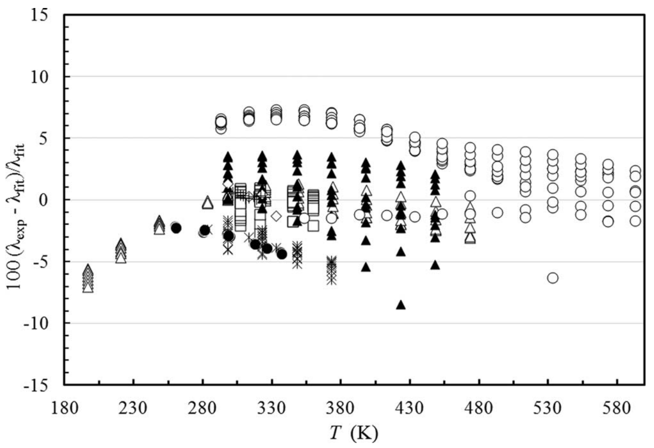

FIG. 9. Percentage deviations of primary experimental data of *n*-hexane from the values calculated by Eqs. (1), (6), and (7) and the empirical enhancement of Eq. (12) as a function of temperature. Watanabe and Seong[7] (●); Tanaka *et al.*[8] (⚹); Assael *et al.*[9] (+); Li *et al.*[10] (□); Kashiwagi *et al.*[11] (◊); Naziev *et al.*[12] (Δ); Mukhamedzyanov and Usmanov[13] (▲); Golubev and Naziev[14] (◯).

3.4. The 0.101325 MPa liquid line

Figure 10 shows the deviations of a selection of primary data at 0.101325 MPa from the proposed scheme of Eqs. (1) and (6)–(11). From the primary data of Table 1, data that exhibited higher uncertainty from the proposed scheme than their quoted uncertainty were excluded. The remaining investigators shown in Fig. 10 are Assael *et al.*[9] and Li *et al.*[10] (extrapolated isotherm to 0.1 MPa) with quoted uncertainties of 0.5% and 0.3%, and Kashiwagi *et al.*[11] and Naziev *et al.*[12] with quoted uncertainties of 2% and 1.5%. The data shown in Fig. 10 exhibit AAD and BIAS of 0.40% and 0.16%, respectively.

The aforementioned thermal conductivity data were fitted to a linear equation in the absolute temperature as

$$\lambda_{0.101\ \mathrm{MPa}} = 215.85 - 0.3199\,T. \qquad (13)$$

This equation represents the selected primary data at 0.101325 MPa, from 280 K to 330 K, with an uncertainty of 1% at the 95% confidence level. Percentage deviations of the values calculated by Eq. (13) from the values obtained from the proposed scheme of Eqs. (1) and (6)–(11), are also shown in Fig. 10.

4. Computer-Program Verification

Table 4 is provided to assist the user in computer-program verification. The thermal-conductivity calculations are based on the tabulated temperatures and densities. Note that Eq. (6) was employed for the dilute-gas correlation.

TABLE 4. Sample points for computer verification of the correlating equations

T (K)	ρ (kg m^{-3})	λ (mW m^{-1} K^{-1})
250.00	700.00	137.62
400.00	2.00	23.558
400.00	650.00	129.28
510.00	2.00	36.772[a]
510.00	2.00	37.105[b]

[a] Computed with modified Olchowy–Sengers critical enhancement; the viscosity at this point for use in Eq. (8) was taken as $\eta = 11.263$ μPa s (see Sec. 3.3.1). All other properties required for the enhancement term are from Span and Wagner.[5]

[b] Computed with empirical critical enhancement Eq. (12).

5. Conclusions

A new wide-ranging correlation for the thermal conductivity of *n*-hexane were developed based on critically evaluated experimental data. The correlation is valid from the triple point to 600 K, and at pressures up to 500 MPa. The correlations are expressed in terms of temperature and density, and the densities were obtained from the equation of state of Span and Wagner,[5] extrapolated to 500 MPa. The overall uncertainty (considered to be estimates of a combined expanded uncertainty with a coverage factor of 2) of the proposed correlation is calculated, for pressures less than 500 MPa and temperatures less than 600 K, to be less than 6%.

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