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GENERALIZATION OF EXPERIMENTAL DATA ON THERMAL CONDUCTIVITY OF PARAFFIN SERIES HYDROCARBONS AND ALCOHOLS

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An expression is obtained for calculating the temperature dependence of the thermal conductivity coefficient of vapors of the paraffin series hydrocarbons and their alcohols over a wide temperature range at pressures of P = 0.1 MPa.

The present state of precise kinetic theory [1] does not provide results accurate enough for practical applications in calculating the thermal conductivity coefficient of multiatomic gases. The theory has been developed only for spherically symmetric molecules without internal degrees of freedom, i.e., monatomic gas molecules.

The absence of a reliable analytical method for calculating λ of multiatomic gases makes experiment the major source of data on thermal conductivity of these substances. However the expensive and inefficient process of purely empirical study of thermal properties of substances with complex molecular structure cannot be extended without limit. It thus becomes necessary to produce computation expressions which permit determination of the transport properties of materials over a wide parameter range with an accuracy close to that of experiment. In the author's opinion the most efficient method of solving this problem is the similarity theory-based method of generalizing experimental data, which makes it possible not only to systematize and evaluate experimental data, but also to predict results for little studied materials. We have performed a generalization of experimental data on the thermal conductivity of vapors of the paraffin series hydrocarbons and their alcohols.

For processing the λ values with a single temperature dependence the expression

$$\frac{\lambda}{\lambda_{T_b}} = F\left(\frac{T}{T_b}\right), \tag{1}$$

was used, where T_b is the boiling point of the substance at normal pressure, K [2]; λ_{T_b} is the thermal conductivity of the material at the boiling point, W/(m·K).

The experimental points fit a single curve well in such coordinates. The maximum deviation from the averaging curve for either the paraffins or the alcohols did not exceed $\pm 2\%$. Aside from the data obtained by the present author in [3], the generalization used data of [4] for hexane, heptane, octane, nonane, and decane, and data from [5, 6] for methyl, ethyl,

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TABLE 1. Comparison of Recommended [12] and Calculated Values of $\lambda \cdot 10^4$, W/(m·K), for Alcohol Vapors

Substance	T, K	$\lambda_{exp}/\lambda_{calc}$	$\frac{\Delta\lambda}{\lambda}$, %	Substance	T, K	$\lambda_{exp}/\lambda_{calc}$	$\frac{\Delta\lambda}{\lambda}$, %
Methanol	380	238/242	+2,1	Ethanol	390	246/245	—0,4
	450	316/326	+3,2		450	316/317	+0,3
	570	468/484	+3,4		570	472/469	—0,6
Isopropanol	390	242/242	0	Propanol	410	251/254	+1,1
	450	310/313	+1,0		450	296/301	+1,7
	560	454/452	—0,4		570	458/449	—2,0
Butanol-1	440	273/274	+0,4	Pentanol-1 (n-alyl)	420	236/237	+0,4
	500	349/345	—1,1		500	326/328	+0,6
	580	450/443	—1,6		580	440/424	—3,6
Hexanol-1	470	274/280	+2,2	Heptanol-1	480	268/278	+3,7
	520	332/337	+1,5		530	326/334	+2,5
	570	395/396	+0,3		600	401/416	+3,7
Octanol-1	480	257/265	+3,1				
	530	312/321	+2,9				
	570	356/366	+2,8				

propyl, and isopropyl alcohols. Analysis of the quality and conditions of the experimental studies of [3-6], and the similar uncertainties of the experiments permit the conclusion that the reliability of their results is identical. Therefore in the mathematical processing all of our data and the results of [3-6] were considered equally.

Processing of the experimental points by the method of least squares yielded the equation:

$$\lambda = (a\tau^2 + b\tau + c)\lambda_{T_b}, \quad (2)$$

where for the alcohols $a = 0.238$, $b = 1.573$, $c = -0.7999$: for the paraffins $a = 0.699$, $b = 0.566$, $c = -0.276$, $\tau = T/T_h$.

It developed that the values of λ_{T_b} could be related to the boiling points of the alcohols and paraffins by the following expressions:

$$\lambda_{T_b} = (0{,}444\,T_b + 41{,}34)\cdot 10^{-4}\ (\text{W/(m·K)}) \quad (3)$$

$$\lambda_{T_b} = (0{,}532\,T_b - 12{,}02)\cdot 10^{-4}\ (\text{W/(m·K)}). \quad (4)$$

Thus, using Eqs. (2)-(4), we obtain expressions for the temperature dependence of thermal conductivity of the alcohols and paraffins:

$$\lambda = (0{,}238\,\tau^2 + 1{,}573\,\tau - 0{,}799)(0{,}444\,T_b - 41{,}34)\cdot 10^{-4}\ (\text{W/(m·K)}), \quad (5)$$

$$\lambda = (0{,}699\,\tau^2 + 0{,}566\,\tau - 0{,}276)(0{,}532\,T_b - 12{,}02)\cdot 10^{-4}\ (\text{W/(m·K)}). \quad (6)$$

Equations (5) and (6) are valid for the temperature range 270-650 K. Comparison of λ values calculated by Eq. (5) with experimental data shows that the equation describes the temperature dependence of thermal conductivity in the alcohol vapors with sufficient accuracy. The deviation of experimental data of various authors [5-11] from calculations by Eq. (5) lies in the limits 1-3%, being greater at only a few points, but never exceeding $\pm$4%.

Table 1 presents a comparison of values of $\lambda \cdot 10^4$, W/(m·K), for alcohol vapors calculated by Eq. (5) with the data recommended in [12].

Equation (6) permits calculating thermal conductivity of gaseous paraffin hydrocarbons from ethane to tridecane inclusive. Comparison of calculated and experimental data [13-17] for both light and heavy members of the series shows that deviations lie mainly in the range 0-3%, increasing to a maximum of $\pm$6% only at a few points near the limits of the interval. Table 2 shows deviations of calculated values of paraffin series vapor thermal conductivities from the recommended data of [12].

The deviation of the calculated thermal conductivity values from experiment for methane are apparently the consequence of the significant differences between the first and subsequent

TABLE 2. Comparison of Recommended [12] and Calculated Values of $\lambda \cdot 10^4$, W/(m·K), for Paraffin Vapors

Substance	T, K	$\lambda_{exp}/\lambda_{calc}$	$\frac{\Delta\lambda}{\lambda}$, %	Substance	T, K	$\lambda_{exp}/\lambda_{calc}$	$\frac{\Delta\lambda}{\lambda}$, %
Ethane	250	156/153	−1,9	Heptane	400	217/212	−2,3
	350	285/285	0		500	335/325	−3,0
	500	530/550	+3,8		600	466/457	−1,9
Propane	300	182/182	0	Octane	420	222/219	−1,4
	400	311/310	−0,3		500	311/307	−1,3
	500	459/468	+2,0		600	437/432	−1,1
Butane	300	161/159	−1,2	Nonane	450	237/238	+0,4
	500	424/414	−2,4		550	350/349	−0,3
	550	502/494	−1,6		600	412/411	−0,2
Pentane	320	166/161	−3,0	Decane	480	254/257	+1,2
	400	260/248	−4,6		550	332/334	+0,6
	470	352/335	−4,8		600	390/393	+0,8
Hexane	400	236/228	−3,4	Undecane	500	263/266	+1,1
	500	360/348	−3,3		550	317/320	+0,9
	600	500/488	−2,4		600	373/378	+1,3

TABLE 3. Comparison of Calculated Values of Thermal Conductivity $\lambda \cdot 10^4$, W/(m·K), of Mixtures of Paraffin Vapors and Their Polymers with Experimental Data

Substance	T, K	λ_{exp}	λ_{calc}	$\frac{\Delta\lambda}{\lambda}$, %	Reference
$0{,}503C_2H_6$—$0{,}497C_3H_8$	305,8	203	204	+0,6	[14]
	367,6	284	287	+1,1	
	427,5	375	379	+1,1	
	478,5	485	467	+1,9	
$0{,}3C_5H_{12}$—$0{,}7C_6H_{14}$	323	155	154	−0,6	[17]
	373	205	204	−0,3	
$0{,}815C_5H_{12}$—	323	163	162	−0,9	
$0{,}185C_6H_{14}$	373	216	214	−1,1	
Isobutane	300	161	164	+1,9	[12]
	400	285	283	−0,7	
	470	388	381	−1,8	
Isopentene	300	146	146	0	
	400	254	253	−0,4	
	460	330	329	−0,3	

members of the series as regards molecular structure. Formation of the homologic paraffin series takes place by replacement of a hydrogen atom in a molecule of the preceding member by a CH_3 radical according to the pattern CH_3–CH_2–CH_2–CH_3. Methane, being the initial member of this series, has a spherically symmetric molecule, while the molecules of the remaining members form chains, the length of which increases with increase in the number of carbon atoms in the molecule. Methane also appeared as an exception to generalization in [15, 18].

Deviation of the calculated λ from experimental [15] for the higher representatives of the paraffin series (tetradecane, hexadecane, octadecane) comprises 3-6%. This is apparently due to a change in the character of molecular interaction caused by an increase in molecular binding energy with increase in boiling point of the substance.

Equation (6) was also used to calculate λ values for ethane–propane, heptane–hexane, and butane and pentane isomer mixtures. The mixture boiling point T_{bm} was determined with the equation

$$T_{bm} = x_1 T_b^1 + x_2 T_b^2, \quad (7)$$

where x_1, x_2 are the molar fractions of the mixture components and T_b^1, T_b^2 are the component boiling points.

Comparison of calculated and experimental [12, 14, 17] values of λ for these materials shows that the deviation of experiment from calculation does not exceed ±2.0% (Table 3).

Thus, based on comparison of experimental data on thermal conductivity of alcohols and paraffin hydrocarbons in the gaseous phase with values calculated with Eqs. (5) and (6), we may conclude that it is possible to use those equations for calculating the temperature dependence $\lambda = f(T)$ of gaseous alcohols, paraffins, and their binary mixtures for engineering calculations in heat and mass transport processes.

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