AIP | Journal of Physical and Chemical Reference Data

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Citation: Journal of Physical and Chemical Reference Data **41**, 023101 (2012); doi: 10.1063/1.3700155
View online: http://dx.doi.org/10.1063/1.3700155
View Table of Contents: http://scitation.aip.org/content/aip/journal/jpcrd/41/2?ver=pdfcov
Published by the AIP Publishing

Reference Correlation of the Thermal Conductivity of Toluene from the Triple Point to 1000 K and up to 1000 MPa

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(Received 4 January 2012; accepted 16 March 2012; published online 20 April 2012)

This paper contains new, representative equations for the thermal conductivity of toluene. 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. Although there are a sufficiently large number of data at normal temperatures, data at very low and very high temperatures as well as near the critical region are scarce. 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 1000 K and pressures up to 1000 MPa. The overall uncertainty (considered to be estimates of a combined expanded uncertainty with a coverage factor of two) of the proposed correlation is estimated, for pressures less than 700 MPa and temperatures less than 550 K, to be less than 3% for the liquid, while for the region 550 K $\leq T \leq$ 700 K the uncertainty is estimated to be 4%. For the region $T > 700$ K and 500 MPa $\leq p \leq$ 1000 MPa, the equations can safely be used with an uncertainty of the order of 10%. Finally, the uncertainty along the saturation line is estimated to be 2% with a coverage factor of two. *© 2012 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.* [http://dx.doi.org/10.1063/1.3700155]

Key words: correlation; critical phenomena; thermal conductivity; toluene; transport properties.

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1. Introduction

Toluene is an important industrial fluid that is used as a solvent, a chemical intermediate for explosives production, and a valuable blending component in high-octane gasolines.[1] It can easily be obtained in high purity, is a liquid over a wide range of temperatures, and is noncorrosive with respect to standard engineering materials, making it potentially of interest as a reference fluid for thermophysical properties such as thermal conductivity.[2] Jamieson *et al.*[3] provided a data survey of liquid thermal conductivity to 1973. Liley[4] surveyed the gas-phase data to 1968. Touloukian[5] surveyed both the gas and liquid phases to 1970 and provided recommended values. More recently, reference correlations for the thermal conductivity at the saturation boundary have been published.[6,7] In 1986, Nieto de Castro *et al.*[7] reviewed and analyzed the available liquid-phase thermal conductivity data for water, toluene, and *n*-heptane and provided two correlations for the thermal conductivity of liquid toluene along the saturation boundary: one for a limited temperature range 230 K $\leq T \leq$ 360 K where the experimental data are of the lowest uncertainty, and a second, wider-range correlation valid for the range 189 K $\leq T \leq$ 360 K that has slightly larger uncertainties. In 2000, Ramires *et al.*[6] provided new reference-quality experimental measurements and proposed a new reference correlation for the saturation boundary valid over the range 189 K $\leq T \leq$ 553 K, which significantly increased the upper temperature range. Vargaftik *et al.*[8] provided tables of recommended values of the thermal conductivity of toluene not only for the liquid at saturation, but also for the gas, liquid, and supercritical regions over a range of pressures up to 150 MPa. It is the goal of this work to review the experimental data, and propose a wide-ranging correlation for the thermal conductivity surface of toluene that is valid over gas, liquid, and supercritical states.

2. Methodology

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

$$\lambda(\rho, T) = \lambda_{\mathrm{o}}(T) + \Delta\lambda(\rho, T) + \Delta\lambda_{\mathrm{c}}(\rho, T), \tag{1}$$

where ρ is the density, T is the temperature, and the first term, $\lambda_{\mathrm{o}}(T) = \lambda(0,T)$, is the contribution to the thermal conductivity in the dilute-gas limit, where only two-body molecular interactions occur. The last term, $\Delta\lambda_{\mathrm{c}}(\rho,T)$, for the critical enhancement, arises from the long-range density fluctuations that occur in a fluid near its critical point, and that contribute to a divergence of the thermal conductivity at that singular point. The remaining term, $\Delta\lambda(\rho,T)$, for the residual thermal conductivity, 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 a transport property in general is useful because it is possible, to some extent, to treat both $\lambda_{\mathrm{o}}(T)$ and $\Delta\lambda_{\mathrm{c}}(\rho,T)$ theoretically. In addition, it is possible to derive information about $\lambda_{\mathrm{o}}(T)$ 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.

It is obvious that the analysis described above must 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 (IATP)] of the International Union of Pure and Applied Chemistry, the primary data are identified by the following criteria:[9]

(i) Measurements must have been made with a primary experimental apparatus, i.e., one for which a complete working equation is available.

(ii) The form of the working equation should be such that sensitivity of the property measured to the principal variables does not magnify the random errors of measurement.

(iii) All principal variables should be measurable to a high degree of precision.
(iv) The published work should include some description of purification methods and a guarantee of the purity of the sample.
(v) The data reported must be unsmoothed data. While graphs and fitted equations are useful summaries for the reader, they are not sufficient for standardization purposes.
(vi) The lack of accepted values of the thermal conductivity of standard reference materials implies that only absolute, and not relative, measurement results can be considered.
(vii) Explicit quantitative estimates of the uncertainty of reported values should be given, taking into account the precision of experimental measurements and possible systematic errors.
(viii) Owing to the desire to produce reference values of low uncertainty, limits must be imposed on the uncertainty of the primary data sets. These limits are determined after critical evaluation of the existing data sets.

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 in practice, such a narrow definition would limit the range of the data representation unacceptably. Consequently, within the primary data set, it is also necessary to include results that extend over a wide range of conditions, albeit with a higher uncertainty, 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.

In the following sections, the individual contributions to the thermal conductivity of toluene are treated separately, in each case subjecting all of the relevant available experimental data to a critical scrutiny in order to compile the primary data set and derive a global correlation of $\lambda(\rho,T)$.

3. The Correlation

Table 1 summarizes, to the best of our knowledge, experimental measurements of the thermal conductivity of toluene reported in the literature. Over 90 sets are included in the table, representing 2539 thermal conductivity measurements. References that present only graphical results or a correlating equation are not included in this summary. Also, references that employed toluene in order to calibrate thermal-conductivity instruments are not included. In addition, two theses or reports that have been mentioned in the literature, but that we were unable to obtain,[105,106] are also not included in Table 1. From the aforementioned sets, 25 were considered as primary data.

TABLE 1. Thermal conductivity measurements of toluene

1st author	Year Publ.	Technique employed[a]	Purity[a] (%)	Uncertainty (%)	No of data	Temperature range (K)	Pressure range (MPa)
Primary data							
Wu[10]	2009	THW-Abs	99.5	2.0	38	274–375	0–0.08
Wu[11]	2005	THW-Abs	99.9	2.0	8	234–373	0–0.08
Sun[12]	2002	THW-Abs	99.95	0.5	24	297–423	3–35
Watanabe[13]	2002	THW-Abs	99.0	0.5	21	260–330	0–0.01
Assael[14]	2001	THW-Abs	99.9	0.5	50	234–336	0.1–18
Perkins[15]	2000	THW-Abs	PurSpect	0.5–1.5	184	300–550	0–3
Lei[16]	1997	THW-Abs	na	0.7	6	253–303	0.1
Watanabe[17]	1997	THW-Abs	99.0	0.5	84	295–319	0–0.008
Ramires[18]	1993	THW-Abs	99.99	0.5	37	299–367	0–0.06
Yamada[19]	1993	THW-Abs	99.7	0.5	70	193–452	0.1–20
Assael[20]	1992	TWH-Abs	99.9	0.5	48	253–335	0.1–27.8
Perkins[21]	1991	THW-Abs	PurSpect	1.0	105	301–554	0.09–19
Ramires[22]	1989	THW-Abs	99.99	0.3	11	299–366	0–0.06
Taxis[23]	1988	THW-Abs	99.9	0.3	28	308–347	0–67
Charitidou[24]	1987	THW-Abs	99.9	0.5	12	307–347	0.1
Shulga[25]	1986	ACHW-Abs	99.5	1.0	87	255–401	0–1000
Nieto de Castro[26]	1983	THW-Abs	99.95	0.3	104	308–360	0.9–585
Kashiwagi[27]	1982	THW-Abs	99.5	1.0	94	273–373	0.1–250
Nagasaka[28,29]	1981	THW-Abs	99.0	0.5	5	274–354	0.1
Zaitseva[30]	1976	CC	na	3.0	17	370–683	0.1
Geller[31]	1974	SSHW	na	1.2	32	183–313	0–60
Kandiyoti[32]	1973	THW-Abs	na	3.5	17	303–364	0.1–633
Mani[33]	1973	THW-Abs	AR	1.0–2.0	81	317–581	0.09–14
McLaughlin[34]	1971	THW-Abs	Analar	0.7–1.5	23	180–400	0–0.15
Akhundov[35]	1970	THW-Abs	99.9	2.0	163	299–673	0.006–30

TABLE 1. Thermal conductivity measurements of toluene—Continued

1st author	Year Publ.	Technique employed[a]	Purity[a] (%)	Uncertainty (%)	No of data	Temperature range (K)	Pressure range (MPa)
Secondary data							
Garnier[36]	2008	THW	99.9	5.0	2	273, 298	0.1
Tomida[37]	2007	THW-Rel	na	2.0	9	294–334	0.1–20
Pan[38]	2004	THW	99.9	2.0	8	234–373	0–0.07
Ould-Lahoucine[39]	2003	ThPr	99.5	3.0	1	298	0.1
Tarzimanov[40]	2002	PHW	na	1.0	5	293–493	0–1.05
Zhang[41]	2001	Cal-Rel	na	3.0	8	292–363	0.1
Will[42]	1998	DLS	99.9	na	65	298–590	0–4
Fujii[43]	1997	THW-Rel	na	2.0	2	295–299	0.1
Frezzotti[44]	1995	CC-Rel	99.9	3.0	10	302–392	0–0.12
Kraft[45]	1995	PCS	99.9	2.5	24	290–520	0–1.6
Tong[46]	1995	SSHW	na	1.0	19	323–523	5–18
Wang[47]	1995	Cal-Rel	na	1.0	1	298	0.1
Kim[48]	1993	THW-Abs	98.0	2.0	3	293–333	0.1
DiGuilio[49]	1992	THW-Rel	na	2.0	7	298–356	0.003–0.04
Gross[50]	1992	THW-Abs	na	2.0	1	293	0.1
Naziev[51]	1991	CC	99.98	2.0	80	197–473	0.1–50
DiGuilio[52]	1990	THW-Rel	HPLC	2.0	4	298–354	0.1
Huang[53]	1989	THW-Rel	na	3.0	3	273–301	0.0008–0.004
Richard[54]	1989	THW-Abs	na	na	4	311–343	0.1
Rowley[55]	1988	THW-Rel	99.99	1.0	3	313	0.1
Knibbe[56]	1987	THW	na	1.0	9	288–445	0–0.4
Rowley[57]	1987	THW-Rel	99.99	1.0	3	293–308	0.1
Ogiwara[58]	1985	PP-Rel	na	2.0	2	298–313	0.1
Baroncini[59]	1984	SSHW-Rel	na	na	2	298–323	0–0.01
Yata[60]	1984	THW	99.90	1.5	5	289–364	0–0.05
Atalla[61]	1981	ACHS	na	2.2	7	283–313	0–0.01
Kitazawa[62]	1981	THW-Abs	99.5	1.6	18	213–352	0.1–25
Nefedov[63]	1980	ACHW	na	2.0	80	300–640	0–30
Ogiwara[64]	1980	SSPP-Rel	na	2.0	6	293–343	0.003–0.03
Spirin[65]	1980	THW-Rel	na	1.5	9	293–453	0–0.5
Leidenfrost[66]	1979	SSHW	na	na	48	253–473	0.5–2.7
Tada[67]	1978	LasFl	99.7	2.6	4	293–303	0.101
Julia[68]	1977	THW-Rel	na	0.3	6	273–353	0–0.04
Trump[69]	1977	THW	na	1.0	3	273–313	0–0.007
Il’in[70]	1976	THW-Rel	na	3.0	8	293–363	0–0.05
Kostrovskii[71]	1974	SSHW	99.96	2.0	30	396–642	0.1–3
Davis[72]	1971	THW-Abs	na	1.0	9	297–403	0–0.17
Venart[73]	1971	THW-Abs	99.96	1.0	22	180–373	0–0.08
Brykov[74]	1970	SSHW-Abs	na	2.0	16	183–333	0–0.01
Rastorguev[75]	1970	SSHF-Abs	HighPur	1.5	70	293–453	0.09–150
Stupak[76]	1970	CC	na	na	4	298–350	0.101
Rastorguev[77]	1969	SSHF-Abs	HighPur	1.3	173	276–453	0.09–49
Rastorguev[78]	1969	SSHF-Abs	HighPur	1.5	74	270–405	0.001–0.98
Tree[79]	1969	CC	99.97	0.8	40	277–368	0.2–2.5
Ganiev[80]	1968	CC	na	1.0	15	299–438	0.4
Geller[81]	1968	SSHW	na	1.2	24	300–473	0.1–0.9
Pittman[82]	1968	THW	Analar	1.0	65	181–396	0.1
Vargaftik[83]	1968	SSHW	na	1.5	13	309–702	0.000001
Poltz[84]	1967	GPP	na	0.5	3	298–328	0.1
Rastorguev[85]	1967	THW-Abs	HighPur	1.0	27	297–428	0.003–0.3
Arrigoni[86]	1966	THW	na	5.0	1	294	0.1
Tufeu[87]	1966	CC	na	1.0	10	273–363	0.1
Tsvetkov[88]	1965	CC	na	na	8	193–363	0–0.05
Venart[89]	1965	RHF-Abs	na	2.0	9	273–353	0–0.04
Horrocks[90]	1963	THW	99.95	0.3	4	298–334	0.1
Ziebland[2]	1961	CC	na	2.0	26	258–384	0.1–4
Frontasev[91]	1959	GHP	na	1.0	1	293	0.1

TABLE 1. Thermal conductivity measurements of toluene—Continued

1st author	Year Publ.	Technique employed[a]	Purity[a] (%)	Uncertainty (%)	No of data	Temperature range (K)	Pressure range (MPa)
Schrock[92]	1958	CS	na	2.0	6	207–288	0–0.002
Briggs[93]	1957	CC	na	3.0	8	293–363	0.1
Challoner[94]	1956	GHP-Abs	na	1.0	5	273–353	0.1
Schmidt[95]	1954	PP	na	na	7	294–352	0.003–0.03
Filippov[96]	1953	CC	na	3.0	9	300–514	0.004–1.4
Riedel[97]	1951	CC	na	na	3	193–353	0.1
Abas-Zade[98]	1949	HW	na	na	26	273–593	0–4.3
Shiba[99]	1931	PB	na	na	1	300	0.1
Smith[100]	1930	CC	na	na	2	303–348	0–0.03
Davis[101]	1924	HTHW	na	5.0	2	292–342	0.1
Bridgman[102]	1923	CC	na	0.8	20	303–348	0.1–882
Goldschmidt[103]	1911	HW	na	na	2	273–293	0.1
Weber[104]	1886	na	na	na	1	293	0.1

[a] Abs, absolute; ACHS, alternating current hot strip; ACHW, alternating current hot wire; Cal, calorimetry; CC, coaxial cylinder; CS, concentric spheres; DLS, dynamic light scattering; GHP, guarded hot plate; GPP, guarded parallel plate; LasFl, laser flash; na, not available; PCS, photon correlation spectroscopy; PHW, pulse-heated wire; PB, piezometer bulb; PP, parallel plate; RHF, radial heat flow; SSHF, steady-state hot filament; SSHW, steady-state hot wire; ThPr, thermistor probe; THW, transient hot wire; Analar, AR, HighPur, HPLC, PurSpect, type of purity quoted.

The data of Sun *et al.*,[12] Watanabe and Seong,[13] Watanabe,[17] Assael and Dalaouti,[14] Assael *et al.*,[20] Perkins *et al.*,[15,21] Lei *et al.*,[16] Ramires *et al.*,[18,22] Yamada *et al.*,[19] Taxis *et al.*,[23] Charitidou *et al.*,[24] Nieto de Castro *et al.*,[26] and Nagasaka and Nagashima,[28] were all performed in transient hot-wire instruments in an absolute way, exhibited very low uncertainty (typically ±0.5%), and fulfill the aforementioned criteria for primary data. The data of Wu *et al.*[10,11] and Kashiwagi *et al.*,[27] performed also in transient hot-wire instruments but of slightly higher uncertainty, were also included in the primary data sets. In addition to these sets, some more sets were included; while they only partially fulfill the aforementioned criteria, they extend the temperature and pressure ranges of application. Thus the measurements of Shulga *et al.*,[25] performed in an AC transient hot-wire instrument, and of Kandiyoti *et al.*,[32] performed in a transient hot-wire instrument, were also included, as they extended the pressure range of application. To extend the temperature range, the measurements of Zaitseva *et al.*,[30] Geller and Zaporozhan,[31] Mani and Venart,[33] McLaughlin and Pittman,[34] and Akhundov and Gasanova[35] were also included, but with a lower statistical weight. The remaining measurements in Table 1 did not fulfill the criteria for primary data, nor did they contribute to extending the experimental coverage, and hence they were considered as secondary data.

Figure 1 shows the temperature and pressure ranges of the primary measurements outlined in Table 1. Temperatures for all data were converted to the ITS-90 temperature scale.[107] The development of the correlation requires densities; the equation of state (EOS) of Lemmon and Span,[108] valid from 178 K to 700 K and pressures up to 500 MPa, was used to provide the density for each experimental state point from the experimental temperature and pressure. Some of the primary data sets (Shulga *et al.*,[25] Nieto de Castro *et al.*,[26] and Kandiyoti *et al.*[32]) exceed the upper pressure limit of the EOS, but we believe the extrapolation behavior of this EOS is reasonable and used it to provide densities at pressures above 500 MPa. We also adopted the values for the critical point and triple point from this EOS; the critical temperature, T_c, the critical pressure, p_c, and the critical density, ρ_c, were taken to be equal to 591.75 K, 4.1263 MPa, and 291.992 kg m^{-3}, respectively.[108] The triple-point temperature is 178 K.[108] It should be noted that, for this EOS, the uncertainty in density from an input of temperature and pressure was reported to be 0.05% in the liquid phase up to 540 K, 0.5% from 540 K up to the critical temperature, 1% at temperatures above 540 K, 0.5% at pressures from 100 MPa to 500 MPa, and 0.2% in the vapor phase. The uncertainty for the saturated liquid density (and densities near atmospheric pressure) approaches 0.01% around 300 K. We also note that the estimated uncertainty in heat capacities is 0.5% and increases to 3% in the critical region.[108]

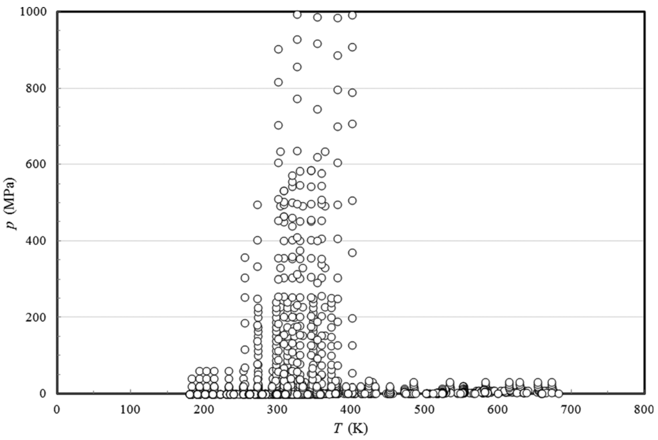

FIG. 1. Temperature and pressure ranges of the experimental thermal conductivity data for toluene.

3.1. The dilute-gas limit

In addition to the data of Zaitseva *et al.*[30] and Akhundov and Gasanova,[35] two other investigators (Nefedov and Filippov[63] in 1980, and Kostrovski and Prostov[71] in 1974) performed measurements near the dilute-gas limit. As these four sets are restricted to the temperature range from 350 K to 700 K, a theoretical based scheme was preferred in order to correlate the dilute-gas limit thermal conductivity, $\lambda_o(T)$, over a much wider temperature range.

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 perfect-gas heat capacity at constant volume, C_{Vo}, through the modified Eucken correlation,[109]

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

In the above equation, M represents the molar mass of toluene (92.140 g mol^{-1}), and R the universal gas constant[110] (8.3144621 J mol^{-1} K^{-1}). To employ the above equation, the dilute-gas viscosity and the perfect-gas heat capacity at constant volume are required. The dilute-gas viscosity can easily be obtained as a function of the reduced collision integral $\Omega^*(T^*)$, as

$$\eta_o(T) = \frac{5}{16}\left[\frac{M\,R\,T}{\pi}\right]^{1/2}\frac{1}{\sigma^2\,\Omega^*(T^*)}, \tag{3}$$

where the collision integral can be calculated[111] as a function of the reduced temperature, $T^* = T(k_B/\varepsilon)$, for the range $0.3 < T^* < 100$, as

$$\begin{aligned}\Omega^*(T^*) = {}& 1.16145(T^*)^{-0.14874} + 0.52487\mathrm{e}^{-0.7732T^*} \\ & + 2.16178\mathrm{e}^{-2.43787T^*} - 6.435\times10^{-4}(T^*)^{0.14874} \\ & \times \sin\left[18.0323(T^*)^{-0.7683} - 7.2371\right],\end{aligned} \tag{4}$$

and the perfect-gas heat capacity at constant volume, C_{Vo}, can be obtained from the heat capacity at constant pressure, C_{po} (J mol^{-1} K^{-1}), since $C_{po} - C_{vo} = R$. C_{po} is calculated according to Lemmon and Span,[108]

$$\frac{C_{po}}{R} = c_0 + \sum_{k=1}^{5} \upsilon_k \left(\frac{u_k}{T}\right)^2 \frac{\exp(u_k/T)}{[\exp(u_k/T) - 1]^2}. \tag{5}$$

The coefficients c_0, υ_k, and u_k for Eq. (5) are provided in Table 2. Equations (2)–(5) form a consistent scheme for the calculation of the dilute-gas limit thermal conductivity. It should be noted that the above equations assume that toluene vapor, although not spherical in shape, behaves like a Lennard–Jones gas, an assumption that has been employed successfully in the prediction and correlation of its viscosity (see for example Vogel and Hendl[112]). Furthermore, the fixed numerical value employed in the modified Eucken correlation, Eq. (2), was preferred, as it was simpler and at the same time produced very good results.

TABLE 2. Coefficients of Eq. (5) for the dilute-gas thermal conductivity of toluene

K	1	2	3	4	5
υ_k (−)	1.6994	8.0577	17.059	8.4567	8.6423
u_k (K)	190.0	797.0	1619.0	3072.0	7915.0
c_0 (−)	4.0				

In the above equations, the only unknowns are the Lennard–Jones parameters, σ (m) and ε/k_B (K). Since only four sets of thermal conductivity measurements exist near the dilute limit, these data were employed in order to optimize these two parameters. The values obtained were $\sigma = 0.524\times10^{-10}$ m and $\varepsilon/k_B = 595$ K. It should be noted that these values predict the viscosity values of Vogel and Hendl[112] within ±5%. The deviations of the present experimental dilute-limit thermal conductivity values from those calculated by the scheme of Eqs. (2)–(5) are shown in Fig. 2.

The values of the dilute-gas limit thermal conductivity, $\lambda_o(T)$, in mW m^{-1} K^{-1}, obtained by the scheme of Eqs. (2)–(5), were fitted for ease of use to a fifth-order polynomial as

$$\begin{aligned}\lambda_o(T) = {}& 5.8808 - 6.1693\times10^{-2}T + 3.4151\times10^{-4}T^2 \\ & - 3.0420\times10^{-7}T^3 + 1.2868\times10^{-10}T^4 \\ & - 2.1303\times10^{-14}T^5.\end{aligned} \tag{6}$$

Values calculated by Eq. (6) do not deviate from the values calculated by the scheme of Eqs. (2)–(5) by more than 1% over the temperature range 175–2000 K (with the largest deviations at the high end). In the same figure, the dilute-gas limit thermal-conductivity values proposed by Vargaftik *et al.*,[8] which are valid between 400 K and 650 K, are also shown. The agreement is excellent. However, due to the uncertainties in the limited data available, we estimate the uncertainty of Eqs. (2)–(5) as well as Eq. (6) to be

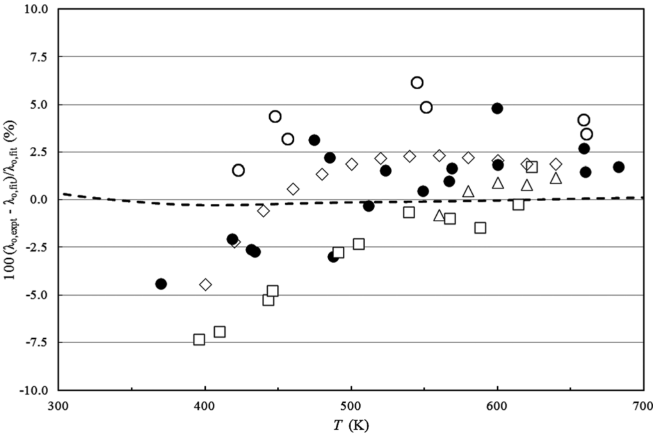

FIG. 2. Percentage deviations of experimental data for dilute-gas toluene from the values calculated by Eqs. (2)–(5). Nefedov and Filippov[63] (△), Zaitseva *et al.*[30] (●), Kostrovskii and Prostov[71] (□), Akhundov and Gasanova[35] (○), Vargaftik *et al.*[8] (◇), Values calculated by Eq. (6) (--).

approximately 5% above 400 K, and larger below 400 K, possibly reaching 10% at the triple point.

Finally it should be added that Abas-Zade[98] also proposed some dilute-gas limit thermal conductivity values in 1948, and these were the basis for some of the earliest compilations of recommended values such as those of Touloukian[5] and of Liley.[4] However, these values are much higher than any other set (by 14%–25%), and hence are not considered further.

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 non-singular residual values far away from the critical point.[113–115] 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. 116) to fit all the primary data simultaneously to the residual thermal conductivity and the critical enhancement, while maintaining the parameters already obtained from the fit of the dilute-gas thermal-conductivity data. The density values employed were obtained by the Helmholtz EOS of Lemmon and Span.[108]

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

$$\Delta\lambda(\rho,T) = \sum_{i=1}^{6}\left(B_{1,i} + B_{2,i}(T/T_c)\right)(\rho/\rho_c)^i. \tag{7}$$

The coefficients $B_{1,i}$ and $B_{2,i}$ are shown in Table 3.

3.3. The critical enhancement

3.3.1. Simplified crossover model

The theoretical based crossover model proposed by Olchowy and Sengers[113–115] 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.[117] The critical enhancement of the thermal conductivity is given by

TABLE 3. Coefficients of Eq. (7) for the residual thermal conductivity of toluene

i	$B_{1,i}$ (W m^{-1} K^{-1})	$B_{2,i}$ (W m^{-1} K^{-1})
1	$-5.185\,30 \times 10^{-2}$	$5.174\,49 \times 10^{-2}$
2	$1.338\,46 \times 10^{-1}$	$-1.219\,02 \times 10^{-1}$
3	$-1.204\,46 \times 10^{-1}$	$1.377\,48 \times 10^{-1}$
4	$5.302\,11 \times 10^{-2}$	$-7.327\,92 \times 10^{-2}$
5	$-1.006\,04 \times 10^{-2}$	$1.729\,14 \times 10^{-2}$
6	$6.334\,57 \times 10^{-4}$	$-1.385\,85 \times 10^{-3}$

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

with

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

and

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

In Eqs. (8)–(10), k_B is Boltzmann's constant and $\bar{\eta}$ is the viscosity that we obtained from a preliminary correlation[118] currently implemented in the REFPROP database[119] that uses the empirical form given by Lemmon and Jacobsen.[120] The method is not tied to any particular viscosity model; other formulations may be used as well. C_p and C_V are the isobaric and isochoric specific heat obtained from the EOS.[108] The effective wavenumber cutoff $\bar{q}_D$ can be determined by fitting thermal conductivity data in the critical region; however, the only data that were perhaps close enough to critical to show an enhancement were six points on the 3.5 MPa isobar of Akhundov *et al.*,[35] which proved insufficient for the regression. We instead used a predictive correlation[121] to obtain the value $\bar{q}_D^{-1} = 6.2 \times 10^{-10}$ m. The correlation length ξ is given by

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

As already mentioned, the coefficients $B_{1,i}$ and $B_{2,i}$ in Eq. (7) were fitted with ODRPACK (Ref. 116) to the primary data for the thermal conductivity of toluene. This crossover model requires the universal constants[117] $R_D = 1.02$, $\nu = 0.63$, and $\gamma = 1.239$, and system-dependent amplitudes Γ and ξ_0. For this work, we adopted the values $\Gamma = 0.05$ and estimated $\xi_0 = 2.2 \times 10^{-10}$ m, using the method that will be presented in Ref 121. The reference temperature T_{ref}, far above the critical temperature where the critical enhancement is negligible, was calculated by $T_{\text{ref}} = (^3/_2)\,T_c$,[122] which for toluene is 887.625 K. In other works, T_{ref} has been set at $2T_c$ (Ref. 113) or even $2.5T_c$ (Ref. 123). The optimal value of the parameter $\bar{q}_D$ will change slightly due to the selection of a different cutoff; we have selected $1.5T_c$ due to the fact that the upper limit of the EOS is 700 K and we want to minimize extrapolations of the EOS.

Table 4 summarizes comparisons of the primary data with the correlation. Here we define the percent deviation as $\text{PCTDEV} = 100*(\lambda_{\text{exp}} - \lambda_{\text{fit}})/\lambda_{\text{fit}}$, where λ_{exp} is the experimental value of the thermal conductivity and λ_{fit} is the value

TABLE 4. Evaluation of the toluene correlation for the primary data

1st author	Year Publ.	AAD (%)	BIAS (%)	STDEV (%)
Wu[10]	2009	0.55	0.26	0.60
Wu[11]	2005	0.71	0.45	0.64
Sun[12]	2002	0.87	−0.87	0.54
Watanabe[13]	2002	0.16	0.16	0.17
Assael[14]	2001	0.17	0.12	0.17
Perkins[15]	2000	1.48	1.03	1.30
Lei[16]	1997	0.54	0.49	0.41
Watanabe[17]	1997	0.49	0.38	0.45
Ramires[18]	1993	0.32	−0.14	0.40
Yamada[19]	1993	0.98	0.18	1.15
Assael[20]	1992	0.44	0.43	0.27
Perkins[21]	1991	0.42	0.01	0.47
Ramires[22]	1989	0.49	−0.28	0.53
Taxis[23]	1988	0.47	−0.46	0.23
Charitidou[24]	1987	0.54	0.51	0.30
Shulga[25]	1986	1.75	−0.79	1.92
Nieto de Castro[26]	1983	0.86	0.23	1.05
Kashiwagi[27]	1982	0.79	−0.06	0.98
Nagasaka[28,29]	1981	0.33	−0.13	0.39
Zaitseva[30]	1976	1.70	0.30	2.00
Geller[31]	1974	1.03	0.93	0.64
Kandiyoti[32]	1973	1.45	0.47	1.58
Mani[33]	1973	0.79	−0.72	0.83
McLaughlin[34]	1971	1.36	1.36	0.89
Akhundov[35]	1970	2.21	−0.64	3.84
Entire data set		**1.13**	**0.25**	**1.81**

calculated from the correlation. The average absolute percent deviation (AAD) is found with the expression $\mathrm{AAD} = (\sum|\mathrm{PCTDEV}|)/n$, where the summation is over all n points, the bias percent is found with the expression $\mathrm{BIAS} = (\sum\mathrm{PCTDEV})/n$, and the standard deviation is $\mathrm{STDEV} = ([n\sum\mathrm{PCTDEV}^2 - (\sum\mathrm{PCTDEV})^2]/n^2)^{1/2}$.

Figure 3 shows the percentage deviations of all primary thermal conductivity data from the values calculated by Eqs. (1)–(11) as a function of the density, while Figs. 4 and 5 show the same deviations but as a function of the temperature and pressure. The primary data for toluene listed in Table 1 cover a wide range of conditions and extend to 1000 MPa. Based on comparisons with the primary data, we estimate the uncertainty (considered to be estimates of a combined expanded uncertainty with a coverage factor of two) for pressures less than 700 MPa and temperatures less than 550 K to be less than 3%; for the region 550 K $\leq T \leq$ 700 K the uncertainty is estimated to be 4%. The region near the saturation boundary (within 0.5 MPa of the saturation pressure) has lower uncertainties and will be treated separately in Sec. 3.4. Uncertainties in the critical region are much larger, since the thermal conductivity approaches infinity at the critical point. The Olchowy–Sengers critical-enhancement model gives the correct behavior, but due to lack of accurate data in the critical region we were unable to provide a detailed assessment of the performance in this region. Finally, we believe the equations may safely be used for extrapolation in the region $T > 700$ K and 500 MPa $\leq p \leq$ 1000 MPa with an uncertainty on the order of 10%.

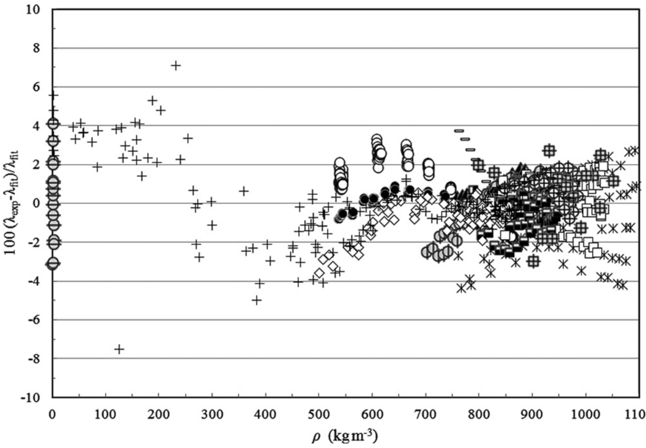

FIG. 3. Percentage deviations of primary experimental data of toluene from the values calculated by the present model as a function of the density. Wu *et al.*[10] (◧), Wu *et al.*[11] (◨), Sun *et al.*[12] (◭), Watanabe and Seong[13] (⊟), Assael and Dalaouti[14] (△), Perkins *et al.*[15] (○), Lei *et al.*[16] (⬘), Watanabe[17] (◫), Ramires *et al.*[18] (⬖), Yamada *et al.*[19] (⦶), Assael *et al.*[20] (▲), Perkins and Roder[21] (●), Ramires *et al.*[22] (⬗), Taxis *et al.*[23] (◆), Charitidou *et al.*[24] (△), Shulga *et al.*[25] (✱), Nieto de Castro *et al.*[26] (□), Kashiwagi *et al.*[27] (⬓) Nagasaka and Nagashima[28,29] (⬒), Zaitseva *et al.*[30] (⊖) Geller and Zaporozhan[31] (⊕) Kandiyoti *et al.*[32] (⊞) Mani and Venart[33] (◇), McLaughlin and Pittman[34] (-), Akhundov and Gasanova[35] (+).

Figures 6 and 7 show the deviations of the secondary data from the values calculated by the proposed scheme. It can be seen that the majority of the secondary data are within 4% of the proposed correlation. Most of the larger deviations refer

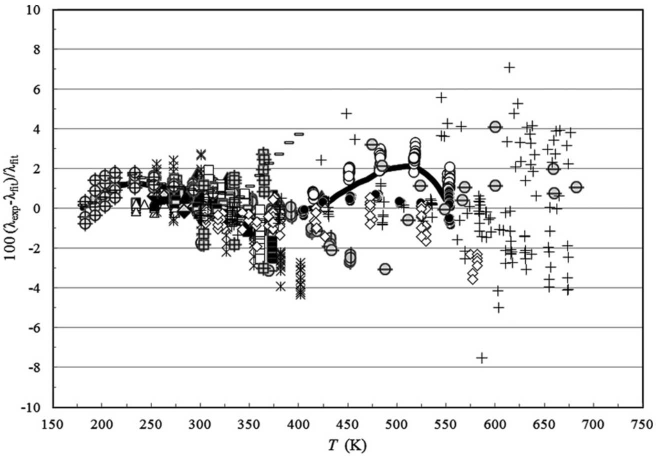

FIG. 4. Percentage deviations of primary experimental data of toluene from the values calculated by the present model as a function of the temperature. Wu *et al.*[10] (◧), Wu *et al.*[11] (◨), Sun *et al.*[12] (◭), Watanabe and Seong[13] (⊟), Assael and Dalaouti[14] (△), Perkins *et al.*[15] (○), Lei *et al.*[16] (⬘), Watanabe[17] (◫), Ramires *et al.*[18] (⬖), Yamada *et al.*[19] (⦶), Assael *et al.*[20] (▲), Perkins and Roder[21] (●), Ramires *et al.*[22] (⬗), Taxis *et al.*[23] (◆), Charitidou *et al.*[24] (△), Shulga *et al.*[25] (✱), Nieto de Castro *et al.*[26] (□), Kashiwagi *et al.*[27] (⬓) Nagasaka and Nagashima[28,29] (⬒), Zaitseva *et al.*[30] (⊖) Geller and Zaporozhan[31] (⊕) Kandiyoti *et al.*[32] (⊞) Mani and Venart[33] (◇), McLaughlin and Pittman[34] (-), Akhundov and Gasanova[35] (+), Reference correlation of Ramires *et al.*[6] (—).

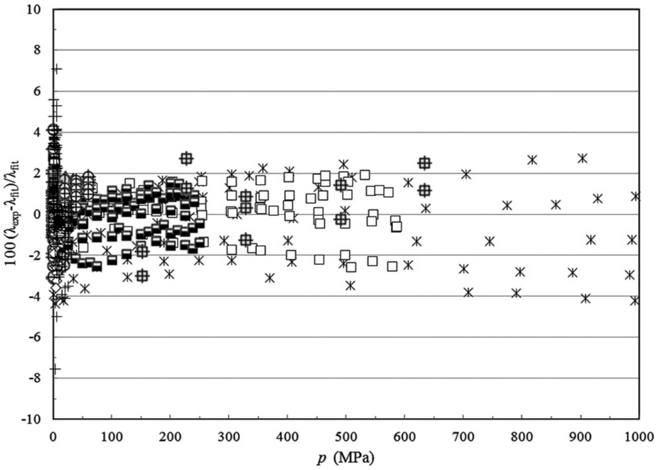

FIG. 5. Percentage deviations of primary experimental data of toluene from the values calculated by the present model as a function of the pressure. Wu *et al.*[10] (◧), Wu *et al.*[11] (◨), Sun *et al.*[12] (◭), Watanabe and Seong[13] (⊟), Assael and Dalaouti[14] (△), Perkins *et al.*[15] (○), Lei *et al.*[16] (⬘), Watanabe[17] (⊞), Ramires *et al.*[18] (◈), Yamada *et al.*[19] (⦶), Assael *et al.*[20] (▲), Perkins and Roder[21] (●), Ramires *et al.*[22] (◈), Taxis *et al.*[23] (◆), Charitidou *et al.*[24] (◭), Shulga *et al.*[25] (⚹), Nieto de Castro *et al.*[26] (□), Kashiwagi *et al.*[27] (⬓), Nagasaka and Nagashima[28,29] (⬒), Zaitseva *et al.*[30] (⊖) Geller and Zaporozhan[31] (⊕) Kandiyoti *et al.*[32] (⊞) Mani and Venart[33] (◇), McLaughlin and Pittman[34] (-), Akhundov and Gasanova[35] (+).

to data in the vicinity of the critical point. In particular, the light-scattering photon correlation spectroscopy (PCS) data of Will *et al.*[47] provide thermal diffusivity data that were converted to thermal conductivity with ρ and C_p calculated from the EOS.[39] This conversion process introduces additional uncertainty in the critical region, where the uncertainty in the calculated C_p increases. Finally, Fig. 8 shows a plot of the thermal conductivity of toluene as a function of the temperature for different pressures.

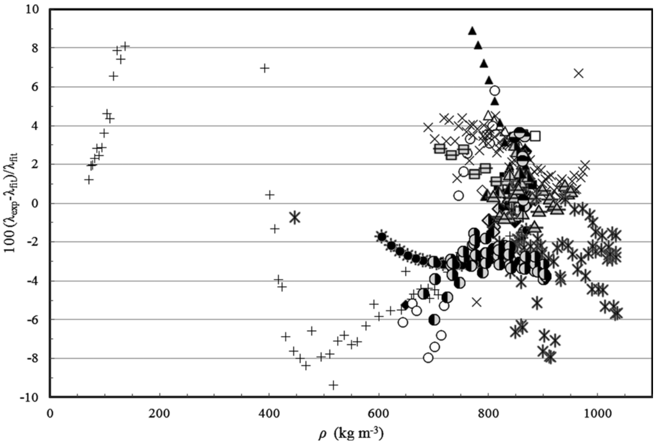

FIG. 6. Percentage deviations of secondary experimental data of toluene from the values calculated by the present model as a function of the density (period 1978–2008). Garnier *et al.*[36] (□), Tomida *et al.*[37] (■), Pan *et al.*[38] (◇), Ould-Lahoucine *et al.*[39] (⊕), Tarzimanov *et al.*[40] (◆), Zhang and Xu[41] (△), Will *et al.*[42] (+), Fujii *et al.*[43] (⊖), Frezzotti *et al.*[44] (▲), Kraft *et al.*[45] (●), Tong and Li[46] (○), Wang and Yang[47] (⦶), Kim *et al.*[48] (⬘), DiGuilio *et al.*[49] (◈), Gross *et al.*[50] (⬘), Naziev *et al.*[51] (X), DiGuilio and Teja[52] (◈), Huang *et al.*[53] (⬓), Richard and Shankland[54] (◧), Rowley and Gubler[55] (⬒), Knibbe and Raal[56] (⊟), Rowley and White[57] (◨), Ogiwara *et al.*[58] (⊞), Baroncini *et al.*[59] (◭), Yata *et al.*[60] (◭), Atalla *et al.*[61] (▲), Kitazawa and Nagashima[62] (⊖), Nefedov and Filippov[63] (⚹), Ogiwara *et al.*[64] (⊖), Spirin[65] (◐), Leidenfrost[66] (◑), Tada *et al.*[67] (◓).

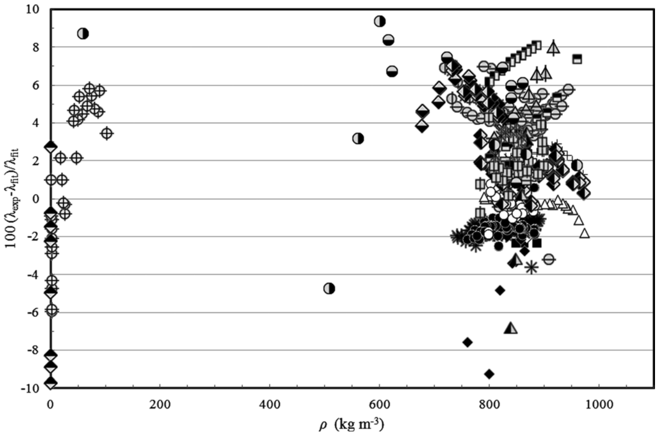

FIG. 7. Percentage deviations of secondary experimental data of toluene from the values calculated by the present model as a function of the density (period 1930–1977). Julia *et al.*[68] (□), Trump *et al.*[69] (■), Il'in[70] (◇), Kostrovskii and Prostov[71] (⊕), Davis *et al.*[72] (◆), Venart and Mani[73] (△), Brykov *et al.*[74] (+), Rastorguev and Pugash[75] (⊖), Stupak *et al.*[76] (▲), Rastorguev *et al.*[77] (⚹), Rastorguev *et al.*[78] (●), Tree and Leidenfrost[79] (○), Ganiev and Rastorguev[80] (⦶), Geller and Rastorguev[81] (⬘), Pittman[82] (◈), Vargaftik *et al.*[83] (⬘), Poltz and Jugel[84] (X), Rastorguev and Geller[85] (◈), Arrigoni[86] (⬓), Tufeu[87] (◧), Tsvetkov[88] (⬒), Venart[89] (⊟), Horrocks and McLaughlin[90] (◨), Ziebland[2] (⊞), Schrock and Starkman[92] (◭), Briggs[93] (◭), Frontasev and Gusakov[91] (◭), Challoner and Powell[94] (◭), Schmidt and Leidenfrost[95] (⚹), Filippov[96] (⊖), Riedel[97] (◐), Abas-Zade[98] (◑), Shiba[99] (◓), Smith[100] (-).

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,

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

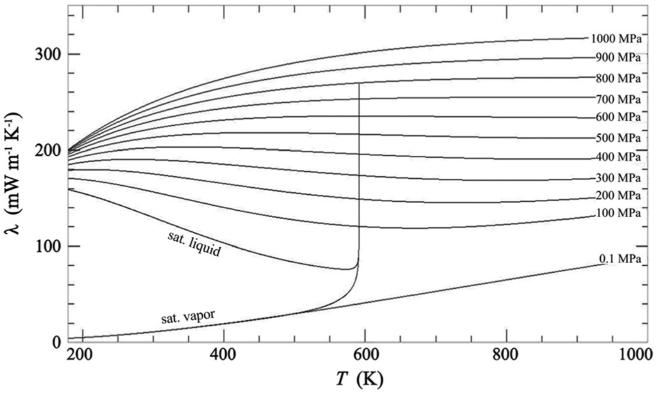

FIG. 8. Thermal conductivity of toluene as a function of the temperature for different pressures.

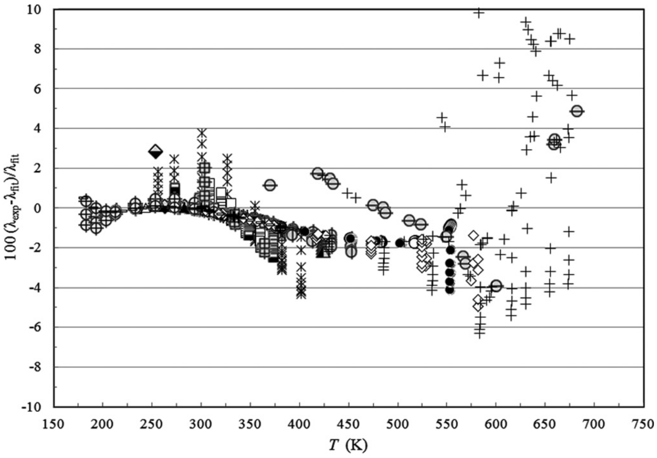

FIG. 9. Percentage deviations of primary experimental data of toluene from the values calculated by Eqs. (1), (6), (7), and (12) as a function of the temperature. Wu *et al.*[10] (◧), Wu *et al.*[11] (◨), Sun *et al.*[12] (◭), Watanabe and Seong[13] (⊟), Assael and Dalaouti[14] (△), Perkins *et al.*[15] (○), Lei *et al.*[16] (⬘), Watanabe[17] (◫), Ramires *et al.*[18] (⬖), Yamada *et al.*[19] (⦶), Assael *et al.*[20] (▲), Perkins and Roder[21] (●), Ramires *et al.*[22] (⬗), Taxis *et al.*[23] (◆), Charitidou *et al.*[24] (◬), Shulga *et al.*[25] (✳), Nieto de Castro *et al.*[26] (□), Kashiwagi *et al.*[27] (⬓) Nagasaka and Nagashima[28,29] (⬒), Zaitseva *et al.*[30] (⊖) Geller and Zaporozhan[31] (⊕) Kandiyoti *et al.*[32] (⊞) Mani and Venart[33] (◇), McLaughlin and Pittman[34] (-), Akhundov and Gasanova[35] (+).

where $\Delta T_c = (T/T_c) - 1$ and $\Delta\rho_c = (\rho/\rho_c) - 1$. This equation requires no accurate information on the compressibility, specific heat, and viscosity of toluene in the critical region, as does the theory of Olchowy and Sengers.[113–115] 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 $C_1 = 0.20 \times 10^{-3}$ W m^{-1} K^{-1}, $C_2 = 4.50 \times 10^{-2}$, and $C_3 = 0.090$. 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. 4 and 10, it can be seen that employing Eq. (12) results in little deterioration in the representation of the data.

3.4. The liquid saturation line

Figure 10 shows the percentage deviations of all primary thermal conductivity data from the values calculated by Eqs. (1)–(11) as a function of the temperature along the liquid saturation line. It can be seen that the proposed correlation represents the data within 2% at a 95% confidence level. In addition to the deviations of the primary data, the deviations of the values calculated by the reference correlation proposed by Ramires *et al.*[6] in 2000 are also shown. This correlation is characterized by uncertainties, at the 95% confidence level, of 1% for 189 K $< T <$ 440 K, 1.5% for 440 K $< T <$ 480 K, and 2% for 480 K $< T <$ 553 K, near the saturation line. The agreement between the two correlations is excellent.

In 1993, Vargaftik *et al.*[8] published two correlations. The first correlation, A, considered a large number of experimental data sets and was characterized by an uncertainty of 1% for 180 K $< T <$ 400 K, 1.5% for 400 K $< T <$ 500 K, and 2%–3% for $T >$ 500 K. Except in the region near 450 K, where the values calculated by that correlation deviate by up to 5% from the proposed one, in all other regions the agreement is considered satisfactory. In the same publication, Vargaftik *et al.*[8] proposed an additional correlation based upon the previously employed data with the exception of the data of Gabulov,[105] Rastorguev and Pugash,[75] and Leidenfrost,[66] which he considered not to be obtained in "sophisticated instruments"; it should be noted that these sets were also not included in the primary data set of the present work. The resulting correlation, B, is also shown in Fig. 10. It can be seen that, at temperatures higher than 450 K, the deviations between the two correlations exceed their mutual uncertainties.

In Table 5, selected values of the thermal conductivity of toluene along the liquid saturation line calculated by the

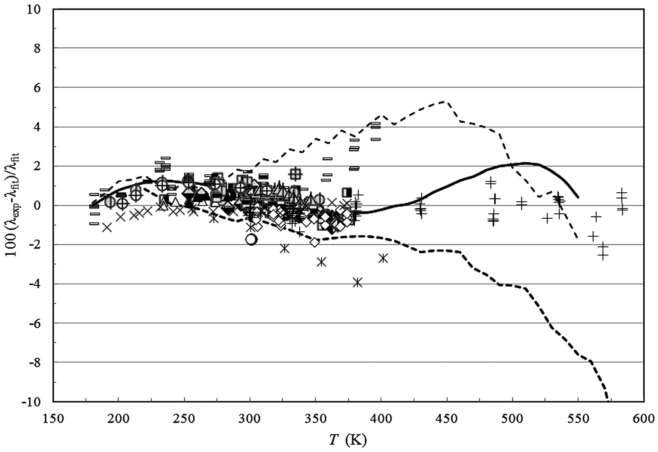

FIG. 10. Percentage deviations of primary experimental data of toluene from the values calculated by the present model as a function of the temperature along the liquid saturation line. Reference correlation of Ramires *et al.*[6] (—); Correlation (A) of Vargaftik *et al.*[8] (- - -); correlation (B) of Vargaftik *et al.*[8] (- - - -), and Wu *et al.*[10] (◧), Wu *et al.*[11] (◨), Watanabe and Seong[13] (⊟), Assael and Dalaouti[14] (△), Perkins *et al.*[15] (○), Lei *et al.*[16] (⬘), Watanabe[17] (◫), Ramires *et al.*[18] (⬖), Yamada *et al.*[19] (⦶), Assael *et al.*[20] (▲), Perkins and Roder[21] (●), Ramires *et al.*[22] (⬗), Taxis *et al.*[23] (◆), Charitidou *et al.*[24] (◬), Shulga *et al.*[25] (✳), Nieto de Castro *et al.*[26] (□), Kashiwagi *et al.*[27] (⬓) Nagasaka and Nagashima[28,29] (⬒), Geller and Zaporozhan[31] (⊕) Kandiyoti *et al.*[32] (⊞) Mani and Venart[33] (◇), McLaughlin and Pittman[34] (-), Venart and Mani[73] (X), Akhundov and Gasanova[35] (+).

TABLE 5. Selected values for the thermal conductivity of toluene along the liquid saturation line, calculated from the present scheme

T (K)	*p* (MPa)	ρ (kg m^{-3})	λ (mW m^{-1} K^{-1})
180	0.000000055336	972.87	158.79
200	0.0000010833	953.54	155.09
250	0.00017649	906.74	143.35
300	0.0041774	860.44	129.81
350	0.034821	812.87	116.07
400	0.15731	762.19	103.22
450	0.48619	705.68	92.115
500	1.1766	638.14	83.384
550	2.4279	544.82	77.383
590	4.0385	366.89	85.764

TABLE 6. Sample points for computer-verification of the correlating equations

T (K)	ρ (kg m^{-3})	λ (mW m^{-1} K^{-1})
298.15	0.000	10.749
298.15	862.948	130.66
298.15	876.804	136.70
595.00	0.000	40.538
595.00	46.512	41.549[a]
595.00	46.512	44.851[b]
185.00	0.000	4.3758
185.00	968.821	158.24

[a] Computed with modified Olchowy–Sengers critical enhancement; the viscosity at this point for use in Eq. (8) was taken as $\eta = 15.660$ μPa s (Ref. 119); all other properties required for the enhancement term are from Lemmon and Span (Ref. 108).

[b] Computed with empirical critical enhancement.

proposed scheme are shown. Values for the saturation pressure and density shown in the same table are obtained by the EOS of Lemmon and Span.[108]

4. Computer-Program Verification

Table 6 is provided to assist the user in computer-program verification. The thermal conductivity calculations are based on the tabulated temperatures and densities.

5. Conclusions

New wide-ranging correlations for the thermal conductivity of toluene were developed based on critically evaluated experimental data. The correlations are valid from the triple point to 1000 K, and at pressures up to 1000 MPa. The correlations are expressed in terms of temperature and density, and the densities were obtained from the EOS of Lemmon and Span.[108]

Acknowledgments

The work described in this paper was carried out under the auspices of the IATP. We thank our colleague Dr. Ilmutdin M. Abdulagatov for assistance with the Russian literature.

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