Reference Correlation for the Thermal Conductivity of *n*-Hexadecane from the Triple Point to 700 K and up to 50 MPa

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Reference Correlation for the Thermal Conductivity of *n*-Hexadecane from the Triple Point to 700 K and up to 50 MPa

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This paper presents a new wide-ranging correlation for the thermal conductivity of *n*-hexadecane based on critically evaluated experimental data. The correlation is designed to be used with a recently developed equation of state, and it is valid from the triple point up to 700 K and pressures up to 50 MPa. We estimate the uncertainty at a 95% confidence level to be 4% over the aforementioned range, with the exception of the dilute-gas range where the uncertainty is 2.7% over the temperature range 583–654 K. The correlation behaves in a physically reasonable manner when extrapolated to the full range of the equation of state, but the uncertainties are larger outside of the validated range, and also in the critical region. *Published by AIP Publishing on behalf of the National Institute of Standards and Technology.* https://doi.org/10.1063/1.5021459

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5 5 7

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Key words: n-hexadecane; thermal conductivity; transport properties.

CONTENTS

1.	Introduction
2.	The Correlation
	2.1. The dilute-gas limit
	2.2. The residual term
	2.3. The critical enhancement term
3.	Recommended Values
4.	Conclusions
	Acknowledgments
5.	References

List of Tables

1.	Thermal conductivity measurements of n-
	hexadecane
2.	Coefficients of Eq. (7) for the residual thermal
	conductivity of <i>n</i> -hexadecane
3.	Evaluation of the <i>n</i> -hexadecane thermal conduc-
	tivity correlation for the primary data
4.	Evaluation of the <i>n</i> -hexadecane thermal conduc-

tivity correlation for the secondary data

5.	Thermal conductivity values of <i>n</i> -hexadecane	
	along the saturation line, calculated by the present	
	correlation	7
6.	Thermal conductivity values of <i>n</i> -hexadecane at	
	selected temperatures and pressures, calculated	
	by the present correlation	7

List of Figures

1.	Temperature-pressure range of the primary ex-	
	perimental thermal conductivity data for n-	
	hexadecane	3
2.	Temperature–density range of the primary exper-	
	imental thermal conductivity data for <i>n</i> -	
	hexadecane	3
3.	Dilute-gas limit thermal conductivity of <i>n</i> -hex-	
	adecane as a function of temperature	4
4.	Percentage deviations of the dilute-gas limit thermal	
	conductivity experimental data of <i>n</i> -hexadecane	
	from Eq. (6) as a function of temperature	4
5.	Percentage deviations of primary thermal con-	
	ductivity experimental data of <i>n</i> -hexadecane from	
	the values calculated by the present correlation as	
	a function of temperature	5
6.	Percentage deviations of primary thermal con-	
	ductivity experimental data of <i>n</i> -hexadecane from	
	the values calculated by the present correlation as	
	a function of pressure	6

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6

7. Percentage deviations of primary thermal conductivity experimental data of *n*-hexadecane from the values calculated by the present correlation as a function of density

1. Introduction

In a series of recent papers, new reference correlations for the thermal conductivity of normal- and parahydrogen,¹ water,² sulfur hexafluoride,³ carbon dioxide,⁴ toluene,⁵ benzene,⁶ *n*-pentane and isopentane,⁷ *n*-hexane,⁸ cyclopentane,⁷ cyclohexane,⁹ *n*-heptane,¹⁰ methanol,¹¹ ethanol,¹² ethene and propene,¹³ ortho-xylene, meta-xylene, para-xylene, and ethylbenzene,¹⁴ and *n*-undecane¹⁵ were reported. The work was also extended to refrigerants; thus, reference correlations for the thermal conductivity of R245fa¹⁶ and R161¹⁷ were reported. In this paper, the methodology adopted in the aforementioned papers is extended to developing a new reference correlation for the thermal conductivity of *n*-hexadecane.

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*-hexadecane that is valid over gas, liquid, and supercritical states and that incorporates densities provided by the new Helmholtz equation of state of Romeo and Lemmon.¹⁸

The analysis that will be described will 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 purposes of comparison. According to the recommendation adopted by the Subcommittee on 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.¹⁹ 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.

2. The Correlation

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

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

where ρ is the density, *T* is the temperature, and the first term, $\lambda_0(T) = \lambda(0,T)$, is the contribution to the thermal conductivity

- 8. Thermal conductivity of *n*-hexadecane as a function of temperature for selected pressures
- 9. Thermal conductivity of *n*-hexadecane as a function of density for selected temperatures 6

6

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 the critical point. 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.

Table 1 summarizes, to the best of our knowledge, the experimental measurements²⁰⁻³⁷ of the thermal conductivity of *n*-hexadecane reported in the literature. The measurements of Assael et al.²² and Wada et al.²³ were performed in absolute transient hot-wire instruments employing a complete theoretical model, that operated with uncertainties of 0.5% and 1%, respectively. Furthermore, measurements from the two groups have already been successfully employed in previous correlations as primary data (Wada et al.²³ in Refs. 5, 10, and 15, and Assael et al.²² in Refs. 1, 5–8, 10–12, and 14). Hence, these two sets were considered as primary data. Mukhamedzyanov²⁴ and Mukhamedzyanov et al.²⁸ also employed a transient hot-wire instrument with an uncertainty of 1.5% and 1%, respectively. Those sets of measurements were also considered as primary data, as measurements from this group have already been successfully employed in previous correlations and provide an additional source of high-temperature vapor-phase data.^{6–8,11–15} Also in the primary data set, the measurements of Vélez et al.,²¹ performed in a transient hotwire instrument with the slightly inferior uncertainty of 2%, were included. The vapor-phase measurements of Tarzimanov and Mashirov,²⁷ performed in a hot-wire instrument, were also included in the primary data set, as they have also been employed in previous reference correlations.^{6,11–13,15} Tarzimanov and Mashirov²⁷ observed decomposition of n-hexadecane at temperatures above 675 K, and thus measurements from 660 K and higher were disregarded and not included in the primary data set. Additionally, the seven liquid-phase measurements of Tarzimanov et al.³¹ were not included in the primary data set, as they are inexplicably lower by up to 15% than all other measurements. The measurements of Feja and Hanzelmann²⁰ were performed in a concentric-cylinder instrument with a 3% uncertainty, and were included in the primary data set, as a full description of the instrument and the calibration procedures was given. Finally, a double calorimeter was employed by Mustafaev^{25,26} for measurements in the vapor and liquid phases with an uncertainty of 2%. As measurements from this investigator have previously been employed in other reference correlations,^{14,15} these sets were also considered as primary data. The remaining sets were considered as secondary.

We also note that the hot-wire measurements of Bogatov *et al.*,³⁶ performed up to 49 MPa with an uncertainty of 2%, were not included in the primary data set as at 0.1 MPa they

TABLE 1.	Thermal	conductivity	measurements	of	n-hexadecane

		Technique				Temperature	Pressure
1st author	Year publ.	employed ^a	Purity (%)	Uncertainty (%)	No. of data	range (K)	range (MPa)
Primary data							
Feja ²⁰	2018	CC	99.00	3.0	18	293-403	0.101
Velez ²¹	2015	THW	99.00	2.0	14	291-348	0.101
Assael ²²	1991	THW	99.00	0.5	10	297-337	0.101
Wada ²³	1985	THW	99.00	1.0	4	295-362	0.101
Mukhamedzyanov ²⁴	1974	THW		1.5	12	313-553	0.101
Mustafaev ²⁵	1973	DCAL		2.0	112	313-693	0.101-50
Mustafaev ^{26,b}	1973	DCAL		2.0	12	583-678	0.101
Tarzimanov ^{27,b}	1970	HW	99.97	4.0	6	584-697	0.097
Mukhamedzyanov ²⁸	1963	THW		1.0	15	307–453	0.101
Secondary data							
Sun ²⁹	2015	TTR		10.0	1	298	0.101
Holmen ³⁰	2002	GHF	99.00	20.0	1	291	0.101
Tarzimanov ³¹	1990	HW		2.0	7	325-524	0.101
Wang ³²	1989	THERM		2.0	13	423-523	5-25
Kravchun ³³	1986	THWPH		2.0	1	297	0.101
Gaitonde ³⁴	1978	PP		1.0	1	298	0.101
Powell ³⁵	1972	ThComp		3.0	1	303	0.101
Bogatov ³⁶	1969	HW		1.5	108	303-473	0.098-49
Sakiadis ³⁷	1952	PP	98.00	1.0	1	316	0.101

^aCC, Concentric Cylinders; DCAL, Double Calorimeter; GHF, Guarded Heat Flow; HW, Hot Wire; PP, Parallel Plate; ThComp, Thermal Comparator; THERM, Thermistor; THW, Transient Hot Wire; THWPH, Transient Hot Wire Periodic Heating; TTR, Transient Thermo-Reflectance.

^bIncludes vapor-phase measurements.

deviate by up to 15% from all other measurements, probably attributed to an improper calibration of the instrument.

Figures 1 and 2 show the range of the primary measurements outlined in Table 1, along with the saturation curve. The development of the correlation requires densities; Romeo and Lemmon¹⁸ developed an accurate, wide-ranging Helmholtz-energy equation of state that is valid from the triple point up to 800 K and 50 MPa, with an uncertainty in saturated liquid density of up to 0.1% in the temperature range 273-490 K, 0.1% in all other densities between 318 and



FIG. 1. Temperature-pressure range of the primary experimental thermal conductivity data for n-hexadecane. (--) saturation curve.



FIG. 2. Temperature-density range of the primary experimental thermal conductivity data for n-hexadecane. (--) saturation curve.

373 K, and pressures up to 28 MPa; and heat capacities 0.3%-0.5% in the temperature range 298–373 K. We also adopt the values for the critical point from their equation of state; the critical temperature, $T_{\rm c}$, and the critical density, $\rho_{\rm c}$, are 722.1 K and 226.441 kg m⁻³, respectively,¹⁸ while the triplepoint temperature is 291.329 K.¹

2.1. The dilute-gas limit

In order to be able to extrapolate the temperature range of the measurements, a theoretically-based scheme was used to correlate the dilute-gas limit thermal conductivity, $\lambda_0(T)$, over a wide temperature range. The traditional kinetic approach for thermal conductivity results in an expression involving three generalized cross sections.^{38,39} However, it is possible to derive an equivalent kinetic theory expression for the thermal conductivity by making use of the approach of Thijsse *et al.*⁴⁰ and Millat *et al.*,⁴¹ where one considers an expansion in terms of total energy, rather than separating translational from internal energy as is done traditionally. In this case, the dilute-gas limit thermal conductivity, $\lambda_o(T)$ (mW m⁻¹ K⁻¹), of a polyatomic gas can be shown to be inversely proportional to a single generalized cross section, $^{38-41} S(10E)$ (nm²), as

$$\lambda_{\rm o}(T) = 1000 \frac{5k_{\rm B}^2(1+r^2)T}{2m\langle\nu\rangle_{\rm o}S(10E)} f_{\lambda},\tag{2}$$

where $k_{\rm B}$ is the Boltzmann constant, T (K) is the absolute temperature, f_{λ} (-) is the dimensionless higher-order correction factor, m (kg) is the molecular mass of n-hexadecane, and $\langle \nu \rangle_{0} = 4\sqrt{k_{\rm B}T/\pi m}$ (m/s) is the average relative thermal speed. The dimensionless quantity r^2 is defined by r^2 = $2C_{int}^{o}/5k_{B}$, where C_{int}^{o} is the contribution of both the

rotational, $C_{\text{rot}}^{\text{o}}$, and the vibrational, $C_{\text{vib}}^{\text{o}}$, degrees of freedom to the isochoric ideal-gas heat capacity C_{v}^{o} .

The recent classical trajectory calculations^{42–44} confirm that, for most molecules studied, the higher-order thermalconductivity correction factor is near unity. One can take advantage of this finding to define the effective generalized cross section S_{λ} (= $S(10E)/f_{\lambda}$) (nm²), and rewrite Eq. (2) for the dilute-gas limit thermal conductivity of *n*-hexadecane, $\lambda_{o}(T)$ (mW m⁻¹ K⁻¹), as

$$\lambda_0(T) = 0.037\,071\,3\frac{\left(C_p^{\rm o}/k_{\rm B}\right)\sqrt{T}}{S_{\lambda}}.$$
(3)

The ideal-gas isobaric heat capacity per molecule, C_p^o (= C_{int}^o + 2.5 k_B) in (J/K), can be obtained from Romeo and Lemmon¹⁸ as

$$\frac{C_p^{\rm o}}{k_{\rm B}} = c_0 + \sum_{k=1}^2 \nu_k \left(\frac{u_k}{T}\right)^2 \frac{\exp(u_k/T)}{\left[\exp(u_k/T) - 1\right]^2},\tag{4}$$

where the values of the coefficients of Eq. (4) are $c_0 = 23.03$, $\nu_1 = 18.91$, $\nu_2 = 76.23$, $u_1 = 420$ K, and $u_2 = 1860$ K. It has been previously noted,⁴¹ and recently confirmed³⁹ for smaller molecules, that the cross section S(10E) exhibits a nearly linear dependence on the inverse temperature. Hence, in order to develop the correlation, we have fitted the effective cross section S_{λ} (nm²), obtained from the only two low-density primary data sets^{26,27} shown in Table 1 by means of Eqs. (3) and (4), as a function of the inverse temperature, as:

$$S_{\lambda} = 0.003\,56 + \frac{1424.045}{T}.$$
 (5)

We note here that since Tarzimanov and Mashirov²⁷ observed decomposition of *n*-hexadecane at 675 K, temperatures above 660 K of both these vapor data sets were not included. Equations (3)–(5) form a consistent set of equations for the calculation of the dilute-gas limit thermal conductivity of *n*-hexadecane.

The values of the dilute-gas limit thermal conductivity, $\lambda_0(T)$ in mW m⁻¹ K⁻¹, obtained by the scheme of Eqs. (3)–(5), were fitted as a function of the reduced temperature $T_r = T/T_c$ for ease of use to the following equation:

$$\lambda_0(T) = \frac{4.255\,47 - 39.3553\,T_{\rm r} + 140.965\,T_{\rm r}^2 - 244.669\,T_{\rm r}^3 + 143.418\,T_{\rm r}^4 - 48.4488\,T_{\rm r}^5 + 6.8884\,T_{\rm r}^6}{0.152\,925 - T_{\rm r}}.$$
(6)

Values calculated by Eq. (6) do not deviate from the values calculated by the scheme of Eqs. (3)–(5) by more than 0.03% over the temperature range from 292 to 1000 K, the range of validity of Eq. (6). Equation (6) is hence employed in the calculations that will follow.

Figure 3 shows the dilute-gas limit thermal conductivity of the selected investigators, and the values calculated by Eq. (6), as a function of the temperature. In Fig. 4, percentage deviations of the dilute-gas limit thermal conductivity of *n*-hexadecane from Eq. (6) are shown. In the same figure, values quoted in the books by Vargaftik *et al.*⁴⁵ and Yaws⁴⁶

are also shown. Furthermore, values calculated from the viscosity data of Lyusternik and Zdanov,⁴⁷ through a modified Eucken equation,⁵ are also shown. They all agree with the present correlation within their mutual uncertainties. Based on these measurements, the uncertainty of the correlation, at the 95% confidence level over the temperature range 583–654 K, is 2.7%. The correlation behaves in a physically reasonable manner over the entire range from the triple point to the highest temperature of the experimental data, 654 K;



Fig. 3. Dilute-gas limit thermal conductivity of *n*-hexadecane as a function of temperature. Mustafaev²⁶ (•), Tarzimanov and Mashirov²⁷ (o), and Eq. (6) (—).



FIG. 4. Percentage deviations of the dilute-gas limit thermal conductivity experimental data of *n*-hexadecane from Eq. (6) as a function of temperature. Mustafaev²⁶ (•), Tarzimanov and Mashirov²⁷ (o), Vargaftik *et al.*⁴⁵ (—), Yaws⁴⁶ (- -), and values calculated from the data of Lyusternik and Zdanov⁴⁷ (Δ).

however, we anticipate the uncertainty may be larger in the areas where data are not available and the correlation is extrapolated.

2.2. The residual term

The thermal conductivity of pure fluids exhibits an enhancement over a large range of densities and temperatures around the critical point and becomes 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.48-50 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 theoretically, 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. 51) to fit all primary data simultaneously to the residual thermal conductivity and the critical enhancement, while maintaining the values of the dilute-gas thermal-conductivity data already obtained. The density values employed were obtained by the equation of state of Romeo and Lemmon.¹⁸ The primary data were weighted in inverse proportion to the square of their uncertainty.

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

$$\Delta\lambda(\rho,T) = \sum_{i=1}^{5} \left(B_{1,i} + B_{2,i} (T/T_{\rm c}) \right) \left(\rho/\rho_{\rm c} \right)^{i}.$$
 (7)

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

2.3. The critical enhancement term

The theoretically based crossover model proposed by Olchowy and Sengers^{48–50} 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.⁵² The critical enhancement of the thermal conductivity from this simplified model is given by

$$\Delta\lambda_{\rm c} = \frac{\rho C_p R_{\rm D} k_{\rm B} T}{6\pi\overline{\eta}\xi} \left(\overline{\Omega} - \overline{\Omega}_0\right),\tag{8}$$

with

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

i	$B_{1,i} (\mathrm{mW} \mathrm{m}^{-1} \mathrm{K}^{-1})$	$B_{2,i} (\mathrm{mW} \mathrm{m}^{-1} \mathrm{K}^{-1})$
1	$-0.372089 imes 10^{-1}$	$0.409~813 imes 10^{-1}$
2	$0.935~694 imes 10^{-1}$	$-0.101\ 536 imes 10^{0}$
3	$-0.313\ 826 imes 10^{-1}$	$0.574~353 imes 10^{-1}$
4	$0.201\ 863 imes 10^{-2}$	$-0.153\ 161 imes 10^{-1}$
5	$0.255\ 103 imes 10^{-3}$	$0.197\ 462 imes 10^{-2}$

$$\overline{\Omega} = \frac{2}{\pi} \left[\left(\frac{C_p - C_v}{C_p} \right) \arctan\left(\overline{q}_{\mathrm{D}} \xi \right) + \frac{C_v}{C_p} \overline{q}_{\mathrm{D}} \xi \right]$$
(9)

and

$$\overline{\Omega}_{0} = \frac{2}{\pi} \left[1 - \exp\left(-\frac{1}{\left(\overline{q}_{\mathrm{D}}\xi\right)^{-1} + \left(\overline{q}_{\mathrm{D}}\xi\rho_{\mathrm{c}}/\rho\right)^{2}/3}\right) \right].$$
(10)

In Eqs. (8)–(10), $\overline{\eta}$ (Pa s) is the viscosity, and C_p and C_v (J kg⁻¹ K⁻¹) are the isobaric and isochoric specific heat obtained from the equation of state. The correlation length ξ (m) is given by

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

As already mentioned, the coefficients $B_{1,i}$ and $B_{2,i}$ in Eq. (7) were fitted with ODRPACK (Ref. 51) to the primary data for the thermal conductivity of *n*-hexadecane. This crossover model requires the universal amplitude, $R_D = 1.02$

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

1st author	Year publ.	AAD (%)	BIAS (%)
Feja ²⁰	2018	2.00	-1.89
Velez ²¹	2015	0.65	0.65
Assael ²²	1991	0.59	-0.44
Wada ²³	1985	0.34	-0.34
Mukhamedzyanov ²⁴	1974	1.88	0.70
Mustafaev ²⁵	1973	1.85	-0.94
Mustafaev ²⁶	1973	0.72	-0.72
Tarzimanov ²⁷	1970	1.95	1.95
Mukhamedzyanov ²⁸	1963	2.16	2.16
Entire data set		1.67	-0.45



Fig. 5. Percentage deviations of primary thermal conductivity experimental data of *n*-hexadecane from the values calculated by the present correlation as a function of temperature. Feja and Hanzelmann²⁰ (•), Velez *et al.*²¹ (□), Assael *et al.*²² (•), Wada *et al.*²³ (△), Mukhamedzyanov²⁴ (★), Mustafaev²⁵ (▲), Mustafaev²⁶ (◇), Tarzimanov and Mashirov²⁷ (◆), Mukhamedzyanov *et al.*²⁸ (■).

(-), the universal critical exponents, $\nu = 0.63$ and $\gamma = 1.239$, and the system-dependent amplitudes Γ and ξ_0 . For this work, we adopted the values $\Gamma = 0.063$ (-) and $\xi_0 = 0.291 \times 10^{-9}$ m, using the universal representation of the critical enhancement of the thermal conductivity by Perkins *et al.*⁵³ When there are sufficient experimental data available in the critical region, the remaining parameter \overline{q}_D^{-1} may be found by regression. In this case, there are no critical-region data available, so we instead use the method of Perkins *et al.*⁵³ to estimate the effective cutoff wavelength \overline{q}_D^{-1} . The estimated value is 9.98×10^{-10} m. The viscosity required for Eq. (8) was obtained by the very recent correlation of Meng *et al.*⁵⁴ The reference temperature $T_{\rm ref}$, far above the critical temperature where the critical enhancement is negligible, was calculated by $T_{\rm ref} = (3/2)T_c$,⁵⁵ which for *n*-hexadecane is 1083.2 K.

Table 3 summarizes comparisons of the primary data with the correlation. The average absolute percent deviation of the



FIG. 6. Percentage deviations of primary thermal conductivity experimental data of *n*-hexadecane from the values calculated by the present correlation as a function of pressure. Feja and Hanzelmann²⁰ (•), Velez *et al.*²¹ (□), Assael *et al.*²² (\bigoplus), Wada *et al.*²³ (\bigtriangleup), Mukhamedzyanov²⁴ (**X**), Mustafaev²⁵ (**A**), Mustafaev²⁶ (\bigotimes), Tarzimanov and Mashirov²⁷ (\bigoplus), Mukhamedzyanov *et al.*²⁸ (□).



FIG. 7. Percentage deviations of primary thermal conductivity experimental data of *n*-hexadecane from the values calculated by the present correlation as a function of density. Feja and Hanzelmann²⁰ (•), Velez *et al.*²¹ (□), Assael *et al.*²² (\bigoplus), Wada *et al.*²³ (\triangle), Mukhamedzyanov²⁴ (**X**), Mustafaev²⁵ (**A**), Mustafaev²⁶ (\bigotimes), Tarzimanov and Mashirov²⁷ (\bigoplus), Mukhamedzyanov *et al.*²⁸ (\blacksquare).

fit is 1.7%, and its bias is -0.47%. We estimate the uncertainty in thermal conductivity at a 95% confidence level to be 4% for the liquid phase over the temperature range 290–700 K at pressures up to 50 MPa.

Figure 5 shows the percentage deviations of all primary thermal conductivity data from the values calculated by Eqs. (1) and (6)–(11), as a function of temperature, while Figs. 6 and 7 show the same deviations but as a function of the pressure and the density. Table 4 shows the average absolute percent deviation (AAD) and the bias for the secondary data. Figure 8 shows a plot of the thermal conductivity of *n*-hexadecane as a function of the temperature for different pressures. The plot demonstrates the smooth extrapolation behavior at conditions outside of the range of experimental data (above 700 K and 50 MPa). Finally, Fig. 9 shows the thermal conductivity of *n*-hexadecane as a function of the temperature for different pressures.

TABLE 4. Evaluation of the *n*-hexadecane thermal conductivity correlation for the secondary data

1st author	Year publ.	AAD (%)	BIAS (%)
Sun ²⁹	2015	2.75	-2.75
Holmen ³⁰	2002	30.9	30.9
Tarzimanov ³¹	1990	8.54	-8.54
Wang ³²	1989	8.21	-8.21
Kravchun ³³	1986	1.10	1.10
Gaitonde ³⁴	1978	5.77	-5.77
Powell ³⁵	1972	3.39	3.39
Bogatov ³⁶	1969	5.22	-5.22
Sakiadis ³⁷	1952	4.09	4.09



Fig. 8. Thermal conductivity of *n*-hexadecane as a function of temperature for selected pressures.



Fig. 9. Thermal conductivity of n-hexadecane as a function of density for selected temperatures.

THERMAL CONDUCTIVITY OF HEXADECANE

T (K)	p (MPa)	$ ho_{ m liq}$ (kg m ⁻³)	$ ho_{ m vap}$ (kg m ⁻³)	$\lambda_{liq} \ (mW \ m^{-1} \ K^{-1})$	$\lambda_{vap} (mW \; m^{-1} \; K^{-1})$
300	2.470×10^{-7}	768.87	2.242×10^{-5}	143.50	6.10
350	2.105×10^{-5}	733.87	1.638×10^{-3}	134.77	8.60
400	4.609×10^{-4}	698.80	3.142×10^{-2}	126.32	11.73
450	4.276×10^{-3}	662.94	2.607×10^{-1}	118.27	15.42
500	2.256×10^{-2}	625.36	1.262×10^{0}	110.63	19.63
550	8.131×10^{-2}	584.62	4.313×10^{0}	103.29	24.31
600	2.258×10^{-1}	538.12	1.190×10^{1}	95.96	29.52
650	5.246×10^{-1}	480.10	2.954×10^{1}	88.03	35.63
700	1.087×10^{0}	389.94	7.882×10^{1}	77.99	46.00

density for different temperatures, including the critical enhancement.

3. Recommended Values

In Table 5, thermal conductivity values are given along the saturated liquid line, calculated from the present proposed correlation between 300 and 700 K, while in Table 6 thermal conductivity values are given for temperatures between 350 and 700 K at selected pressures. Saturation pressure and

TABLE 6. Thermal conductivity values of n-hexadecane at selected temperatures and pressures, calculated by the present correlation

p (MPa)	<i>T</i> (K)	ho (kg m ⁻³)	$\lambda \ (mW \ m^{-1} \ K^{-1})$
0.1	300	768.94	143.53
	350	733.96	134.80
	400	698.92	126.36
	450	663.10	118.32
	500	625.54	110.68
	550	584.69	103.30
	600	4.813	29.510
	650	4.367	35.083
	700	4.010	40.981
10	300	775.36	146.53
	350	742.24	138.25
	400	709.71	130.33
	450	677.41	122.93
	500	644.98	116.13
	550	612.06	109.95
	600	578.18	104.36
	650	542.82	99.31
	700	505.43	94.80
25	300	784.21	150.94
	350	753.27	143.21
	400	723.48	135.89
	450	694.61	129.16
	500	666.49	123.09
	550	639.00	117.72
	600	612.04	113.05
	650	585.52	109.08
	700	559.38	105.81
50	300	797.17	157.99
	350	768.87	151.02
	400	742.12	144.45
	450	716.72	138.45
	500	692.52	133.10
	550	669.40	128.42
	600	647.29	124.41
	650	626.10	121.07
	700	605.77	118.37

saturation density values for selected temperatures, as well as the density values for the selected temperature and pressure, are obtained from the equation of state of Romeo and Lemmon.¹⁸

4. Conclusions

A new wide-ranging correlation for the thermal conductivity of *n*-hexadecane was developed based on critically evaluated experimental data. The correlation is expressed in terms of temperature and density and is designed to be used with the equation of state of Romeo and Lemmon.¹⁸ The estimated uncertainty at the 95% confidence level is estimated to be 4% from the triple point to 700 K and up to 50 MPa, with the exception of the dilute-gas range where the uncertainty is 2.7% over the temperature range 583–654 K. The correlation behaves in a physically reasonable manner when extrapolated to the full range of the equation of state (to 800 K and 50 MPa), but the uncertainties are larger outside of the validated range, and also in the critical region.

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