Thermophysical Properties of Dilute Hydrogen Sulfide Gas

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ABSTRACT: New, simple, and practical correlations for shear viscosity, self-diffusion coefficient, bulk viscosity, and thermal conductivity of hydrogen sulfide in the limit of zero density are provided, together with a correlation for the second pressure virial coefficient. The correlations are based on the values of thermophysical properties generated from a highly accurate, fully quantum-mechanical, ab initio potential energy surface. The validation of the computed values of thermophysical properties against the rather scarce experimental data demonstrates an excellent agreement with the most accurate data sets. The analysis undertaken indicates that the correlated values provide the most reliable, accurate, and internally consistent representation of thermophysical properties of hydrogen sulfide. The correlations extend over the temperature range (180 to 2000) K. The behavior of each transport property is represented by an independent correlation of the appropriate effective collision cross section as a function of temperature, while the behavior of the second pressure virial coefficient is directly represented as a function of temperature. The uncertainty of the proposed transport property correlations varies from ± 0.4 % for the shear viscosity in the temperature range (300 to 700) K to ± 5.0 % for the bulk viscosity. The uncertainty of the second pressure virial coefficient correlation is estimated to be of the order of ± 1 $cm^3 \cdot mol^{-1}$ at temperatures above 400 K, decreasing to ± 30 $cm^3 \cdot mol^{-1}$ at 180 K.
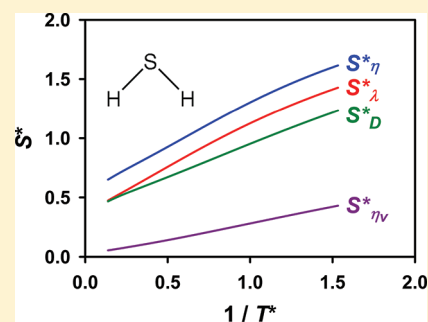
INTRODUCTION

There is considerable demand for accurate and reliable values of thermophysical properties of a wide variety of fluids over extensive ranges of density and temperature as has been demonstrated in a number of studies.[1] The economic case for improving the accuracy with which the properties are determined is strong; however, the wide range of possible fluids and their mixtures and of conditions of interest precludes obtaining the relevant data by experimental means alone. There is, therefore, a clear need for predictive methods and correlations that are accurate, reliable, and internally consistent. In this context the thermophysical properties in the limit of zero density provide the essential basis for the correlation and for the prediction of the properties over a wider range of thermodynamic states.[2] The aim of this paper is to fill the gap that exists in our knowledge about the properties of hydrogen sulfide and to provide correlations for transport properties in the limit of zero density and for the second pressure virial coefficient.

Hydrogen sulfide is an important constituent of sour natural gas, and environmental and safety considerations require its removal. The sweetening of natural gas results in streams of pure H_2S or of mixtures with CO_2 that require either further treatment or carbon capture and storage (CCS) injection. As the world moves toward cleaner energy and natural gas enters the "golden age"[3] as part of an intermediate solution, there has been a marked interest in the thermophysical properties of H_2S. However, accurate and reliable experimental data are rather scarce, as the handling of H_2S requires special safety considerations. The lack of hydrogen sulfide experimental data is not likely to change in the near future, and other means of obtaining accurate and reliable data are required.

We have recently determined an accurate, ab initio intermolecular potential energy hypersurface (PES) for hydrogen sulfide based on high-level quantum-mechanical computations.[4] The partial validation of the PES was performed by calculating the thermophysical properties of H_2S and by comparing them with the available experimental data.[4] For this purpose we calculated the second pressure virial coefficient, shear viscosity, and thermal conductivity of H_2S. The second pressure virial coefficient was evaluated by means of the Takahashi and Imada approach,[5] while the transport properties in the zero-density limit were evaluated by utilizing the kinetic theory of molecular gases[6−8] and the classical-trajectory method.[9] The agreement with the most accurate experimental data and correlations turned out to be excellent.[4] For instance, the calculated second pressure virial coefficients agree to within ± 1 $cm^3 \cdot mol^{-1}$ with the values obtained from the currently recommended equation of state (EOS) for H_2S above 400 K.[10] Furthermore, the experimental viscosity values of Vogel[11] were reproduced to within ± 0.1 % over the whole measured temperature range of (292 to 682) K. Such a good agreement, together with the evidence from other fluids,[12−17] indicates that the current computational methodology can provide values of thermophysical properties that are commensurate with the best available experimental data. Furthermore, as has been argued before,[4,15−17] at low and high temperatures, where the experimental data are by necessity of lower accuracy, the present computational means provide a more accurate estimate of thermophysical properties. Taking into account

the scarcity and quality of currently available H_2S experimental data, it can be argued that, notwithstanding the recent viscosity data by Vogel,[11] the data calculated from the ab initio potential energy surface currently represent the most accurate estimates for the thermophysical properties of hydrogen sulfide in the zero-density limit.

To facilitate the modification of the current H_2S viscosity correlation[18] and the development of future transport property correlations that are functions of both density and temperature, we provide in this paper reliable and accurate transport property correlations, valid in the zero-density limit, for the shear viscosity, self-diffusion coefficient, bulk viscosity, and thermal conductivity of H_2S in the temperature range from (180 to 2000) K. We also provide a correlation for the second pressure virial coefficient in the same temperature range. Although H_2S is not stable at the highest temperatures considered and does dissociate, any high-temperature application will require the knowledge of thermophysical properties of all species present in equilibrium to characterize the mixture. All of the correlations developed in this work are based on the values of thermophysical properties computed previously[4] using the ab initio PES of H_2S.

■ METHODOLOGY

The shear viscosity of a polyatomic gas in the limit of zero density can be expressed as[8]

$$\eta = \frac{k_B T}{\langle v \rangle_0} \frac{f_\eta}{S(2000)} \tag{1}$$

where $\langle v \rangle_0 = 4(k_B T/\pi m)^{1/2}$ is the average relative thermal speed, m is the molecular mass, T is the temperature, k_B is Boltzmann's constant, f_η is the higher-order correction factor, and $S(2000)$ is a generalized cross section. The generalized cross sections include all of the information about the dynamics of the binary collisions that govern transport properties and in turn are governed by the intermolecular potential energy surface. The notation and conventions employed in labeling the generalized cross sections are fully described elsewhere.[8] In line with our previous work[19,20] and to introduce a more practical correlation equation for hydrogen sulfide, we have rewritten eq 1 as

$$\eta/\mu\text{Pa·s} = 0.87721 \frac{\sqrt{T/\text{K}}}{S^*_\eta(T^*)} \tag{2}$$

by combining the generalized cross section $S(2000)$ and the higher-order correction factor f_η into a single reduced effective cross section $S^*_\eta(T^*)$, which is a function of a reduced temperature T^* ($T^* = k_B T/\varepsilon$) and has been normalized with respect to $\pi\sigma^2$. The choice of the length scaling parameter σ and the temperature scaling parameter ε/k_B will be discussed in more detail in the section on the correlations. However, it is worth pointing out that the constant in eq 2 already contains the chosen numerical value of the length scaling parameter σ.

In the first-order approximation of kinetic theory the product of the mass density and the self-diffusion coefficient, ρD, and the bulk viscosity η_V of a polyatomic gas are also inversely proportional to a single generalized cross section[8] that can be easily replaced in each case, for correlative purposes, by a reduced

effective cross section. For hydrogen sulfide the resulting expressions are as follows,

$$\rho D/\mu\text{Pa·s} = \frac{k_B T}{\langle v \rangle_0} \frac{f_D}{S'(1000)} = 0.87721 \frac{\sqrt{T/\text{K}}}{S^*_D(T^*)} \tag{3}$$

$$\eta_V/\mu\text{Pa·s} = \frac{2}{3}\left(\frac{r^2}{0.6 + r^2}\right)^2 \frac{k_B T}{\langle v \rangle_0} \frac{f_{\eta V}}{S(0010)}$$

$$= 0.58481\left(\frac{r^2}{0.6 + r^2}\right)^2 \frac{\sqrt{T/\text{K}}}{S^*_{\eta V}(T^*)} \tag{4}$$

The quantity r^2 is defined by $r^2 = 2c_{int}/5k_B$, where c_{int} is the contribution of both the rotational, c_{rot}, and the vibrational, c_{vib}, degrees of freedom to the isochoric heat capacity c_V. For brevity we will refer to eq 3 as the correlation for the self-diffusion coefficient in the rest of the paper.

For thermal conductivity the traditional kinetic theory approach results in an expression involving three generalized cross sections.[8] This is not surprising since the thermal conductivity is strongly influenced by the presence of internal degrees of freedom. However, it is possible to derive an equivalent kinetic theory expression for thermal conductivity by making use of the Thijsse et al. approach,[21,22] where one considers expansion in terms of total energy, rather than separating translational from internal energy as is done traditionally. In this case, the thermal conductivity of a polyatomic gas can be shown to be inversely proportional to a single generalized cross section,[8,20−22]

$$\lambda = \frac{5k_B^2 T}{2m\langle v \rangle_0} \frac{(1 + r^2)}{S(10E)} f_\lambda \tag{5}$$

One can take advantage of the Thijsse formulation and the observation that the higher−order correction factor is a weakly temperature-dependent, near unity quantity, to express the thermal conductivity in terms of a single reduced effective cross section,

$$\lambda/\text{mW·m}^{-1}\cdot\text{K}^{-1} = 0.53502 \frac{(1 + r^2)\sqrt{T/\text{K}}}{S^*_\lambda(T^*)} \tag{6}$$

Data Generation. The transport properties of hydrogen sulfide in the limit of zero density and the second pressure virial coefficient were calculated directly from the ab initio intermolecular potential as described in ref 4. A six-dimensional PES for two interacting rigid hydrogen sulfide molecules was determined from high-level quantum-mechanical ab initio computations. A total of 4016 points for 405 different angular orientations of two molecules were calculated utilizing the counterpoise-corrected supermolecular approach at the CCSD(T) level of theory and extrapolating the calculated interaction energies to the complete basis set limit. An analytical site−site potential function with 11 sites per hydrogen sulfide molecule was fitted to the interaction energies. The PES was validated[4] by computing the second pressure virial coefficient, shear viscosity, and thermal conductivity and comparing with the available experimental data.

The second pressure virial coefficient was determined classically including quantum corrections. The quantum effects were incorporated by means of the Takahashi and Imada approach,[5] which involved replacing the full potential by a

temperature-dependent effective potential. For transport properties all of the generalized cross sections have been evaluated by means of the classical-trajectory approach.[9] The accuracy and usefulness of this approach has been demonstrated in a number of studies by evaluating transport and relaxation properties of N_2,[23] CO,[24,25] CO_2,[12−14] CH_4,[15,16] and H_2O.[17] All of the calculations were performed on the assumption that both hydrogen sulfide molecules behave as rigid asymmetric tops. This assumption was dictated by the nature of the available intermolecular potential, which was developed using the zero-point vibrationally averaged configuration. To include the effects of vibrationally active modes we employed the approximation described in our previous work[13,26] to correct, where necessary, the generalized cross sections. Overall, up to 160 000 classical trajectories were evaluated at each energy of interest, and each generalized cross section was obtained by integrating over total energy by using 25 energy pivot points within the Chebyshev quadrature.

In general, the agreement with the primary second pressure virial coefficient, viscosity, and thermal conductivity experimental data is within the experimental error for temperatures higher than 300 K.[4] However, the scatter of the primary experimental data of different workers for the second pressure virial coefficient and thermal conductivity indicates that they are most likely less accurate than claimed. For temperatures lower than room temperature the lack of reliable data indicates that the values calculated in this work are currently the most accurate estimates for the thermophysical properties of hydrogen sulfide.[4] The same is true for temperatures higher than (500 to 700) K.

The generalized cross sections evaluated in the previous work[4] were used to generate the shear viscosity, self-diffusion, bulk viscosity, and thermal conductivity values in the temperature range (180 to 2000) K by means of eqs 1, 3, 4, and 5, respectively. For shear and bulk viscosity the higher-order corrections up to the third order were included, while thermal conductivity was evaluated up to the second order, as the expressions for higher orders are not yet available. The lack of a higher-order correction resulted in the use of the first-order expression for the self-diffusion coefficient. As previously discussed,[4] the higher-order correction factors used for shear viscosity, bulk viscosity, and thermal conductivity are close to unity, indicating convergence. Based on previous calculations for other fluids,[12−17,23−25] convergence criteria, and comparison with the available primary experimental data on hydrogen sulfide, we have estimated the uncertainty of the calculated shear viscosity, self-diffusion coefficient, bulk viscosity, and thermal conductivity to be of the order of $\pm$ (0.4 to 1.0) %, $\pm$ (1 to 2) %, $\pm$ 5 %, and $\pm$ (1 to 3) %, respectively. The uncertainty of the second pressure virial coefficient is estimated to be of the order of $\pm$ 1 $cm^3 \cdot mol^{-1}$ at temperatures above 400 K, $\pm$ 5 $cm^3 \cdot mol^{-1}$ at 300 K, and $\pm$ 30 $cm^3 \cdot mol^{-1}$ at 180 K.

Correlation. Separate correlations as a function of temperature have been developed for each thermophysical property of interest (shear viscosity, self-diffusion coefficient, bulk viscosity, thermal conductivity, and second pressure virial coefficient). In each case the thermophyscial property values computed from the ab initio PES were used as input data. The correlations were developed in terms of reduced temperature as this leads to more "practical" coefficients that are of similar magnitude. In developing the transport property correlations for hydrogen sulfide, the values of the effective cross sections as a function of temperature have been calculated by means of eqs 2 to 4 and 6

for each transport property of interest. Reduced effective cross sections for the shear viscosity, self-diffusion coefficient, bulk viscosity, and thermal conductivity were then fitted to the functional form

$$S_j^*(T^*) = \sum_{n=0}^{5} \frac{a_n}{T^{*n}} \qquad j = \eta, D, \eta_V, \lambda \tag{7}$$

as a function of reduced temperature T^*. The goodness of fit does not depend on the choice of the temperature scaling parameter ε/k_B. To keep to the spirit of the original calculation[4] a value of 276 K was chosen. This corresponds to the well depth of the spherically averaged ab initio potential energy surface that was used to compute the values of the thermophyscial properties of hydrogen sulfide.[4] Conversely, the length scaling parameter σ, which is already incorporated in the numerical constants in eqs 2 to 4 and 6, was chosen to be 0.377 nm, which corresponds to the separation at which the spherically averaged potential is equal to zero.

To generate the reduced effective cross sections for the bulk viscosity and thermal conductivity, $S^*_{\eta V}$ and S^*_{λ}, it is necessary to have a subsidiary representation of the isochoric heat capacity. For this purpose we have made use of the ideal-gas heat capacity representation used by Lemmon and Span[10] when they developed the short reduced Helmholtz energy equation of state (EOS) for hydrogen sulfide. As knowledge of the isochoric heat capacity is essential to be able to use the bulk viscosity and thermal conductivity correlations developed in this work, we here reproduce the relevant representation,

$$\frac{c_V}{k_B} = \frac{c_{int}}{k_B} + \frac{3}{2} = 3.0 + b_1 T^{1.5} + \sum_{i=2}^{3} b_i \frac{X_i^2 \exp(X_i)}{[\exp(X_i) - 1]^2} \tag{8}$$

$$X_i = \frac{d_i}{T} \tag{9}$$

where the temperature is in K and the coefficients b_i and d_i are given in Table 1. Unlike the transport properties, the second

Table 1. Coefficients in the Ideal-Gas Isochoric Heat Capacity Expression

b_1	$1.4327 \cdot 10^{-6}$
b_2	1.1364
b_3	1.9721
d_2	1823.0
d_3	3965.0

pressure virial coefficient of hydrogen sulfide was directly fitted to the functional form

$$B / cm^3 \cdot mol^{-1} = \sum_{n=0}^{5} \frac{a_n}{T^{*n}} \tag{10}$$

using the same temperature scaling parameter as for the effective cross sections.

■ RESULTS

The effective cross sections and the second pressure virial coefficient were fitted to the functional forms given by eqs 7

and 10, respectively. The optimal coefficients for each correlation are listed in Table 2. In each case the goodness of fit, as

Table 2. Coefficients for the Representation of the Effective Cross Sections and of the Second Pressure Virial Coefficient (ε/k_B = 276 K)

	S^*_η	S^*_D	$S^*_{\eta V}$	S^*_λ	B
a_0	0.53242	0.36776	0.02691	0.37199	39.828
a_1	0.93715	0.82138	0.18521	0.71765	−83.002
a_2	−0.69339	−0.86347	0.10169	0.21117	−206.830
a_3	1.16432	1.21172	−0.03327	−0.22191	101.510
a_4	−0.84306	−0.75362		0.04669	−64.443
a_5	0.20534	0.16942			

measured by R^2, was better than 0.9999. The fit reproduces the shear viscosity and self-diffusion coefficient values to within ± 0.1 %, while for bulk viscosity and thermal conductivity the deviations are only slightly larger, amounting to ± 0.2 %. The values of the second pressure virial coefficient are reproduced to within ± 0.2 cm^3·mol^{-1}. Figure 1 illustrates the behavior of
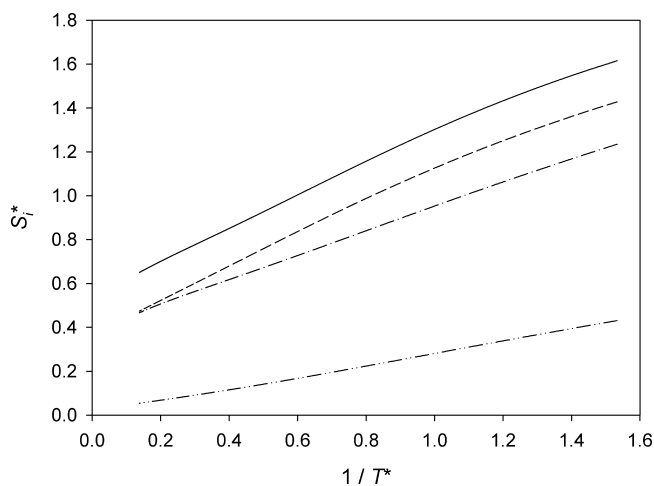

Figure 1. Reduced effective cross sections as a function of inverse reduced temperature, $1/T^*$, for: —, shear viscosity; ·–·, self-diffusion coefficient; ---, thermal conductivity; ·····, bulk viscosity.

the four reduced effective cross sections as a function of inverse reduced temperature. It is interesting to observe that for hydrogen sulfide all four effective cross sections manifest a nearly linear dependence. This has been previously noted for other fluids, but only for the thermal conductivity effective cross section.[27] In fact the linear form only slightly reduces the goodness of fit to $R^2 = 0.997$ for the four transport properties studied.

Table 3 lists the recommended values of thermophysical properties of hydrogen sulfide at selected temperatures within the temperature range (180 to 2000) K. The values listed are based on the correlations developed in this work and can be used, if required, to allow the checking of computer coding of the present correlations.

As has been previously noted,[4,18] the experimental thermophysical data for hydrogen sulfide are rather scarce. The comparison of the computed values with the experimental data for second pressure virial coefficient, shear viscosity, thermal conductivity, and bulk viscosity has been already performed; there were no data on the self-diffusion coefficient. As the developed correlations reproduce the computed values very

Table 3. Recommended Values for the Thermophysical Properties of H$_2$S Based on the Correlations Developed in This Work

T		B	η	ρD	η_V	λ
K	r^2	cm^3·mol^{-1}	µPa·s	µPa·s	µPa·s	mW·m^{-1}·K^{-1}
180	0.6032	−564.0	7.279	9.525	4.586	8.065
200	0.6058	−435.5	8.080	10.73	5.370	8.996
220	0.6097	−349.0	8.878	11.92	6.232	9.963
240	0.6153	−287.5	9.690	13.12	7.173	10.97
260	0.6226	−241.8	10.52	14.32	8.198	12.01
280	0.6315	−206.6	11.35	15.53	9.310	13.09
298.15	0.6409	−181.0	12.12	16.62	10.40	14.09
300	0.6419	−178.7	12.20	16.73	10.51	14.20
320	0.6536	−156.2	13.04	17.93	11.80	15.34
340	0.6664	−137.5	13.88	19.12	13.19	16.52
360	0.6801	−121.9	14.71	20.28	14.66	17.72
380	0.6945	−108.6	15.54	21.44	16.22	18.95
400	0.7096	−97.18	16.36	22.58	17.87	20.20
420	0.7251	−87.24	17.17	23.69	19.60	21.48
440	0.7410	−78.54	17.97	24.80	21.42	22.78
460	0.7572	−70.86	18.75	25.88	23.32	24.10
480	0.7738	−64.03	19.53	26.95	25.29	25.44
500	0.7905	−57.92	20.29	28.00	27.35	26.79
550	0.8333	−45.17	22.16	30.56	32.82	30.26
600	0.8768	−35.12	23.97	33.03	38.73	33.82
650	0.9208	−27.03	25.71	35.42	45.05	37.47
700	0.9649	−20.39	27.40	37.73	51.73	41.19
750	1.0085	−14.85	29.04	39.99	58.74	44.97
800	1.0514	−10.17	30.63	42.18	66.03	48.79
850	1.0931	−6.171	32.18	44.31	73.55	52.64
900	1.1335	−2.720	33.68	46.40	81.26	56.51
950	1.1724	0.286	35.15	48.44	89.13	60.39
1000	1.2097	2.924	36.59	50.43	97.13	64.26
1100	1.2789	7.329	39.36	54.30	113.38	71.95
1200	1.3411	10.85	42.02	58.02	129.83	79.52
1300	1.3967	13.72	44.57	61.61	146.35	86.93
1400	1.4461	16.11	47.03	65.08	162.84	94.16
1500	1.4902	18.11	49.40	68.44	179.3	101.2
1600	1.5294	19.82	51.70	71.71	195.5	108.1
1700	1.5645	21.29	53.93	74.88	211.7	114.7
1800	1.5959	22.57	56.09	77.96	227.6	121.2
1900	1.6243	23.69	58.19	80.97	243.4	127.5
2000	1.6499	24.68	60.23	83.90	258.9	133.6

well, there is no advantage in reproducing the comparison, and the reader is referred to ref 4 for the full analysis. However, for illustrative purposes and to indicate the quality of the experimental data available, we briefly examine the agreement with viscosity and thermal conductivity values. Figure 2 illustrates the deviations of the selected primary experimental viscosity and thermal conductivity data from the correlations developed in this work.

The agreement with the recent viscosity data of Vogel,[11] measured with an all-quartz oscillating-disk viscometer, is excellent. The experimental values are reproduced within ± 0.2 % over the whole measured temperature range of (292 to 682) K. As the agreement is better than the claimed experimental uncertainty of ± 0.2 %, the match is most likely fortuitous, but it allows us to ascribe an uncertainty of ± 0.4 % to the correlated values in this temperature range. The identical temperature dependence of the experimental and computed viscosity values is a further strong validation of the proposed correlation.
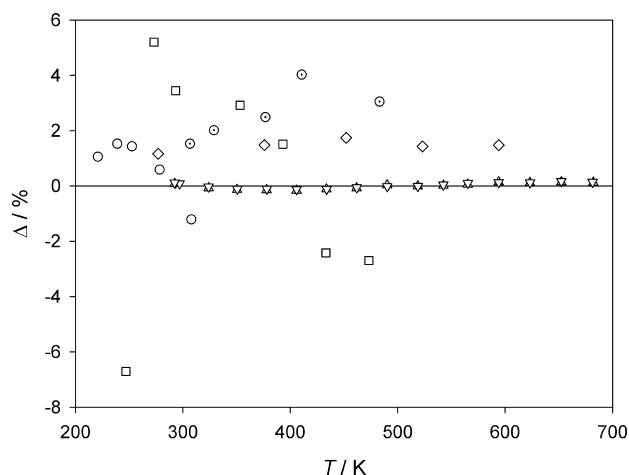
Figure 2. Deviations, $\Delta = (X_{exp} - X_{cor})/X_{cor}$ with $X = \eta$ or λ, of the selected primary experimental viscosity and thermal conductivity data from the present correlations. Experimental viscosity data: △, Vogel, first series of measurements;[11] ▽, Vogel, second series of measurements;[11] ⊙, Pal and Barua;[28] ○, Bhattacharyya et al.[29] Experimental thermal conductivity data: ◇, Correia et al.;[30] □, Barua et al.[31]

The viscosity data of Pal and Barua[28] and Bhattacharyya et al.,[29] that were also measured with an oscillating-disk viscometer, are reproduced somewhat outside the joint claimed uncertainty. However, not only do these data display a different temperature trend to the proposed correlation, but also a different trend between two data sets is observed, which is surprising as both viscosity data sets come from the same laboratory. The available experimental thermal conductivity data of hydrogen sulfide are in general of lower accuracy than the commensurate viscosity data. The agreement with the experimental thermal conductivity data of Correia et al.[30] is very good. Not only does the proposed correlation reproduce the temperature trend of the data of Correia et al.,[30] but the deviations are of the order of +(1 to 2) % only. The agreement with the thermal conductivity data of Barua et al.[31] above room temperature is better than 5 %, but the deviations increase with decreasing temperature. At the lowest temperature of 195 K, not shown in the plot, the thermal conductivity as measured by Barua et al.[31] is nearly 40 % smaller than the recommended correlated value proposed in this work.

Although the main aim of the paper is to provide the practical correlations of thermophysical properties of hydrogen sulfide, it is useful to also examine certain ratios which play an important part in engineering applications. In particular we focus on the Prandtl number,

$$Pr = \frac{c_p \eta}{m\lambda} \tag{11}$$

and $A*$ ratio,

$$A* = \frac{5}{6} \frac{S(2000)}{S'(1000)} \cong \frac{5}{6} \frac{\rho D}{\eta} \tag{12}$$

The usefulness of knowing the Prandtl number is self-evident in different branches of engineering, while $A*$ is primarily used by kinetic theory practitioners to infer the value of diffusion coefficients from the knowledge of viscosity. Figure 3 illustrates the behavior of the Prandtl number and $A*$ as a function of temperature. As expected the Prandtl number decreases with temperature, the rate of change decreasing with increasing
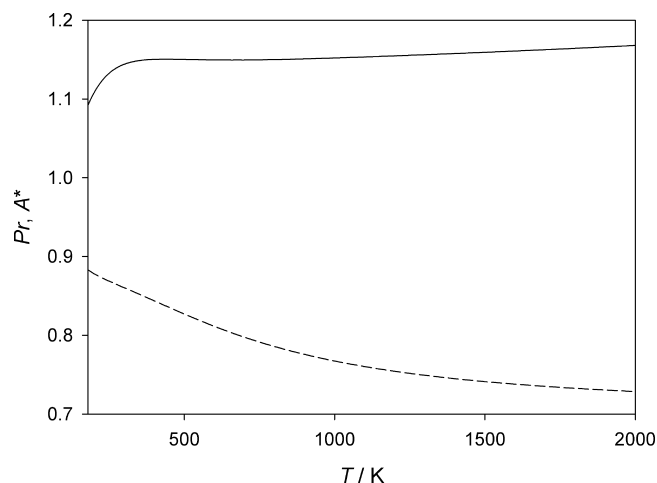

Figure 3. Prandtl number, Pr, and the ratio $A*$ as a function of temperature, T: —, $A*$; ---, Pr.

temperature. However, only at the highest temperatures it is approaching a nearly constant value. The rate of change of the Prandtl number for hydrogen sulfide at high temperatures is marginally higher than that observed for other gases studied so far.[20,32] The value of $A*$ initially increases with temperature from 1.092 at 180 K to 1.144 at about 300 K. The rate of change slows down with increasing temperature, and $A*$ reaches a value of 1.168 at 2000 K. The magnitude and the temperature variation of $A*$ for hydrogen sulfide are in line with what has been observed for other gases.[12,15,33]

■ CONCLUSIONS

Correlations for the shear viscosity, self-diffusion coefficient, bulk viscosity, and thermal conductivity in the zero-density limit and a correlation for the second pressure virial coefficient of H_2S have been presented. They are valid in the temperature range from (180 to 2000) K. The correlations have been validated against the available experimental data. For the shear viscosity correlation we estimate the uncertainty to be of the order of ± 0.4 % in the temperature range (300 to 700) K, increasing to ± 1 % at the lowest (180 K) and highest (2000 K) temperatures considered. For the thermal conductivity and self-diffusion correlations we estimate the uncertainty to be of the order of ± 1 % in the temperature range (300 to 500) K, increasing to ± 3 % and ± 2 %, respectively, at both (180 and 2000) K. For the bulk viscosity correlation the estimated uncertainty is of the order of ± 5 % over the entire temperature range. The uncertainty of the second pressure virial coefficient correlation is estimated to be of the order of ± 1 $cm^3 \cdot mol^{-1}$ at temperatures above 400 K, ± 5 $cm^3 \cdot mol^{-1}$ at 300 K, and ± 30 $cm^3 \cdot mol^{-1}$ at 180 K.

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Notes
The authors declare no competing financial interest.

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