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Vapor Pressures of *n*-Heptane Determined by Comparative Ebulliometry

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The vapor pressures of *n*-heptane have been measured using comparative ebulliometry with water as the reference substance. The measurements cover the temperature and pressure range (372 K and 102 kPa) to (537 K and 2621 kPa) and were correlated by a Wagner-type equation with a standard deviation of 16 Pa in the vapor pressure. The critical pressure was treated as an adjustable parameter, and the value $p_c = 2734$ kPa was obtained using a selected critical temperature, $T_c = 540.13$ K. The calculated normal boiling temperature is $T_b = 371.552$ K, and an extrapolation to the triple point pressure at $T_{tp} = 182.59$ K predicts a pressure, $p_{tp} = 0.178$ Pa.

Introduction

Comparative ebulliometry is an accurate and rapid method to measure vapor pressures. The condensation temperatures of the substance under study and of a reference material, in our case water, are measured when the two liquids are boiling at the same pressure. The vapor pressure is deduced from the known $p(T)$ behavior of the reference fluid. The method avoids the necessity of measuring the pressure directly, and the fluids are degassed by boiling.[1−3]

The great majority of vapor pressure measurements by the ebulliometric method have been restricted to pressures below 200 kPa by the use of glass containers, but work with stainless steel vessels in different laboratories has extended the pressure range considerably over the past decade.[4−11] In this paper, we report 43 vapor pressures over the temperature and pressure range from (371.6 K, 102 kPa) to (537.2 K, 2621 kPa), which is about 3 K and 113 kPa below the critical point of *n*-heptane, and give an equation for use between the triple point and the critical point.

Measurement Section

Materials. HPLC grade heptane obtained from a commercial supplier with a stated purity greater than 99.5 mol % was distilled, without preliminary purification, in a 91 cm × 2.54 cm diameter Podbielniak heligrid column operating at total reflux and about 100 theoretical plates.

Samples of volume 45 cm^3 were removed periodically from the still and stored under argon and sealed in ampules. The purity of the distillate was monitored using the normal boiling temperature T_b, which was measured to 1 mK in a glass ebulliometer.[2,3]

This was a particularly appropriate and fast way to assess the purity of samples for vapor pressure measurements, and fractions with T_b agreeing to 2 mK were combined and set aside for use. A final sample of *n*-heptane with a volume of 200 cm^3 was collected and used for measurements. Analysis by GLC showed that the mole fraction purity was better than 0.999. Dionized and triple distilled water was used as the reference fluid, and helium was used as the buffer gas.

Apparatus and Procedures. The details of the apparatus have been published before; therefore, only a brief description is given here.[7] The sample and reference ebulliometers were constructed from 316 stainless steel tubing, each one has a re-entrant thermometer well (320 mm long for the sample and 450 mm long for the reference) with double radiation shields that provide a very generous depth of immersion for the long-stem platinum thermometer. Both ebulliometers have a welded sidearm and a reflux condenser that is connected to a common pressure line through a cold trap filled with solid CO_2 to avoid any cross contamination. A cylindrical band heater was fitted to the base of the ebulliometer, and thermocouples were attached along the main body of the vessel to monitor the progress of the condensation level until equilibrium was achieved.

The sample ebulliometer was cleaned by boiling 40 cm^3 of purified *n*-heptane for several hours, evacuated, and dried by heating and pumping for several hours before the final 200 cm^3 sample of pure *n*-heptane was introduced under an atmosphere of argon. A similar procedure was followed to clean and charge the water ebulliometer.

The thermometers were calibrated on the ITS-90 by NPL, and their resistance at the triple point of water was checked regularly during the project. Small head corrections were applied to account for the differences between the gaseous densities of heptane and water. The vapor pressures of water were calculated from the correlation published by Wagner.[12]

Results and Discussion

Table 1 lists our 43 vapor pressures measured for *n*-heptane together with the percentage deviations of these results from the final eq 5, which is discussed below. The uncertainty of our temperature measurements is 2 mK, while the uncertainty in the vapor pressure of water, which ultimately restricts the accuracy of our measurements, is 0.025 % at the pressures used here as reported in graphical form by the International Association for the Properties of Water and Steam.[13]

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Table 1. Experimental Vapor Pressures p of n-Heptane Obtained by Comparative Ebulliometry at Temperatures T on ITS-90 Together with Percent Deviations, $100(p_{exp} - p_{cal})/p_{exp}$ from Eq 5 Using the Coefficients Given in Table 2

T/K	p/kPa	$100(p_{exp} - p_{cal})/p_{exp}$	T/K	p/kPa	$100(p_{exp} - p_{cal})/p_{exp}$
372.080	102.902	−0.004	469.841	925.230	0.000
374.500	110.393	−0.004	473.394	983.899	0.000
377.683	120.888	−0.003	476.107	1030.553	0.000
384.393	145.556	−0.002	479.566	1092.410	−0.003
389.406	166.406	−0.002	483.665	1169.382	−0.001
393.585	185.495	−0.001	487.361	1242.283	0.004
396.700	200.787	−0.001	490.812	1313.388	0.005
401.258	224.890	−0.002	494.112	1384.190	0.001
405.442	248.924	0.000	496.771	1443.398	0.002
409.660	275.088	−0.001	500.015	1518.182	−0.001
413.799	302.765	0.001	503.591	1604.134	0.000
419.168	341.763	0.002	507.388	1699.505	0.000
423.851	378.798	0.002	510.952	1793.008	0.000
428.687	420.153	0.000	515.266	1911.603	−0.001
433.814	467.647	0.000	518.993	2019.086	−0.001
438.862	518.271	0.000	522.220	2116.113	−0.001
443.495	568.273	0.000	525.530	2219.702	0.000
447.955	619.765	−0.001	528.304	2309.807	0.000
451.804	666.967	−0.001	531.468	2416.500	−0.001
456.351	726.159	−0.001	534.573	2525.679	−0.001
459.776	773.289	−0.002	537.195	2621.761	0.002
465.068	850.621	0.000			

Over the past century, many equations have been proposed to relate vapor pressures of pure compounds to temperature, but perhaps the most successful has been the Wagner equation,[14] which generates a family of equations suitable for representing vapor pressures. Wagner applied regression techniques to vapor pressure data to produce equations for which both the coefficients and the functional form are adjustable.[15] The general form of the equation is

$$\ln(p/p_c) = (T_c/T)\sum c_i\tau^i \tag{1}$$

where T_c and p_c are the critical temperature and the critical pressure, respectively, and

$$\tau = 1 - T/T_c \tag{2}$$

is a reversed reduced temperature variable. In principle, any set of exponents i may be used to produce a wide variety of functional forms. However, in practice, the equations always have the first two terms in τ and $\tau^{3/2}$ with two or more further terms in τ^i whose exponents are restricted to integer and half-integer values. Equation 1 can be rewritten to treat $\ln p_c$ as an adjustable parameter leaving $\ln p$ as the objective function, and this is the approach we have adopted in the analysis of n-heptane.

The critical temperature (T_c) is required for an analysis using the generalized Wagner equation, and rather than measure T_c ourselves, we have relied on the literature where around nine measurements of the critical point of heptane have been reported in the last 30 years. Ambrose and Tsonopoulos[16] reviewed these results and recommended a critical point of $T_c = (540.2 \pm 0.3)$ K and $p_c = (2740 \pm 30)$ kPa. However, we have preferred Brunner's measurements,[17] which gave $T_c = (540.13 \pm 0.10)$ K and $p_c = (2734 \pm 5)$ kPa because they have lower uncertainties.

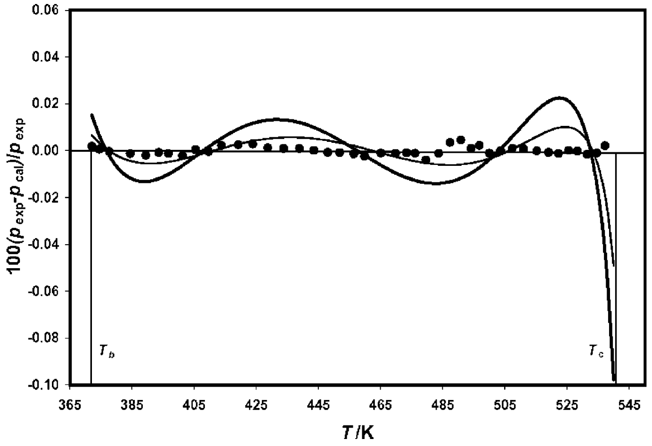

Figure 1. Percent deviations from different Wagner equations fitted to the experimental vapor pressures from Table 1: ●, Wagner eq 4; thin solid line, Wagner eq 3; thick solid line, Wagner equation with terms in τ^3 and τ.[6] T_b and T_c are respectively the normal boiling temperature and the critical temperature.

Figure 1 shows the experimental vapor pressures fitted to different forms of the Wagner equation. The standard form, which is widely used in data banks,[18]

$$\ln p = \ln p_c + (T_c/T)(c_1\tau + c_{1.5}\tau^{1.5} + c_{2.5}\tau^{2.5} + c_5\tau^5) \tag{3}$$

fits our results with a fractional standard deviation of $\sigma(\ln p) = \{\sigma(p)/p\} = 63 \times 10^{-6}$, but it shows some systematic deviations, and the predicted critical pressure is $p_c = 2732.9$ kPa. Another popular form,[14] with terms in τ^3 and τ^6 in place of $\tau^{2.5}$ and τ^5, shows very strong systematic deviations with $\sigma(\ln p) = 138 \times 10^{-6}$ and $p_c = 2731.6$ kPa. The equation that best represents our 43 measurements has the form:

$$\ln p = \ln p_c + (T_c/T)(c_1\tau + c_{1.5}\tau^{1.5} + c_2\tau^2 + c_{4.5}\tau^{4.5}) \tag{4}$$

which was used by Wagner for methane,[19] and gives for n-heptane $\sigma(\ln p) = 18 \times 10^{-6}$ with a calculated critical pressure $p_c = 2734.3$ kPa. The agreement with Brunner's directly measured value of p_c is excellent. Table 2 shows the coefficients of the different forms of the Wagner equations together with the calculated critical pressures (p_c) and standard deviations in p and $\ln p$ obtained through regression analysis.

At the time, we did not measure the vapor pressures of n-heptane below atmospheric pressure, although these metal ebulliometers have since produced results at pressures as low as 5 kPa, which are of comparable quality to those measured in glass containers.[7–10,20] Low pressures measurements are necessary for extrapolation purposes so we have selected the results obtained by Rossini and coworkers[21] and by Smith,[22] both working at NBS with comparative glass ebulliometers, to define the low-pressure region. All measurements were converted to the ITS-90 temperature scale. In the case of Rossini, who produced

Table 2. Critical Pressures, p_c, Coefficients, c_i, of the Wagner Eqs 3, 4, and 5 and Standard Deviations $\sigma(p)$ and $\sigma\{\ln(p)\}$ Obtained by Regression Analysis of the Vapor Pressures, p, in Table 1 Using the Critical Temperature T_c = 540.13 K

p_c/kPa	c_1	$c_{1.5}$	c_2	$c_{2.5}$	c_3	c_4	$c_{4.5}$	c_5	c_6	$10^6\sigma\{\ln(p)/\text{kPa}\}$	$\sigma(p)$/Pa
2732.9	−7.775245	1.849619		−2.788053				−3.556263		63	125
2731.6	−7.699935	1.468769			−3.953889				1.370138	138	269
2734.3	−7.889373	2.779687	−2.710918				−4.742493			18	21
2734.4	−7.897398	2.866000	−2.990959		1.196037	−4.925711				56	16

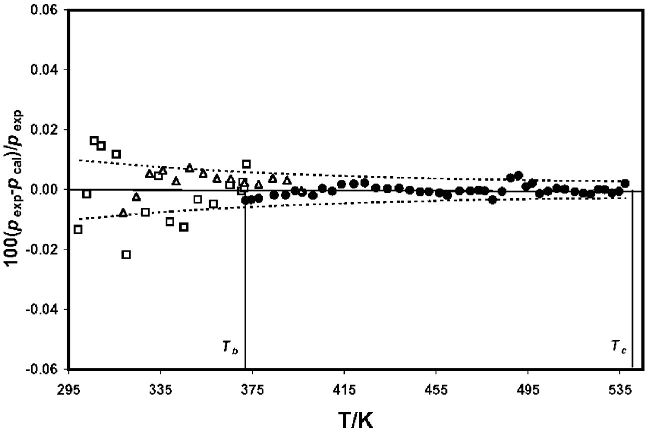

Figure 2. Percent deviations from the Wagner eq 5 for *n*-heptane: ●, this work; □, Willingham et al.;[21] △, Smith;[22] The dot lines show values of 100 $\Delta p/p$ for $\Delta T = \pm$ 2 mK. T_b and T_c are respectively the normal boiling temperature and the critical temperature.

two series of measurements on heptane, we are using his series with the more recent date. The results were combined, with all points receiving equal weight, to give a combined data set for *n*-heptane that covers the experimental temperature and pressure range (298.9 K, 6.3 kPa) to (537 K, 2621 kPa) or $0.55 < T_r < 0.99$ in terms of reduced temperature (T_r). Regression analysis with eq 4 now produced systematic deviations similar to those depicted in Figure 1 for the forms with $\tau^{2.5}$ and τ^5 or the form with τ^3 and τ^6. We encountered this situation before when fitting the vapor pressures of cyclohexane,[8] octane,[9] and acetonitrile[10] and found that an additional term, statistically significant, was needed to account for the behavior at low pressures and to avoid these systematic deviations. Figure 2 shows the deviation plot of our final eq 5 with five adjustable parameters in τ plus the critical pressure p_c, given by

$$\ln p = \ln p_c + (T_c/T)(c_1\tau + c_{1.5}\tau^{1.5} + c_2\tau^2 + c_3\tau^3 + c_4\tau^4) \tag{5}$$

which represents the experimental vapor pressures with standard deviations of $\sigma(p) = 16$ Pa and $\sigma(\ln p) = 56 \times 10^{-6}$. The predicted critical pressure is $p_c = 2734.3$ kPa, which agrees very well with the value measured directly by Brunner[17] and is well within the experimental uncertainty of the critical pressure recommended by Ambrose.[16] The coefficients of eq 5 are shown in Table 2.

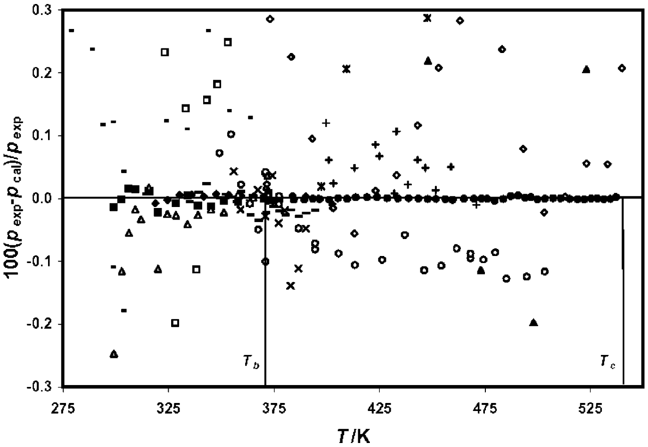

Figure 3. Percent deviations from the Wagner eq 5 for *n*-heptane: ●, this work; ■, Willingham et al.;[21] ◆, Smith;[22] ×, sample 1, Weber;[5] —, sample 2, Weber;[5] ○, sample 3, Weber;[5] +, Wisniewska et al.;[6] ∗, Olson;[11] ◇, McMicking and Key;[23] ▲, Zawisza and Vejrosta;[24] -, Sipowska and Wieczorek;[25,26] △, series 1,Willingham et al.;[21] □, Saez et al.[27] T_b and T_c are respectively the normal boiling temperature and the critical temperature.

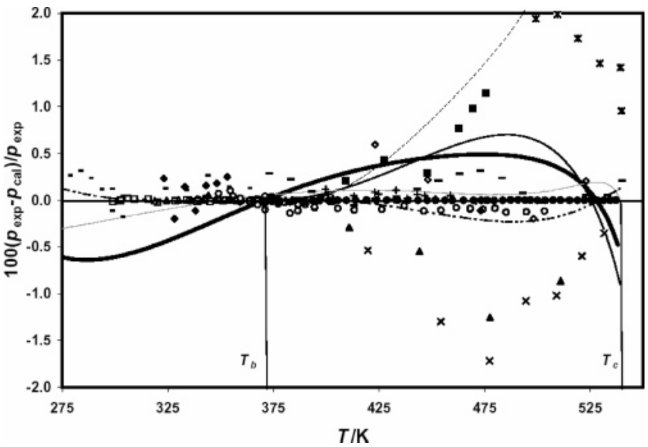

Figure 4. Percent deviations from the Wagner eq 5 for *n*-heptane: ●, this work; □, Willingham et al.;[21] △, Smith;[22] ○, Weber;[5] +, Wisniewska et al.;[6] —, McMicking and Key;[23] ◇, Zawisza and Vejrosta;[24] −, Sipowska and Wieczorek;[25,26] ■, Olson;[11] ◇, de Loos et al.;[30] ◆, Saez et al.;[27] ×, Kay;[28] ▲, Nichols et al.;[29] thin solid line, NIST/TRC;[31] dash line, Dykyj et al.;[32] thick solid line, DIPPR;[33] dot line, Span;[34] dot-dot-dash line, ThermoData Engine.[35] T_b and T_c are respectively the normal boiling temperature and the critical temperature.

The vapor pressures of heptane have been measured by different researchers, and Figures 3 to 5 compare their values with those calculated from eq 5. We included the three sets of results employed to obtain eq 5 and note that they show a high level of internal consistency as compared with the other data from the literature. The vapor pressures measured by Weber[5] (most recent results), Malanowski and co-workers,[6] and Olson[11] were all obtained using metal ebulliometers. In the case of Weber, three different samples with slightly different composition were used in the measurements without further purification. Samples 1 and 3 were reported to have an additional volatile impurity picked up from the apparatus. The vapor pressures of these three samples were adjusted by Weber for the presence of the impurities and are depicted in Figure 3 with different symbols. Sample 2 agrees with eq 5 to about 0.02 %. Samples 1 and 3 show a greater scatter than 0.04 %, but the average deviation is −0.1 %. All of Weber's results agree with eq 5 to within his estimated uncertainties, which range from 0.04 % at 350 K increasing to about 0.1 % at 500 K.[5] Malanowski and co-workers'[6] ebulliometric results were not obtained in the comparative mode, instead a pressure gauge was used to measure the vapor pressures. Their vapor pressures are scattered within 0.1 %. Olson's[11] measurements deviate from eq 5 by less than 0.3 % at low pressures, but his three points above 463 K are high by up to 1 %, as shown in Figure 4. McMicking and Kay[23] agree well at the normal boiling point, but the deviations of the remaining measurements oscillate between 0.3 % and −0.06 % with the critical pressure 0.2 % higher than the value calculated from eq 5. Zawisza and Vejrosta,[24] Sipowska and Wieczorek,[25,26] and Saez et al.[27] agree quite well with eq 5: the deviations are between 0.25 % and −0.2 %. Figure 4 makes a comparison on a less sensitive scale. The vapor pressure of Kay[28] and Nichols et al.[29] at 477 K is lower than eq 5 by −1.5 %, while the results of de Loos et al.,[30] whose sample was 98 % pure, lie above eq 5 by 5 % at their lowest

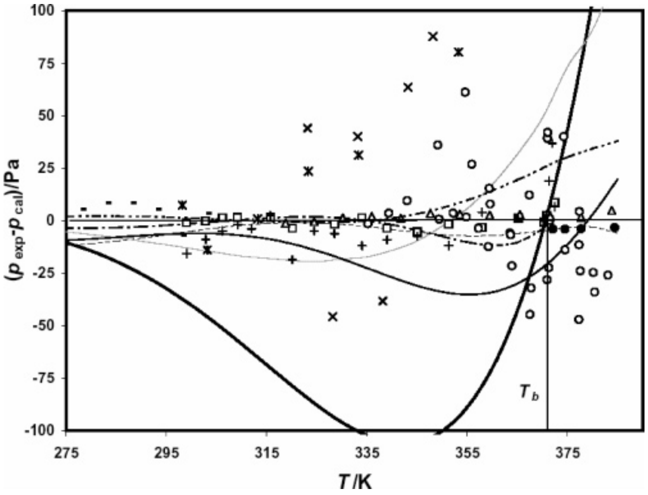

Figure 5. Deviations Δp of the vapor pressure of *n*-heptane from eq 5: ●, this work; □, Willingham et al.;[21] △, Smith;[22] ○, Weber;[5] +, series 1, Willingham et al.;[21] −, Sipowska and Wieczorek;[25] ∗, Sipowska and Wieczorek;[26] ×, Saez et al.;[27] thin solid line, NIST/TRC;[31] dash line, Dykyj et al.;[32] thick solid line, DIPPR;[33] dot line, Span;[34] dot-dot-dash line, ThermoData Engine;[35] dot−dash line, Ruzicka and Mejer.[36] T_b is the normal boiling temperature.

temperature, 429 K, with the deviations diminishing to about 1 % near the critical point.

Several correlations have been proposed for the vapor pressures of heptane, and the most popular are also shown in Figures 4 and 5 as deviations from eq 5. The Landolt−Bornstein[31] equation agrees well at the normal boiling temperature (T_b), but the deviation increases to 5 % near the critical point. The deviations from eq 5 of the DIPPR[33] and NIST/TRC[31] correlations increase above T_b to about 0.6 % near 480 K and then fall as the critical point is approached, to about −0.05 % in the case of the DIPPR correlation and about −0.8 % for the NIST/TRC equation. The behavior of these equations is shown in Figure 5 for pressures below atmospheric. The equation proposed by Span[34] agrees quite well with our final equation, although his predictions are about 60 Pa higher near the normal boiling temperature as shown in Figure 5. Another correlation obtained from ThermoData Engine[35] is shown in Figure 4. This correlation uses a Wagner equation in the standard form (see eq 3) and has a deviation of 0.03 % in the temperature range of 300 K to 420 K. It increases to −0.2 % at 490 K and for temperatures near the critical point is around 0.1 %.

Fractional deviations are known to change rapidly at low pressures, so Figure 5 shows absolute deviations Δp below (385 K, 148 kPa) to assess the pressure measurements and the different correlations. In the plot we have included the data on which we based eq 5: Rossini and co-workers,[21] Smith,[22] and four of our lowest pressures. The absolute deviation from the proposed equation is always less than 5 Pa, except at the highest pressure reported by Rossini and co-workers[21] where it is 9 Pa. At the lower temperature range, the results by Sipowska and Wieczorek[25] agree with our eq 5 to within less than 9 Pa. Another set of measurements from the same group[26] produced vapor pressures, three of which agree quite well with us at low temperatures but at higher temperatures they are above eq 5. Ruzicka and Majer[36] used the vapor pressures of Rossini and co-workers;[21] therefore, their equation agrees quite well with ours. In general, the correlations agree in this temperature range within 25 Pa except for the DIPPR correlation, which at 342 K deviates 106 Pa and agrees quite well with our equation at the normal boiling, but at higher temperatures the deviation increases.

If we take the triple point temperature $T_{\mathrm{tp}} = 182.59$ K proposed by Ruzicka and Majer,[36] then eq 5 predicts a pressure, $p_{\mathrm{tp}} = (0.178 \pm 0.002)$ Pa; the combined standard uncertainty of p_{tp} (0.002 Pa) was obtained by applying the law of propagation of uncertainty to eq 5. The equation proposed by Span[34] calculates $p_{\mathrm{tp}} = (0.1766 \pm 0.0004)$ Pa, the equation obtained by Weber[5] gives $p_{\mathrm{tp}} = (0.173 \pm 0.001)$ Pa, ThermoData Engine[35] predicts $p_{\mathrm{tp}} = (0.179 \pm 0.003)$ Pa, and Ruzicka and Majer[36] have $p_{\mathrm{tp}} = (0.169 \pm 0.008)$ Pa. The uncertainties quoted above are reported by the authors. Consequently, we believe that our final eq 5 gives the vapor pressures of *n*-heptane over the whole fluid range with an excellent agreement with other correlations at the lowest pressures.

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