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Calculation of Viscosity and Diffusion Coefficients for Two Binary Gaseous Mixtures Using the Semi-empirical Inversion Method

Hamid Reza Rafiee*, Mina Rastgar, Neda Heidari

Faculty of Chemistry, Razi University, Kermanshah 67149, Iran

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The accurate reduced potential energies for two binary gas mixtures including benzene-methanol and methane-tetrafluoromethane at low density have been obtained by direct inversion of the viscosity collision integral equations. The kinetic theory along with the extended principle of corresponding-states has been used to calculate the viscosity and diffusion coefficients over a wide range of temperature and composition. Good agreements between calculated and experimental data are obtained.

Key words: Inversion method, Viscosity, Diffusion, Gaseous mixture

I. INTRODUCTION

Transport properties of gaseous mixtures are very important in process design, mass and energy transfer because the mixtures are often encountered more than pure gases. From the theoretical point of view, due to the absence of data over a wide range of temperature, pressure and composition, the semi-empirical methods are interested. For example, the semi-empirical inversion method has extensively been used to extract the pair potential function and then predict transport properties of pure and mixtures of gases [1–10]. The results of kinetic and statistical-mechanical theories provide theoretical expressions for various equilibrium and non-equilibrium properties in terms of the potential energy of interaction between a pair of molecules [11]. Thus the evaluation of such quantities from a known pair potential function is a reliable procedure and the problem is how to gain the intermolecular potential. Due to the facts of availability and measurability, transport properties of gases at low density are an important source of the information about the interactions at the molecular level. The viscosity is the probably easier to be measured and more accurate than others. The general method which has been used to infer intermolecular potential from transport properties was adopting a model potential with a number of adjustable parameters which were varied until a good fit was obtained to a given set of experimental data. The main disadvantage of this method is that the parameters determined from one property, such as viscosity, are slightly different from those obtained from other ones, like diffusion.

A desirable and reliable manner of solving the prob-

lem would be to obtain potential energy $\mu(r)$, directly from the experimental data without explicit assumption of a mathematical model for $\mu(r)$, is the semi-empirical inversion method which is developed by Smith and co-workers [12–15].

The present work while describes an iterative method for generating the effective pair potential energy for gaseous binary mixtures of methane-tetrafluoromethane and benzene-methanol systems, then uses them to predict the low density transport properties over a wide range of temperature and composition. The accuracies for viscosity and diffusion coefficients are within 2% and 3%, respectively.

II. COMPUTATION METHOD

A. Kinetic theory of gases

According to the kinetic theory of gases and the Chapman-Enskog solution [16, 17] of the Boltzmann transport equation [18], the transport properties of gases at low density can be related to a series of collision integrals $\Omega^{(l,s)}$ which depend on the intermolecular potential energy $\mu(r)$. The superscripts l and s appearing in Ω denote weighting factors those account for the mechanism of transport by molecular collision. They are $l=2$ and $s=2$ for viscosity and $l=1$ and $s=1$ for diffusion, respectively [11]. The collision integrals are defined as:

$$\Omega^{(l,s)}(T) = \frac{1}{(s+1)!(kT)^{(s+2)}} \cdot \int_0^\infty Q^{(l)}(E) \exp\left(-\frac{E}{kT}\right) E^{s+1} dE \quad (1)$$

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

* Author to whom correspondence should be addressed. E-mail: rafieehr@yahoo.com, Tel./FAX: +98-831-4274559

θ is the scattering angle, $Q^{(l)}(E)$ is the transport collision integral, b the impact parameter, and E the relative kinetic energy of colliding partners. The deflection angle is given by:

$$\theta(b, g) = \pi - 2b \int_{r_m}^{\infty} \frac{dr}{r^2} \left[1 - \frac{2V(r)}{\mu g^2} - \frac{b^2}{r^2} \right]^{-1/2} \quad (3)$$

The definition of collision integrals as dimensionless reduced quantities makes the calculations of transport properties more convenient. The reduced collision integral is defined as:

$$\Omega^{*(l,s)} = \frac{\Omega^{(l,s)}}{\pi \sigma^2} \quad (4)$$

where σ , the range parameter, denotes the intermolecular separation for which the potential is zero. Numerical differentiation of the mentioned collision integrals and usage of recursion relation can generate collision integrals higher than the ones mentioned. That is:

$$\Omega^{*(l,s+1)} = \Omega^{*(l,s)} \left[1 + \frac{1}{s+2} \frac{d \ln \Omega^{*(l,s)}}{d \ln T^*} \right] \quad (5)$$

$$T^* = \frac{kT}{\varepsilon} \quad (6)$$

where T^* is reduced temperature, the energy parameter ε represent the depth of the potential energy well.

We have shown that three successive numerical integrations are done to obtain collision integrals. The potential energy would serve as the input information required in calculating the collision integrals and consequently the transport properties. Kinetic theory expressions for the transport properties in term of the collision integrals for pure gases and gaseous mixture are as following [11]:

Pure gas, viscosity,

$$\eta = \frac{5}{16} \left(\frac{mKT}{\pi} \right)^{1/2} \frac{f_\eta}{\sigma^2 \Omega^{*(2,2)}(T^*)} \quad (7)$$

$$f_\eta = 1 + \frac{3}{196} (8E^* - 7)^2 \quad (8)$$

Self-diffusion coefficient,

$$D = \frac{3}{8P} \left[\frac{(kT)^3}{\pi m} \right]^{1/2} \frac{f_D}{\sigma^2 \Omega^{*(1,1)}} \quad (9)$$

$$f_D = 1 + \frac{1}{8} \frac{(6C^* - 5)^2}{2A^* + 5} \quad (10)$$

The ratios of the calculated collision integrals have been

determined by the following equations:

$$A^* = \frac{\Omega^{*(2,2)}}{\Omega^{*(1,1)}} \quad (11)$$

$$B^* = \frac{5\Omega^{*(1,2)} - 4\Omega^{*(1,3)}}{\Omega^{*(1,1)}} \quad (12)$$

$$C^* = \frac{\Omega^{*(1,2)}}{\Omega^{*(1,1)}} \quad (13)$$

$$E^* = \frac{\Omega^{*(2,3)}}{\Omega^{*(2,2)}} \quad (14)$$

$$F^* = \frac{\Omega^{*(3,3)}}{\Omega^{*(1,1)}} \quad (15)$$

$$H^* = \frac{3B^* + 6C^* - 35/4}{6C^* - 5} \quad (16)$$

These ratios are weak functions of T^* and their magnitudes are approximately unity and exactly one for rigid spheres. Collision integrals and their ratios are functions of temperature and the parameters of the selected model for intermolecular forces.

For gaseous mixtures the equations for viscosity are:

$$[\eta_{\text{mix}}] = - \frac{\begin{vmatrix} H_{11} & H_{12} & H_{13} & \dots & H_{1v} & x_1 \\ H_{12} & H_{22} & H_{23} & \dots & H_{2v} & x_2 \\ H_{13} & H_{23} & H_{33} & \dots & H_{3v} & x_3 \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ H_{1v} & H_{2v} & H_{3v} & \dots & H_{vv} & x_v \\ x_1 & x_2 & x_3 & \dots & x_v & 0 \end{vmatrix}}{\begin{vmatrix} H_{11} & H_{12} & H_{13} & \dots & H_{1v} \\ H_{12} & H_{22} & H_{23} & \dots & H_{2v} \\ H_{13} & H_{23} & H_{33} & \dots & H_{3v} \\ \cdot & \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ H_{1v} & H_{2v} & H_{3v} & \dots & H_{vv} \end{vmatrix}} \quad (17)$$

where,

$$H_{ii} = \frac{x_i^2}{[\eta_i]} + \sum_{\substack{k=1 \\ k \neq i}}^v \frac{2x_i x_k}{[\eta_{ik}]} \frac{m_i m_k}{(m_i + m_k)^2} \left(\frac{5}{3A_{ik}^*} + \frac{m_k}{m_i} \right) \pi \quad (18)$$

$$H_{ij} = - \frac{2x_i x_j}{\eta_{ij}} \frac{m_i m_j}{(m_i + m_j)^2} \left(\frac{5}{3A_{ij}^*} - 1 \right), \quad (i \neq j) \quad (19)$$

$$\eta_{ij} = \frac{5}{16} \left(\frac{2m_i m_j}{m_i + m_j} \frac{kT}{\pi} \right)^{1/2} \frac{1}{\sigma_{ij}^2 \Omega_{ij}^{*(2,2)}(T_{ij}^*)} \quad (20)$$

A_{ij}^* is the ratio of the collision integrals, x is the molar fraction of components, and η_{ij} is the interaction viscosity. Subscripts i and j represent the heavier and lighter component of the i - j pair, respectively.

For diffusion we have:

$$D_{ij} = \frac{3}{8} \left(\frac{m_i + m_j}{2m_i m_j} \frac{kT}{\pi} \right)^{1/2} \frac{kT}{P} \frac{1 + \Delta_{ij}}{\sigma_{ij}^2 \Omega_{ij}^{*(1,1)}} \quad (21)$$

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

$$\Delta_{ij} = 1.3 (6C_{ij}^* - 5)^2 \frac{a_{ij}x_{ij}}{1 + b_{ij}x_{ij}} \quad (22)$$

$$a_{ij} = \frac{\sqrt{2} \Omega_{ij}^{*(1,1)}(T_{ij}^*)}{8 \left(1 + 1.8 \frac{m_j}{m_i}\right)^2 \Omega_{jj}^{*(2,2)}(T_j^*)} \quad (23)$$

$$b_{ij} = 10a_{ij} \left[1 + 1.8 \frac{m_j}{m_i} + 3 \left(\frac{m_j}{m_i}\right)^2\right] - 1 \quad (24)$$

$$x_{ij} = \frac{x_i}{x_i + x_j} \quad (25)$$

B. Inversion method

The inversion method uses a given set of experimental reduced viscosity collision integrals, $\Omega^{*(2,2)}$, over a wide range of temperatures to invert a pair of values ($\Omega^{*(2,2)}$, T) to V/ε as a function of r/σ using the relations:

$$r^* = \frac{r}{\sigma} = \left[\Omega^{*(2,2)}\right]^{1/2} \quad (26)$$

$$V^* = \frac{V}{\varepsilon} = GT^* \quad (27)$$

G is the inversion function which is a function of T^* and can be calculated by using a model system whose intermolecular potential is known. The values of G for the Lennard-Jones 12-6 potential as the initial model have been determined from Viehland *et al.* [19]. The new potential energies are closer approximations to the true potential than the potential of the initial model. This then can be used for calculations of improved collision integrals by the integrals of Eqs. (1)–(3) and the computer program developed by O'Hara and Smith [20, 21]. This process is repeated by an iterative manner until convergence occurs. The convergence condition is the degree to which the calculated collision integrals for a given iteration are close to the experimental correlation within experimental accuracy. In this work convergence occurred after two iterations.

C. Extended principle of corresponding states

The law of corresponding states is based on this idea that the equilibrium and transport properties of substances whose molecules obey a potential function with two scaling parameters, energy scaling factor ε , and length scaling factor σ , can be expressed in terms of functions that are nearly universal when written in terms of scaling factors. The works on viscosity of noble gases [22] and also binary gas mixtures [23, 24] showed that the function $\Omega^{*(2,2)}$ is universal. The extended law

of corresponding state is a revised principle of corresponding states that characterizes each binary interaction with the aid of five scaling parameters instead of two. The five scaling parameters are: σ , ε , ρ^* , C_6^* , V_0^* ; also a quantum mechanical parameter Λ^* maybe come into play. The dimensionless parameter C_6^* , characterizes the long-range region of the potential energy curve and dimensionless parameters ρ^* and V_0^* characterize the short range repulsive wall. The Λ^* becomes significant when the molecular partners are small and/or the temperature is low.

In our work the correlation function proposed by Najafi and co-workers was applied in order to calculate the unlike pair potential energy [25]. The proposed viscosity correlation function is as following:

$$\Omega^{*(2,2)}(T^*) = \exp \sum_{i=0}^6 la_i (\ln T^*) \quad (28)$$

For $0.8 < T^* < 500$

$$\begin{aligned} a_0 &= 0.4369 \pm 7.8 \times 10^{-4} \\ a_1 &= -0.4505 \pm 1.3 \times 10^{-3} \\ a_2 &= 5.326 \times 10^{-2} \pm 8.1 \times 10^{-4} \\ a_3 &= 3.519 \times 10^{-2} \pm 9.2 \times 10^{-4} \\ a_4 &= -1.751 \times 10^{-2} \pm 4.0 \times 10^{-4} \\ a_5 &= 2.773 \times 10^{-3} \pm 7.0 \times 10^{-5} \\ a_6 &= -1.529 \times 10^{-4} \pm 4.3 \times 10^{-6} \end{aligned}$$

III. RESULTS AND DISCUSSION

The extraction of information about the forces by analyzing the bulk properties will be done if the interaction potential energy is available. The degree of success then depends on the accuracy of both the measurements and theory connecting the forces to macroscopic properties. The transport properties of dilute gases, in special viscosity, which depends on the binary interactions, satisfy the above requirements. In this relation also inversion procedure plays an important role for generating an unlike-molecule potential from the viscosity data and their corresponding states correlations. This, in turn permits us to calculate collision integrals and consequently the transport properties is possible by correlations of the corresponding states.

In the case of the corresponding states principle it should be mentioned that since the functional equation obtained from this principle apply in a more limited form to molecular gases than to noble gases, the arithmetic mean of the function should be used for gases 1 and 2. Also we are confined ourselves to $T^* \geq 1$, consequently in order to proceed to the next iteration which is necessary to extrapolate $V(r)$ at the long-range region (low temperature). The extrapolation function that we

TABLE I The reduced collision integrals and their ratios for benzene-methanol system.

$\lg T^*$	$\Omega^{*(1,1)}$	$\Omega^{*(2,2)}$	A^*	B^*	C^*	E^*	F^*
0	1.362594	1.521943	1.116943	1.190904	0.856426	0.890396	0.930544
0.099991	1.23778	1.379164	1.114225	1.167666	0.865887	0.89626	0.93744
0.200002	1.132638	1.258302	1.110949	1.146855	0.877397	0.904904	0.945634
0.300008	1.044969	1.158073	1.108238	1.132509	0.889521	0.915031	0.954844
0.400002	0.97175	1.076051	1.107333	1.121018	0.901434	0.925315	0.965093
0.500003	0.911211	1.008995	1.107314	1.112058	0.911463	0.934736	0.974596
0.600003	0.859796	0.953669	1.109181	1.106819	0.92014	0.942538	0.983671
0.700002	0.815655	0.907157	1.112181	1.104103	0.927041	0.948542	0.991605
0.800002	0.777003	0.866959	1.115772	1.10279	0.932206	0.95281	0.998343
0.900001	0.742444	0.831271	1.11964	1.102711	0.935897	0.95562	1.003751
1	0.710923	0.79874	1.123523	1.103783	0.938359	0.957473	1.007981
1.099991	0.681628	0.7685	1.127446	1.10608	0.939731	0.958643	1.011046
1.200002	0.653932	0.740025	1.131657	1.109895	0.940072	0.959301	1.01299
1.300008	0.627302	0.712822	1.136343	1.114901	0.939399	0.959236	1.014172
1.400002	0.601293	0.686245	1.141309	1.119961	0.937975	0.958055	1.015304
1.500003	0.575725	0.659548	0.63379	0.619324	0.51378	0.955606	0.560587
1.600003	0.550643	0.632176	0.635157	0.618657	0.513025	0.952297	0.561718
1.700002	0.526359	0.604078	1.147731	1.114817	0.934781	0.949054	1.021703
1.800002	0.503391	0.575743	1.143847	1.10438	0.936378	0.946865	1.024184
1.900001	0.48226	0.548055	1.136645	1.091798	0.939681	0.946407	1.025815
2	0.46334	0.521961	1.126926	1.079108	0.944377	0.948048	1.026308

used is $V^* = -C_6 u^6$, where C_6 is the dispersion coefficient and u is the reciprocal of the intermolecular distance, both in atomic units. It is remarkable to mention that the inversion procedure is insensitive to the nature of the extrapolating function [26].

In this work we obtained accurate reduced potential energies for two binary gas mixtures at low density by direct inversion of the viscosity collision integral equations. The result for the benzene-methanol system is shown in Fig.1. These accurate potential energies then have been used to produce improved collision integrals which in turn serve to calculate the transport properties.

Tables I and II give the results of collision integrals and their ratios for two studied systems (benzene-methanol and methane-tetrafluoromethane).

In Table III the predicted viscosity coefficients for methane-tetrafluoromethane system at different molar fractions and temperatures are compared with the experimental reported values [27]. Deviations are calculated according to:

$$\text{Dev}\% = \frac{X_{\text{exp.}} - X_{\text{calc.}}}{X_{\text{exp.}}} \quad (29)$$

In Table IV the calculated diffusion coefficients of methane-tetrafluoromethane and benzene-methanol system are compared with experimental values [27, 28].

Table V shows the calculated and experimental [28] viscosity coefficients for methane-tetrafluoromethane system at different compositions and temperatures.

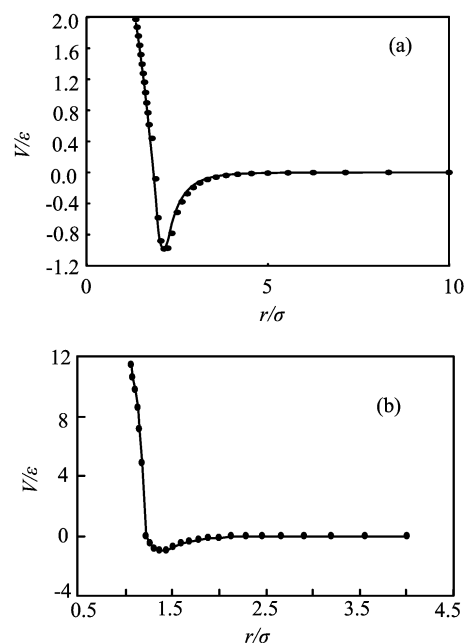


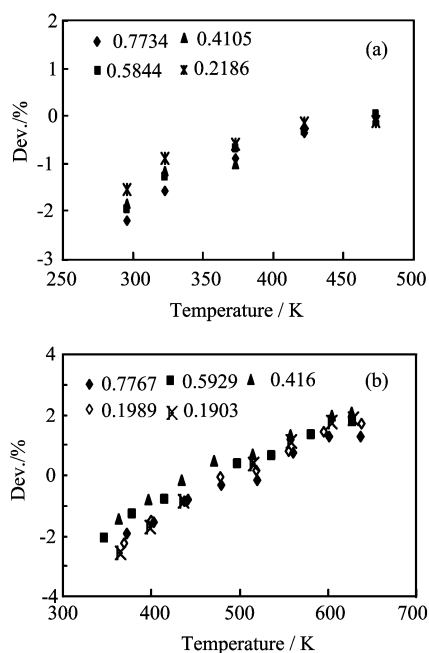
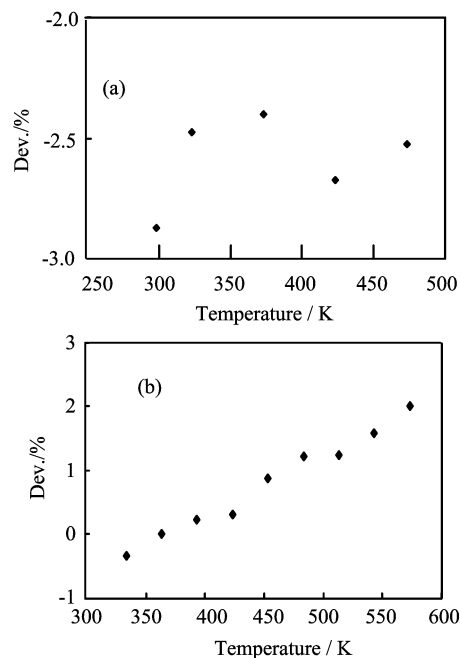
FIG. 1 (a) Improved energy potential obtained by the inversion method for the benzene-methanol system. (b) Initial crude L - J potential.

In Figs. 2 and 3 we show the deviation plots for the calculated properties of these systems.

As can be seen the most deviations points are within

TABLE II The reduced collision integrals and their ratios for methane-tetrafluoromethane system.

$\lg T^*$	$\Omega^{*(1,1)}$	$\Omega^{*(2,2)}$	A^*	B^*	C^*	E^*	F^*
0	1.364617	1.523185	1.1162	1.194339	0.853146	0.887152	0.928771
0.099991	1.236912	1.376548	1.112891	1.168386	0.862953	0.89371	0.936125
0.200002	1.129867	1.253639	1.109545	1.146521	0.8753	0.903544	0.945345
0.300008	1.041264	1.152939	1.107249	1.129659	0.888393	0.914706	0.955606
0.400002	0.968186	1.071241	1.106441	1.117659	0.900866	0.92556	0.966037
0.500003	0.907577	1.004791	1.107114	1.109974	0.911787	0.935174	0.975912
0.600003	0.856624	0.950123	1.109148	1.105364	0.920729	0.943063	0.984751
0.700002	0.813016	0.904217	1.112176	1.103186	0.927625	0.949088	0.992296
0.800002	0.774776	0.864653	1.116004	-14.92250	0.932737	0.953463	0.99871
0.900001	0.740533	0.829551	1.120207	6.068851	5.149236	0.95641	1.003907
1	0.709161	0.797643	1.12477	6.078457	5.160855	0.958294	1.007996
1.099991	0.679824	0.768013	1.129723	6.095311	5.16655	0.959468	1.011057
1.200002	0.651942	0.740138	1.135282	6.119430	5.16644	0.960076	1.013331
1.300008	0.624962	0.713424	1.141549	6.148011	5.161109	0.959871	1.015364
1.400002	0.598517	0.686183	1.146473	6.173078	5.152216	0.958786	1.017683
1.500003	0.57249	0.660497	1.153727	6.186210	5.142357	0.955616	1.020401
1.600003	0.546989	0.633081	1.157392	6.181350	5.134745	0.952291	1.023096
1.700002	0.522251	0.604989	1.158425	6.156605	5.132471	0.949281	1.025438
1.800002	0.498684	0.576772	1.156589	6.110412	5.137825	0.973109	1.027215
1.900001	0.476669	0.548996	1.151741	6.040727	5.152756	0.946003	1.028529
2	0.456464	0.522334	1.144327	5.950618	5.178657	0.900468	1.029403

FIG. 2 Deviation plot for the calculated viscosity coefficients at different temperatures and compositions in gaseous binary mixtures of (a) $\text{CF}_4\text{-CH}_4$ and (b) benzene-methanol.FIG. 3 Deviation plot for the calculated diffusion coefficients of equimolar binary gaseous mixtures of (a) $\text{CF}_4\text{-CH}_4$ and (b) benzene-methanol at different temperatures.

0–2.5% for viscosity and to maximum 3% for diffusion coefficient. This is of great importance to note that the benzene-methanol mixture is a nonpolar-polar sys-

tem which includes large and nonspherical molecule and the results show the ability of inversion method for describing this system in addition to nonpolar-spherical

TABLE III Comparison of calculated and experimental values of viscosity coefficients for methane-tetrafluoromethane system.

T/K	X_{CF_4}	$\eta/(\mu Pa \cdot s)$		Dev. %
		Exp. [27]	Calc.	
296.15	0.7734	16.68	17.05	-2.20
	0.5844	15.97	16.28	-1.97
	0.4105	15.04	15.32	-1.83
	0.2186	13.60	13.81	-1.54
323.15	0.7734	18.03	18.31	-1.58
	0.5844	17.27	17.49	-1.29
	0.4105	16.26	16.45	-1.16
	0.2186	14.70	14.83	-0.88
373.15	0.7734	20.32	20.50	-0.89
	0.5844	19.46	19.59	-0.69
	0.4105	18.26	18.44	-0.10
	0.2186	16.55	16.65	-0.59
422.15	0.7734	22.46	22.54	-0.35
	0.5844	21.48	21.55	-0.31
	0.4105	20.24	20.28	-0.21
	0.2186	18.29	18.32	-0.16
468.15	0.7734	24.53	24.56	-0.12
	0.5844	23.49	23.48	0.02
	0.4105	22.10	22.12	-0.07
	0.2186	19.96	19.98	-0.12

TABLE IV Calculated and experimental values of diffusion coefficients for equimolar binary gaseous mixtures of methane-tetrafluoromethane system and benzene-methanol system at different temperatures.

T/K	$10^4 D_{exp.}^a / (m^2/s)$	$10^4 D_{calc.} / (m^2/s)$	Dev. %
Methane-tetrafluoromethane			
298.15	0.139	0.143	-2.88
323.15	0.161	0.161	-2.48
373.15	0.209	0.214	-2.39
423.15	0.261	0.268	-2.68
473.15	0.318	0.326	-2.52
Benzene-methanol system			
333.15	0.0738	0.0740	-0.34
363.15	0.0873	0.0873	0.00
393.15	0.1022	0.1019	0.22
423.15	0.1183	0.1179	0.30
453.15	0.1356	0.1344	0.87
483.15	0.1542	0.1523	1.22
513.15	0.1739	0.1717	1.24
543.15	0.1948	0.1917	1.58
573.15	0.2168	0.2124	2.01
603.15	0.2400	0.2345	2.27

^a $D_{exp.}$ for methane-tetrafluoromethane and benzene-methanol systems from Ref.[27] and Ref.[28] respectively.

TABLE V Comparison of calculated and experimental values of viscosity coefficients for the gaseous binary mixtures of benzene- methanol system.

$X_{benzene}$	T/K	$\eta/(\mu Pa \cdot s)$		Dev. /%	
		Exp. [28]	Clac.		
0.7767	372	9.882	10.074	-1.94	
	403	10.708	10.874	-1.55	
	441.02	11.720	11.812	-0.79	
	479.02	12.735	12.777	-0.33	
	520.19	13.821	13.845	-0.18	
	561.06	14.940	14.831	0.73	
	601.21	16.038	15.833	1.28	
	637.03	16.988	16.766	1.30	
	0.5929	346.82	9.653	9.852	-2.06
		378	10.522	10.655	-1.26
		414.56	11.545	11.640	-0.82
		497.36	13.848	13.799	-0.35
536.29		14.926	14.833	-0.62	
580.96		16.179	15.963	1.32	
627.38		17.514	17.209	1.74	
0.416		363.21	10.592	10.747	-1.46
		396.37	11.569	11.620	-0.80
		433.88	12.672	12.693	-0.17
		470.94	13.754	13.691	0.46
		514.91	15.044	14.940	0.69
	557.93	16.308	16.089	1.34	
	604.38	17.693	17.347	1.96	
	626.65	18.353	17.973	2.07	
	0.1989	369.33	11.396	11.650	-2.23
		400.23	12.377	12.564	-1.51
		436.94	13.523	13.640	-0.86
		478.47	14.831	14.835	-0.03
518.76		16.088	16.060	0.17	
555.66		17.250	17.114	0.79	
595.42		18.520	18.251	1.45	
637.82		19.863	19.520	1.73	
0.1903		364.67	11.261	11.549	-2.56
		398.32	12.333	12.542	-1.69
		436.44	13.546	13.664	-0.87
		515.66	16.071	16.010	0.38
	558.25	17.427	17.236	1.10	
	604.62	18.907	18.574	1.76	
	628.89	19.670	19.302	1.87	

(noble) gas mixtures where the method is proposed at first [22]. The results represent the advantage of the method used for predicting transport properties without introducing complicated potential functions and related mathematical problems and its ability to predict a transport property (diffusion) by having another one (viscosity) with acceptable accuracy.

IV. CONCLUSION

According to kinetic theory of gases and using the semi-empirical inversion method we extract the pair potential functions in the binary gaseous mixtures of benzene-methanol and methane-tetrafluoromethane systems. Then using collision integrals and the extended corresponding-states law we calculated viscosity and diffusion coefficients in these mixtures over a wide range of temperature and composition. It is worthwhile to note that we selected a mixture having large and nonspherical molecule (benzene) and also test the polar-nonpolar system to examine the ability of the inversion treatment. The results show that accuracy of method in mixtures is acceptable meanwhile the advantage of using a property (viscosity) to predict another one (diffusion coefficient) even for mixtures including polar molecules, is demonstrated as well.

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