THERMAL AND CALORIFIC PROPERTIES OF SIX AROMATIC HYDROCARBONS

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Experimental p, v, and T data are used to derive standard-form equations of state for six aromatic hydrocarbons giving their thermal and calorific properties over a temperature range of 298-673°K and a pressure range of P_s to 500 bars with errors not exceeding the experimental ones.

Detailed experimental invesigations of the thermal properties of the first six members of the aromatic hydrocarbon series over a temperature range of 298-673°K and a pressure range of 1-500 bars [1-5] have been carried out in the last 10 years in view of the fact that the fluid state of substances, in general, and of aromatic hydrocarbons, in particular, had been little studied. The experiments cover the vapor, two-phase, fluid, and supercritical regions of the parameters of state.

The subject of this article is the mathematical processing of the data obtained in the fluid phase.

There are at present no purely theoretical equations of state for the region indicated as a result of the complexity of the fluid state. There are, however, several equations of state for dense gases and fluids [6] which are derived with the aid of fairly sound physical considerations. Lennard-Jones and Devonshire [7] apply the so-called "consistent field" method to the theory of fluids and use the theory of cells as a basis for deriving equations of state for dense gases and fluids. According to their theory, we obtain the following expression for the free energy of one molecule:

$$\varepsilon = -kT\ln\left[\frac{(2\pi mkT)^{3/2}}{h^3}v\right] + \Phi(v), \tag{1}$$

where v is the volume of spherical cell and $\Phi(v)$ is the function of cell volume, identical in significance to the mean value of the energy of the consistent field. The first term in this expression takes account of the kinetic energy and the second, of the influence of the forces of intermolecular interaction. Since it is difficult to calculate the $\Phi(v)$ function accurately, it is assumed that the Lennard-Jones potential (6-12) is valid for the fluid and the function is represented as

$$\Phi(v) = -\frac{\alpha}{v^{\mu}} + \frac{\beta}{v^{\nu}}, \tag{2}$$

where $\mu = m/3$ and $\nu = n/3$. Using the well-known statistical physics formula

$$p = -\left(\frac{\partial\psi}{\partial V}\right)_{T,N}, \tag{3}$$

where $\psi = N\varepsilon$ is the free energy of the whole system, the Lennard-Jones and Devonshire equation of state is obtained in the following form:

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TABLE 1. Values for Constants b_i and h_i of the Polynomials in (7)

Coefficient	Substance					
	benzene	toluene	ethylbenzene	o-xylene	m-xylene	p-xylene
b_0	$8{,}590429\cdot10^{-1}$	$3{,}668361\cdot10^{0}$	$2{,}840787\cdot10^{0}$	$-9{,}701306\cdot10^{1}$	$1{,}728613\cdot10^{1}$	$8{,}242412\cdot10^{0}$
b_1	$-8{,}876854\cdot10^{-2}$	$-8{,}641821\cdot10^{0}$	$-6{,}242733\cdot10^{0}$	$3{,}263168\cdot10^{1}$	$-4{,}919754\cdot10^{1}$	$-2{,}041260\cdot10^{1}$
b_2	$-2{,}009060\cdot10^{0}$	$7{,}972158\cdot10^{0}$	$5{,}668062\cdot10^{0}$	$-3{,}789908\cdot10^{1}$	$5{,}327513\cdot10^{1}$	$1{,}948024\cdot10^{1}$
b_3	$-5{,}586733\cdot10^{-1}$	$-5{,}834985\cdot10^{0}$	$-5{,}009793\cdot10^{0}$	$1{,}599335\cdot10^{1}$	$-2{,}825520\cdot10^{1}$	$-1{,}098297\cdot10^{1}$
b_4	$1{,}452896\cdot10^{-1}$	$1{,}122755\cdot10^{0}$	$9{,}849698\cdot10^{-1}$	$-2{,}706896\cdot10^{0}$	$5{,}158793\cdot10^{0}$	$1{,}957337\cdot10^{0}$
h_0	$1{,}898012\cdot10^{2}$	$1{,}620769\cdot10^{2}$	$2{,}458299\cdot10^{2}$	$2{,}400854\cdot10^{2}$	$5{,}650882\cdot10^{1}$	$1{,}451956\cdot10^{2}$
h_1	$-4{,}385832\cdot10^{2}$	$-3{,}248872\cdot10^{2}$	$-5{,}336785\cdot10^{2}$	$-5{,}548862\cdot10^{2}$	$-2{,}209282\cdot10^{1}$	$-2{,}712121\cdot10^{2}$
h_2	$4{,}135845\cdot10^{2}$	$2{,}738259\cdot10^{2}$	$4{,}705393\cdot10^{2}$	$5{,}217978\cdot10^{2}$	$-3{,}496343\cdot10^{1}$	$2{,}230382\cdot10^{2}$
h_3	$-1{,}737849\cdot10^{2}$	$-1{,}014583\cdot10^{2}$	$-1{,}819293\cdot10^{2}$	$-2{,}160793\cdot10^{2}$	$3{,}600189\cdot10^{1}$	$-8{,}066874\cdot10^{1}$
h_4	$2{,}753657\cdot10^{1}$	$1{,}414698\cdot10^{1}$	$2{,}631820\cdot10^{1}$	$3{,}349571\cdot10^{1}$	$-8{,}330058\cdot10^{0}$	$1{,}110499\cdot10^{1}$
T_{cr} K	562,60	593,95	619,55	631,59	619,15	618,15

$$p = \frac{kT}{v} + \frac{\mu\alpha}{v^3} - \frac{\nu\beta}{v^5}. \tag{4}$$

In deriving Eq. (4), α and β are assumed to be independent of temperature, i.e., the $\Phi(v)$ function is not dependent on the temperature, which contradicts experimental data. By using Eq. (4) to describe the experimental p, v, and T data of individual pure fluids, however, it is possible to define more precisely the form of the intermolecular interaction function for different groups of fluids, as well as to establish the temperature dependences of the coefficients of the equation. To this end, the equation of state (4) is used to describe the experimental data on the p, v, and T of the first six members of the aromatic series – benzene, toluene, ethylbenzene, o-, m-, and p-xylene – for temperatures ranging from 298 to 673°K and pressures ranging from 1 to 500 bars.

Satisfactory results are obtained only within the temperature limits of 298-498°K and pressure limits of up to 200 bars. Calculations made for these temperature and pressure ranges using the equation of state (4) show that the mean discrepancy with experimental data on specific volume is ±0.5-0.6%.

The range of parameters of state to be described can be extended and the accuracy of the equation of state (4) can be improved by taking into account the fact that the Lennard-Jones intermolecular potential function of interaction (6-12), which is used in the derivation, is not the only possible function. The exponents for v in the second and third terms of expression (4) can be varied by using other potential functions as the basis for the derivation or by taking different values for m and n in expression (2), i.e., the values of the exponents for specific volumes in Eq. (4) can be altered as a function of the properties of the specific fluid.

It is established by our investigations that the equation of state

$$p = \frac{RT}{v} + \frac{B_1(T)}{v^2} + \frac{H_1(T)}{v^8} \tag{5}$$

or

$$\frac{z-1}{\rho} = B(T) + H(T)\rho^6 \tag{6}$$

describes with a high degree of accuracy the experimental p, v, and T data of the aromatic hydrocarbons within the temperature limits of 293-673°K and pressure limits of up to 500 bars when $\omega \geqslant 1.9$.

The B and H coefficients of Eq. (6) are found for each temperature by the method of least squares using all the experimental points at a given isotherm.

TABLE 2. Comparison between Values for Density of Benzene, Toluene, Ethylbenzene, ortho-, meta-, and para-Xylene Calculated from Equation of State (6) and Experimental Data [1-5]

Benzene			Toluene			Ethylbenzene		
p, bars	$\rho_{Eq.(6)}$	$\Delta\rho$, %	p, bars	$\rho_{Eq.(6)}$	$\Delta\rho$, %	p, bars	$\rho_{Eq.(6)}$	$\Delta\rho$, %
			298,15 K					
13,874	0,87423	+0,01	8,700	0,86380	0,00	19,500	0,86380	+0,02
106,35	0,88173	—0,01	106,12	0,87123	0,00	145,01	0,86279	+0,04
305,09	0,89615	+0,01	298,45	0,88439	0,00	307,12	0,88326	—0,01
490,53	0,90798	+0,01	496,51	0,89634	0,00	485,42	0,89365	+0,01
			373,15 K					
11,386	0,79173	+0,06	22,107	0,79283	+0,06	14,890	0,79634	+0,02
107,01	0,80482	+0,04	104,74	0,80279	+0,06	112,88	0,80732	+0,02
301,28	0,82662	+0,03	305,00	0,82318	+0,06	298,49	0,82509	+0,02
506,13	0,84521	+0,04	481,85	0,83810	+0,06	498,13	0,84111	—0,09
			473,15 K					
105,64	0,69052	—0,08	7,807	0,67650	—0,03	9,040	0,69591	—0,05
252,05	0,72470	—0,12	153,38	0,71416	—0,04	105,97	0,71865	—0,05
347,79	0,74126	—0,11	350,58	0,74697	—0,05	304,55	0,75150	—0,07
483,84	0,76044	—0,06	501,42	0,76580	—0,07	492,08	0,77416	—0,11
			573,15 K					
253,11	0,61505	+0,15	176,73	0,61212	+0,18	104,10	0,60732	+0,02
350,51	0,64638	+0,03	275,06	0,64537	+0,06	254,76	0,65986	—0,08
403,45	0,65943	+0,06	374,33	0,66884	+0,12	399,38	0,68998	+0,02
472,74	0,67396	+0,10	501,71	0,69177	+0,22	497,04	0,70564	+0,05
			673,15 K					
351,42	0,55070	—0,04	276,17	0,55017	—0,04	208,69	0,54568	—0,03
404,43	0,57228	—0,19	346,48	0,58025	—0,32	299,44	0,58755	—0,34
451,64	0,58779	—0,18	401,48	0,59783	—0,20	400,13	0,61724	—0,18
505,27	0,60251	—0,09	499,31	0,62216	+0,03	484,22	0,63587	+0,01
o-Xylene			m-Xylene			p-Xylene		
			298,15 K					
1,368	0,87544	+0,07	6,071	0,86053	+0,07	—	—	—
148,14	0,88537	+0,07	145,06	0,87053	+0,01	—	—	—
303,15	0,89486	+0,07	301,05	0,88068	0,00	—	—	—
492,80	0,90541	+0,08	500,11	0,89229	+0,02	—	—	—
			373,15 K					
5,203	0,81068	+0,07	13,512	0,79861	+0,03	4,726	0,79029	—0,03
105,04	0,82119	+0,08	120,47	0,81002	+0,00	103,91	0,80169	—0,03
302,24	0,83896	+0,06	302,03	0,82658	—0,01	255,00	0,81669	—0,02
495,74	0,85369	+0,04	400,18	0,83447	0,00	405,58	0,82958	—0,05
			473,15 K					
12,795	0,71572	—0,24	25,582	0,69748	+0,05	21,576	0,69216	+0,04
105,58	0,73482	—0,15	124,51	0,71897	—0,02	105,45	0,71169	+0,05
312,99	0,76619	—0,10	301,03	0,74713	—0,03	307,51	0,74529	+0,02
496,92	0,78701	—0,09	500,17	0,77077	+0,01	451,93	0,76322	0,00
			573,15 K					
104,80	0,62587	+0,24	100,77	0,60287	—0,06	100,56	0,59900	+0,22
252,33	0,67392	+0,07	249,18	0,65537	+0,02	300,42	0,66541	—0,07
398,76	0,70351	+0,06	350,27	0,67772	—0,01	404,31	0,68583	—0,03
483,87	0,71697	+0,09	500,21	0,70276	0,00	506,95	0,70216	+0,02
			673,15 K					
206,36	0,55873	+0,28	308,55	0,58772	+0,23	306,53	0,58431	+0,12
299,55	0,60138	—0,35	351,26	0,60209	—0,10	404,07	0,61419	—0,02
403,14	0,63162	—0,38	400,98	0,61619	—0,02	455,28	0,62646	+0,01
508,69	0,65423	—0,27	501,80	0,63916	+0,04	500,00	0,63591	+0,01

The temperature dependences of the coefficients B(T) and H(T) for all six substances are described with a fairly high degree of accuracy by the polynomials

$$B(T)=\sum_{i=0}^{4}\frac{b_i}{\tau_i},\quad H(T)=\sum_{i=0}^{4}\frac{h_i}{\tau_i}; \tag{7}$$

the values of the constants in (7) for all six substances are given in Table 1.

Data calculated from the proposed equation of state (6) taking into account the relationships in (7) are compared in Table 2 with experimental data.

TABLE 3. Values for Specific Volumes of Saturated Benzene, Toluene, Ethylbenzene, ortho-, meta-, and para-Xylene Fluids Calculated from the Equation of State (6) and the Discrepancy between Them and Experimental Values

T, K	Benzene		Toluene		Ethylbenzene	
	$v_{\text{Eq.(6)}}$	Δv, %	$v_{\text{Eq.(6)}}$	Δv, %	$v_{\text{Eq.(6)}}$	Δv, %
298,15	1,1453	−0,02	1,1585	+0,09	1,1596	−0,05
303,15	1,1524	0,00	1,1650	+0,04	1,1649	−0,08
313,15	1,1669	0,00	1,1782	+0,02	1,1765	+0,07
323,15	1,1819	−0,06	1,1819	−0,02	1,1890	+0,03
333,15	1,1975	0,00	1,2056	−0,01	1,2022	−0,04
343,15	1,2136	0,00	1,2200	−0,04	1,2158	−0,11
348,15	1,2214	−0,03	1,2284	+0,02	1,2227	−0,14
353,15	1,2305	0,00	1,2349	−0,06	1,2297	−0,17
363,15	1,2461	0,00	1,2502	−0,06	1,2440	−0,20
373,15	1,2663	−0,10	1,2662	+0,02	1,2585	−0,22
383,15	1,2853	0,00	1,2828	−0,06	1,2734	−0,22
393,15	1,3054	0,00	1,3002	−0,06	1,2888	−0,18
398,15	1,3160	−0,11	1,3092	−0,09	1,2966	−0,19
403,15	1,3267	0,00	1,3183	−0,04	1,3046	−0,18
413,15	1,3490	0,00	1,3372	0,00	1,3211	−0,14
423,15	1,3728	−0,11	1,3572	−0,03	1,3383	−0,10
433,15	1,3980	0,00	1,3783	+0,06	1,3563	−0,04
443,15	1,4253	0,00	1,4005	+0,12	1,3753	0,00
448,15	1,4393	−0,10	1,4121	−0,15	1,3852	0,00
453,15	1,4543	0,00	1,4240	+0,18	1,3954	+0,07
463,15	1.4869	0,00	1,4496	+0,22	1,4168	+0,12
473,15	1,5224	−0,10	1,4768	+0,15	1,4396	+0,17
483,15	1,5614	0,00	1,5066	+0,32	1,4642	+0,21
493,15	1,6078	0,00	1,5393	+0,34	1,4908	0,25
498,15	1,6347	−0,18	1,5586	+0,30	1,5049	+0,26
503,15	1,6626	−0,17	1,5758	+0,33	1,5197	+0,27
513,15	1		1,6171	+0,27	1,5514	+0,29
523,15			1,6652	+0,09	1,5807	+0,28
533,15			1,7246	+0,34	1,6262	+0,23
543,15					1,6709	+0,09
548,15					1,6977	−0,03
553,15					1,7261	−0,20

T, K	o-Xylene		m-Xylene		p-Xylene	
298,15	1,1424	−0,08	1,1627	+0,10	1,1698	+0,10
303,15	1,1464	+0,08	1,1681	−0,04	1,1749	+0,04
313,15	1,1560	+0,24	1,1790	+0,02	1,1860	−0,04
323,15	1,1673	+0,24	1,1902	−0,01	1,1979	−0,07
333,15	1,1797	+0,20	1,2018	+0,03	1,2104	+0,02
343,15	1,1928	+0,07	1,2140	+0,06	1,2236	+0,01
348,15	1,1996	+0,10	1,2204	−0,05	1,2304	+0,01
353,15	1,2064	−0,02	1,2268	+0,07	1,2373	−0,03
363,15	1,2202	−0,08	1,2403	+0,07	1,2515	−0,07
373,15	1,2344	−0,13	1,2545	+0,05	1,2662	−0,10
383,15	1,2487	−0,14	1,2695	+0,02	1,2815	−0,10
393,15	1,2633	+0,13	1,2853	−0,02	1,2974	−0,08
398,15	1,2707	+0,13	1,2934	−0,10	1,3056	+0,01
403,15	1,2782	+0,10	1,3018	−0,06	1,3140	−0,06
413,15	1,2936	+0,06	1,3193	−0,08	1,3312	−0,04
423,15	1,3095	+0,02	1,3376	−0,11	1,3492	−0,03
433,15	1,3260	+0,03	1,3569	−0,13	1,3681	−0,01
443,15	1,3434	−0,07	1,3773	−0,13	1,3880	−0,02
448,15	1,3523	−0,09	1,3878	−0,04	1,3983	−0,01
453,15	1,3616	−0,12	1,3987	−0,13	1,4090	−0,02
463,15	1,3809	−0,16	1,4213	−0,12	1,4312	−0,03
473,15	1,4015	−0,20	1,4453	−0,10	1,4549	−0,04
483,15	1,4235	−0,24	1,4708	−0,08	1,4802	−0,06
493,15	1,4473	−0,27	1,4982	−0,05	1,5075	−0,08
498,15	1,4600	−0,28	1,5126	−0,09	1,5220	−0,09
503,15	1,4732	−0,29	1,5276	−0,05	1,5372	−0,10
513,15	1,5014	−0,31	1,5597	−0,03	1,5698	−0,10
523,15	1,5326	−0,31	1,5950	−0,16	1,6061	−0,09
533,15	1,5676	−0,26	1,6345	+0,02	1,6473	−0,03
543,15	1,6073	−0,15	1,6798	+0,10	1,6953	+0,12
548,15	1,6295	−0,05	1,7055	+0,07	1,7229	+0,27
553,15	1,6536	+0,08	1,7338	+0,29		

It can be seen from the table that the densities of the six fluid hydrocarbons under investigation can be calculated with a high degree of accuracy using the equation of state (6) within the temperature limits of 298-673°K and the pressure limits of P_s to 500 bars. The mean discrepancy is ±0.07% for benzene, ±0.08% for toluene, ±0.06% for ethylbenzene, ±0.15% for o-xylene, ±0.03% for m-xylene, and ±0.04% for p-xylene. The maximum discrepancy is 0.38% for o-xylene at 673°K.

The relatively large discrepancy between the values calculated using (6) and the experimental values when $T \geqslant T_{cr}$ is due to the fact that in this parameter range the equation operates at the lower limit of density at which it is still valid. In other words, the equation of state is valid for specific volumes not exceeding double the volume of the substance in the state, so that as the radius increases up to $2r_i$, the concept of the consistent field which forms the basis of the derivation of the equation of state ceases to be sound, since the molecule can easily move out of the cell formed by neighboring particles.

The densities of the fluid at the saturation line are also calculated using (6) and are compared with experimental data (Table 3). As shown by this comparison, the equation of state (6) can be recommended for calculating v' up to $0.89T_{cr}$ with an error of ±0.0-0.20%.

It should be noted that the calorific properties of the fluid aromatic hydrocarbons under examination can also be described with a fairly high degree of accuracy by using the proposed equation of state.

By using the differential relationship

$$\left(\frac{\partial c_p}{\partial p}\right)_T = -T\left(\frac{\partial^2 v}{\partial T^2}\right)_p$$

or

$$c_p(p,\ T) = c_{p_1}(p_1,\ T) - T\int\limits_{p_1}^{p_2}\left(\frac{\partial^2 v}{\partial T^2}\right)_p dp$$

and in accordance with the equation of state (6), the following expression [8] is obtained for specific heat at a constant temperature:

$$c_p(p,\ T) - c_{p_1}(p_1 T) = R\left\{2TB' - T^2B''\right)\left(\frac{1}{v} - \frac{1}{v_1}\right) + \frac{1}{7}(2TH' + T^2H'')\left(\frac{1}{v^7} - \frac{1}{v_1^7}\right) + \\ + \frac{\left[1 + (B + TB')\frac{1}{v} + (H + TH')\frac{1}{v^7}\right]^2}{1 + \frac{2B}{v} + \frac{8H}{v^7}} + \frac{\left[1 + (B + TB')\frac{1}{v_1} + (H + TH')\frac{1}{v_1^7}\right]^2}{1 + \frac{2B}{v_1} + \frac{8H}{v_1^7}}\right\}. \qquad (8)$$

A comparison between c_p values calculated for toluene using (6) within the temperature limits of 25-400°C and pressure limits of up to 250 bars and experimental values [8] shows that the discrepancy over the whole range is not greater than ± 0.5% and is basically less than ± 0.2%.

Thus, the standard-form equation of state which has been formulated can be used over a wide range of temperatures (298-673°K) and pressures (P_s to 500 bars) to establish with a high degree of accuracy the thermal and calorific properties of six fluid hydrocarbons of the aromatic series.

NOTATION

ε, free energy of one molecule; ψ, free energy of the whole system; N, number of particles in volume V; v_0, volume of spherical cell; $\Phi(v_0)$, cell volume function, identical in significance with mean value of consistent field energy; f, pressure; T, temperature; T_{cr}, critical temperature; v, specific volume; ρ, density; ρ_s, density of saturated fluid; R, gas constant; z, compressibility; α, β, coefficients in Eq. (4); B_1, H_1 and B, H, coefficients in

Eqs. (5) and (6), temperature-dependent; τ, corrected temperature; b_i, h_i, coefficients of polynomials in (7); c_p, specific heat at constant temperature; c_{p_1}, v_1, parameters of a point at a given isotherm for a selected pressure p_1; B', H' and B'', H'', first and second temperature derivatives of coefficients B and H according to (7).

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CALCULATING THE TIME OF ISOTHERMAL SATURATION OF A SPHERE

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Results of a numerical solution of the inverse Stefan problem are presented for a sphere with boundary conditions of the third kind. Expressions are derived for calculating the time of total diffusion saturation of a spherical core, taking into account the rate of interaction of the gas phase with the surface of the solid.

In many fields of technology it is important to know the time of isothermal diffusion saturation of solid particles whose material is used to form a target product. A characteristic case is provided by saturation of particles of spherical form and separation of the original material from the target product by a moving boundary of phase separation. Usually, the diffusing matter penetrates the solid from a gaseous or liquid phase. The depth of saturation is determined by the rate of mass transfer in the solid and in the surrounding medium. The diffusion coefficient in the liquid or gas is many orders greater than in the solid. Therefore, in the first approximation of the process description we can confine ourselves to the solution of the interior problem of mass transfer, i.e., to the analysis of the reaction diffusion within the solid.

The problem concerned with diffusion saturation of a sphere for an arbitrary kinetic relationship of the motion of the phase separation boundary is solved in [1, 2]. However, the use of the methods of these investigations, to determine the depth of saturation of the sphere, i.e., the solution of the inverse problem, constitutes considerable difficulties. We have made an attempt to numerically solve the problem of isothermal saturation of a sphere-shaped particle as a result of a reaction diffusion within the solid phase, taking into ac-

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