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Thermodynamic Properties of n-Dodecane

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An equation of state has been developed to represent the thermodynamic properties of all liquid, vapor, and supercritical states of *n*-dodecane. Experimental data used to develop the equation included pressure—density—temperature state points, vapor pressures, isobaric and saturation heat capacities, heats of vaporization, and speeds of sound. The uncertainties of properties calculated using the equation are as follows: 0.2% in density at pressures up to 200 MPa, and 0.5% at higher pressures up to 500 MPa; 1% in heat capacity; 0.5% in the speed of sound; and 0.2% in vapor pressure. Deviations of calculated properties from available experimental data in the critical region are higher for all properties except vapor pressure.

Introduction

The modeling of petroleum based rocket and jet fuels often requires the use of surrogate mixtures with a limited number of components to represent the thermodynamic and transport properties of the actual mixture (see, for example, Edwards and Maurice¹). The thermophysical properties of dodecane are similar to those of aviation kerosene, and accurate knowledge of its characteristics is a precursor to modeling rocket fuels. Khasanshin et al.² reported equations for calculating the thermodynamic properties of dodecane in the liquid phase based primarily on their own speed-of-sound measurements and, to a lesser degree, on the measurements of others.

Equations of state for pure fluid properties are often expressed as fundamental equations explicit in the Helmholtz energy, with the density and temperature as independent variables. From these equations, most single-phase thermodynamic properties can be calculated using density or temperature derivatives of the Helmholtz energy. The location of the saturation boundaries requires an iterative solution using the so-called Maxwell criterion, i.e., equal pressures and Gibbs energies at constant temperature during phase changes. An equation of state that can be used to calculate the thermodynamic properties of dodecane at liquid, vapor, and supercritical states is given here, and transport equations are given in a companion paper (Huber et al.³).

Equation of State

The generalized functional form developed in the work of Span and Wagner⁴ was used here as a starting point

to fit an equation to represent the thermodynamic properties of dodecane. They developed a single equation for nonpolar fluids by fitting multiple properties over all liquid and vapor states, including the critical region. Their technical equations were developed with much insight into the proper behavior of an equation of state. The number of terms in their equation was kept to a minimum, thus decreasing the intercorrelation between terms and the possibility of overfitting. The objective of Span and Wagner was not the determination of a functional form that described the data sets as well as possible, but rather the development of the best functional form that considered the data for all the substances simultaneously.

To describe the properties of *n*-dodecane more accurately, the temperature exponents reported in the work of Span and Wagner⁴ were fitted as variables in addition to the coefficients of the equation. This allowed for greater flexibility, especially because dodecane has a longer saturation boundary (greater range of temperature between the triple point and the critical point) than that of many of the fluids fitted in their work. In addition, because there is a limited amount of experimental data in the vapor phase and at high temperatures, the shorter functional form with fixed exponents on density aids the ability of the equation to extrapolate into these areas. Graphical techniques were used to ensure that the behavior in the vapor phase was similar to that of other fluids (such as propane, where vapor phase data are available). Nonlinear techniques used in the development of the R-125 equation of state (from Lemmon and Jacobsen⁵) were also used to improve the behavior outside the regions characterized by experimental data.

The values of temperature and density at the critical point are two of the most important properties required in the development of equations of state. However,

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Table 1. Summary of Critical Points for n-Dodecane

source	critical temperature (K)	critical pressure (MPa)	critical density (mol/dm³)
Allemand et al. ⁸ (1986)	658.154	1.8239	
Ambrose and Townsend ⁹ (1968)	658.281	1.824	
Ambrose et al. 10 (1960)	658.281		
Anselme et al. ⁷ (1990)	658.154		1.3268
Gomez-Nieto and Thodos ¹¹ (1977)	653.855	1.8066	
Mogollon et al. 12 (1982)	657.655		
Pak and Kay ¹³ (1972)	658.904	1.8602	
Rosenthal and Teja ¹⁴ (1989)	658.754	1.810	
Teja et al. ¹⁵ (1989)	658.154		
this work	658.1	1.817	1.33

measurements of the critical point are often scarce and vary widely for the heavier hydrocarbons such as dodecane. In addition, the number of measurements of the critical density are substantially fewer than those for the critical temperature. The critical density is difficult to determine accurately by experiment, because of the infinite compressibility at the critical point and the associated difficulty of reaching thermodynamic equilibrium. For dodecane, the critical temperature lies in the same region as the limits of dissociation, thus increasing the uncertainties in experimental temperature values. However, several methods have been proposed that fit temperature, pressure, or density as a function of the carbon number to best represent the critical values. The ones used here for the critical temperature and pressure were published by Lemmon and Goodwin.⁶ The critical density was taken from Anselme et al.⁷ These values are

$$T_c = 658.1 \text{ K}$$
 (1)

$$p_c = 1.817 \text{ MPa}$$
 (2)

$$\rho_{\rm c} = 1.33 \text{ mol/dm}^3 \tag{3}$$

The published values of critical parameters and sources for dodecane are listed in Table 1. The selected triple point temperature of Finke et al. 16 is 263.60 K and is used as the lower limit of the equation of state. An additional value of 263.51 K was reported by Huffman et al.17

The equation of state expressed in its fundamental form, explicit in the Helmholtz energy, is widely used for calculating thermodynamic properties with high accuracy for many fluids. The independent variables in the functional form are density and temperature:

$$a(\rho, T) = a^{0}(\rho, T) + a^{r}(\rho, T)$$
(4)

where a is the molar Helmholtz energy, $a^0(\rho, T)$ the ideal gas contribution to the Helmholtz energy, and $a^{r}(\rho, T)$ the residual Helmholtz energy that corresponds to the influence of intermolecular forces. In many applications, the functional form is explicit in the dimensionless Helmholtz energy α , using independent variables of dimensionless density and temperature. The form of this equation is

$$\frac{a(\rho, T)}{RT} = \alpha(\delta, \tau) = \alpha^{0}(\delta, \tau) + \alpha^{r}(\delta, \tau)$$
 (5)

where $\delta = \rho/\rho_c$, $\tau = T_c/T$, and T_c and ρ_c are the critical parameters given above and in Table 1.

The dimensionless Helmholtz energy of the ideal gas can be represented by

$$\alpha^{0} = \frac{h_{0}^{0}\tau}{RT_{c}} - \frac{s_{0}^{0}}{R} - 1 + \ln\left(\frac{\delta\tau_{0}}{\delta_{0}\tau}\right) - \frac{\tau}{R}\int_{\tau_{0}}^{\tau} \frac{c_{p}^{0}}{\tau^{2}} d\tau + \frac{1}{R}\int_{\tau_{0}}^{\tau} \frac{c_{p}^{0}}{\tau} d\tau$$
(6)

where $\delta_0 = \rho_0/\rho_c$ and $\tau_0 = T_c/T_0$. T_0 and p_0 are arbitrary constants, and ρ_0 is the ideal gas density at T_0 and p_0 $(\rho_0 = p_0/(T_0 R))$. The arbitrary datum state values for h_0^0 and s_0^0 are chosen based on common conventions in a particular industry. For hydrocarbons, the enthalpy and entropy are often set to zero for the liquid at the normal boiling point.

The calculation of thermodynamic properties from the ideal gas Helmholtz energy requires an equation for the ideal gas heat capacity, c_p^0 . These values can be obtained from heat capacity measurements extrapolated to zero pressure, gaseous speed-of-sound measurements, or calculations from statistical methods using fundamental frequencies. Values calculated from statistical techniques are available from the Thermodynamics Research Center (TRC; see Marsh et al. 18) for temperatures in the range of 200–1000 K. Their values were fitted to the expression

$$\frac{c_p^0}{R} = c_0 + \sum_{k=1}^4 c_k \left(\frac{u_k}{T}\right)^2 \frac{\exp(u_k/T)}{\left[\exp(u_k/T) - 1\right]^2}$$
(7)

where the ideal gas constant, R, is 8.314472 J mol⁻¹ K^{-1} . The Einstein functions containing the terms u_k

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Table 2. Coefficients of the Ideal-Gas Heat-Capacity **Equations**

	_	
\boldsymbol{k}	c_k	u_k
0	23.085	
1	37.776	1280
2	29.369	2399
3	12.461	5700
4	7.7733	13869

were used so that the behavior of the ideal gas heat capacity as a function of temperature would be similar to that derived from statistical methods. However, these are empirical coefficients and should not be confused with the fundamental frequencies.

The ideal gas Helmholtz energy equation, derived from eqs 6 and 7, is

$$\alpha^{0} = a_{1} + a_{2}\tau + \ln \delta + (c_{0} - 1) \ln \tau + \sum_{k=1}^{5} c_{k} \ln \left[1 - \exp \left(-\frac{u_{k}\tau}{T_{c}} \right) \right]$$
(8)

where a_1 and a_2 can be any arbitrary values set by the definition of the reference state for enthalpy and entropy. The coefficients of these equations are given in Table 2.

The functional form used for the Helmholtz energy equation of state is given as

$$\begin{split} \alpha^{\mathrm{r}}(\delta,\tau) &= n_{1}\delta\tau^{0.32} + n_{2}\delta\tau^{1.23} + n_{3}\delta\tau^{1.5} + n_{4}\delta^{2}\tau^{1.4} + \\ &n_{5}\delta^{3}\tau^{0.07} + n_{6}\delta^{7}\tau^{0.8} + n_{7}\delta^{2}\tau^{2.16}\exp^{-\delta} + \\ &n_{8}\delta^{5}\tau^{1.1}\exp^{-\delta} + n_{9}\delta\tau^{4.1}\exp^{-\delta^{2}} + n_{10}\delta^{4}\tau^{5.6}\exp^{-\delta^{2}} + \\ &n_{11}\delta^{3}\tau^{14.5}\exp^{-\delta^{3}} + n_{12}\delta^{4}\tau^{12.0}\exp^{-\delta^{3}} \end{aligned} \tag{9}$$

The coefficients n_k of the residual portion of the equation of state are given in Table 3. The functions used for calculating pressure (p), enthalpy (h), entropy (s), isochoric heat capacity (c_v) , isobaric heat capacity (c_p) , and the speed of sound (w) from eq 5 are given in eqs 10-15. The molar mass (*M*) is 170.33484 g/mol.

$$p = \rho RT \left[1 + \delta \left(\frac{\partial \alpha^{r}}{\partial \delta} \right)_{\tau} \right]$$
 (10)

$$\frac{h}{RT} = \tau \left[\left(\frac{\partial \alpha^0}{\partial \tau} \right)_{\delta} + \left(\frac{\partial \alpha^r}{\partial \tau} \right)_{\delta} \right] + \delta \left(\frac{\partial \alpha^r}{\partial \delta} \right)_{\tau} + 1 \qquad (11)$$

$$\frac{s}{R} = \tau \left[\left(\frac{\partial \alpha^0}{\partial \tau} \right)_{\delta} + \left(\frac{\partial \alpha^{r}}{\partial \tau} \right)_{\delta} \right] - \alpha^0 - \alpha^{r}$$
 (12)

$$\frac{c_{v}}{R} = -\tau^{2} \left[\left(\frac{\partial^{2} \alpha^{0}}{\partial \tau^{2}} \right)_{\delta} + \left(\frac{\partial^{2} \alpha^{r}}{\partial \tau^{2}} \right)_{\delta} \right]$$
(13)

$$\frac{c_p}{R} = \frac{c_v}{R} + \frac{\left[1 + \delta(\partial \alpha^r / \partial \delta)_\tau - \delta \tau(\partial^2 \alpha^r / \partial \delta \partial \tau)\right]^2}{1 + 2\delta(\partial \alpha^r / \partial \delta)_\tau + \delta^2(\partial^2 \alpha^r / \partial \delta^2)_\tau}$$
(14)

$$\frac{w^{2}M}{RT} = 1 + 2\delta \left(\frac{\partial \alpha^{r}}{\partial \delta}\right)_{\tau} + \delta^{2} \left(\frac{\partial^{2}\alpha^{r}}{\partial \delta^{2}}\right)_{\tau} - \frac{\left[1 + \delta(\partial \alpha^{r}/\partial \delta)_{\tau} - \delta\tau(\partial^{2}\alpha^{r}/\partial \delta\partial\tau)\right]^{2}}{\tau^{2} \left[(\partial^{2}\alpha^{0}/\partial\tau^{2})_{\delta} + (\partial^{2}\alpha^{r}/\partial\tau^{2})_{\delta}\right]} (15)$$

Equations for additional thermodynamic properties such as the isothermal compressibility and the Joule-Thomson coefficient can be found in Lemmon and Jacobsen. 19

Table 3. Coefficients of the Equation of State

k	n_k	k	n_k	
1	1.38031	7	0.956627	
2	-2.85352	8	0.0353076	
3	0.288897	9	-0.445008	
4	-0.165993	10	-0.118911	
5	0.0923993	11	-0.0366475	
6	0.000282772	12	0.0184223	

The derivatives of the ideal gas Helmholtz energy (given in eq 8) and the residual Helmholtz energy required by the equations for the thermodynamic properties are given in Span and Wagner.4

Experimental Data and Comparisons to the Equation of State

The units adopted for this work were kelvins (International Temperature Scale of 1990, ITS-90) for temperature, megapascals for pressure, and moles per cubic decimeter for density. Units of the experimental data were converted as necessary from those of the original publications to these units. Where necessary, temperatures reported on IPTS-68 and IPTS-48 were converted to ITS-90 (see Preston-Thomas²⁰).

Multiple data types over much of the fluid surface are often used in the development of equations of state. Not all data are used in the fitting of the equation, although comparisons are made to all available experimental data to estimate the uncertainties. These uncertainty values are determined by statistical comparisons of property values calculated using the equation of state to the experimental data. These statistics are based on the percent deviation in any property, X, which is defined as

$$\% \Delta X = \left(\frac{X_{\text{data}} - X_{\text{calc}}}{X_{\text{data}}}\right) \times 100 \tag{16}$$

Using this definition, the average absolute deviation is defined as

$$AAD = \frac{1}{n} \sum_{i=1}^{n} \left| \% \Delta X_i \right| \tag{17}$$

where n is the number of data points. The average absolute deviations between experimental data and the equation of state are given in Table 4. Data sets that contain only one or two data points for vapor pressure

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Table 4. Summary and Comparisons of Experimental Data for n-Dodecane

Table 4. Summar	ry and Con	inparisons of Experime	ental Data for <i>II</i>	-Douecane	
reference	number of point	s range (K)	pressure range (MPa)	density range (mol/dm³)	AAD (%)
		-Density-Temperature,			
Boelhouwer ³⁰ (1960)	28	303-393	0 - 118	3.96 - 4.7	0.107
Caudwell et al. ³² (2003)	85	298 - 473	0.1 - 192	3.57 - 4.81	0.038
Cutler et al. ³⁴ (1958)	78	311 - 408	0.1 - 689	3.89 - 5.13	0.953
Dymond et al. ³⁸ (1981)	32	298-373	0.1 - 502	4.05 - 5.17	0.139
Dymond et al. ³⁹ (1982)	35	298-373	0.1 - 442	4.05 - 5.1	0.071
Gouel ⁴⁷ (1978)	90	298 - 394	5.17 - 40.6	3.98 - 4.52	0.492
Landau and Wuerflinger ⁵³ (1980)	88	268-313	10 - 250	4.35 - 4.94	0.124
Rousseaux et al. ⁶⁷ (1983)	18	323-423	0 - 30.6	3.82 - 4.4	0.046
Snyder and Winnick ⁷¹ (1970)	96	298-358	0.101 - 417	4.11 - 5.04	0.169
Takagi and Teranishi ⁷² (1985)	3	298	0.1 - 100	4.37 - 4.69	0.061
Tanaka et al. ⁷³ (1991)	21	298-348	0.1 - 151	4.16 - 4.72	0.056
		Vanan Duaganna			
Allemand et al. ⁸ (1986)	19	Vapor Pressure	0 0 004		1.17
	21	298-390	0-0.004		
Beale and Docksey ²⁷ (1935)		300-658	0-1.77		1.9
Dejoz et al. 35 (1996)	38	344-502	0-0.134		0.15
Gierycz et al. 44 (1985)	13	378-418	0.003-0.013		0.84
Houser and Van Winkle ⁴⁸ (1957)	5	401-441	0.007 - 0.027		0.055
Keistler and Van Winkle ⁴⁹ (1952)	8	363 - 486	0.001 - 0.101		1.59
Krafft ⁵¹ (1882)	6	364 - 488	0.001 - 0.101		5.49
Maia de Oliveira et al. ⁵⁴ (2002)	10	432 - 489	0.02 - 0.102		0.063
Morgan and Kobayashi ⁶⁰ (1994)	13	353-588	0.001 - 0.671		0.261
Sasse et al. ⁶⁸ (1988)	37	264-371	0 - 0.002		1.65
Viton et al. ⁷⁶ (1996)	35	264 - 468	0 - 0.058		0.871
Willingham et al. ⁷⁸ (1945)	20	400 - 491	0.006 - 0.104		0.057
8					
Aigart et al 21 (1001)		Saturated Liquid Density		400 407	0.035
Aicart et al. ²¹ (1981) Aminabhavi and Gopalkrishna ²³ (1994)	4 3	298 - 333 $298 - 318$		4.23 - 4.37 $4.29 - 4.38$	
Aminabhavi and Gopaikrishna ²⁵ (1994)	ა ი				0.06
Aminabhavi and Banerjee ²² (2001)	3 3	298-308		4.33-4.38	0.11
Aminabhavi and Patil ²⁴ (1997)	3	298-308		4.33 - 4.38	0.057
Aralaguppi et al. ²⁵ (1999)	4	298-308		4.34 - 4.38	0.087
Asfour et al. ²⁶ (1990)	4	293-313		4.31 - 4.39	0.106
Bingham and Fornwalt ²⁹ (1930)	8	273-373		4.04 - 4.48	0.183
Boelhouwer ³⁰ (1960)	4	303-393		3.96 - 4.35	0.026
Cutler et al. ³⁴ (1958)	6	311-408		3.89 - 4.32	0.045
Diaz Pena and Tardajos ³⁶ (1978)	4	298-333		4.22 - 4.37	0.04
Dornte and Smyth ³⁷ (1930)	12	263-483		3.51 - 4.53	0.062
Dymond and Young ⁴⁰ (1980)	9	283-393		3.97 - 4.44	0.059
Findenegg ⁴¹ (1970) Francis ⁴² (1957)	6	286 - 333		4.22 - 4.43	0.054
Francis ⁴² (1957)	28	373-643		2.2 - 4.05	0.181
Garcia et al. ⁴³ (2002)	5	278-318		4.29 - 4.46	0.073
Gomez-Ibanez and Liu ⁴⁶ (1961)	5 3	288-308		4.33 - 4.42	0.04
Landau and Wuerflinger ⁵³ (1980)	7	268-313		4.3-4.5	0.183
Mansker et al. 55 (1987)	3	298-338		4.19-4.38	0.12
Meeussen et al. ⁵⁶ (1967)	3	298-328		4.24 - 4.37	0.079
Nayak et al. ⁶¹ (2001)	3	298-308		4.33-4.37	0.111
Ortega et al. (2001)	4	288-318		4.29-4.43	0.05
Quayle et al. (1966)	3	293-313		4.31-4.4	0.04
Schiessler et al. (1344) Schiessler et al. (1344)		273-372		4.05 - 4.48	0.054
	5				
Schmidt et al. ⁷⁰ (1966) Trenzado et al. ⁷⁵ (2001)	4	298-313		4.31-4.37	0.037
	5	283-313		4.31-4.44	0.019
Vogel ⁷⁷ (1946)	4	293-359		4.12-4.4	0.175
Wu et al. ⁷⁹ (1998)	4	293-313		4.31 - 4.4	0.03
		Heat of Vaporization			
Melaugh et al. ⁵⁷ (1976)	1	298			0.343
Morawetz ⁵⁸ (1968)	8	298			1.84
Morawetz ⁵⁹ (1972)	ĺ	298			0.445
,	_				
D 1 128 (0000)	~~	Isobaric Heat Capacity	0.4.400		0.70
Bessieres et al. ²⁸ (2000)	77	313-373	0.1 - 100	G : **	0.59
Costas and Patterson ³³ (1985)	3	283-313		Sat. Liq.	0.22
Lainez et al. ⁵² (1989)	1	298		Sat. Liq.	1.27
Tardajos et al. ⁷⁴ (1986)	1	298		Sat. Liq.	0.224
	•	Saturation Heat Capacity			
Finke et al. 16 (1954)	80	11.8–317			0.302
Huffman et al. (1934)	19	93.3-298			0.843
ramman et al. (1991)					0.043
		Isochoric Heat Capacity			
Polikhronidi et al. ⁶⁵ (2002)	55	324 - 377		4.05-4.27	4.16
		Speed of Sound			
Aminabhavi and Gopalkrishna ²³ (1994)	3	298-318		Sat. Liq.	0.194
Boelhouwer ³¹ (1967)	85	273-473	10-140	Sat. Liq.	0.194
Golik and Ivanova ⁴⁵ (1962)			10 140	Cat I:a	
	6	293-343	0.1 40.1	Sat. Liq.	0.09
Khasanshin and Shchemelev ⁵⁰ (2001)	30	303-433	0.1 - 49.1	C I	0.161
Neruchev et al. 62 (1969)	19	293-653		Sat. Liq.	0.94
Plantier et al. ⁶⁴ (2000)	9	293-373		Sat. Liq.	0.145
Takagi and Teranishi ⁷² (1985)	3	298	0.1 - 100		0.454
Tardajos et al. ⁷⁴ (1986)	1	298		Sat. Liq.	0.138
				-	

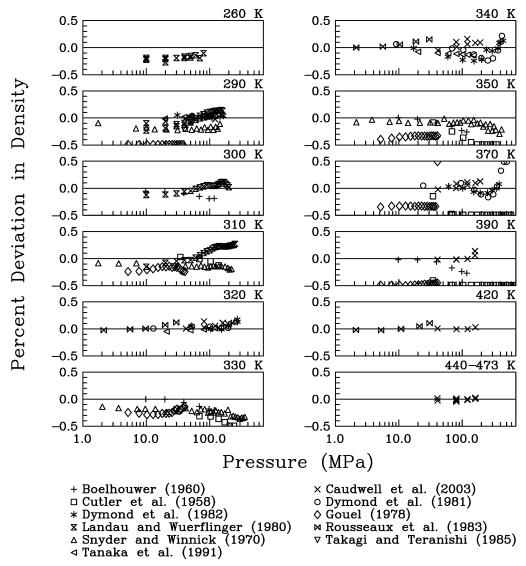


Figure 1. Comparison of densities calculated with the equation of state to the experimental data for n-dodecane.

or saturated liquid density are not shown. The comparisons given below for the various data sets compare

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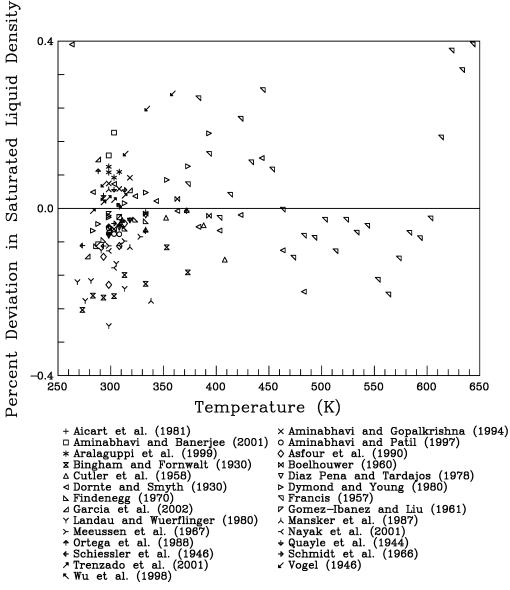


Figure 2. Comparison of saturated liquid densities calculated with the equation of state to the experimental data for *n*-dodecane.

eq 17. In the figures, data of a given type are generally separated into temperature increments of 10 K; the temperatures listed at the top of each small plot are the

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lower bounds of the data in the plot. Data points off scale are shown at the top or bottom of each plot.

Experimental measurements for dodecane and deviations of properties calculated using the equation of state from these data are given in Table 4 and shown in Figures 1 through 4. Figure 1 compares the equation of state to experimental pressure-density-temperature $(p-\rho-T)$ data in the liquid phase (no data are available in the vapor phase or at supercritical temperatures). The equation was fitted primarily to the data of Caudwell et al.³² in the liquid phase. The equation represents the data of Caudwell et al.,32 Dymond and co-workers,39,40 Rousseaux et al.,67 Takagi and Teranishi,72 and Tanaka et al.⁷³ generally all within 0.1%, with several

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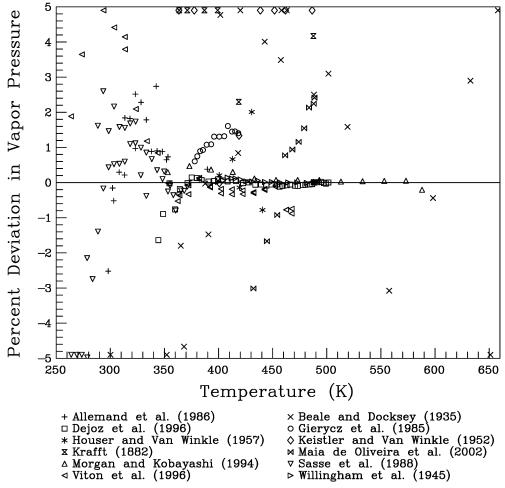


Figure 3. Comparison of vapor pressures calculated with the equation of state to the experimental data for *n*-dodecane.

outliers at 340 K. The data of Snyder and Winnick⁷¹ are consistently 0.1%-0.2% lower than that given by the equation of state. The data of Landau and Wuerflinger⁵³ are generally within 0.2% of the equation of state, with some of the data above and some below. Differences are up to 2% for the data of Cutler et al.³⁴ and 1.5% for the data of Gouel;⁴⁷ these data overlap other high-accuracy data in the liquid phase. Of the 150 data points available for the saturated liquid density (see Figure 2), the deviations of 122 of these points are within 0.15%. However, the temperatures for all but two of the data sets are <410 K.

The scatter in the vapor pressure measurements is significantly higher than that for densities, as shown in Figure 3. Disregarding the multiple outliers, vapor pressures are represented to within 0.2% at temperatures >350 K. The average absolute errors at these higher temperatures are 0.06% for the data of Dejoz et al., 35 0.16% for the data of Morgan and Kobayashi, 60 0.04% for the data of Willingham et al., 78 and 0.3% for the data of Viton et al. 76 The scatter in the data increases substantially as the temperature decreases, approaching 5% at 300 K. However, the vapor pressure is 21 Pa at this temperature, and small absolute differences represent significant percentages of the values at these low pressures.

The isobaric heat capacity of dodecane was measured by Bessieres et al. 28 from 313 K to 373 K at pressures up to 100 MPa. There are also five data points in the liquid phase at <313 K measured by other researchers.

In addition, saturation heat capacities are numerically similar to isobaric heat capacities at low temperatures; there are 15 points between 266 K and 317 K. The equation of state represents almost all of these data points to within 1%. The data of Bessieres et al. were obtained after the equation of state was finalized and provide a good indication of the extrapolation abilities of the equation (because other c_p data were limited to temperatures of <317 K at saturation conditions only). These new data all lie between 0.4% and 0.8% below the equation of state, within the equation's estimated uncertainty of 1%. The deviations of these data from the equation show no temperature dependence. At 313 K, these data differ from the data point of Costas and Patterson³³ by 0.65%, with the point of Costas and Patterson situated 0.25% higher than that given by the equation of state.

The deviation for the heat of vaporization data point of Melaugh et al. 57 is +0.3%, whereas the average deviation for the data of Morawetz is approximately -1.8%. The speed of sound in the liquid phase generally differs from the equation of state by up to 0.5%, as shown in Figure 4, except for values obtained at temperatures of <340 K, where the differences are as much as 1%.

Estimated Uncertainty of Calculated Properties

The equation of state for dodecane is valid from the triple point to 700 K at pressures to 500 MPa. The

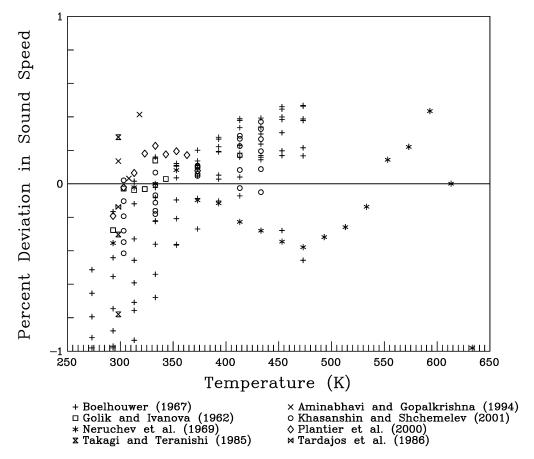


Figure 4. Comparison of speed-of-sound values calculated with the equation of state to the experimental data for *n*-dodecane.

Table 5. Calculated Property Values for Algorithm Verification

temperature (K)	pressure (MPa)	density (mol/dm³)	$(J \text{ mol}^{C_V} \text{ K}^{-1})$	$(J \text{ mol}^{-1} \text{ K}^{-1})$	speed of sound (m/s)
300.0	0.0	0.0	271.3952	279.7096	122.8511
300.0	7.161946	4.4	311.1937	377.1307	1316.614
600.0	0.7228018	0.2	488.1173	526.2322	123.5851
600.0	120.2532	4.0	499.9857	539.3864	1255.247
658.2	1.820055	1.33	547.6852	128753.9	49.76424

uncertainties (where the uncertainties can be considered to be estimates of a combined expanded uncertainty with a coverage factor of 2) of density values calculated using the equation of state in the liquid phase (including at saturation) are 0.2% for pressures of <200 MPa and 0.5% for higher pressures. The uncertainty for heat capacities is 1%, and that for the speed-of-sound values is 0.5%. The estimated uncertainties of vapor pressures calculated using the Maxwell criterion are 0.2% for temperatures of >350 K and approach 5% as the temperature decreases to the triple point temperature. These estimated uncertainties for calculated properties are consistent with the experimental accuracies of the various available experimental data. If additional data

are measured in the future, it is reasonable to expect that the overall accuracy of the correlation can be improved, consistent with the accuracy of the new data. As an aid to those using computer programs to calculate the properties of dodecane, calculated values of properties from the equation of state are given in Table 5. The number of digits displayed in the table does not indicate the accuracy in the values but is given only for validation of computer code.

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