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반실험적 반전 방법을 이용한 이성분계 기체 혼합물의 점도와 확산계수 계산

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

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요 약. 넓은 범위의 온도와 조성 하에 있는 벤젠-톨루엔, 벤젠- 페놀, 벤젠- p-자일렌의 이성분계 기체 혼합물에 대한 점도와 확산계수를 반실험적 반전 방법을 사용하여 예측하였다. 점도와 확산계수에 대한 정확도는 각각 3%와 4% 이내이다.
주제어: 반전 방법, 운반 성질, 점도, 확산계수

ABSTRACT. Viscosity and diffusion coefficients for the gaseous binary mixtures of benzene- toluene, benzene-phenol and benzene-p-xylene over a wide range of temperature and composition have been predicted using the semi-empirical inversion method. The accuracies are within 3% and 4% for viscosities and diffusion coefficients, respectively.
Keywords: Inversion method, Transport properties, Viscosity, Diffusion coefficient

INTRODUCTION

Transport properties of gaseous mixtures are of great importance 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 absent of data over a wide range of temperature, pressure and composition, the semi-empirical methods are interested. The semi-empirical inversion method has been used extensively 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 fact 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 probably easiest to measure and most 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, for example viscosity, are slightly different from those obtained from other ones, say diffusion.

A desirable and reliable manner of solving the problem would be to obtain potential energy u(r), directly from the experimental data without explicit assumption of a mathematical model for u(r), is the semi-empirical inversion method which is developed by Smith and coworkers.[12-15]

The present work while describes an iterative method for generating the effective pair potential energy for gaseous binary mixtures of benzene-toluene, benzene-phenol and benzene-p-xylene systems, then use 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 3% and 4%, respectively.

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, u(r). The superscripts l and s appearing in Ω denote weighting factors that 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:

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

Where,

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

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:

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

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 range parameter σ 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:

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

where reduced temperature T^* is defined as:

$$T^* = kT/\varepsilon, \quad (6)$$

in which the energy parameter ε represent the depth of the potential energy well.

We have shown that three successive numerical integrations (equations 1-1 to 1-3) should be 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:

Pure gas,

Viscosity,

$$\eta = \frac{5}{16}\left(\frac{mKT}{\pi}\right)^{\frac{1}{2}}\frac{f_\eta}{\sigma^2\Omega^{*(2,2)}(T^*)} \quad f_\eta = 1+\left(\frac{3}{196}\right)(8E^*-7)^2 \quad (7)$$

Self-diffusion coefficient,

$$D = \frac{3}{8P}\left(\frac{(kT)^3}{\pi m}\right)^{\frac{1}{2}}\frac{f_D}{\sigma^2\Omega^{*(1,1)}} \quad f_D = 1+\frac{1}{8}\frac{(6C^*-5)^2}{2A^*+5} \quad (8)$$

The ratios of the calculated collision integrals have been determined by the following equations:

$$A^* = \frac{\Omega^{*(2,2)}}{\Omega^{*(1,1)}} \quad (9)$$

$$B^* = \frac{\left\lfloor 5\Omega^{*(1,2)} - 4\Omega^{*(1,3)}\right\rfloor}{\Omega^{*(1,1)}} \quad (10)$$

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

$$E^* = \frac{\Omega^{*(2,3)}}{\Omega^{*(2,2)}} \quad (12)$$

$$F^* = \frac{\Omega^{*(3,3)}}{\Omega^{*(1,1)}} \quad (13)$$

$$H^* = \frac{\left(3B^*+6C^*-\frac{35}{4}\right)}{(6C^*-5)} \quad (14)$$

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:

$$[\eta_{mix}] = -\frac{\begin{bmatrix} H_{11} & H_{12} & H_{13} & \dots & H_{1\upsilon} & x_1 \\ H_{12} & H_{22} & H_{23} & \dots & H_{2\upsilon} & x_2 \\ H_{13} & H_{23} & H_{33} & \dots & H_{3\upsilon} & x_2 \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ H_{1\upsilon} & H_{2\upsilon} & H_{3\upsilon} & \dots & H_{\upsilon\upsilon} & x_\upsilon \\ x_1 & x_2 & x_3 & \dots & x_\upsilon & 0 \end{bmatrix}}{\begin{bmatrix} H_{11} & H_{12} & H_{13} & \dots & H_{1\upsilon} \\ H_{12} & H_{22} & H_{23} & \dots & H_{2\upsilon} \\ H_{13} & H_{23} & H_{33} & \dots & H_{3\upsilon} \\ \cdot & \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ H_{1\upsilon} & H_{2\upsilon} & H_{3\upsilon} & \dots & H_{\upsilon\upsilon} \end{bmatrix}} \tag{15}$$

Where,

$$H_{ii} = \frac{x_i^2}{[\eta_i]} + \sum_{\substack{k=1 \\ k\neq 1}}^{\upsilon} \frac{2x_i x_k}{[\eta_{ik}]} \frac{m_i m_k}{(m_i+m_k)^2}\left[\frac{5}{3A_{ik}^*} + \frac{m_k}{m_i}\right]\pi \tag{16}$$

$$H_{ij}(i\neq j) = -\left(\frac{2x_i x_j}{\eta_{ij}}\right)\left(\frac{m_i m_j}{(m_i+m_j)^2}\right)\left(\frac{5}{3A_{ij}^*} - 1\right) \tag{17}$$

$$\eta_{ij} = \frac{5}{16}\left[\left(\frac{2m_i m_j}{(m_i+m_j)^2}\right)\frac{kT}{\pi}\right]^{\frac{1}{2}} \frac{1}{\sigma_{ij}^* \Omega_{ij}^{(2,2)*}(T_{ij}^*)}. \tag{18}$$

A_{ij}^* is the ratio of the collision integrals defined by equation (1.9), x is the mole 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:

$$D_{ij} = \frac{3}{8}\left[\left(\frac{m_i+m_j}{2m_i m_j}\right)\frac{kT}{\pi}\right]^{\frac{1}{2}} \frac{kT}{P}\left(\frac{1+\Delta_{ij}}{\sigma_{ij}^2 \Omega_{ij}^{(1,1)*}}\right), \tag{19}$$

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

$$\Delta_{ij} = 1.3(6C_{ij}^* - 5)^2 \frac{a_{ij}x_{ij}}{1+b_{ij}x_{ij}}, \tag{20}$$

where

$$a_{ij} = \frac{\sqrt{2}}{8\left[1+1.8\left(\frac{m_j}{m_i}\right)\right]^2} \frac{\Omega_{ij}^{(1,1)*}(T_{ij}^*)}{\Omega_{jj}^{(2,2)*}(T_j^*)}, \tag{21}$$

$$b_{ij} = 10a_{ij}\left[1+1.8\left(\frac{m_j}{m_i}\right)+3\left(\frac{m_j}{m_i}\right)^2\right]-1 \tag{22}$$

$$x_{ij} = \frac{x_i}{x_i+x_j} \tag{23}$$

The 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:

$$r^* = r/\sigma = (\Omega^{*(2,2)})^{1/2}, \tag{24}$$

$$V^* = V/\sigma = G\ T^* \tag{25}$$

G is the inversion function which is a function of reduced temperature (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 using the integrals of equations (1.1) to (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. Our result obtained converged after two iterations.

The 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[25] was applied in order to calculate the unlike pair potential energy. The proposed viscosity correlation function is as following:

$$\Omega^{*(2,2)}(T^*) = \exp\sum_{i=0}^{6} a_i(\ln T^*) \quad (26)$$

For $0.8<T^*<500$,

where

$a_0=4.369\times10^{-1}\pm7.8\times10^{-4}$
$a_1=-4.505\times10^{-1}\pm1.3\times10^{-3}$ $a_2=5.326\times10^{-2}\pm8.1\times10^{-4}$
$a_3=3.519\times10^{-2}\pm9.2\times10^{-4}$ $a_4=-1.751\times10^{-2}\pm4.0\times10^{-4}$
$a_5=2.773\times10^{-3}\pm7.0\times10^{-5}$ $a_6=-1.529\times10^{-4}\pm4.3\times10^{-6}$

RESULTS AND DISCUSSION

The extraction of information about the forces by analyzing the bulk properties will be done if the interaction potential energy be 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 more accurately than 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 $T^*\geq1$, consequently in order to proceed to the next iteration it is necessary to extrapolate $V(r)$ at the long- range region (low temperature). The extrapolation function that we used is $V^*=-C_6u^6$, 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 three binary gas mixtures at low density by direct inversion of the viscosity collision integral equations. These accurate potential energies then have been used to produce improved collision integrals which in turn serve to calculate the transport properties.

Tables 1-3 contain the results of collision integrals and their ratios for three studied gaseous mixtures (benzene-phenol, benzene-toluene and benzene-pxylene).

***Table* 1.** The reduced collision integrals and their ratios for Benzene-Phenol system

Log T*	$\Omega^{*(1,1)}$	$\Omega^{*(2,2)}$	A*	B*	C*	E*	F*
0	1.367913	1.52346	1.113712	1.196872	0.851868	0.8861	0.925861
0.099991	1.238705	1.375504	1.110437	1.170127	0.861581	0.89269	0.93318
0.200002	1.130447	1.25161	1.107181	1.147355	0.873938	0.902734	0.942522
0.300008	1.040931	1.150372	1.105137	1.129947	0.887212	0.914308	0.953129
0.400002	0.9672	1.068633	1.104873	1.118024	0.89994	0.925494	0.964095
0.500003	0.906153	1.00243	1.106248	1.110324	0.911036	0.93528	0.974527
0.600003	0.854899	0.948037	1.108947	1.106132	0.920093	0.94327	0.983806
0.700002	0.811005	0.902383	1.112673	1.104561	0.926999	0.949343	0.99168
0.800002	0.772497	0.86306	1.117237	1.1049	0.931931	0.953594	0.998175
0.900001	0.737885	0.828105	1.122275	1.106553	0.935134	0.956402	1.003435
1	0.706026	0.796184	1.127711	1.109264	0.936917	0.958071	1.007626
1.099991	0.676092	0.76636	1.133536	1.113063	0.937516	0.958915	1.010873
1.200002	0.647458	0.738002	1.139873	1.118093	0.937069	0.959084	1.013347
1.300008	0.619648	0.710542	1.146717	1.123766	0.935708	0.958352	1.015561
1.400002	0.59234	0.683194	1.153403	1.127962	0.933776	0.956079	1.018312
1.500003	0.565494	0.654937	1.158173	1.127486	0.932061	0.951837	1.022188
1.600003	0.539422	0.62494	1.158521	1.119478	0.931727	0.946236	1.026927
1.700002	0.514858	0.593236	1.152206	1.10332	0.933857	0.940935	1.031257
1.800002	0.492657	0.560947	1.138586	1.081129	0.93911	0.938108	1.033799
1.900001	0.473615	0.529968	1.118961	1.056786	0.947252	0.939287	1.033766
2	0.458209	0.50225	1.096098	1.034103	0.957298	0.944766	1.031335

***Table* 2.** The reduced collision integrals and their ratios for Benzene-Toluene system

Log T*	$\Omega^{*(1,1)}$	$\Omega^{*(2,2)}$	A*	B*	C*	E*	F*
0	1.356781	1.536988	1.132976	1.202151	0.86163	0.88857	0.942235
0.099991	1.235327	1.38945	1.124797	1.176803	0.867722	0.893177	0.94432
0.200002	1.131019	1.264257	1.11779	1.153428	0.877296	0.902233	0.950188
0.300008	1.043105	1.161153	1.113144	1.135001	0.888667	0.913259	0.95848
0.400002	0.969727	1.077356	1.110966	1.121421	0.900088	0.923952	0.967508
0.500003	0.908346	1.008982	1.110772	1.114071	0.910383	0.933456	0.976191
0.600003	0.856412	0.952592	1.112295	1.109601	0.918931	0.941411	0.984113
0.700002	0.8117	0.905247	1.115244	1.107802	0.925531	0.947728	0.99117
0.800002	0.772328	0.864609	1.119482	1.107809	0.930307	0.952176	0.997479
0.900001	0.736893	0.82846	1.124261	1.108444	0.933531	0.954769	1.003227
1	0.704368	0.795018	1.128702	1.108232	0.935708	0.955488	1.00863
1.099991	0.674168	0.762898	1.131629	1.105802	0.937467	0.95477	1.013666
1.200002	0.64607	0.731339	1.132037	1.100801	0.939399	0.95344	1.017955
1.300008	0.620094	0.700298	1.129527	1.09366	0.941897	0.952417	1.02115
1.400002	0.596377	0.670177	1.12425	1.084881	0.945089	0.952196	1.023149
1.500003	0.575056	0.641444	1.116556	1.074733	0.948998	0.95282	1.024298
1.600003	0.556259	0.614484	1.106679	1.063049	0.953659	0.954164	1.02492
1.700002	0.540118	0.589615	1.094674	1.049816	0.959086	0.956284	1.02499
1.800002	0.526721	0.567257	1.080852	1.035932	0.965282	0.959446	1.024262
1.900001	0.516086	0.547881	1.065944	1.022559	0.971974	0.963907	1.022576
2	0.508078	0.531895	1.051127	1.011105	0.978758	0.96957	1.020093

***Table* 3.** The reduced collision integrals and their ratios for Benzene-p Xylene system

Log T*	$\Omega^{*(1,1)}$	$\Omega^{*(2,2)}$	A*	B*	C*	E*	F*
0	1.366743	1.524735	1.115599	1.19757	0.85218	0.885646	0.92655
0.099991	1.237821	1.376018	1.111646	1.1709	0.861644	0.892235	0.933436
0.200002	1.129637	1.251601	1.107967	1.148233	0.873857	0.902312	0.942457
0.300008	1.040045	1.149956	1.105678	1.130973	0.887026	5.02547	0.952856
0.400002	0.966199	1.067924	1.105284	1.118917	0.899592	5.087449	0.963682
0.500003	0.904965	1.00149	1.106662	1.111391	0.910609	0.935083	0.974044
0.600003	0.853496	0.947007	1.109563	1.107439	0.919559	0.943125	0.983298
0.700002	0.809338	0.901307	1.113635	1.106273	0.926335	0.949255	0.991158
0.800002	0.77051	0.861981	1.118716	1.107251	0.931063	0.953538	0.997649
0.900001	0.735479	0.827012	1.124455	1.109729	0.934002	0.956314	1.002935
1	0.70309	0.795003	1.130727	1.113319	0.935437	0.957765	1.007257
1.099991	0.672505	0.764856	1.137324	1.117448	0.935678	0.95812	1.010837
1.200002	0.643143	0.735761	1.144008	1.121806	0.935021	0.95754	1.01387
1.300008	0.614648	0.707107	1.150425	1.125545	0.933775	0.956027	1.016685
1.400002	0.586865	0.678292	1.155788	1.127007	0.93239	0.953416	1.019782
1.500003	0.559889	0.648711	1.158643	1.123852	0.93156	0.949573	1.023565
1.600003	0.534094	0.617969	1.157043	1.114188	0.932242	0.944971	1.02788
1.700002	0.51012	0.586271	1.149281	1.097574	0.935316	0.940904	1.03175
1.800002	0.488733	0.554645	1.134862	1.075914	0.941176	0.93917	1.033904
1.900001	0.470568	0.524727	1.115092	1.052687	0.949558	0.941083	1.033634
2	0.455986	0.498195	1.092568	1.031232	0.959511	0.946877	1.031133

According to these collision integrals and their ratios we calculated the viscosities of binary mixtures using equations 1-15 to 1-18 and then compared to experimental ones.[27,28] *Tables* 4-6 contain the calculated and experimental values of viscosity coefficients for studied mixtures. The absolute deviation for quantity X is calculated according to:

$$\text{Dev } \% = \frac{\left| X^{\exp.} - X^{calc.} \right|}{X^{\exp}} \times 100$$

Experimental data for viscosity and diffusion coefficients for mixtures of benzene-toluene and benzene-p-xylene are taken from Ref. 27 and for benzene-phenol mixtures from Ref. 28.

***Table* 4.** Comparison of calculated and experimental* values of viscosity coefficients for benzene-toluene system

T(K)	η_{exp}(μPas)	η_{calc}(μPas)	Dev %
$X_{benzene}$=0.2313			
348.85	8.208	8.271	-0.77
356.37	8.381	8.439	-0.69
375.71	8.828	8.882	-0.61
417.03	9.784	9.773	0.11
459.04	10.758	10.659	0.92
496.02	11.616	11.445	1.47
539.71	12.621	12.304	2.51
572.74	13.375	12.956	3.13
614.00	14.334	13.786	3.82
632.20	14.753	14.117	4.31
$X_{benzene}$= 0.4174			
328.88	7.897	7.997	-1.27
344.19	8.251	8.336	-1.03
355.49	8.509	8.590	-0.95
383.98	9.174	9.253	-0.86
424.96	10.138	10.146	-0.08
469.70	11.190	11.112	0.70
516.18	12.275	11.873	3.27
556.00	13.201	12.892	2.34
596.69	14.139	13.719	2.97
629.16	14.887	14.324	3.78
$X_{benzene}$=0.5689			
329.38	8.007	8.150	-1.18
341.60	8.296	8.423	-1.53
354.89	8.604	8.724	-1.39
386.04	9.345	9.454	-1.17
433.32	10.474	10.506	-0.30
473.72	11.433	11.393	0.35
514.51	12.412	12.279	1.07
554.05	13.338	13.085	1.90
590.63	14.198	13.834	2.56
629.64	15.110	14.626	3.20
$X_{benzene}$=0.7872			
335.80	8.318	8.515	-2.37
344.62	8.533	8.715	-2.13
365.75	9.044	9.205	-1.78
401.95	9.928	10.071	-1.44
437.52	10.797	10.880	-0.77
475.88	11.733	11.738	-0.04
516.00	12.705	12.649	0.44
556.10	13.675	13.487	1.37
592.44	14.540	14.245	2.03
625.75	15.321	14.946	2.45

*Experimental data are taken from [27].

***Table* 5.** Comparison of calculated and experimental* values of viscosity coefficients for benzene-phenol system

T(K)	η_{exp}(μPas)	η_{calc}(μPas)	Dev %
$X_{benzene}$=0.2114			
399.77	9.963	10.223	-2.61
410.48	10.225	10.489	-2.58
430.88	10.729	10.959	-2.14
475.04	11.816	11.972	-1.32
518.47	12.884	13.004	-0.93
557.90	13.848	13.854	-0.04
596.70	14.793	14.700	0.63
637.12	15.782	15.601	1.15
$X_{benzene}$=0.3943			
402.43	9.950	10.231	-2.82
411.90	10.178	10.460	-2.77
437.11	10.791	11.035	-2.26
479.31	11.816	12.020	-1.73
518.46	12.767	12.947	-1.41
559.34	13.758	13.837	-0.57
597.62	14.700	14.688	0.08
634.41	15.591	15.521	0.45
$X_{benzene}$=0.6055			
405.65	9.925	10.251	-3.28
411.70	10.066	10.394	-3.26
435.98	10.646	10.949	-2.85
473.77	11.549	11.838	-2.50
512.67	12.483	12.762	-2.23
553.75	13.482	13.672	-1.41
591.09	14.381	14.514	-0.92
626.95	15.249	15.350	-0.66
$X_{benzene}$=0.695			
435.28	10.551	10.911	-3.41
449.79	10.894	11.248	-3.25
457.33	11.078	11.426	-3.14
497.91	12.049	12.415	-3.04
542.01	13.120	13.397	-2.11
583.31	14.129	14.327	-1.40
611.47	14.816	14.985	-1.14
634.81	15.382	15.519	-0.89
$X_{benzene}$=0.8231			
442.72	10.626	11.050	-3.99
458.00	10.985	11.410	-3.87
478.26	11.471	11.900	-3.74
520.80	12.488	12.900	-3.30
558.4	13.393	13.740	-2.59
593.43	14.243	14.550	-2.15
626.81	15.080	15.350	-1.79

*Experimental data are taken from [28].

Also according to equations 1-19 to 1-23 we calculated diffusion coefficients for equimolar binary gaseous mixtures at different temperatures in 1 atmosphere pressure. Then we compared these values with experimental reported

***Table* 6.** Comparison of calculated and experimental* values of viscosity coefficients for benzene-p-xylene system.

T(K)	η_{exp}(μPas)	η_{calc}(μPas)	Dev %
$X_{benzene}$=0.1578			
428.50	9.327	9.559	-2.91
462.76	10.079	10.260	-1.79
504.85	11.001	11.114	-1.03
524.35	11.428	11.519	-0.80
543.13	11.838	11.910	-0.61
574.39	12.513	12.475	0.03
601.93	13.109	12.982	0.97
$X_{benzene}$=0.3250			
362.19	8.151	8.378	-2.78
382.03	8.587	8.801	-2.49
415.39	9.318	9.542	-2.40
429.31	9.625	9.849	-2.33
452.86	10.154	10.319	-1.62
473.21	10.596	10.729	-1.25
488.62	10.948	11.046	-0.89
530.24	11.858	11.924	-0.55
566.01	12.643	12.616	0.21
596.29	13.309	13.186	0.92
626.39	13.971	13.765	1.47
$X_{benzene}$=0.5142			
354.84	8.240	8.464	-2.72
374.61	8.688	8.894	-2.37
399.70	9.258	9.460	-2.18
437.99	10.132	10.313	-1.79
441.19	10.204	10.378	-1.70
472.59	10.924	11.028	-0.95
508.35	11.745	11.797	-0.44
542.41	12.517	12.525	-0.06
578.13	13.321	13.211	0.82
609.85	14.073	13.833	1.71
$X_{benzene}$=0.7292			
344.61	8.295	8.637	-2.92
368.55	8.859	9.073	-2.41
397.00	9.530	9.736	-2.16
436.53	10.465	10.644	-1.71
470.29	11.266	11.368	-0.90
506.62	12.125	12.179	-0.44
543.34	12.990	12.980	0.08
547.45	13.086	13.061	0.19
579.04	13.821	13.692	0.93
606.61	14.459	14.254	1.42

*Experimental data are taken from [27].

data. Results are depicted in *Tables* 7-9.

Also deviation plots based on deviation values are demonstrated in *Figs.* 1-6.

As can be seen the most deviations points are within 0-3% for viscosity and to maximum 4% for diffusion coefficient. This is of great importance to note that the benzene-phenol mixture is a nonpolar-polar system which includes large and nonspherical molecules and the results show the ability of inversion method for describing this system in addition to nonpolar-spherical (noble) gas mix-

***Table* 7.** Calculated and experimental* values of diffusion coefficients for equimolar binary gaseous mixtures of benzene- toluene at different temperatures.

T(K)	10^4 D_{exp} (m^2 s^{-1})	10^4 D_{calc} (m^2 s^{-1})	Dev %
363.15	4.08	4.16	-1.96
393.15	4.76	4.86	-2.10
423.15	5.51	5.59	-1.45
453.15	6.31	6.35	-0.63
483.15	7.17	7.18	-0.14
513.15	8.08	8.04	0.49
543.15	9.04	8.94	1.11
573.15	10.05	9.87	1.79
603.15	11.12	10.86	2.34
633.15	12.23	11.88	2.86

*Experimental data are taken from [27].

***Table* 8.** Calculated and experimental* values of diffusion coefficients for equimolar binary gaseous mixtures of benzene-phenol at different temperatures.

T(K)	10^4 D_{exp} (m^2 s^{-1})	10^4 D_{calc} (m^2 s^{-1})	Dev %
443.15	0.0612	0.0633	-3.41
463.15	0.0668	0.0689	-3.11
483.15	0.0727	0.0748	-2.86
503.15	0.0787	0.0809	-2.79
523.15	0.0850	0.0872	-2.56
543.15	0.0916	0.0934	-1.96
563.15	0.0984	0.1000	-1.67
583.15	0.1054	0.1068	-1.33
603.15	0.1126	0.1140	-1.25
623.15	0.1202	0.1214	-1.00

*Experimental data are taken from [28].

***Table* 9.** Calculated and experimental* values of diffusion coefficients for equimolar binary gaseous mixtures of benzene-p-xylene at different temperatures.

T(K)	10^4 D_{exp} (m^2 s^{-1})	10^4 D_{calc} (m^2 s^{-1})	Dev %
393.15	4.29	4.43	-3.47
423.15	4.96	5.12	-3.30
453.15	5.68	5.83	-2.57
483.15	6.45	6.57	-1.92
513.15	7.28	7.38	-1.36
543.15	8.14	8.217	-0.95
573.15	9.05	9.07	-0.22
603.15	10.00	9.97	0.30

*Experimental data are taken from [27].

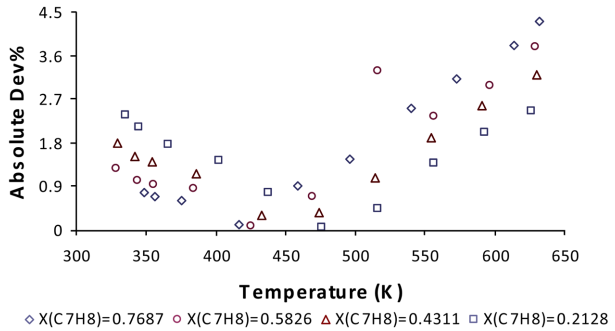

***Fig.* 1.** Deviation plot for viscosities of benzene-toluene mixtures at different compositions and temperatures.

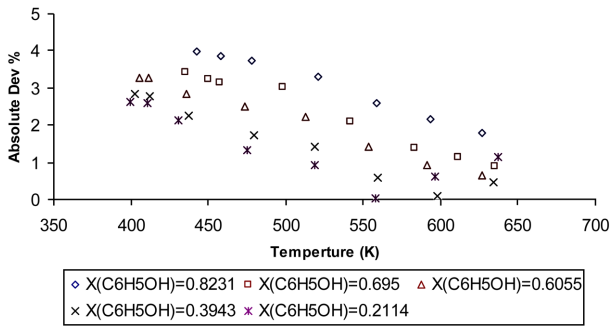

***Fig.* 2.** Deviation plot for viscosities of benzene-phenol mixtures at different compositions and temperatures.

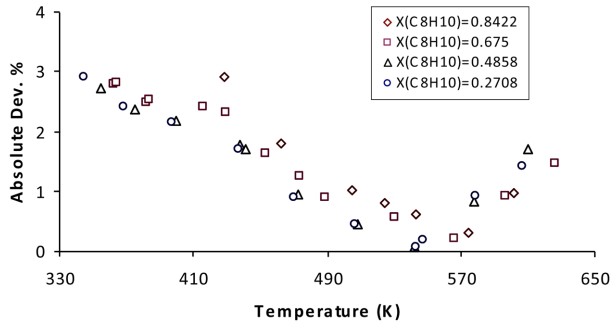

***Fig.* 3.** Deviation plot for viscosities of benzene-p-xylene mixtures at different compositions and temperatures.

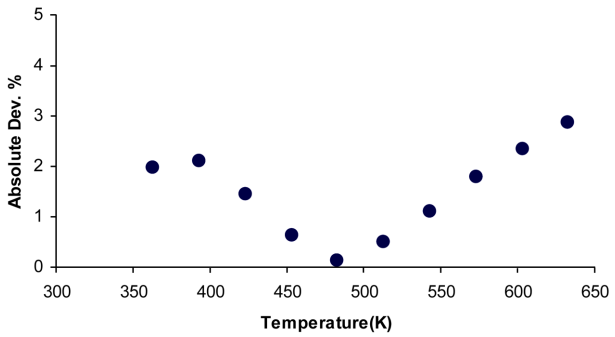

***Fig.* 4.** Deviation plot for diffusion coefficients of equimolar mixtures of benzene-toluene at different temperatures.

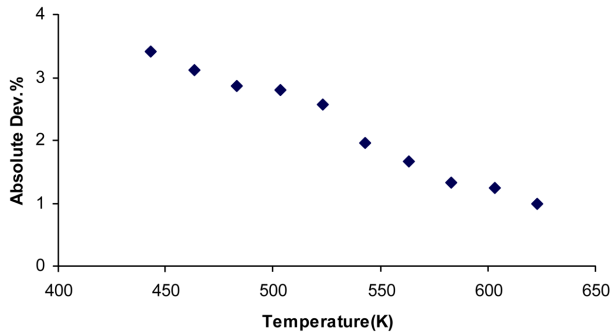

***Fig.* 5.** Deviation plot for diffusion coefficients of equimolar mixtures of benzene-phenol at different temperatures.

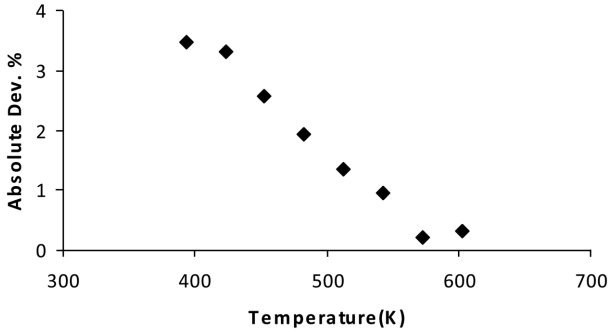

***Fig.* 6.** Deviation plot for diffusion coefficients of equimolar mixtures of benzene-p-xylene at different temperatures.

tures where the method is proposed at first.[22] The other two studied systems are also including large and nonspherical molecules but the result represents the advantage of the method used for predicting transport properties without introducing complicated potential functions and related mathematical difficulties.

CONCLUSION

According to kinetic theory of gases and using the semi-empirical inversion method we extract the pair potential function in the binary gaseous mixtures of benzene-toluene, benzene-p-xylene and benzene-phenol systems. Then using collision integrals and the extended corresponding-states law we calculated viscosity and diffusion coefficients in mixtures over a wide range of temperature and composition. It is worthwhile to note that we selected mixtures having large and nonspherical molecules and also test the polar-nonpolar system to examine the ability of the inversion treatment. The results showed 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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