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GENERALIZATION AND CALCULATION OF THE THERMAL DIFFUSION FACTOR OF BINARY HYDROGEN-CONTAINING GASEOUS MIXTURES

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The results of generalization of experimental data on the thermal diffusion factor α_T of hydrogen-containing gaseous mixtures within the framework of similarity theory have been given. The calculated relation which makes it possible to predict the thermal diffusion factor of hydrogen-containing mixtures of nonpolar gases with a limited body of data on the substance has been obtained. The α_T values of mixtures of hydrogen with inert gases, including radon Rn, and with N_2, SiH_4, and GeH_4 in the temperature interval 100–1500 K have been calculated.

Keywords: *thermal diffusion factor, gaseous mixtures, hydrogen, inert gases, nitrogen, silane, german, similarity theory, generalization of data.*

Introduction. Gaseous mixtures with hydrogen at relatively low pressures play an important role in various processes in nature, engineering, and technologies. In particular, many gas-transport processes of growing of materials in electronic engineering are accompanied by the concentration and thermal diffusion of the components in a hydrogen medium. In this connection, investigation and generalization of data on the transport properties of hydrogen-containing gaseous mixtures are important both scientifically and practically.

For many gaseous systems containing hydrogen, thermal diffusion characteristics have not been studied at all or have been investigated not quite adequately. In this situation where there is a shortage of information it is important to know methods for calculation and prediction of the properties of mixtures from incomplete or indirect experimental data.

In the presented work, we have obtained a calculated relation for the thermal diffusion factor of hydrogen-containing gaseous mixtures on the basis of generalization (processing) of results of experimental investigations of α_T within the framework of similarity theory.

We have included, into the data array for the generalization, the α_T values of binary mixtures of hydrogen with inert gases and nitrogen, since there is the greatest number of experimental points for these mixtures, according to the review of literature data.

In the earlier works, the results on thermal diffusion were presented in the form of the separation value of the gaseous mixture (Δx_1) as a function of the ratio of the temperatures of the hot T_1 and cold T_2 regions. For these data, the values of the thermal diffusion factor α_T were calculated and referred to the logarithmic mean temperature T determined from the Brown formula [1]:

$$T = \frac{T_1 T_2}{T_1 + T_2} \ln \frac{T_1}{T_2} .$$

The error in the results of investigations of thermal diffusion characteristics which was evaluated by the authors of works on mixtures of hydrogen with inert gases at a nearly normal pressure was within ±(1–10%).

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TABLE 1. Potential Parameters for Different Gases: ε/k (Lennard-Jones model) and σ (solid spheres)

Gas	Force constants*		Gas	Force constants*	
	ε/k, K	σ, nm		ε/k, K	σ, nm
He	10.22	0.218	Xe	229.0	0.486
Ne	35.7	0.260	H_2	33.3	0.273
	27.5			38.0	
Ar	124.0	0.364	N_2	91.5	0.375
	116.0			79.8	Kr
Kr	190.0	0.416			

*For Ne, Ar, H_2, and N_2, the upper values of the parameter ε/k correspond to the temperature interval 80–300 K, whereas the lower ones correspond to the interval 300–1000 K.

The α_T values of the selected gaseous mixtures of equimolar concentration were used for processing.* Not only were the experimental data included, but the interpolation results and smoothed α_T values in the presence of the wide scatter in experimental data were also included.

The experimental α_T values for each gaseous mixture were preprocessed using the least-squares method to evaluate their reliability; all data were considered as being equally accurate. Results differing from the averaged ones by more than 10–15% were eliminated from further processing, and the remaining data were averaged again.

The resulting averaged values of α_T for the considered mixtures of H_2 with He, Ne, Ar, Kr, Xe, and N_2 were combined into a single data array with the aim of processing it within the framework of similarity theory; as applied to the thermophysical properties of substances it is common to call this theory the "law of corresponding states."

Generalization of the Data on α_T. According to the two-parametric law of corresponding states, the temperature dependence of the thermal diffusion factor in reduced form can be written as follows [2]:

$$\alpha_T^* = \frac{\alpha_T}{\alpha_{T(\mathrm{h.s})}} = f(T^*) \,, \tag{1}$$

where $\alpha_T = \alpha_{T(\mathrm{exp})}$, $\alpha_{T(\mathrm{h.s})}$ is dependent on the collision diameter of the interacting hard spheres σ and on the molecular masses of the components, and $T^* = kT/\varepsilon_{12}$.

The values of $\alpha_{T(\mathrm{h.s})}$ for the binary gaseous mixture are calculated from the relation

$$\alpha_{T(\mathrm{h.s})} = \frac{S_1 x_1 - S_2 x_2}{Q_1 x_1^2 + Q_{12} x_1 x_2 + Q_2 x_2^2} \,, \tag{2}$$

where

$$S_1 = \frac{2}{5} \frac{m_1}{m_2} \sqrt{\frac{2m_2}{m_1 + m_2}} \frac{\sigma_1^2}{\sigma_{12}^2} - \frac{8}{5} \frac{m_1 m_2}{(m_1 + m_2)^2} - \frac{3m_2 (m_2 - m_1)}{(m_1 + m_2)^2} \,;$$

$$Q_1 = \frac{2}{5} \frac{2}{(m_1 + m_2)\, m_2} \sqrt{\frac{2m_2}{m_1 + m_2}} \frac{\sigma_1^2}{\sigma_{12}^2} \left(3m_2^2 + m_1^2 + \frac{8}{5} m_1 m_2 \right);$$

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*The thermal diffusion factor α_T can be computed with the use of the separation value Δx_1 from the formula $\alpha_T = \dfrac{\Delta x_1}{x_1 x_2 \ln (T_1/T_2)}$ and the separation coefficient q from the formula $\alpha_T = \dfrac{\ln q}{\ln (T_1/T_2)}$, where $q = (x_1/x_2)_{T_1}/(x_1/x_2)_{T_2}$. The difference in α_T values here is the smallest for the equimolar concentration.

TABLE 2. Coefficients a and b of the Dependence $\alpha_{T(\mathrm{h.s})}^{-1} = a + bx_1$ for Mixtures of Hydrogen with Inert Gases and Nitrogen

Gaseous mixture	Coefficients		Gaseous mixture	Coefficients	
	a	*b*		*a*	*b*
H_2–He	4.272513	–0.63253	H_2–Kr	0.73943	1.280831
H_2–Ne	1.425718	0.637969	H_2–Xe	0.595798	1.418686
H_2–Ar	0.906703	1.131872	H_2–N_2	0.91011	1.14826

$$Q_{12} = \frac{2}{5}\left(\frac{15\,(m_1 - m_2)^2}{(m_1 + m_2)^2} + \frac{32 m_1 m_2}{(m_1 + m_2)^2} + \frac{8}{5}\,\frac{m_1 + m_2}{(m_1 m_2)^{1/2}}\,\frac{\sigma_1^2 \sigma_2^2}{\sigma_{12}^4}\right).$$

Expressions for the quantities S_2 and Q_2 involved in (2) are obtained by the corresponding replacement of the subscripts in the expressions for S_1 and Q_1. The values of σ_{12} and ε_{12}/k are determined from the data on σ and ε/k for pure components using the combination rules

$$\sigma_{12} = \frac{\sigma_1 + \sigma_2}{2}\,, \quad \varepsilon_{12} = (\varepsilon_1 \varepsilon_2)^{1/2}\,.$$

Table 1 indicates the values of potential parameters, which were used in processing the data on α_T, for inert gases and nitrogen. The ε/k values (borrowed from [2]) for pure gases have been obtained from data on the coefficient of dynamic viscosity for the Lennard-Jones potential model (12–6). The collision diameters σ of the mixtures' components, which are necessary for calculating $\alpha_{T(\mathrm{h.s})}$, have been determined from data obtained at 273 K on the coefficient of viscosity [2].

The best description of the formed array on α_T^* (85 points) in the interval of the reduced temperatures $T^* = 1.4$–38 is obtained, with the least-squares method, in logarithmic coordinates in the form of the polynomial

$$\ln \frac{1}{\alpha_T^*} = C_1 + C_2 \ln T^* + C_3 \frac{1}{\ln T^*}\,, \tag{3}$$

which, with allowance for the coefficients of the polynomial for calculation of the generalized values of the thermal diffusion factor, yields the expression

$$\alpha_T = \alpha_{T(\mathrm{h.s})}\left[\exp\left(-\,0.61087698 + 0.26355851 \ln T^* + 1.5166357 \frac{1}{\ln T^*}\right)\right]^{-1}. \tag{4}$$

The calculated $\alpha_{T(\mathrm{h.s})}$ values of the mixtures are also processed by the least-squares method. According to [3], the dependence of the reciprocal of $\alpha_{T(\mathrm{h.s})}$ on the concentration of the heavy component x_1 of binary gaseous mixtures can be approximated by the linear function

$$\alpha_{T(\mathrm{h.s})}^{-1} = a + bx_1\,. \tag{5}$$

The coefficients a and b of Eq. (5) for the considered pairs of components are given in Table 2.

The general pattern of approximation of experimental data on the reduced thermal diffusion factor for mixtures of hydrogen with inert gases and nitrogen using (4) is shown in Fig. 1. We emphasize that the experimental data on α_T of the systems in question lie mainly in the interval 90–500 K in the region of the reduced temperatures $T^* > 1$. For all pairs with hydrogen (except for He), the de Buhr parameter $\Lambda^* = h/\sigma\sqrt{2m\varepsilon}$ characterizing the role of quantum effects in thermophysical properties is approximately the same and is equal to ~1. The "quantum" thermal diffusion factor at 100 K is almost 10% higher than the classical one. It may be considered in the first approximation that dependence (4) generalizing the experimental data to an extent is representative, at low temperatures, of the role

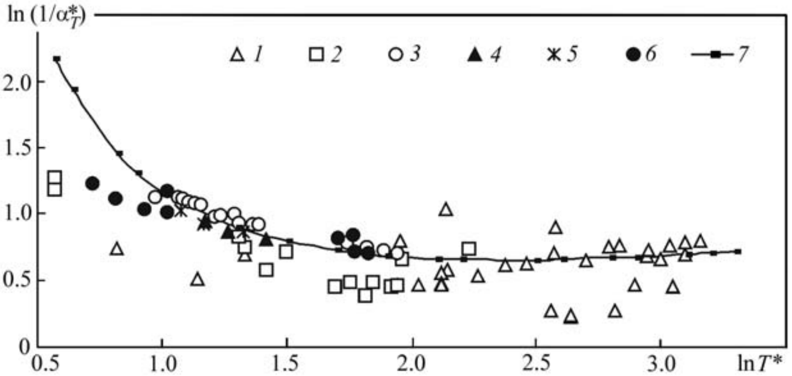


Fig. 1. ln $(1/\alpha_T^*)$ vs. ln T^* for the binary mixtures of hydrogen with inert gases and nitrogen ($x_{H_2} \simeq 0.5$): 1) H_2–He, 2) H_2–Ne, 3) H_2–Ar, 4) H_2–Kr, 5) H_2–Xe, and 6) H_2–N_2; 7) generalized sphere curve obtained from polynomial (4).

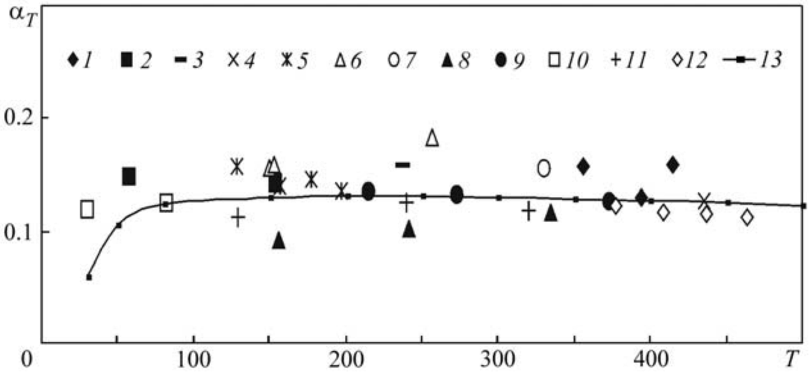


Fig. 2. Temperature dependence of α_T of the H_2–He mixture ($x_{H_2} \sim 0.5$). Experimental data: 1 and 5) [9], 2) [5], 3) [1, 10], 4) [11], 6) [12–14], 7) [15], 8) [16, 17], 9) [18], 10) [4], 11) [19], 12) [20], 13) calculated data obtained from polynomial (4) ($x_{H_2} = 0.5$). T, K.

of the quantum effect for the mixture "hydrogen–heavy inert gases." For the H_2–He mixture, the same estimates at a temperature of ~50 K give a correction of the order +30%, which will be taken into account further in calculations of the recommended data on α_T.

Calculation of the Thermal Diffusion Factor α_T. The dependences (calculated from polynomial (4)) of the thermal diffusion factor on temperature for the mixtures of H_2 with He, Ne, Ar, Kr, Xe, and N_2 are given in Figs. 2–7 compared to the experimental data on $\alpha_T(x_{H_2} \simeq 0.5)$. To compare them to the calculation results we have also used the tabulated α_T values for mixtures of hydrogen with Ne, Ar, Kr, and Xe; these values were obtained in [6] in generalizing the data, primarily the data on the viscosity of these mixtures.

H_2–He Mixture. The temperature dependence of the thermal diffusion factor of the H_2–He mixture ($x_{H_2} \simeq 0.5$) is presented in Fig. 2. The disagreement in experimental data of different authors amounts to more than 10%. The α_T values calculated from polynomial (4) in the range of the temperatures T = 150–500 K diminish with growth in the temperature only slightly, which corresponds to the analogous dependence of the experimental data. Unlike the experimental data of [4, 5], we observe a sharp decrease in the calculated data on α_T with temperature ($T < 100$ K). The high values of α_T of the H_2–He mixture at T = 25–100 K are explained in [4, 5] by the distinctive features of the behavior of hydrogen and helium at low temperatures, which are determined by quantum effects and inelastic collisions. Calculation of α_T at temperatures lower than 80 K is carried out with the use of the potential parameters ε/k obtained from the second virial coefficient [2]: $\varepsilon/k(H_2)$ = 29.2 K and $\varepsilon/k(\mathrm{He})$ = 6.03 K.

H_2–Ne Mixture. For mixtures of H_2 with Ne, as for those with He, the experimental data on α_T obtained in different works with an error of ±(2–5%) have a disagreement of more than 10%. Figure 3 compares results of cal-

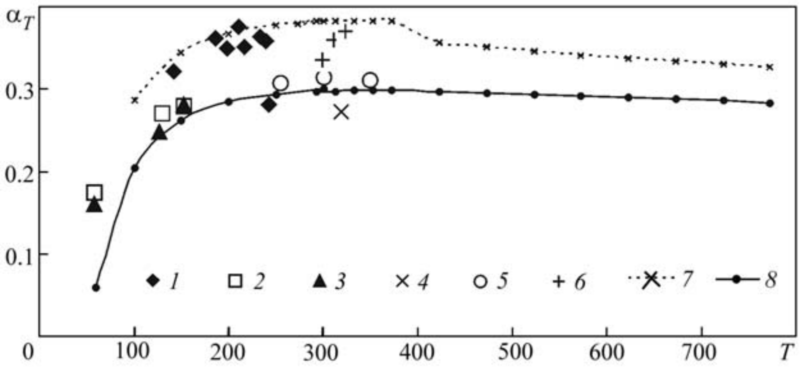


Fig. 3. Temperature dependence of α_T of the H_2–Ne mixture (x_{H_2} = 0.5). Experimental data: 1) [21], 2) interpolated data [22], 3) interpolated data [12], 4) interpolated data [23], 5) [24], and 6) [25]. Calculated data: 7) tabulated data [6] and 8) data obtained from polynomial (4). *T*, K.

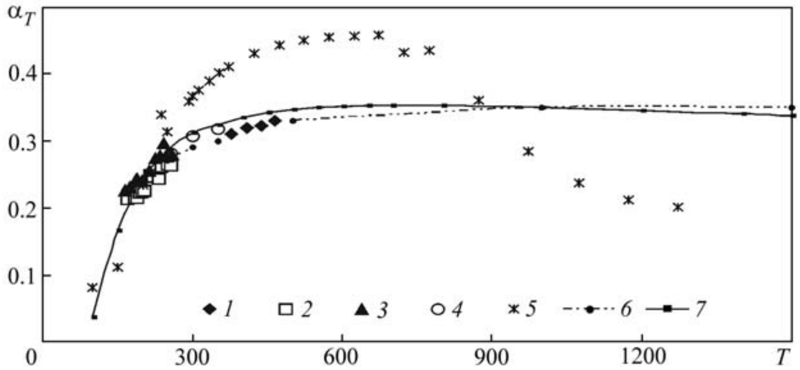


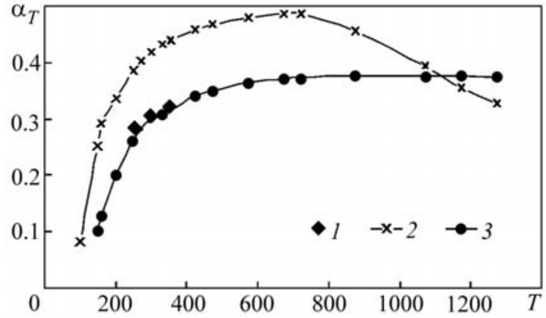
Fig. 4. Temperature dependence of α_T of the H_2–Ar mixture ($x_{H_2} \simeq 0.5$). Experimental data: 1) [20], 2 and 3) [26], and 4) [24]. Calculated data (x_{H_2} = 0.5): 5) tabulated data [6], 6) data obtained from the regions of molecular-kinetic theory using the selected parametric models [7], and 7) data obtained from polynomial (4). *T*, K.

culation from polynomial (4) and experimental values of α_T (including those interpolated for the concentration x_{H_2} = 0.5), and also tabulated data [6]. As is seen in Fig. 3, in the temperature region 100–400 K, the calculation performed from polynomial (4) fairly well (within 1–6%) describes most of the experimental values of α_T (including the precision data of [24]) and is inconsistent with the results of [6]. For the temperature region <100 K, the calculation from polynomial (4) gives understated α_T values relative to the interpolated data [12, 22].

H_2–Ar Mixture. The temperature dependence of α_T of this mixture is given in Fig. 4. Calculations performed according to molecular-kinetic theory with the use of potential parameters obtained by statistical processing of experimental data on transport properties [7] and from polynomial (4) are consistent with experimental results on α_T within ~2–7%. The tabulated data in [6] in the temperature range 250–800 K are, conversely, overstated (have their maximum); at higher temperatures, they are understated by nearly 30% relative to the results of our calculations.

H_2–Kr and H_2–Xe Mixtures. Figures 5 and 6 compare the α_T values of mixtures of H_2 with Kr and Xe of equimolar concentration, which have been calculated from polynomial (4), and tabulated data [6] to the experimental results on α_T. From the calculated data of [6] in the temperature range *T* = 200–800 K, there is a maximum of α_T plotted as a function of the temperature, which is inconsistent with experimental data and with the data calculated from polynomial (4). Table 3 compares the calculated values of α_T for these mixtures and certain experimental data for different concentrations of H_2.

H_2–N_2 Mixture. The temperature dependence of α_T of this mixture of equimolar concentration is given in Fig. 7. The calculations performed from polynomial (4) and from the relations of molecular-kinetic theory using



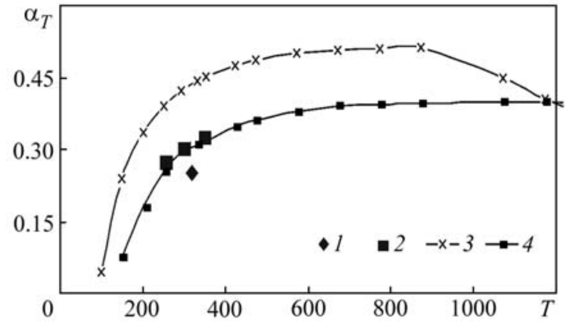


Fig. 5. Temperature dependence of α_T of the H_2–Kr mixture (x_{H_2} = 0.5). Experimental data: 1) [24]. Calculated data: 2) tabulated data [6] and 3) data obtained from polynomial (4). T, K.

Fig. 6. Temperature dependence of α_T of the H_2–Xe mixture (x_{H_2} = 0.5). Experimental data: 1) [24] and 2) interpolated data [23]. Calculated data: 3) tabulated data [6] and 4) data obtained from polynomial (4). T, K.

TABLE 3. Comparison of the α_T Values of H_2–Kr and H_2–Xe Mixtures, Calculated from Polynomial (4), and Certain Experimental Data

Gaseous mixture	$x(H_2)$	T_m	$\alpha_{T(exp)}$	$\alpha_{T(calc)}$ from polynomial (4)	δ^*, %	Literature source of experimental data
H_2–Kr	0.82	255.3	0.385	0.380	–1.3	[24]
		350	0.428	0.448	4.5	
	0.23	255.3	0.226	0.214	–5.6	
		350	0.261	0.252	–3.6	
	$x_{Kr} \to 0$	236.9	0.457	0.465^{**}	1.7	[27]
		345.4	0.563	0.583	3.4	
		422.5	0.575	0.633	9.2	
		461.8	0.583	0.65	10.3	
H_2–Xe	0.2	318.6	0.197	0.224	12.5	[23]
	0.4		0.232	0.268	13.4	
	0.6		0.277	0.333	16.8	
	0.7		0.309	0.380	18.7	
	$x_{Xe} \to 0$	300	0.56	0.619^{**}	9.5	
		400	0.69	0.741	6.9	
		500	0.77	0.803	4.1	
		700	0.86	0.854	0.7	

$^*\delta = (\alpha_{T(calc)} - \alpha_{T(exp)})/\alpha_{T(calc)}$. **Calculation of α_T was peformed for the concentration x_{Kr} and x_{Xe} = 0.001.

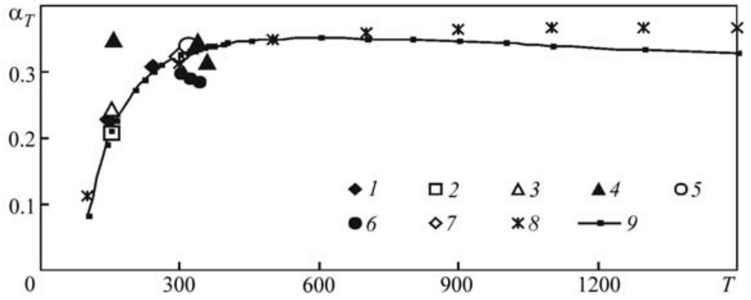


Fig. 7. Temperature dependence of α_T of the H_2–N_2 mixture ($x_{H_2} \simeq 0.5$). Experimental data: 1) interpolated data [26], 2) [28], 3) [12], 4) interpolated data [11], 5) [23], 6) [29], and 7) [30]. Calculated data (x_{H_2} = 0.5): 8) from molecular-kinetic theory [8] and 9) data obtained from polynomial (4). T, K.

TABLE 4. Potential Parameters for SiH_4, GeH_4, and Rn: ε/k (Lennard-Jones model) and σ (hard spheres)

Gas	Force constants		Literature source (reference)
	ε/k, K	σ, nm	
SiH_4	265	0.48	[32]
	207.6		[33]
	330		[31]*
GeH_4	285	0.443	[32]
	237		[33]
	515.8		[31]*
Rn	400	0.4	[34]

*ε/k have been calculated from ε_{12}/k obtained from the data on α_T.

TABLE 5. Coefficients a and b in the Dependence $\alpha_{T(\mathrm{h.s})} = (a + bx)^{-1}$ for H_2–SiH_4, H_2–GeH_4, and H_2–Rn Mixtures

Gaseous mixture	Coefficients	
	a	b
H_2–SiH_4	0.661709	1.395176
H_2–GeH_4	0.76209	1.259707
H_2–Rn	0.8339	1.1742

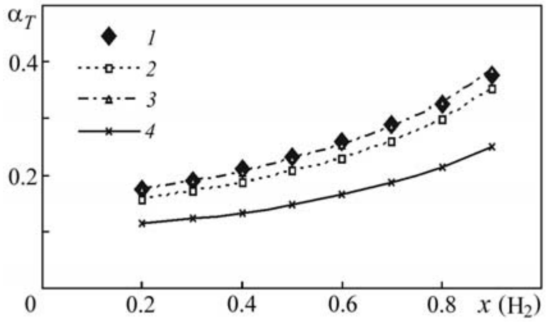


Fig. 8. Concentration dependence of α_T of the H_2–SiH_4 mixture at T_1 = 293 K and T_2 = 195 K (T_m = 237.4). Experimental data: 1) [31]. Calculated data were obtained from polynomial (4) with the use of the potential parameters: 2) ε/k (SiH_4) = 265 K [32] and ε/k (H_2) = 37 [2], 3) ε/k (SiH_4) = 207.6 K [33] and ε/k (H_2) = 37 [2], and 4) ε/k (SiH_4) = 330 K [31] and ε/k (H_2) = 37 [2].

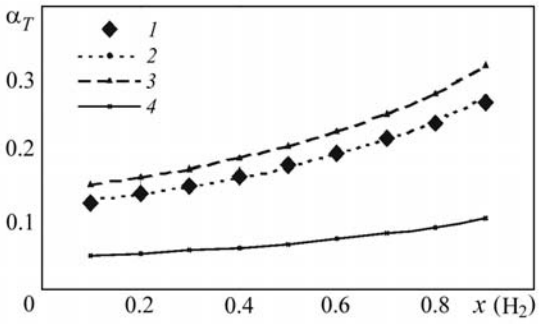


Fig. 9. Concentration dependence of α_T of the H_2–GeH_4 mixture at T_1 = 293 K and T_2 = 195 K (T_m = 237.4). Experimental data: 1) [31]. Calculated data were obtained from polynomial (4) with the use of the potential parameters: 2) ε/k (GeH_4) = 285 K [32] and ε/k (H_2) = 37 [2], 3) ε/k (GeH_4) = 237 K [33] and ε/k (H_2) = 37 [2], and 4) ε/k (GeH_4) = 515.8 K [31] and ε/k (H_2) = 37 [2].

the selected parametric models [8] are consistent with each other and with experimental data in the interval of temperatures T = 100–700 K. At higher temperatures, the calculated data have a slight disagreement. In this region of temperatures to T = 1500 K, there are virtually no experimental data on the thermal diffusion factor for most hydrogen-containing gaseous mixtures.

To check the predicting capacity of the generalized equation obtained (polynomial (4)) we have calculated the thermal diffusion factor α_T of mixtures of H_2 with molecules (SiH_4, GeH_4), which are widely used in the processes of gas-phase deposition of substances (silicon, germanium) and have a limited amount of experimental data, and with radon (Rn). Mixtures of gases with radon are of interest for medicine, metallurgy, and geology.

TABLE 6. Temperature Dependence of the Thermal Diffusion Factor α_T of Mixtures of Hydrogen with Inert Gases Including Rn, H_2, SiH_4, and GeH_4 ($x_{H_2} = 0.5$)

T, K	H_2–He	H_2–Ne	H_2–Ar	H_2–Kr	H_2–Xe	H_2–Rn	H_2–N_2	H_2–SiH_4	H_2–GeH_4
100	0.122	0.192	0.036	–	–	–	0.082	–	–
200	0.132	0.280	0.244	0.202	0.182	0.071	0.272	0.174	0.114
300	0.130	0.296	0.311	0.300	0.298	0.186	0.324	0.286	0.242
400	0.127	0.298	0.335	0.333	0.339	0.262	0.343	0.335	0.303
500	0.124	0.295	0.347	0.356	0.367	0.303	0.349	0.358	0.335
600	0.121	0.291	0.352	0.367	0.383	0.328	0.351	0.371	0.352
700	0.119	0.287	0.353	0.373	0.391	0.342	0.350	0.378	0.362
800	0.117	0.283	0.353	0.376	0.396	0.352	0.348	0.381	0.368
900	0.114	0.279	0.352	0.377	0.398	0.358	0.345	0.383	0.371
1000	0.112	0.275	0.350	0.377	0.399	0.362	0.343	0.383	0.373
1200	0.109	0.268	0.345	0.375	0.398	0.365	0.337	0.381	0.374
1400	0.106	0.262	0.341	0.371	0.395	0.366	0.331	0.378	0.372
1500	0.105	0.259	0.338	0.369	0.393	0.366	0.328	0.376	0.371

Data on the concentration dependence of α_T of H_2–SiH_4 and H_2–GeH_4 mixtures, obtained by the two-bulb method at T_1 = 293 K and T_2 = 195 K, are given in [31]. From the results of α_T measurements, Devyatykh et al. have determined the values of the constant ε_{12}/k for the Lennard-Jones potential (12–6).*

For calculation of the thermal diffusion factor α_T of H_2–SiH_4, H_2–GeH_4, and H_2–Rn mixtures using the generalized equation (4), we used the potential parameters ε/k and σ (determined in [31–35]) for SiH_4 and GeH_4 and for Rn (in [34]) (Table 4). Table 5 gives a and b coefficients of Eq. (5) for mixtures H_2–SiH_4, H_2–GeH_4, and H_2–Rn. As is seen in Table 4, for SiH_4 and GeH_4, the parameters ε/k computed in [32] from the data on viscosity are more than 20% higher that the data on ε/k given in [33].

Figures 8 and 9 compare the α_T values of H_2–SiH_4 and H_2–GeH_4 mixtures, which have been calculated from polynomial (4) and have been obtained with the use of different potential parameters, and experimental data. For the H_2–SiH_4 mixtures, the best description of the experimental values of α_T has been obtained using calculated data obtained with the use of the potential parameters of [33] (curve 3, Fig. 8).

For the H_2–GeH_4 mixture, the experimental values of α_T are in better agreement with the calculated data obtained with the use of the potential parameters of [32] (curve 2, Fig. 9). The use of the potential parameters obtained from individual thermal diffusion measurements in calculating α_T (curves 4, Figs. 8 and 9) leads to understated α_T values.

Table 6 gives the generalized α_T values (calculated from polynomial (4)) of the gaseous mixtures under study in the temperature range 100–1500 K for the concentration x_{H_2} = 0.5.

CONCLUSIONS

1. We have been able, with the use of the two-parametric law of corresponding states, to generalize experimental data on the thermal diffusion factor of binary mixtures of hydrogen with inert gases and nitrogen at temperatures higher than 100 K within the errors of their determination.

2. For these systems, we have calculated the recommended data on α_T, in particular, at $T > 600$ K, i.e., in the temperature region where there are no experimental data. We have predicted the thermal diffusion factor for H_2–Rn, H_2–SiH_4, and H_2–GeH_4 mixtures based on the law of corresponding states. The developed method of generalization of data can be extended to other mixtures of hydrogen with nonpolar gases.

3. The method of corresponding states is an efficient means for generalizing and predicting data on the thermal diffusion factor of mixtures of nonpolar gases and hydrogen.

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*The procedure for determining the values from data on the thermal diffusion factor assumes the presence of a generalized temperature dependence for a certain mixture or a certain class of mixtures.

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NOTATION

a, b, and C, coefficients of polynomials; h, Planck constant, J·s; k, Boltzmann constant; m_1 and m_2, molecular masses, kg·kmole^{-1}; m, reduced mass of a particle pair, kg·kmole^{-1}; q, separation coefficient of the gaseous mixture; T_1 and T_2, temperatures of the hot and cold regions of the thermal diffusion apparatus, K; T, logarithmic-mean temperature, K; T^*, reduced temperature; x, mole fraction of the component in the mixture; Δx_1, separation value of the gaseous mixture; α_T, thermal diffusion factor; $\alpha_{T(\exp)}$ and $\alpha_{T(\mathrm{h.s})}$, experimental value of the thermal diffusion factor and theoretical value calculated for the hard-sphere model respectively; δ, relative error, %; ε (or ε/k), parameter of the potential function of intermolecular interaction, J (or K); σ, effective collision diameter of a molecule, nm; Λ^*, parameter characterizing the role of quantum effects. Subscripts: 1 and 2, components of the mixture; exp, experimental; h.s, hard spheres; *, reduced.

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