



Fluid Dynamics and Transport Phenomena

Transport properties of dilute ammonia-noble gas mixtures from new intermolecular potential energy functions



Farshid Zargari^{1,2,*}, Delara Mohammad-Aghaie¹, Maryam Lotfi¹, Masoume Ghorbanipour³,
 Mohammad Mehdi Alavianmehr¹, Omolbanin Shahraki^{4,**}

¹ Department of Chemistry, Shiraz University of Technology, Shiraz, Iran

² Medicinal and Natural Products Chemistry Research Center, Shiraz University of Medical Sciences, Shiraz, Iran

³ Department of Physical Chemistry, University of Tabriz, Tabriz, Iran

⁴ Zahedan University of Medical Sciences, Zahedan, Iran

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ABSTRACT

Previously we have determined the dilute mixture transport properties of slightly polar fluorocarbons using the inverted intermolecular potential energies (*Ind. Eng. Chem. Res.* 45 (2006) 9211–9223). In the present paper, the corresponding states correlations for reduced viscosity collision integrals were employed to obtain effective unlike interaction potential models for dilute binary mixtures of highly polar molecule ammonia with noble gases. The inverted potentials were fitted to the Morse–Spline–van der Waals (MSV), model potential. The method of least-squares fitting was then applied to identify best consistence force parameters for each ammonia-noble gas mixture, taking advantage of experimental viscosities, diffusion coefficients and thermal conductivities. The proposed potential models were compared with those obtained from other sources, in order to assess the extent of their validity.

The potentials were later employed to calculate transport properties of the studied mixtures. Then, results were compared with those reported in the literature, which led to the acceptable agreement.

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1. Introduction

Transport properties of matters in different thermo-physical states are important features, required in different engineering design problems, such as simulations of viscous flows through channels and combustion chambers of various technical devices, such as flows in rocket engines, chemical reactors and shock tubes. There is a growing demand for more accurate transport properties, in response to the worldwide need for higher efficiency, process integration and energy awareness in the industry [1].

Three principal transport properties of industrial interest are the viscosity, η , the diffusivity, D , and the thermal conductivity, λ , which characterize the dynamics of fluids, involving the momentum transport

related to the pressure difference, the mass transport related to the concentration difference, and the heat transport related to the temperature difference, respectively [2].

Prediction and determination of equilibrium and non-equilibrium properties of a matter, and interpretation of most phenomena involving atoms and molecules, depend on knowledge of intermolecular forces. Once the interaction potential is known, evaluation of thermophysical properties of fluids will be straightforward. This reduces the need for experimentation considerably. Various methods of determining intermolecular potentials have been used, either theoretical, based on experimental information, or combining both approaches [3,4].

Among these methods, inversion of dilute gas properties has been of particular importance. The semi-empirical method of inversion, developed by Maitland and co-workers, determines unique potential energy function from thermophysical properties, without explicit assumption of a mathematical model [5–8].

The Chapman–Enskog solution of the Boltzmann equation of gas kinetic theory, provides expressions to relate the transport coefficients of gases to interaction potential energy, through collision integrals, $\Omega^{(Ls)}(T^*)$ [9,10]. For noble gases, with spherically symmetric potentials, inversion of experimental second virial coefficients, $B_2(T)$, is directly related to the pair potential $U(r)$. Combining this result with other

* Correspondence to: F. Zargari, Department of Chemistry, Shiraz University of Technology, Shiraz, Iran, Medicinal and Natural Products Chemistry Research Center, Shiraz University of Medical Sciences, Shiraz, Iran.

** Correspondence to: O. Shahraki, Zahedan University of Medical Sciences, P.O. Box: 98167-43463, Zahedan, Iran.

E-mail addresses: f.zargari@sutech.ac.ir (F. Zargari), o.shahraki@gmail.com (O. Shahraki).

experimental sources such as viscosity and diffusion coefficients, and quantum mechanical calculations, provides an accurate knowledge of $U(r)$ for these simple substances [11–14].

However, the Chapman–Enskog theory for transport properties of polyatomic gases with non-spherical interactions is fundamentally different from that of monatomic molecules, due to the possibility of inelastic collisions, which makes change in the rotational and vibrational energies [15].

Another approximation has been proposed by Mason and Monchick [16] who assumed that the molecules have a fixed relative orientation, during a collision. The physical basis for this assumption is that most of the interaction in a collision occurs in the vicinity of the distance of the closest approach, during which the relative orientation does not change much, so that one relative orientation dominates in each collision. Therefore the Chapman–Enskog theory of polyatomic molecules retains its original form, but the collision integrals must be averaged over all possible orientations, occurring in collisions.

In the important case of dilute polar gases, Mason and Monchick [17] applied this approximation, considering the facts that these molecules have an angle-dependent potential and the possible rotational-energy transfers on every collision must be taken into account. In order to calculate the collision integrals of some polar gases, they employed the Stockmayer potential as interaction potential and related it to the collision integrals $\Omega^{(ls)}$, using the following equations:

$$\theta = \pi - 2b \int_{r_m}^{\infty} \frac{r^{-2} dr}{\left\{ 1 - \left(\frac{b^2}{r^2} \right) - \left[\frac{2U(r)}{mw^2} \right] \right\}^{1/2}} \quad (1)$$

$$Q^{(l)}(E) = 2\pi \left[1 - \frac{1 + (-1)^l}{2(1+l)} \right]^{-1} \int_0^{\infty} (1 - \cos^l \theta) b db \quad (2)$$

$$\Omega^{(ls)}(T) = \left[(s+1)!(kT)^{s+2} \right]^{-1} \int_0^{\infty} Q^{(l)}(E) \exp(-E/kT) E^{s+1} dE \quad (3)$$

where θ is the classical deflection angle for $U(r)$ interaction potential, b the impact parameter, r_m the distance of the closest approach in a collision, w the relative velocity of colliding partners and $Q^{(l)}(E)$ the collision cross section, corresponding to the l moment. They used the experimental viscosities and dipole moments of a number of polar gases to determine the potential parameters necessary to calculate other properties of these gases. Over-all agreement between the experiment and their model, makes the Stockmayer potential for polar gases, comparable to the Lennard-Jones (12-6) model for non-polar gases. It has been shown that effective total interaction energy between a polar molecule and non-polar molecule, has the same form as that of two non-polar molecules which are spherically symmetric [15], so in mixtures of polar and non-polar gases, the polar–nonpolar interactions have essentially a non-polar nature.

Ammonia has a widespread use in many industrial sectors and it is one of the chemicals with the largest production volume in the world. Its main uses are in fertilizers, industrial refrigeration systems, explosives, as well as in plastic and pharmaceutical product manufacturing [18]. Furthermore ammonia is often the subject of experimental and theoretical studies, because of its ability to form hydrogen bonds and its simple symmetric molecular structure.

Reliable data for mixtures with ammonia are of special interest in the field of refrigeration. Furthermore, the correct description of the intermolecular interactions in such systems is a challenging task from a theoretical point of view due to the intramolecular inversion behavior of the ammonia molecule.

Recently, Papari *et al.* have applied the inversion method based on the law of corresponding states, to infer the intermolecular potential energies of non-polar polyatomic molecules [19,20] and their mixtures

with noble gases [21–28], and predict their collision integrals, required to calculate transport properties. Their method was also applied to pure refrigerants [23,29] and refrigerant mixtures [30,31] as slightly polar molecules to obtain the effective and isotropic pair potential energies of this class of fluids.

The novelty of the present work is that the Papari *et al.*'s scheme is extended to a highly polar molecule ammonia and its mixtures with noble gases at low density. The numerical values of the inverted potential energies of ammonia–noble gas binary mixtures are then fitted to an analytical MSV model potential. The experimental viscosity, diffusion coefficient and thermal conductivity data, together with an iterative least squares method are used to obtain the best force parameters, ε_{12} and σ_{12} for each binary system.

Generated intermolecular potential energies are evaluated by comparison of our model potential with those obtained from other sources, both experimental and theoretical. In addition, the dilute gas transport coefficients (except thermal conductivity) of the studied mixtures, encompassing a wide range of temperatures, are predicted using the Chapman–Enskog version of the kinetic theory [9,10] and compared with the literature data. Computation of thermal conductivities for the studied mixtures through Schreiber *et al.* method [32] and comparing the results with literature data, provide a further test for the inverted potential energy functions.

2. Transport Properties of Gaseous Mixtures

Expressions for the viscosity η , thermal conductivity λ , and diffusion coefficient D of pure substances are given in Ref. [19]. The mixture transport properties of dilute gases are obtained by the following relationships:

2.1. Viscosity

The viscosity of an arbitrary multicomponent mixture of dilute gases can be evaluated from the following equations:

$$\eta_{\text{mix}} = - \begin{vmatrix} H_{11} & H_{12} & \dots & x_1 \\ H_{21} & H_{22} & \dots & x_2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1 & x_2 & \dots & 0 \end{vmatrix} / \begin{vmatrix} H_{11} & \dots & H_{1\nu} \\ H_{21} & \dots & H_{2\nu} \\ \vdots & \ddots & \vdots \\ H_{\nu 1} & \dots & H_{\nu\nu} \end{vmatrix} \quad (4)$$

where

$$H_{ij}(i \neq j) = - \frac{2x_i x_j}{\eta_{ij}} \frac{m_i m_j}{(m_i + m_j)^2} \left(\frac{5}{3A_{ij}^*} - 1 \right) \quad (5)$$

$$H_{ii} = - \frac{x_i^2}{\eta_i} + \sum_{k \neq i}^{\nu} \frac{2x_i x_k}{\eta_{ik}} \frac{m_i m_k}{(m_i + m_k)^2} \left(\frac{5}{3A_{ik}^*} - \frac{m_k}{m_i} \right) \quad (6)$$

$$\eta_{ij}^0 = \frac{5}{16} \left[\left(\frac{2m_i m_j}{m_i + m_j} \right) \frac{k_B T}{\pi} \right]^{1/2} \frac{1}{\sigma_{ij}^2 \Omega_{ij}^{*(2,2)}(T_{ij}^*)} \quad (7)$$

where A_{ij}^* is the ratio of the collision integrals, defined by Eq. (11) in Ref. [19], x_i the mole fraction of component i , and m_i the molecular mass of the component i . $k_B T$ is the molecular thermal energy, σ the distance at which the potential energy is zero, and η_{ij}^* the interaction viscosity. Subscripts i and j denote the heavier and lighter components of the i – j pair, respectively.

2.2. Diffusion

Diffusion in multicomponent mixtures is entirely described in terms of binary diffusion coefficients, D_{ij} [15]:

$$D_{ij} = \frac{3}{8} \left[\left(\frac{m_i + m_j}{2m_i m_j} \right) \frac{k_B T}{\pi} \right]^{1/2} \frac{k_B T}{P} \frac{1 + \Delta_{ij}}{\sigma_{ij}^2 \Omega_{ij}^{*(1,1)}(T_{ij}^*)} \quad (8)$$

where P is the pressure and Δ_{ij} is a higher order correction term of the binary diffusion coefficient, which can be defined as:

$$\Delta_{ij} \approx 1.3 \left(6C_{ij}^* - 5 \right)^2 \frac{a_{ij} x_{ij}}{1 + b_{ij} x_{ij}} \quad (9)$$

where

$$a_{ij} = \frac{\sqrt{2}}{8 \left[1 + 1.8 \left(\frac{m_j}{m_i} \right) \right]^2} \frac{\Omega_{ij}^{*(1,1)}(T_{ij}^*)}{\Omega_{ij}^{*(2,2)}(T_{ij}^*)}, \quad (10)$$

$$b_{ij} = 10a_{ij} \left[1 + 1.8 \left(\frac{m_j}{m_i} \right) + 3(m_j/m_i)^2 \right] - 1, \quad (11)$$

$$x_{ij} = \frac{x_i}{x_i + x_j}. \quad (12)$$

2.3. Thermal diffusion factor

A tendency of a convection-free mixture to separate under a thermal (or temperature) gradient is known as the thermal diffusion process or Soret effect. In this process, the transport of matter takes place (*i.e.* a concentration gradient of the mixture constituents develops) with the temperature gradient. The thermal diffusion coefficient is the measure of this effect, and its sign determines the direction of the thermal diffusion [33].

The Chapman–Enskog expression for the thermal-diffusion factor, α_T , of a binary mixture is:

$$\alpha_T = \left(6C_{ij}^* - 5 \right) \left(\frac{x_1 S_1 - x_2 S_2}{x_1^2 Q_1 + x_2^2 Q_2 + x_1 x_2 Q_{12}} \right) (1 + k_T), \quad (13)$$

where k_T is a higher order correction term for the thermal-diffusion factor. This term is usually negligible compared with experimental uncertainties in α_T . The corresponding formulas of quantities S_1 , Q_1 , and Q_{12} in Eq. (13) can be found in Ref. [31], Eqs. (23)–(25).

The expressions for S_2 and Q_2 are obtained from those of S_1 and Q_1 by interchanging subscripts 1 and 2. The sign convention for α_T requires that subscript 1 denotes the heavier component.

2.4. Thermal conductivity

The dependence of thermal conductivity of polyatomic molecular gases, on the internal degrees of freedom and the inherent details of inelastic collisions, prevents the application of Chapman Enskog theory for the calculation of this property. In this respect, the thermal conductivity of a multicomponent polyatomic gas mixture at zero density can be expressed in the form analogous to that for a mixture, consisting of monatomic species [32]:

$$\lambda = - \left| \begin{array}{ccc|ccc} L_{11} & \cdots & L_{1n} & x_1 & & \\ \vdots & & \vdots & \vdots & & \\ L_{n1} & \cdots & L_{nn} & x_n & & \\ \hline x_1 & \cdots & x_n & 0 & & \end{array} \right| / \left| \begin{array}{ccc} L_{11} & \cdots & L_{1n} \\ \vdots & & \vdots \\ L_{n1} & \cdots & L_{nn} \end{array} \right| \quad (14)$$

where, x_i is the mole fraction of species i and the symbol λ , indicates the full formal first-order kinetic theory result, obtained by means of expansion in Thijssse basis vectors [34]. Studies have shown that accurate and

relatively simple expressions for pure polyatomic gases [35], atom–diatom mixtures [36], and atom–molecule mixtures [37] can be obtained by means of the Thijssse approximation, which identifies the total energy, as the dominant factor in determining thermal conductivity.

Employing the Thijssse *et al.* [34] and spherical approximations to the full results, gives rise to the following determinant elements, L_{ij} [32]:

$$L_{qq} = \frac{x_q^2}{\lambda_q} + \sum_{\mu \neq q} \frac{25x_q x_\mu}{8A_{q\mu}^* \lambda_{q\mu}} \left(\frac{R}{C_{pq}^0} \right)^2 \left[\frac{25}{4} y_\mu^4 + \frac{15}{2} y_q^4 - 3y_\mu^4 B_{q\mu}^* + 4y_q^2 y_\mu^2 A_{q\mu}^* + \left(\frac{C_{pq}^0}{R} - 2.5 \right) \right] \quad (15)$$

$$L_{qq'} = - \frac{25x_q x_{q'} y_q^2 y_{q'}^2}{8A_{qq'}^* \lambda_{qq'}} \left(\frac{R}{C_{pq}^0} \right) \left(\frac{R}{C_{pq'}^0} \right) \left[\frac{55}{4} - 3B_{qq'}^* - 4A_{qq'}^* \right] \quad (16)$$

where λ_q is the thermal conductivity of pure molecular species q , $\lambda_{qq'}$, is the interaction thermal conductivity, C_{pq}^0 , is the ideal-gas isobaric heat capacity of q , R is the gas constant, and the quantities A^* and B^* are ratios of effective cross-sections, given by Eqs. (11) and (14) in Ref. [19]. In addition y_q is the mass ratio of species q , given by:

$$y_q^2 = \frac{M_q}{(M_q + M_{q'})} \quad (17)$$

Here, M_q is the relative molecular mass of species q . The interaction thermal conductivity can be related to the more readily available interaction viscosity, $\eta_{qq'}$, through the equation below:

$$\lambda_{qq'} = \frac{15}{8} R \frac{(M_q + M_{q'})}{M_q M_{q'}} \eta_{qq'} \quad (18)$$

Inspection of above equations reveals that in order to obtain the thermal conductivity of a multi-component polyatomic gas mixture, knowledge of the thermal conductivity and the isobaric heat capacity of each of the pure species is required. This information is readily available for a large number of fluids as a function of temperature, either in terms of correlations or directly from experimental information. Three binary interaction parameters, namely, $\eta_{qq'}$, A^* and B^* , as functions of temperature, are the remaining required quantities which in the present work correspond to the interaction viscosity and collision integral ratios, obtained from the inversion method.

3. Results and Discussion

Detailed iterative inversion technique was employed in this study to define the intermolecular pair interaction potential energies of five NH_3 -noble gas mixtures, from corresponding states correlations of viscosity. Implementation of the full inversion procedure, requires the extension of experimental data over as wide temperature range as possible. To achieve this, we considered the corresponding states correlation for functional viscosity collision integrals, $\Omega^{*(2,2)}$ of noble gases proposed in Ref. [38], together with the one given for ammonia in Ref. [17], to obtain the mixed interaction functional $\langle \Omega^{*(2,2)} \rangle_{ij}$ for NH_3 -noble gas mixtures by employing the following simple combining rule:

$$\frac{2}{\langle \Omega^{*(2,2)} \rangle_{ij}} = \frac{1}{\langle \Omega^{*(2,2)} \rangle_i} + \frac{1}{\langle \Omega^{*(2,2)} \rangle_j} \quad (19)$$

Resulting $\langle \Omega^{*(2,2)} \rangle_{ij}$ values were employed to perform the inversion procedure in order to generate effective interaction potentials for considered systems. The inverted potential energy values were then fitted to an analytical multi-parameter MSV potential model. This model potential includes a Morse function and the van der Waals dispersion expansion that is respectively used for short range and long range

interactions, along with a Spline function responsible for joining them smoothly.

The reduced form of MSV potential function reads as:

$$\langle U^*(r) \rangle = \frac{\langle U(r) \rangle}{\varepsilon} \quad (20)$$

$$= \exp[2\beta(1-\gamma x)] - 2 \exp[\beta(1-\gamma x)] \quad x \leq x_1 \quad (21)$$

$$= a_1 + (x-x_1)(a_2 + (x-x_2)[a_3 + (x-x_1)a_4]) \quad x_1 < x < x_2 \quad (22)$$

$$= -\left(\frac{C_6^*}{x^6} + \frac{C_8^*}{x^8} + \frac{C_{10}^*}{x^{10}}\right) x_2 \leq x \leq \infty \quad (23)$$

where $x = r/\sigma$, $x_1 = 1.071444$, and $x_2 = 1.405981$.

Table 1

Calculated parameters of MSV potential function (Eqs. (24)–(27)) for NH₃–noble gas mixtures

	Mixture				
	NH ₃ –He	NH ₃ –Ne	NH ₃ –Ar	NH ₃ –Kr	NH ₃ –Xe
ε/k_B	56.05	81.2	205.15	212.6	239.1
$\sigma(A)$	2.89	3.03	3.210	3.35	3.514
r_1^*	1.071444	1.071444	1.071444	1.071444	1.071444
r_2^*	1.405981	1.405981	1.405981	1.405981	1.405981
β	6.3800	6.4080	6.3770	6.3084	6.3345
$\gamma = \sigma/r_m$	0.8894	0.8887	0.8897	0.8893	0.8891
C_6^*	6.483	3.106	5.171	3.433	5.448
C_8^*	3.192	4.281	−5.42	1.51	−7.022
C_{10}^*	−6.939	−7.573	3.477	−3.717	5.489
a_1	−0.7797	−0.7838	−0.7867	−0.764	−0.7847
a_2	0.0009534	0.07491	0.142	−0.1569	0.2018
a_3	20.48	20.38	20.34	22.37	20.36
a_4	−115.6	−112.6	−109.9	−133	−106.6

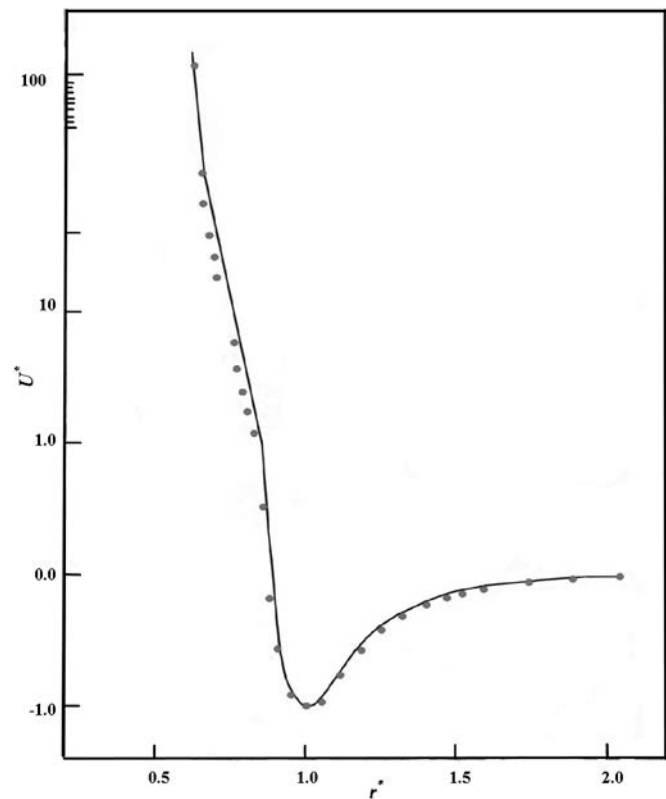


Fig. 1. Reduced MSV potential model of NH₃–Ne mixture (●) obtained by inversion of reduced viscosity collision integrals compared with improved Lennard-Jones (ILJ) potential model of Pirani *et al.* [39] (—).

A nonlinear least squares method was performed for all studied binary mixtures, where the outcome of the fittings has been reported in Table 1. Our model potentials for mixtures of NH₃ with Ne, Ar, He and Kr have been compared with those obtained from molecular beam scattering measurements and infrared spectroscopic observations [39] in Figs. 1 and 2 and S1 and S2 of supplementary data, respectively. The acceptable accordance, confirms the validity of our inverted potential energy functions for aforementioned mixtures.

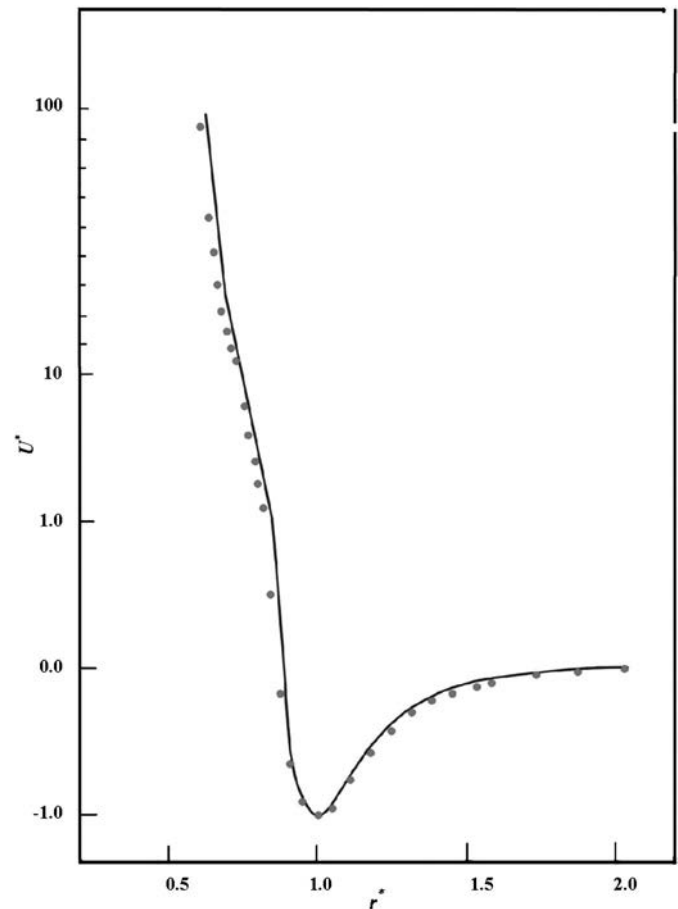


Fig. 2. Reduced MSV potential model of NH₃–Ar mixture (●) obtained by inversion of reduced viscosity collision integrals compared with improved Lennard-Jones (ILJ) potential model of Pirani *et al.* [39] (—).

As a further test to assess the reliability of our proposed potential models for the present systems, mixture transport properties in low density region were computed. To achieve this, the effective potential energies obtained from the inversion method were used to perform the integration over the whole range, in turn, to evaluate the improved kinetic theory collision integrals over the given range, using Eqs. (1)–(3). The results for the most commonly needed collision integrals and their ratios, obtained from Eqs. (11)–(15) in Ref. [19], for binary mixtures of NH₃–Ne, NH₃–Ar, NH₃–He, NH₃–Kr and NH₃–Xe have been tabulated in Tables 2 and 3 and S1, S2 and S3 of supplementary material, respectively.

To calculate mixture transport properties, we needed to know the binary potential parameters, σ_{ij} and ε_{ij} of studied mixtures. Unlike interaction parameters characterizing binary interactions can be obtained from like parameters, σ_{ii} , ε_{ii} and σ_{jj} , ε_{jj} by means of the combining rules. In this study, in order to obtain ε_{12} and σ_{12} for NH₃–noble gas mixtures, we employed experimental viscosity, diffusion coefficient and thermal conductivity data as reference properties. Our determination method of effective pair potential parameters, involved minimizing

Table 2The reduced collision integrals and their ratios for NH₃–Ne mixture

lgT*	$\Omega^{*(1,1)}$	A*	B*	C*	E*	F*
–0.6	2.7850	1.0640	1.2687	0.8624	0.9128	0.9172
–0.5	2.5220	1.0804	1.2869	0.8502	0.9045	0.9094
–0.4	2.2644	1.0963	1.2944	0.8381	0.8928	0.9030
–0.3	2.0175	1.1083	1.2876	0.8284	0.8803	0.8991
–0.2	1.7884	1.1144	1.2678	0.8236	0.8708	0.8982
–0.1	1.5834	1.1150	1.2385	0.8249	0.8671	0.9006
0.0	1.4061	1.1118	1.2062	0.8325	0.8702	0.9069
0.1	1.2575	1.1072	1.1748	0.8451	0.8791	0.9169
0.2	1.1359	1.1029	1.1483	0.8608	0.8920	0.9295
0.3	1.0377	1.1001	1.1278	0.8775	0.9062	0.9434
0.4	0.9588	1.0991	1.1141	0.8935	0.9201	0.9570
0.5	0.8952	1.1001	1.1058	0.9072	0.9322	0.9691
0.6	0.8429	1.1028	1.1019	0.9182	0.9421	0.9795
0.7	0.7990	1.1068	1.1007	0.9265	0.9492	0.9884
0.8	0.7610	1.1115	1.1009	0.9323	0.9539	0.9958
0.9	0.7273	1.1164	1.1017	0.9362	0.9568	1.0018
1.0	0.6966	1.1211	1.1030	0.9387	0.9585	1.0065
1.1	0.6681	1.1256	1.1047	0.9402	0.9593	1.0102
1.2	0.6412	1.1299	1.1064	0.9408	0.9596	1.0132
1.3	0.6156	1.1338	1.1076	0.9410	0.9592	1.0158
1.4	0.5909	1.1371	1.1082	0.9409	0.9585	1.0181
1.5	0.5673	1.1396	1.1081	0.9408	0.9576	1.0201
1.6	0.5445	1.1413	1.1073	0.9409	0.9569	1.0218
1.7	0.5228	1.1424	1.1063	0.9411	0.9565	1.0231
1.8	0.5020	1.1429	1.1054	0.9414	0.9563	1.0239
1.9	0.4821	1.1431	1.1046	0.9418	0.9563	1.0243
2.0	0.4632	1.1429	1.1040	0.9421	0.9564	1.0245
2.1	0.4451	1.1426	1.1033	0.9425	0.9565	1.0247
2.2	0.4278	1.1421	1.1022	0.9430	0.9565	1.0251
2.3	0.4114	1.1408	1.0992	0.9437	0.9559	1.0262

Table 3The reduced collision integrals and their ratios for NH₃–Ar mixture

lgT*	$\Omega^{*(1,1)}$	A*	B*	C*	E*	F*
–0.6	2.7876	1.0640	1.2698	0.8588	0.9096	0.9103
–0.5	2.5187	1.0798	1.2872	0.8473	0.9017	0.9039
–0.4	2.2573	1.0952	1.2941	0.8357	0.8908	0.8998
–0.3	2.0084	1.1074	1.2862	0.8268	0.8796	0.8983
–0.2	1.7788	1.1143	1.2643	0.8228	0.8712	0.8996
–0.1	1.5745	1.1160	1.2344	0.8250	0.8682	0.9038
0.0	1.3988	1.1137	1.2022	0.8334	0.8716	0.9108
0.1	1.2520	1.1096	1.1723	0.8465	0.8803	0.9206
0.2	1.1320	1.1052	1.1467	0.8623	0.8927	0.9326
0.3	1.0352	1.1018	1.1273	0.8789	0.9067	0.9456
0.4	0.9573	1.1003	1.1141	0.8945	0.9203	0.9583
0.5	0.8943	1.1008	1.1063	0.9079	0.9325	0.9697
0.6	0.8424	1.1035	1.1029	0.9186	0.9423	0.9797
0.7	0.7986	1.1076	1.1021	0.9265	0.9495	0.9883
0.8	0.7605	1.1128	1.1029	0.9320	0.9542	0.9956
0.9	0.7266	1.1183	1.1046	0.9356	0.9570	1.0015
1.0	0.6955	1.1238	1.1067	0.9376	0.9585	1.0063
1.1	0.6664	1.1292	1.1091	0.9386	0.9590	1.0102
1.2	0.6388	1.1343	1.1112	0.9389	0.9588	1.0134
1.3	0.6123	1.1388	1.1125	0.9387	0.9579	1.0164
1.4	0.5869	1.1423	1.1126	0.9385	0.9566	1.0189
1.5	0.5624	1.1445	1.1118	0.9384	0.9553	1.0210
1.6	0.5390	1.1456	1.1100	0.9386	0.9545	1.0225
1.7	0.5167	1.1458	1.1081	0.9391	0.9542	1.0236
1.8	0.4955	1.1454	1.1063	0.9398	0.9543	1.0242
1.9	0.4754	1.1448	1.1049	0.9405	0.9547	1.0246
2.0	0.4564	1.1440	1.1040	0.9413	0.9552	1.0247
2.1	0.4384	1.1432	1.1029	0.9420	0.9557	1.0249
2.2	0.4213	1.1422	1.1010	0.9428	0.9558	1.0255
2.3	0.4051	1.1402	1.0969	0.9438	0.9551	1.0269

the relative root mean square deviations (RMSD's) between reference transport properties and those predicted through Chapman–Enskog expressions for calculating viscosity, diffusion and thermal conductivity of binary mixtures. (Eqs. (24)–(26)). In fact, the least squares fitting method was employed to determine most consistent potential parameters,

able to reproduce all mentioned transport properties within experimental accuracies.

$$\eta_{ij}^0 = \frac{5}{16} \left[\left(\frac{2m_i m_j}{m_i + m_j} \right) \frac{k_B T}{\pi} \right]^{1/2} \frac{1}{\sigma_{ij}^2 \Omega_{ij}^{*(2,2)}} \quad (24)$$

$$D_{ij}^0 = \frac{3}{8} \left(\frac{(m_i + m_j) k_B^3 T^3}{2\pi m_i m_j} \right)^{1/2} \frac{(1 + \Delta_{ij})}{\sigma_{ij}^2 \Omega_{ij}^{*(1,1)}} \quad (25)$$

$$\lambda_{ij}^0 = \frac{75}{64} \left(\frac{(m_i + m_j) k_B^3 T}{2\pi m_i m_j} \right)^{1/2} \quad (26)$$

Our predicted potential parameters, obtained from the above procedure have been reported in Table 4. For comparison we have added the same parameters from two references [40,41], calculated merely based on the viscosity and diffusion coefficients, respectively.

Table 4Potential parameters (ε_{12} and σ_{12}) of studied mixtures

System	NH ₃ –He	NH ₃ –Ne	NH ₃ –Ar	NH ₃ –Kr	NH ₃ –Xe
σ	0.289 ^① 0.270 ^②	0.303 ^① 0.303 ^②	0.3210 ^① 0.2890 ^②	0.331 ^① 0.367 ^②	0.3514 ^① 0.327 ^②
ε/k	56.05 ^① 51.5 ^②	84.7 ^① 84.7 ^②	205.15 ^① 216.0 ^②	245.8 ^① 271.6 ^②	239.1 ^① 242.8 ^②
			212.3 ^③	264.95 ^③	

① This work.

② From experimental viscosity data reference [42].

③ From diffusion coefficient reference [43].

As previously mentioned, the validity of any potential energy function is confirmed by its ability to reproduce thermophysical properties, within acceptable accuracies. Having the binary potential parameters, we employed the inverted pair potential energies of all five systems to the Chapman–Enskog [9,10] method to compute viscosity coefficients,

Table 5Predicted low density transport properties of equimolar NH₃–Ne mixture

T/K	$10^6 \eta / \text{Pa} \cdot \text{s}$	$10^4 D_{12} / \text{m}^2 \cdot \text{s}^{-1}$	α_T	$10^3 \lambda / \text{mW} \cdot \text{mK}^{-1}$
200	14.9460	0.1939	–0.00180	80.993
250	18.0250	0.2904	–0.00222	35.641
273.15	19.3790	0.3400	–0.00238	37.868
293.15	20.5170	0.3854	–0.00249	39.992
300	20.9000	0.4014	–0.00253	40.753
313.15	21.6280	0.4328	–0.00259	42.26
333.15	22.7140	0.4824	–0.00268	44.649
353.15	23.7780	0.5341	–0.00276	47.141
373.15	24.8220	0.5877	–0.00283	49.718
423.15	27.3470	0.7305	–0.00298	56.44
473.15	29.7690	0.8850	–0.00309	63.397
523.15	32.1030	1.0510	–0.00317	70.399
573.15	34.3590	1.2280	–0.00324	77.257
623.15	36.5460	1.4158	–0.00329	83.877
673.15	38.6710	1.6139	–0.00333	89.612
723.15	40.7400	1.8223	–0.00336	
773.15	42.7590	2.0405	–0.00339	
873.15	46.6600	2.5060	–0.00343	
973.15	50.4010	3.0089	–0.00345	
1073.15	54.0030	3.5477	–0.00347	
1173.15	57.4840	4.1214	–0.00349	
1273.15	60.8570	4.7288	–0.00350	
1773.15	76.4450	8.2427	–0.00352	
2273.15	90.5090	12.4940	–0.00353	
2773.15	103.5600	17.4270	–0.00353	
3273.15	115.8700	23.0030	–0.00353	

binary diffusion coefficients, and thermal diffusion factors of equimolar NH_3 –noble gas mixtures at low density.

Moreover, the thermal conductivities of aforementioned binary gas mixtures were obtained using the Schreiber *et al.* method [33]. The outcome of these computations for NH_3 –Ne, NH_3 –Ar, NH_3 –He, NH_3 –Kr and NH_3 –Xe mixtures, in a wide temperature range $250 \leq T \leq 3273.15$ K, was tabulated respectively in Tables 5 and 6 and S4, S5 and S6 of supplementary material.

Table 6

Predicted low density transport properties of equimolar NH_3 –Ar mixture

T/K	$10^6 \eta/\text{Pa} \cdot \text{s}$	$10^4 D_{12}/\text{m}^2 \cdot \text{s}^{-1}$	α_T	$10^3 \lambda/\text{mW} \cdot \text{mK}^{-1}$
200	8.9532	0.1042	−0.0008	26.422
250	11.2490	0.1623	0.0162	18.380
273.15	12.3030	0.1931	0.0241	19.715
293.15	13.2050	0.2216	0.0308	20.974
300	13.5130	0.2317	0.0330	21.422
313.15	14.1010	0.2517	0.0373	22.299
333.15	14.9870	0.2835	0.0434	23.672
353.15	15.8650	0.3169	0.0493	25.081
373.15	16.7330	0.3518	0.0549	26.520
423.15	18.8620	0.4455	0.0676	30.210
473.15	20.9290	0.5479	0.0787	33.981
523.15	22.9350	0.6585	0.0882	37.783
573.15	24.8820	0.7770	0.0965	41.566
623.15	26.7730	0.9030	0.1036	45.326
673.15	28.6100	1.0362	0.1098	48.835
723.15	30.3970	1.1764	0.1151	
773.15	32.1370	1.3234	0.1198	
873.15	35.4880	1.6369	0.1274	
973.15	38.6850	1.9757	0.1331	
1073.15	41.7480	2.3388	0.1376	
1173.15	44.6910	2.7254	0.1410	
1273.15	47.5300	3.1348	0.1437	
1773.15	60.4910	5.5061	0.1502	
2273.15	71.9880	8.3812	0.1520	
2773.15	82.4980	11.7220	0.1523	
3273.15	92.2880	15.4990	0.1522	

Table 7

The non-linear least squares parameters, standard errors (SE) and correlation coefficients (R) of Eq. (27)

Mixture	a_η	b_η/K	c_η/K^2	d_η	SE_η	R_η
He– NH_3	0.6326	−120.7	9059	−0.563	1.33×10^{-3}	0.9999
Ne– NH_3	0.6544	−55.55	1789	−0.5276	2.6×10^{-4}	0.9999
Ar– NH_3	0.6242	−186.5	1.19×10^4	−0.4641	3.9×10^{-3}	0.9999
Kr– NH_3	0.6180	−84.2	−2290	3.568×10^{-3}	3.2×10^{-3}	0.9999
Xe– NH_3	0.5892	−177.1	8253	0.1812	2.1×10^{-3}	0.9999

Table 8

The non-linear least squares parameters, standard errors (SE) and correlation coefficients (R) of Eq. (28)

Mixture	a_D	b_D/K	c_D	SE_D	R_D
He– NH_3	1.656	−19.24	−9.57	6.73×10^{-4}	0.9999
Ne– NH_3	1.658	−28.12	−10.27	1.14×10^{-3}	0.9999
Ar– NH_3	1.642	−91.06	−10.52	1.48×10^{-3}	0.9999
Kr– NH_3	1.654	−101.7	−10.80	2.64×10^{-3}	0.9999
Xe– NH_3	1.648	−104	−10.88	2.79×10^{-3}	0.9999

Table 9

The non-linear least squares parameter, standard errors (SE) and correlation coefficients (R) of Eq. (30)

Mixture	$a_\lambda/\text{W} \cdot \text{mK}^{-1}$	$b_\lambda/\text{W} \cdot \text{mK}^{-2}$	$c_\lambda/\text{W} \cdot \text{mK}^{-3}$	$d_\lambda/\text{W} \cdot \text{mK}^{-4}$	$e_\lambda/\text{W} \cdot \text{mK}^{-5}$	SE_λ	R_λ
He– NH_3	41.28	0.2322	5.062×10^{-4}	3.418×10^{-6}	-8.44×10^{-9}	1.5×10^{-2}	0.9
Ne– NH_3	13.36	0.2334	-17.2×10^{-4}	7.567×10^{-6}	-1.54×10^{-8}	1.5×10^{-2}	0.9
Ar– NH_3	21.2	−0.1164	5.795×10^{-4}	-5.81×10^{-7}	-5.7×10^{-10}	4.0×10^{-4}	1
Kr– NH_3	18.1	−0.124	5.96×10^{-4}	-8.58×10^{-7}	2.09×10^{-10}	2.7×10^{-4}	0.9
Xe– NH_3	16.47	−0.1227	5.626×10^{-4}	-8.85×10^{-7}	4.42×10^{-10}	1.7×10^{-4}	1

The interaction viscosity of dilute gas mixtures, η_{12} , which is the hypothetical viscosity of a gas of mass $\mu = m_1 m_2 / (m_1 + m_2)$ in which only unlike interactions take place, was obtained through using Eq. (7) and our model potential energies. The quantity was correlated for all five studied mixtures with the following equation:

$$\ln(\eta/\eta_0) = a_\eta \ln(T/T_0) + b_\eta/T + c_\eta/T^2 + d_\eta \quad (27)$$

where, $\eta_0 = 1 \mu\text{Pa} \cdot \text{s}$, and $T_0 = 1$ K.

Further, the binary diffusion coefficients, thermal diffusion factors and also thermal conductivities of the five equimolar NH_3 –noble gas mixtures were correlated with Eqs. (27)–(30), respectively.

$$\ln(PD/P_0 D_0) = a_D \ln(T/T_0) + b_D/T + c_D \quad (28)$$

$$\ln \alpha_T^{-1} = a_\alpha / T^* + b_\alpha / T^{*2} + c_\alpha \ln T^* + d_\alpha (\ln T^*)^2 + e_\alpha / \ln T^* + f_\alpha / (\ln T^*)^2 + g_\alpha / (\ln T^*)^3 \quad (29)$$

$$\lambda = a_\lambda + b_\lambda T + c_\lambda T^2 + d_\lambda T^3 + e_\lambda T^4 \quad (30)$$

where $P_0 = 101325$ Pa and $D_0 = 1 \text{ cm}^2 \cdot \text{s}^{-1}$. Parameters of the Eqs. (27)–(30) were allowed to vary for all five systems, using nonlinear least-squares method and listed in Tables 7–9 and S7 of supplementary data.

In order to assess the reliability of predicted transport properties and also our inverted potential energy functions, resulting transport properties were checked against the literature data. Calculated viscosities for the NH_3 –Ne, –Ar, –He, –Kr and –Xe mixtures were compared with experimental data [42,44–46] and the results depicted as deviation plots, in Figs. 3 and 4 and S3–S5 of supplementary material, respectively. The average absolute deviations (AADs) of the calculated viscosities for aforementioned mixtures, from the experimental ones [42,44–46] were found to be 3.73%, 3.57%, 2.72%, 4.79% and 2.68%, respectively.

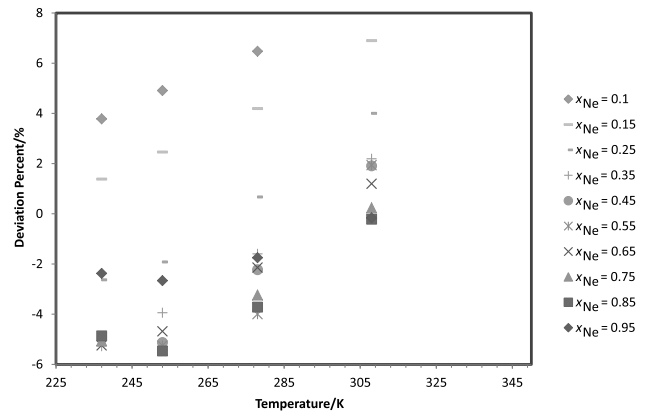


Fig. 3. Deviation plot for the dilute viscosity coefficients of NH_3 –Ne gaseous mixture in terms of temperature at different mole fractions of Ne: (◆) $x_{\text{Ne}} = 0.1$; (◼) $x_{\text{Ne}} = 0.15$; (◻) $x_{\text{Ne}} = 0.25$; (◊) $x_{\text{Ne}} = 0.35$; (●) $x_{\text{Ne}} = 0.45$; (⊗) $x_{\text{Ne}} = 0.55$; (⊗) $x_{\text{Ne}} = 0.65$; (▲) $x_{\text{Ne}} = 0.75$; (■) $x_{\text{Ne}} = 0.85$; (◆) $x_{\text{Ne}} = 0.95$ compared with experiment [42,44].

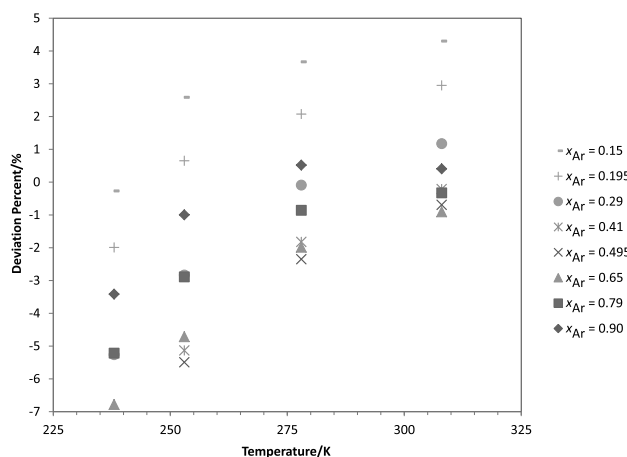


Fig. 4. Deviation plot for the dilute viscosity coefficients of NH_3 –Ar gaseous mixture in terms of temperature at different mole fractions of Ar: (■) $x_{\text{Ar}} = 0.15$; (+) $x_{\text{Ar}} = 0.195$; (●) $x_{\text{Ar}} = 0.29$; (×) $x_{\text{Ar}} = 0.41$; (○) $x_{\text{Ar}} = 0.495$; (▲) $x_{\text{Ar}} = 0.65$; (■) $x_{\text{Ar}} = 0.79$; (◆) $x_{\text{Ar}} = 0.90$, compared with experiment [42,44–46].

It should be mentioned that these viscosity measurements have been performed, using an oscillating disk viscometer at atmospheric pressure and in the nominal temperature range, from -35°C to 35°C . The accuracy of the measurements has been claimed to be of 1% for NH_3 –He, –Ne, –Kr and –Xe mixtures. In the case of NH_3 –Ar mixture, the precision of measured viscosities by Rakshit *et al.* [46] is 1% at -35°C to 35°C temperature range, and it varies from 0.2% for argon-rich to 1.5% for ammonia-rich mixture, in Iwasaki *et al.* reported data [45].

Predicted diffusion coefficients of ammonia-noble gas mixtures at several temperatures have been compared with experimental ones reported in the literature [43]. Relative deviations of the diffusion coefficients, for NH_3 –Ar and NH_3 –Kr mixtures from experimental data [43] are plotted in Fig. 5. The AADs for these mixtures were found to be 7.39% and 8%, respectively. Diffusion coefficients for mixtures of ammonia with argon and krypton have been measured using two-bulb technique in the temperature range of -20 to 60°C where the accuracy has been claimed to be within $\pm 1\%$.

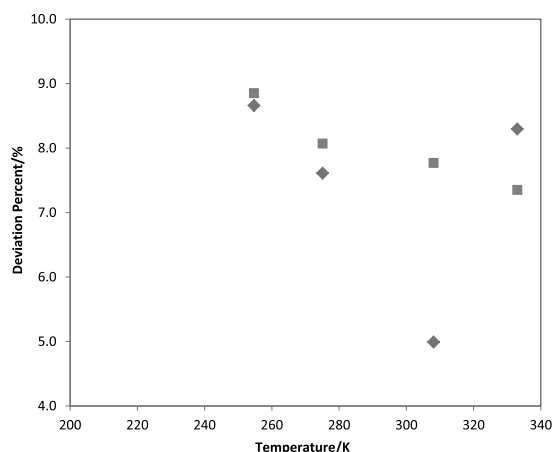


Fig. 5. Deviation plot for the diffusion coefficients of NH_3 –Ar and NH_3 –Kr gaseous mixtures at different temperatures, compared with literature data [43]: (◆) NH_3 –Ar, (■) NH_3 –Kr.

The thermal diffusion factor describes, physically, the actual extent of the spatial separation of an initially uniform gaseous mixture of different molecular partners, which takes place whenever that mixture is subject to a temperature gradient. Unfortunately we have not found any literature values of this property for the studied mixtures. Therefore, we could not evaluate our calculated thermal diffusion factors using the MSV model potential.

Thermal conductivities and heat capacities of pure species required by the Schreiber *et al.*'s method [32], were taken from NIST data [47]. In order to assess the validity of predicted thermal conductivities of NH_3 –noble gas binary mixtures, Figs. 6 and 7 and S6 of supplementary data depict the relative deviations of the calculated thermal conductivities of, NH_3 –Ne, NH_3 –Ar and NH_3 –He mixtures from the experimental values [48], respectively. It should be cited that the hot-wire method has been used in this reference [48] to measure the thermal conductivities of aforementioned mixtures with the experimental uncertainty within 1%–1.5% at temperatures, 39–199.6 $^\circ\text{C}$. The AAD values of our calculated thermal conductivities for NH_3 –He, NH_3 –Ne and NH_3 –Ar mixtures from the experimental values (each for 20 data points) were found to be 7.57%, 7.83% and 10.63%, respectively.

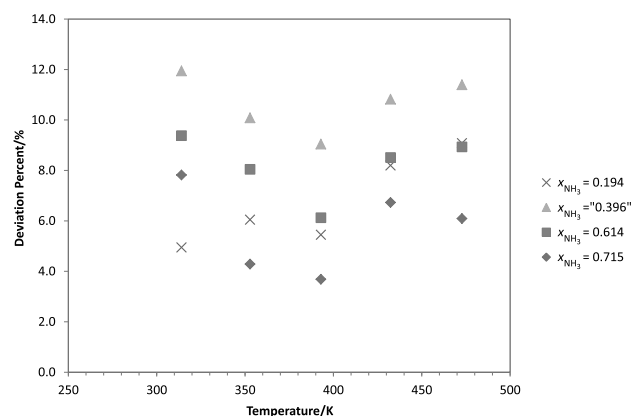


Fig. 6. Deviation plot for the thermal conductivities of NH_3 –Ne gaseous mixture at different temperatures, compared with experiment [48]: (×) $x_{\text{NH}_3} = 0.194$; (▲) $x_{\text{NH}_3} = 0.396$; (■) $x_{\text{NH}_3} = 0.614$; (◆) $x_{\text{NH}_3} = 0.715$.

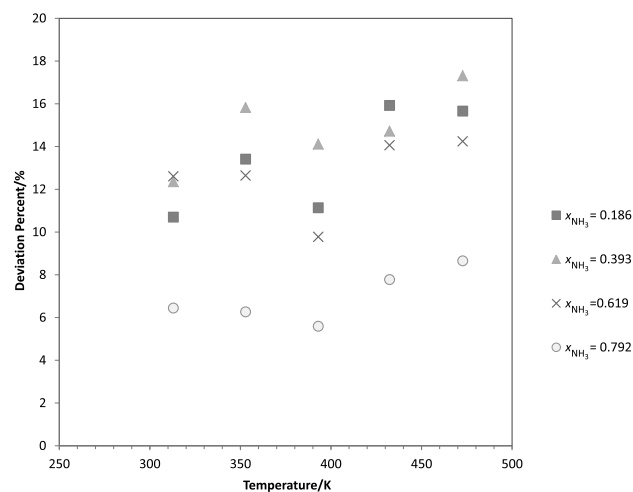


Fig. 7. Deviation plot for the thermal conductivities of NH_3 –Ar gaseous mixture at different temperatures, compared with experiment [48]: (■) $x_{\text{NH}_3} = 0.186$; (▲) $x_{\text{NH}_3} = 0.393$; (×) $x_{\text{NH}_3} = 0.619$; (○) $x_{\text{NH}_3} = 0.792$.

4. Conclusions

In this study the pair interaction energies of NH_3 -noble gas mixtures were obtained using the inversion method, based on the corresponding states correlations of viscosity, and fitted to the MSV model potentials. Our inverted potential functions showed reasonable agreement with previously obtained potential energies, based on the molecular beam scattering measurements and infrared spectroscopic observations.

Viscosities, diffusion coefficients, thermal diffusion factors and thermal conductivities of studied mixtures were calculated at low density and compared with literature data, where available. The acceptable agreement between calculated and experimental transport properties, provided further evidence to support the reliability of our inverted potentials for NH_3 -noble gas mixtures. The most important features of the inversion method are its independence on the explicit assumption about the functional form of potential model, the establishment of unique potentials, and leading to collision integrals which are prerequisite for determination of thermophysical properties.

Supplementary Material

Supplementary data to this article can be found online at <http://dx.doi.org/10.1016/j.cjche.2017.07.007>.

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