Experimental Vapor Pressures of Six *n*-Alkanes (C_{21}, C_{23}, C_{25}, C_{27}, C_{29}, C_{30}) in the Temperature Range between 350 K and 460 K

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Vapor pressures of six normal alkanes (heneicosane, tricosane, pentacosane, heptacosane, nonacosane, and triacontane) were measured from 0.5 Pa to 600 Pa using a static apparatus. The experimental data ($P-T$) were smoothed using the Antoine equation and compared with the available literature values. Pressures were then calculated by means of a modified Peng−Robinson equation of state and compared with experimental values. The model represents the experimental results quite well.

Introduction

Vapor pressures are fundamental data required in the petroleum industry to develop thermodynamic models. Abundant and reliable information is available for *n*-alkanes of low and medium molar mass, but much less data are published for the higher molar mass necessary for characterizing higher boiling petroleum fractions.

In this work, we carried out a study of the vapor pressure of six normal alkanes. The purity of the different compounds, purchased from Fluka, was better than 99.5 %. They were used without further purification. We measured the vapor pressures down to 0.5 Pa using a static apparatus designed and built in our laboratory.[1] Experimental results were correlated by the Antoine equation and compared with the available literature data.

A thermodynamic model based on a modified Peng−Robinson equation of state—described in detail in previous studies[2,3]—was used to predict the vapor pressures of the alkanes studied. The calculated pressures were compared with the experimental results.

Experimental Section

Static Apparatus. Vapor pressures were measured using the static apparatus shown in Figure 1. It allows reliable measurements within a very large pressure range: 0.5 Pa to 200 kPa. The description of the apparatus and the experimental procedure can be found elsewhere,[4−7] so only the most salient information is given here.

The apparatus was equipped with a differential manometer from Datametrics (Wilmington, MA; model 1173). The pressure measurement consists of applying the vapor pressure of the sample on the measurement side of the gauge. The reference side was continuously pumped. The residual pressure was 10^{-4} Pa and therefore can be neglected. For pressures above 1.5 kPa, some air was introduced into the reference part of the gauge. Two pressure gauges (Rosemount) were used for an accurate determination of the air pressure. In this way, the pressure range of the apparatus was increased up to 200 kPa. In this study, only the Datametrics gauge was used as the alkanes studied were not very volatile ($P < 1.3$ kPa). The estimated uncertainty of the pressure determination was as follows: 0.05 for the pressure range ($0.3 < P/\text{Pa} < 10$), 0.02 ($10 < P/\text{Pa} < 130$), 0.01 ($130 < P/\text{Pa} < 1300$). Temperature measurements were carried out using a copper−constantan thermocouple calibrated against a 25 Ω platinum resistance standard thermometer (± 0.001 K, IPTS 90) and a Leeds & Northrup bridge ($\pm 10^{-4}$ Ω). During measurements, the stability of the temperature is ± 0.02 K.

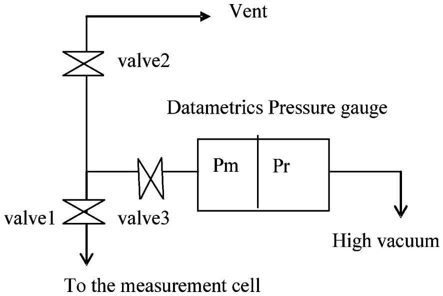

Figure 1. Simplified diagram of the static apparatus.

Degassing Procedure. The measurement cell has been already described.[4] It consisted of two parts, namely: an upper part connected permanently to the apparatus, a condensation coil was welded on this part; and a lower part that was the sample reservoir. When degassing, the lower part of the cell was heated, and cold water was circulated through the coil so as to minimize the loss of the compound during vapor venting. Trapped air and volatile impurities that were the principle sources of error in pressure measurements were thereby eliminated.

Results

Comparison with Literature Data. The experimental T and P values of the different alkanes are reported in Tables 1 to 6. The data were fit using the Antoine equation:

$$\log P/\text{Pa} = A - \frac{B}{C + T/\text{K}} \tag{1}$$

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Table 1. Experimental Vapor Pressure of Heneicosane (n-$C_{21}H_{44}$) and Comparison with Literature Data

T/K	P/Pa	$\Delta P/P^a$	$\Delta P/P^b$	$\Delta P/P^c$	$\Delta P/P^d$	$\Delta P/P^e$	$\Delta P/P^f$	$\Delta P/P^g$	$\Delta P/P^h$
351.54	0.396		−0.0025		−0.27	−0.32			0.0894
361.52	0.971		0.014		−0.29	−0.47			0.0699
371.42	2.20		0.015		−0.39	−0.58	0.11		0.0415
381.65	4.98		0.037		−0.52		−0.003		0.0420
391.86	10.6		0.046		−0.75		0.14		0.0380
402.05	21.3	0.12	0.044						0.0285
422.19	75.1	0.066	0.032						0.0215
432.27	133	0.047	0.018					−0.37	0.0173
442.30	228	0.036						−0.28	0.0180
452.22	378	0.035		−0.0028				−0.21	0.0224
461.96	611	0.046						−0.13	0.0382
	d	0.058	0.026	0.0028	0.49	0.46	0.084	0.25	0.0388

[a] Comparison with ref 8. [b] Comparison with ref 9. [c] Comparison with ref 10. [d] Comparison with ref 11. [e] Comparison with ref 12. [f] Comparison with ref 13. [g] Comparison with ref 14. [h] Comparison with ref 16.

Table 2. Experimental Vapor Pressure of Tricosane (n-$C_{23}H_{48}$) and Comparison with Literature Data

T/K	P/Pa	$\Delta P/P^a$	$\Delta P/P^b$	$\Delta P/P^c$	$\Delta P/P^d$	$\Delta P/P^e$
412.18	12.9	0.146		−0.24		0.0688
422.26	24.8	0.104				0.0526
422.29	24.7	0.099				0.0525
432.34	46.1	0.075				0.0438
442.33	83.9	0.072			−0.51	0.0561
452.22	143	0.050	0.55		−0.42	0.0442
461.99	242	0.056	0.57		−0.32	0.0612
	d	0.086	0.56	0.24	0.42	0.0545

[a] Comparison with ref 8. [b] Comparison with ref 12. [c] Comparison with ref 13. [d] Comparison with ref 14. [e] Comparison with ref 16.

Table 3. Experimental Vapor Pressure of Pentacosane (n-$C_{25}H_{52}$) and Comparison with Literature Data

T/K	P/Pa	$\Delta P/P^a$	$\Delta P/P^b$	$\Delta P/P^c$	$\Delta P/P^d$	$\Delta P/P^e$	$\Delta P/P^f$	$\Delta P/P^g$
381.69	0.331	0.36	0.003			−0.20		0.0732
391.91	0.783	0.28	0.005			−0.22		0.0354
402.03	1.78	0.20	0.016	−0.020		−0.23		0.0242
411.75	3.83	0.17	0.044	0.12		−0.21		0.0410
411.78	3.83	0.17	0.042	−0.12		−0.21		0.0410
422.02	8.02	0.13	0.040	−0.24		−0.23		0.0389
432.21	15.8	0.088	0.018			−0.28		0.0284
442.33	29.6	0.053			−0.34	−0.34		0.0145
442.34	29.9	0.060			−0.32	−0.32		0.0145
452.24	54.1	0.045			−0.20			0.0262
452.25	53.4	0.031			−0.21			0.0272
461.95	92.6	0.024			−0.10		−0.96	0.0180
461.98	92.3	0.019			−0.11		−0.10	0.0172
461.98	93.8	0.034			−0.092		−0.083	0.0185
d		0.13	0.021	0.125	0.20	0.25	0.093	0.0333

[a] Comparison with ref 8. [b] Comparison with ref 9. [c] Comparison with ref 11. [d] Comparison with ref 12. [e] Comparison with ref 13. [f] Comparison with ref 14. [g] Comparison with ref 16.

Table 4. Experimental Vapor Pressure of Heptacosane (n-$C_{27}H_{56}$) and Comparison with Literature Data

T/K	P/Pa	$\Delta P/P^a$	$\Delta P/P^b$	$\Delta P/P^c$	$\Delta P/P^d$
401.68	0.592	0.35		0.31	0.0760
401.69	0.590	0.35		0.31	0.0760
411.78	1.29	0.26	0.11	0.23	0.0253
411.81	1.30	0.26	0.12	0.24	0.0253
421.93	2.69	0.17	−0.058	0.15	−0.0225
421.95	2.72	0.18	−0.48	0.16	−0.0225
432.03	5.56	0.071	−0.22	0.11	−0.0265
442.18	11.0	0.080			−0.0325
452.27	21.4	0.070			−0.0092
462.27	40.1	0.087			0.0194
462.27	40.5	0.084			0.0196
	d	0.18	0.11	0.22	0.0302

[a] Comparison with ref 8. [b] Comparison with ref 13. [c] Comparison with ref 15. [d] Comparison with ref 16.

Table 5. Experimental Vapor Pressure of Nonacosane (n-$C_{29}H_{60}$) and Comparison with Literature Data

T/K	P/Pa	$\Delta P/P^a$	$\Delta P/P^b$
422.10	0.970		0.1146
422.10	0.971		0.1146
432.12	2.06	−0.099	0.0877
442.17	4.21	−0.048	0.0669
442.19	4.17	−0.060	0.0.68
452.20	8.24	−0.22	0.0481
452.23	8.19	−0.23	0.0478
	d	0.13	0.0793

[a] Comparison with ref 13. [b] Comparison with ref 16.

Table 6. Experimental Vapor Pressure of Triacontane ($C_{30}H_{62}$) and Comparison with Literature Data

T/K	P/Pa	$\Delta P/P^a$	$\Delta P/P^b$	$\Delta P/P^c$
432.36	1.15	0.097	0.10	0.0246
432.37	1.13	0.080	0.087	0.0245
442.48	2.33	−0.0075	−0.10	−0.034
452.32	4.57	−0.073	−0.32	−0.0663
452.34	4.51	−0.089	−0.45	−0.0662
d		0.069	0.21	0.0424

[a] Comparison with ref 8. [b] Comparison with ref 13. [c] Comparison with ref 16.

by minimizing the objective function S:

$$S = \sum_{i=1}^{n} \left(\frac{P_{\text{exp}} - P_{\text{cal}}}{P_{\text{exp}}} \right)^2 \tag{2}$$

The constants A, B, and C determined from least-squares fitting and the mean relative deviations d (n, number of experimental points) are reported in Table 7:

$$d = \frac{1}{n} \sum \frac{|P_{\text{exp}} - P_{\text{lit}}|}{P_{\text{exp}}} \tag{3}$$

For n-C_{21}, our experimental data are in a good agreement with the TRC tables[8] (d, mean relative deviation is 0.058) except at 402.05 K where the relative deviation on pressure $\Delta P/P = 0.12$.

The pressure range measured by Grenier-Loustalot et al.[9] is between 0.4 Pa to 133 Pa. Our data agree with these authors in the entire range investigated ($d = 0.026$).The single common point with Mazee[10] is at 452.22 K, and the agreement with his experimental value is very good ($\Delta P/P = 0.0028$). Piacente and co-workers[11,12] measured n-C_{21} using three different methods—torsion, Knudsen, and transpiration methods. Our data are in total disaccord with the values these authors obtained with the different methods ($d = 0.49$ and $d = 0.46$). In 1994, Piacente et al.[13] published some new points using the torsion method; the deviations with our results are much smaller than those cited

Table 7. Constants of the Antoine Equation and *d* (mean relative deviation)

n-alkane	*T*/K	*A*	*B*	*C*	*d*
heneicosane	351.54 to 461.962	10.6059	2982.1	−80.69	0.0045
tricosane	401.97 to 461.992	12.0889	4168.2	−32.51	0.0038
pentacosane	381.69 to 461.983	10.6117	3136.9	−99.04	0.0078
heptacosane	401.68 to 462.272	16.9409	8694.7	104.76	0.0044
nonacosane	422.10 to 452.232	11.4783	3942.0	−79.06	0.0031
triacontane	432.36 to 452.342	14.3019	6465.8	21.53	0.0066

previously ($d = 0.084$). In the same way, our data do not agree with the data from Stull[14] ($d = 0.25$).

Concerning n-C_{23}, our results are in a quite good agreement with the TRC tables[8] ($d = 0.09$) and in total disagreement with the data of both Piacente and co-workers[11,12] and Stull[14] ($d =$ 0.56, 0.24, and 0.42, respectively).

The experimental results of n-C_{25} were compared with the TRC tables.[8] Our values are in a good agreement with the data compilated at pressures above 30 Pa. The discrepancy increases when the pressure decreases and reaches $\Delta P/P = 0.36$ at 0.3 Pa. On the other hand, our data are in a very good agreement with Grenier-Loustalot et al.[9] vapor pressures ($d = 0.021$). In this case our results are in total disagreement with the vapor pressures reported by Piacente and co-workers[11−13] ($d = 0.20$, 0.25, and 0.12 respectively). Our experimental values present a mean relative deviation of 0.093 when compared to the Stull[14] measurements.

In case of n-C_{27}, our pressure values are in quite good agreement with the TRC tables[8] in the range between 6 Pa and 40 Pa. The deviation with our experimental data increases with decreasing pressures. For only one temperature our vapor pressure is in accord with the value reported by Piacente et al.:[13] at $T = 421.93$ K ($\Delta P/P = 0.05$). Our experimental pressures are in total disaccord with Morecroft[15] data ($d = 0.22$).

For n-C_{29}, the sole comparison data are from TRC tables.[8] The relative deviation with our data is $\Delta P/P = 0.13$.

For n-C_{30}, the comparison with the TRC tables[8] shows a quite good agreement (mean relative deviation with experimental values is 0.07). The mean relative deviation with Piacente et al.[13] values is $d = 0.21$.

The main goal of the present study is to provide the existing database with high-quality experimental vapor pressures. For this reason, we did not carry out comparisons with calculated values using the different correlations of the literature except the one developed by Chickos and Hanshaw[16] based on a correlation gas chromatography. The comparison with our experimental values shows a good agreement (Tables 1 to 6). The mean relative deviation for C_{21}, C_{23}, C_{25}, C_{27}, C_{29}, and C_{30} is $d = 0.04$, 0.05, 0.03, 0.03, 0.08, and 0.04, respectively.

Prediction of Vapor Pressures by a Group Contribution Method. The proposed model was developed to represent and predict thermophysical properties of heavy hydrocarbons such as vapor pressures, heats of vaporization, and saturated liquid heat capacities.[2,3] The model was used successfully for the prediction of vapor pressures[4−7] of different kind of molecules such as cycloalkanes, aromatic hydrocarbons, sulfides, etc. In the present study, the group contribution method is used to predict vapor pressures of the alkanes studied in order to compare the calculated values to the experimental results.

As described previously,[3] the model uses a volume translated Peng−Robinson equation of state:

$$P = \frac{RT}{\tilde{v} - \tilde{b}} - \frac{a(T)}{\tilde{v}(\tilde{v} - \gamma\tilde{b})} \tag{4}$$

with $\gamma = 2(1 + \sqrt{2})$ where $\tilde{v}$ is the pseudo-volume, $\tilde{b}$ is the pseudo-covolume, and $a(T)$ is a temperature-dependent function. The pseudo-covolume $\tilde{b}$ is estimated from Bondi's method[17] as follows:

Table 8. Values of Group Contributions for Pseudo-Covolume $\tilde{b}$ and Parameter *m*, Increment for Parameter *m*

groups	$V_{w,j}$/cm^3·mol^{-1}	M_j
CH_3	13.67	0.04125
CH_2	10.23	0.04303

increment	δm_k
CH_3 and CH_2	0.04523

$$\tilde{b} = \tilde{b}_{CH_4}[\sum_{j=1}^{2} V_{w,j}N_j/V_{w,CH_4}] \tag{5}$$

with $\tilde{b}_{CH_4} = 15.68$ cm^3·mol^{-1}and $V_{w,CH_4} = 17.12$ cm^3·mol^{-1}, $V_{w,j}$ is the contribution of group j to the van der Waals volume, and N_j is the number of CH_3 groups ($j = 1$) and CH_2 groups ($j = 2$).

The form of the function $a(T)$ is given by

$$a(T) = a(T_b)\left\{1 + m_1\left[1 - \left(\frac{T}{T_b}\right)^{1/2}\right] - m_2\left(1 - \frac{T}{T_b}\right)\right\} \tag{6}$$

where $a(T_b)$ is the value of parameter $a(T)$ at the normal boiling point, m_1 and m_2 are calculated by the following equations:

$$m_1 = 12.5295 + 41.3891m_2 \tag{7}$$

$$m_2 = 0.93505m - 0.58579 \tag{8}$$

The parameter m, which takes into account the shape of a molecule, serves as substitute for the acentric factor. It is calculated by a group contribution method such as

$$m = 0.34190 + S - 0.18473S^2 \tag{9}$$

with

$$S = \sum_{j=1}^{2} M_jN_j + \delta m_k I_k \tag{10}$$

$$\delta m_k = 0.04523 \quad (k = 1)$$

M_j is the contribution of group j to m, and δm_k is the kth-type increment in m. Here two groups are necessary, CH_3 and CH_2, and only one increment is considered such as:

$$I_k = (N_C)^{-0.5} \tag{11}$$

where (N_C) is the total number of carbon atoms.

The values of $V_{w,j}$, M_j, and δm_k, reported in Table 8 and already published,[3] have been adjusted on a wide variety of hydrocarbons (134 compounds) from the literature in the pressure range between 1 Pa to $2 \cdot 10^5$ Pa. These compounds, cited in ref 3, constitute the database of the model. To predict vapor pressures of the normal alkanes studied, the only necessary datum for the model is the normal boiling temperature, T_b. The normal boiling temperatures of the database compounds as well as the substances studied were taken from TRC tables[8] and from Lide.[18] These T_b data were deduced from compilations. On the other hand, as parameter m is known (deduced from group contribution), the model is capable of estimating T_b (eq 5) using an iterative method by minimizing the average relative deviations of our experimental vapor pressures for a given n-alkane.

Table 9. Comparison between Experimental Vapor Pressures and Those Predicted by the Group Contribution Method[a]

n-alkane	n^b	$\tilde{b}$/cm^3·mol^{-1}	*m*	T_b/K^c	100 *d*	T_b/K^d	100 *d*	T_b/K^e	100 *d*
C_{21}	11	203.30	1.09889	629.65	3.99	629.70	4.21	628.83	1.04
C_{23}	9	222.06	1.15437	653.25	4.59	653.20	4.39	652.18	1.09
C_{25}	15	240.82	1.20717	674.95	1.59	675.10	2.26	674.55	0.82
C_{27}	11	259.59	1.25729	695.05	5.25			693.72	2.99
C_{29}	7	278.35	1.30742	713.55	1.78	714.00	2.41	713.60	1.76
C_{30}	5	287.73	1.32741	722.35	15.49	722.90	12.54	725.58	2.97

[a] *d*, mean relative deviation. [b] Number of experimental points. [c] Predicted by the group contribution method. [d] From ref 18. [e] From ref 8.

Table 10. Comparison of Experimental Vapor Pressures between Morgan and Kobayashi[19] and Those Predicted by the Group Contribution Method[a]

n-alkane	n^b	$\tilde{b}$/cm^3·mol^{-1}	*m*	pressure range/bar	T_b/K^c	100 *d*
C_{10}	13	100.12	0.74701	0.009−6.0	447.31	0.30
C_{12}	11	118.88	0.81667	0.007−3.75	489.47	0.33
C_{14}	14	137.64	0.88390	0.004−2.60	526.73	0.38
C_{16}	19	156.40	0.94858	0.003−1.30	560.01	0.53
C_{18}	17	175.16	1.01068	0.003−0.98	589.45	1.03
C_{19}	15	184.54	1.01074	0.0025−0.52	603.05	1.85
C_{20}	31	193.92	1.07014	0.0024−0.38	616.95	0.93
C_{22}	12	212.68	1.12696	0.0024−0.20	641.75	1.02
C_{24}	13	231.44	1.18111	0.0009−0.17	664.35	0.47
C_{28}	14	268.97	1.28134	0.0008−0.06	704.45	0.70

[a] *d*, mean relative deviation. [b] Number of experimental points. [c] From ref 8.

In Table 9, we report the mean relative deviation between experimental and predicted vapor pressures using T_b from the literature[8,18] and T_b estimated by the model.

For five compounds, *n*-C_{21} to *n*-C_{29}, the average absolute deviation between the estimated normal boiling temperatures and those of literature is less than 1 K, which indicates that the model is quite accurate. The predicted pressures are in good agreement with the experimental data; the mean relative deviation ranges between 0.01 and 0.03.

For *n*-$C_{30,}$ the mean relative deviation is respectively $d = 0.15$ and $d = 0.13$ when T_b is taken from the TRC tables[8] or from Lide;[18] $d = 0.03$ when T_b is estimated from our work, the later value of T_b being much higher. For this compound, we have only five points between 1 Pa and 5 Pa where two points are doubled. On the other hand, the two investigated points are at the measurement limit of the apparatus, which perhaps explains the observed deviation.

We have applied our group contribution method to 10 compounds measured by Morgan and Kobayashi[19] (Table 10). These compounds do not belong to the database. Their normal boiling temperature T_b is taken from the TRC tables.[8] The model represents the vapor pressures of the 10 substances satisfactorily: the mean relative deviation is between $d = 0.003$ and $d = 0.01$. Usually the model reproduces the measured data correctly in a pressure range of 1 Pa to $2 \cdot 10^{5}$ Pa. In case of C_{10}, C_{12}, C_{14}, and C_{16}, the model enables extrapolation until $6 \cdot 10^{5}$ Pa.

Conclusions

We report vapor pressures for six *n*-alkanes (*n*C_{21} to *n*C_{30}) between 0.5 Pa to 600 Pa. Our measurements are in a good agreement with TRC[8] and Grenier-Loustalot et al.[9] values; the accord with calculated pressures by Chickos and Hanshaw[16] is very good too. The group contribution model reproduces our experimental vapor pressures quite well. Triacontane constitutes the largest *n*-alkane that could be measured with our static apparatus.

Since we have reached the limit of our static apparatus, to satisfy industrial requirements (particularly petroleum and agrochemical industries) of vapor or sublimation pressure measurements on larger molecular weight compounds, we have developed a new apparatus. A paper describing this new technique will be forthcoming.

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