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Thermal conductivity of gaseous and liquid n-hexane

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ABSTRACT

Absolute measurements of the thermal conductivity of n-hexane performed in a coaxial cylinder cell operating under steady state conditions are reported. The measurements of the thermal conductivity of n-hexane were carried out in the liquid along nine quasi-isotherms below the critical temperature ($T_c = 507.82$ K), in the low-pressurized gas at some temperatures below the critical temperature, and in the compressed gas along nine quasi-isotherms above the critical temperature. Additional thermal conductivity measurements were also performed in the liquid and the gas along the isobar at 0.101325 MPa and in the vapor close to the saturation curve for temperatures below the boiling temperature ($T_b = 341.865$ K). The present 577 data cover roughly the temperature range from 293 K to 612 K and the pressure range from 0.01 to 40 MPa. An analysis of the different sources of error leads to an estimated uncertainty of approximately 1.5%. The experimental results are correlated separating the additional contributions of the temperature effect and the density effect (in the density range from 0 to 670 kg m^{-3}). A brief comparison is shown with previous experimental measurements of the thermal conductivity of n-hexane.

1. Introduction

The purpose of this work is to report a new set of experimental data and to provide wide-ranging correlations for the thermal conductivity of n-hexane, which are valid over gas and liquid states. Normal hexane is very often used in industrial products. One of the most common applications of n-hexane is its use as a solvent, especially as a degreaser and industrial grade cleaner, paint diluent and alcohol denaturant. It is also commonly used in quality cleaning products. Other common applications include its use in shoe glue and leather, as its combination with insoluble compounds makes it an excellent adhesive.

In the food industry, n-hexane is frequently used to extract edible vegetable oils from oilseeds such as soybeans, cottonseeds, rapeseeds (canola), flaxseeds (linseed), mustard seeds, peanuts, safflower seeds and corn germs, which are then processed into food for human or livestock for animal.

Normal-hexane is an excellent reactive medium of polymerization, used as a raw material for the manufacture of polymers such as polypropylene or polyethylene. It can be also used to achieve complex three-dimensional structures of silver nanocrystals using near-critical fluid processing [1]. The silver nanoparticles were synthesized stabilizing droplets of water-solution in n-hexane by a monolayer of bis (2-ethyl-hexyl) sulfosuccinate (AOT) acting as a surfactant to form the so-called reverse micelles. At the end of the process, n-hexane is removed by subcritical CO_2.

Despite this widely use of n-hexane in the chemical industry developments, there are very few measurements of the thermal conductivity of n-hexane by comparison to other industrial fluids. Nevertheless, accurate experimental data of thermal conductivity are required over wide ranges of temperature and pressure to develop correlations that can represent this transport property, in order to design and improve efficient chemical processes and equipment. In Table 1, are reviewed a selected set of the experimental measurements of the thermal conductivity of n-hexane reported in the literature [2–13], which are considered in this work. The main goal is to compare the reliability of the measurements obtained from different methods for a future development of an improved wide-ranging correlation. Table 1 gives the range of measurements, the method used and the uncertainty. However for

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Table 1
Experimental studies of the thermal conductivities of n-hexane reported in the literature and considered in the present paper.

Year	Authors	Technique used[a]	Uncertainty[b] (%)	Temperature range K	Pressure range MPa	Ref.
1962	Golubev and Naziev	CC(Abs)	na	293–633	0.1–50	[2]
1969	Bogatov	HW	1.0	293–473	0.1–49	[3]
1972	Mukhamedzyanov et al.	HW(Abs)	2.0	298–448	0.1–220.5	[4]
1980	Kravchun	HW	na	282–576	0.1–30	[5]
1981	Naziev et al.	CC(Abs)	1.5	196–473	0.1–50	[6]
1982	Kashiwagi et al.	THW(Rel)	2.0	298–333	0.1	[7]
1983	**Shashkov et al.**	HF(Abs)	1.5	332–370	0.1	[8]
1984	Naziev et al.	CC(Abs)	na	423–623	0.1–2	[9]
1984	Li et al.	THW(Abs)	0.3	307–360	1.8–643	[10]
1987	Assael et al.	THW(Abs)	0.5	300–325	0.1	[11]
1988	Tanaka et al.	THW(Abs)	1.0	283–373	0.1–250	[12]
2002	Watanabe et al.	THW(Abs)	0.5	297–334	0.1	[13]
1994	Vargaftik et al.	COR.		200–470	0.1–40	[14]
2013	Assael et al.	COR.		178–600	0.1–500	[15]

[a] Abs, absolute; Rel, relative; CC, coaxial cylinder; HF, hot filament; HW, hot wire; THW, transient hot wire; COR, correlation.
[b] na: not available.

a reader interested in a more extended literature review of the thermal conductivity measurements in n-hexane, a larger set of publications on the thermal conductivity measurements of n-hexane can be found in Refs. [14] and [15], where are proposed correlations of the n-hexane thermal conductivity data, which can be easily completed using the TRC/NIST SOURCE DATA archive Thermolit for n-hexane case.

As shown in Table 1, most of the selected experimental data have been reported in the liquid state and are performed with hot filament (HF), hot wire (HW), or transient hot wire (THW) apparatuses. The data of Li et al. [10], Assael et al. [11], Tanaka et al. [12], Watanabe et al. [13], were measured in an absolute transient hot-wire (THW) instrument with an uncertainty of less than 1.0%. The absolute measurements of Mukhamedzyanov et al. [4], and those of Kashiwagi et al. [7], using respectively hot wire (HW) and transient hot wire (THW) techniques, were reported both with an uncertainty of 2%. However, the comparison between these different sets of data, which enter in the selected primary data of Ref. [15], shows that the mutual deviations are much larger that the claimed uncertainties, as confirmed from the statistical evaluations of their correlation reported in Table 3 of Ref. [15]. Here the data of Bogatov [3] and Kravchun [5], which use similar hot-wire (HW) techniques, and those of Shashkov et al. [8] using hot-filament (HF) technique are also introduced in these comparative evaluations. As mentioned just above, an additional goal of this work was then to determine which set of data provided from hot wire (HW), hot filament (HF), and transient hot wire (THF) instruments gives the better agreement with our data obtained with a different instrument, namely, the coaxial cylinder (CC) apparatus, and to compare our data to the ones of Refs [2] [6], and [9] obtained using similar CC techniques.

2. Experimental apparatus and procedure

The thermal conductivity measurements of homogeneous liquid and gas n-hexane were carried out as a function of temperature and pressure using a concentric cylinder apparatus, operating in the steady-state mode. These experimental apparatus and procedure were described and used in several publications [16–27]. Here we recall that the fluid was in the annular gap between two coaxial cylinders with the axis in the vertical direction. The thermal conductivity was determined by measuring the temperature difference between the inner and the outer cylinders as a function of the energy dissipated by the inner cylinder. The temperature difference between the two cylinders was varied from 0.5 K (vapor) to 1.0 K (liquid); this temperature difference was measured with an uncertainty of approximately 0.003 K. During the experiments, the stability of the temperature was better than 0.05 K and the uncertainty of temperature measurements was ±0.02 K. The pressure was measured with a precision pressure transducer with uncertainty of 0.02%. To determine the thermal conductivity, we needed to consider the corrections due to heat transferred by radiation, spurious heat flow from the inner to the outer cylinder through the solid centering pins and the wires, heat transferred by convection, and the effects of a possible temperature jump at the boundaries of the fluid layer and surfaces of the cylinders. We calculated the radiation correction from the Stefan-Boltzmann radiation law, assuming that the absorption of radiation by the fluid could be neglected. The correction for heat losses through the solid parts of the cell was determined from a set of calibration measurements with argon, neon, and helium, for which the thermal conductivity was known with considerable precision. These calibrations were performed at pressures of 1 MPa for argon, 5 MPa for neon, and 10 MPa for helium, i.e., at pressures for which any temperature jump can be neglected. The convection which takes place in the cell was assumed to be laminar and was approximated following a relation reported in Ref. [16].

The sample of anhydrous n-hexane was supplied by Sigma-Aldrich with the following product specification: product name: hexane, mixture of isomers anhydrous, > = 99%, formula: C_6H_{14}, formula weight: 86.18, liquid purity (gc area %) ≥ 99.0%, 99.9% remarks on gc purity: as mixture of hexane isomers plus methylcyclopentane, remarks on gc ≥ 65.0% n-hexane 98.2%, refractive index n20/d 1.373–1.381 1.375, water (coulometr.) ≤ 0.005% H_2O (100 ml unit size only), ≤0.001% H_2O (remaining unit sizes) < 0.001%, residue (evaporation) ≤ 0.0005% < 0.0001%, infrared spectrum conforms to structure.

3. Experimental results

The thermal conductivity measurements of n-hexane have provided 577 data covering the temperature range from 293 K to 612 K and pressures up to 40 MPa. Fig. 1 shows the data points in the p-T diagram. 250 data correspond to measurements in the homogeneous liquid region (*full blue squares* in Fig. 1). 269 data correspond to measurements in the gaseous state in Fig. 1, separating 195 data (*open green triangles*) for $\rho > 432\ kg\ m^{-3}$, 55 data (*open green squares*) for $\rho < 20\ kg\ m^{-3}$, and 19 data (*red plus sign*) for $27\ kg\ m^{-3} < \rho < 432\ kg\ m^{-3}$ (see comment below). In addition, 53 data correspond to measurements at atmospheric pressure in the liquid (22 *full red circles*) and the gaseous (31 *open red circles*) region covering the temperature range 315–612 K. 5 data (5 *open purple diamonds*) correspond to measurements in the gas phase along the