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Theoretical Calculation of Transport Properties of the Noble Gases He and Ne and Their Binary Mixtures at Low Density

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Using the Tang–Toennies potential model and a set of expressions given by J. Kestin *et al.*, we calculate the transport properties of the two noble gases He and Ne and of their binary mixtures, based upon the calculation of the interaction potential. Our calculated results for the transport properties are restricted to low densities but cover the full temperature interval extending from 50 K to the onset of ionization; the mole fraction of the binary mixtures is $x_1{:}x_2 = 0.25{:}0.75$. Our results are comparable to the best theoretical results given by J. Kestin *et al.*

1. INTRODUCTION

In their research on transport properties Chapman and Cowling (1939) derived the equations for the viscosity, diffusion, and thermal diffusion of multicomponent mixtures of gases. Kestin *et al.* (1984) reported a set of easy-to-program expressions for the calculation of the thermodynamic and transport properties of the noble gases and of their binary and multicomponent mixtures for the various integrals of 15 pair potentials as functions of temperature and composition. Each pair potential is characterized by material constants which have been accurately determined by a complex numerical fit to a selected body of experimental data with considerable additional input from theory, mainly of quantum mechanical character. Thus, they calculated all properties over the whole range of temperature from absolute zero to the onset of ionization and over the complete composition range of any one of the binary and multicomponent mixtures. Until now there has been no other theoretical calculation based on the calculation of accurate interaction poten-

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tials to check the correctness of the results given by Kestin *et al.* Experimentally it is also difficult to test their results, especially near the ionization.

In this paper, based upon the accurate calculation of the interaction potential between the noble gas atoms using the Tang–Toennies potential model (Tang and Toennies, 1984), we calculate the transport properties of the two noble gases He and Ne and of their binary mixtures over the whole range of temperature from 50 K to ionization with a set of expressions given by Kestin *et al.* (1984). Our calculation also goes a long way beyond the ranges covered by direct measurements, but the secure theoretical formulation makes such an extrapolation both possible and reliable. In Section 2, we briefly describe the Tang–Toennies potential model and present our calculated potential parameters, in which the van der Waals coefficients C_6, C_8, and C_{10} are evaluated by employing Padé approximation, and the Born–Mayer parameters are determined by considering the Tang–Toennies model and the well depth and the location selected from the experimental results. In Section 3, we describe the calculation method for the transport properties as functions of temperature. In Section 4, our calculated results are compared with the best results given by Kestin *et al.* (1984). Furthermore, from the point of view of atomic and molecular physics, we point out that the different transport properties of gases are related to the different parts of the interaction potential of the corresponding systems.

2. CALCULATION OF THE INTERACTION POTENTIAL BETWEEN GASEOUS ATOMS

2.1. The Tang–Toennies Potential Model

In the Tang–Toennies model, the potential is expressed as a sum of the SCF short-range potential and the long-range attractive dispersion potential plus a correction term:

$$V(R) = V_{\mathrm{SCF}}(R) + V_{\mathrm{disp}}(R) + V_{\mathrm{corr}}(R) \qquad (1)$$

where $V_{\mathrm{SCF}}(R)$ is obtained from an accurate SCF calculation and can often be fitted by a Born–Mayer form

$$V_{\mathrm{SCF}}(R) = A_{\mathrm{SCF}} \exp(-bR) \qquad (2)$$

The dispersion potential is given by the damped dispersion series

$$V_{\mathrm{disp}}(R) = \sum_{n\geq 3} f_{2n}(R) C_{2n} R^{-2n} \qquad (3)$$

where $f_{2n}(R)$ is the so-called damping function. The undamped dispersion series is divergent mainly because of the charge overlap. The proper damping function should remove the singular point at $R = 0$ and turn the asymptotic series into a convergent series. According to Tang and Toennies (1984), these damping functions can be expressed as

$$f_{2n}(R) = 1 - e^{-bR} \sum_{k=0}^{2n} \frac{(bR)^k}{k!} \tag{4}$$

where b is the same range parameter as in the repulsive potential of equation (2). Thus these are parameter-free universal damping functions. They satisfy the boundary conditions

$$f_{2n}(R) \to 1 \qquad \text{as} \quad R \to \infty$$

$$f_{2n}(R) \to 0 + O(R^{2n+1}) \qquad \text{as} \quad R \to 0$$

It has been shown that for the H–H and H–He interaction they agree with the "exact" damping functions very well (Tang and Toennies, 1984; Tang and Yang, 1990), especially for the most important terms of $2n = 6$, 8, 10. Gutowski *et al.* (1987) carried out an elaborate *ab initio* calculation of the He–He interaction and showed that the "exact" damping functions for that system agree with equation (4) better than with any other proposed damping functions. These damping functions have been applied to several chemically different types of van der Waals interaction with vastly different dispersion coefficients; not only is satisfactory convergence of the dispersion series obtained for all of them, when added to the repulsive potential the different shapes of the potentials are also successfully predicted. The most important terms in equation (3) are C_6, C_8, and C_{10}. The higher terms can be estimated from the recursion relation (Tang and Toennies, 1984)

$$C_{2n} = \left(\frac{C_{2n-2}}{C_{2n-4}}\right)^3 C_{2n-6} \tag{5}$$

In our calculation the series is terminated at $n = 9$ and results are not significantly different from the ones obtained with the series terminated at $n = 10$, since the series is convergent.

The correction term V_{corr} represents all other contributions to the potential, such as exchange dispersion, intraatomic correlation, and higher order terms, that is,

$$V_{\text{corr}} = V_T - V_{\text{SCF}} - V_{\text{disp}} \tag{6}$$

where V_T is the true potential; it is a small term, but is very difficult to calculate. Fortunately this term is important only in the region of the potential well. This is the flexible part of the model where the interplay between theory and experiment can take place. With the major part of the potential determined by physically meaningful quantities, we can approximate this small remaining term with the help of experiment. It is reasonable to choose the same functional form for this term as either V_{SCF} or V_{disp}. In either case, V_{corr} can be absorbed into one of these terms. Therefore the complete potential model is written as

$$V(R) = Ae^{-bR} - \sum_{n\geq 3}\left(1 - e^{-bR}\sum_{k=0}^{2n}\frac{(bR)^k}{k!}\right)\frac{C_{2n}}{R^{2n}} \tag{7}$$

If A, b, C_6, C_8, and C_{10} for any system are accurately known, it has been found that the potential in the region of the potential well can be described by equation (7) with

$$A = (1 + \alpha)A_{\mathrm{SCF}} \tag{8}$$

where α is a small number varying between 0.13 and 0.19. This means that

$$V_{\mathrm{corr}} = \alpha A_{\mathrm{SCF}}e^{-bR} \tag{9}$$

The Tang–Toennies potential model offers the following principal advantages over earlier work and over most of the other models used to predict or fit van der Waals potentials. This model expression is of a simple closed form and analytic. All five parameters (A, b, C_6, C_8, and C_{10}) which are of principal importance have a simple physical meaning and in part are available from *ab initio* theory. Alternatively, we can use the dispersion coefficients and the experimentally measured well depth and the location of the well minimum R_m to determine the Born–Mayer parameters A and b (Tang and Toennies, 1978). The modified Tang–Toennies model can predict the potentials for ion–atom systems (Ahlrichs *et al.*, 1988; Skullerud and Larsen, 1990).

2.2. The van der Waals Coefficients

In this paper the upper and lower bounds of the van der Waals coefficients for the noble gas atoms are obtained by employing the [2, 1], [1, 0] Padé approximation (Langhoff and Karplus, 1976). The data for the sum rule, excitation energy, and static polarizability for the noble gases are selected from Standard and Certain (1985). Our calculated van der Waals coefficients C_6, C_8, and C_{10} are in good agreement with those of Tang *et al.*, (1976).

2.3. The Born–Mayer Parameters A and b

To find A and b we assume that R_m, ϵ, and C_{2n} are all given (Tang and Toennies, 1984), and we set $x = R/R_m$ and $U(x) = V(R)/\epsilon$, where

$$U(x) = A^*\exp(-b^*x) - \sum_{n\geq 3}^{\infty}\left[1 - \sum_{k=0}^{2n}\frac{(b^*x)^k}{k!}\exp(-bx)\right]\frac{c^*_{2n}}{x^{2n}} \tag{10}$$

where

$$A^* = A/\epsilon$$

$$b^* = bR_m$$

$$C_{2n}^* = C_{2n}/\epsilon R_m^{2n}$$

We use the reduced form of the potential (10) at the minimum $U(x)|_{x=1} = -1$ and $[dU(x)/dx]|_{x=1} = 0$. We get

$$A^* = \sum_{n \geq 3} e^{b^*} - \sum_{k=0}^{2n} \frac{(b^*)^k}{k!} \frac{2n}{b^*} C_{2n}^* - \sum_{n \geq 3} \frac{(b^*)^{2n}}{(2n)!} C_{2n}^* \qquad (11)$$

$$\sum_{n \geq 3} \left[1 - e^{-b^*} \sum_{k=0}^{2n} \frac{(b^*)^k}{k!} \left(\frac{2n}{b^*} - 1 \right) C_{2n}^* \right] - \sum_{n \geq 3} e^{-b^*} \frac{(b^*)^{2n}}{(2n)!} C_{2n}^* + 1 = 0 \qquad (12)$$

We use the above two equations to determine A^* and b^*; our results are in good agreement with those of Tang and Toennies (1984); see Table I.

Our results for the interaction potential between the noble gas atoms are in good agreement with those of the experiments. This shows that the Tang–Toennies model can take account of the divergence of the dispersion expansion and the influence of charge overlap.

3. CALCULATION OF TRANSPORT PROPERTIES

Once the interaction potential is known, the transport coefficients of noble gases can be obtained from the Chapman–Enskog solution of the integrodifferential Boltzmann equation. According to this method, the transport properties of the noble gases can be expressed as algebraic functions of the collision integrals. In this section, we summarize the formulas and numerical procedures used to compute the properties of the noble gases and their binary mixtures at low density. Low density means that their properties are determined by binary collisions.

The collision integrals are Boltzmann-like averages of transport cross section having the form (Hirschfelder *et al.*, 1964)

$$\Omega^{(l,s)}(T) = \int_0^\infty \exp(-\chi)\chi^{s+1} Q^{(l)}(KT\chi)\, d\chi \qquad (13)$$

where K is the Boltzmann constant, T is the absolute temperature, μ is the reduced mass of the colliding partners, and χ is a dimensionless quantity given in terms of the initial kinetic energy of collision E,

$$\chi = E/kT = \mu v^2/2kT \qquad (14)$$

For present purposes, it is sufficient to calculate the collision cross sections classically. The classical definition for $Q^{(l)}$ is

$$Q^{(l)} = 2\pi \int_0^\infty (1 - \cos^l\theta)b\,db \tag{15}$$

where b is the impact parameter and θ is the classical angle of deflection, which is given by

$$\theta = \pi - 2b \int_{R_0}^\infty \frac{dR}{R\{[1 - V(R)/E]R^2 - b^2\}^{1/2}} \tag{16}$$

where R_0 is the distance of closest approach, which is the largest root of

$$[1 - V(R_0)/E]R_0^2 = b^2 \tag{17}$$

The calculation of the collision integrals involves three successive integrations, all of which were carried out numerically. The collision integrals and collision cross sections are evaluated with the 15-point Gauss–Laguerre quadrature (Abramowitz and Stegun, 1970). Because there is a singularity at $R = R_0$ in the integrant of equation (16), the deflection angles were calculated by the Gauss–Mehler quadrature (Hildebrand, 1956), which is especially suited for the evaluation of such integrals. Substituting $x = R/R_0$ in (16), we obtain

$$\theta = \pi - \frac{2b}{R_0} \int_0^1 \frac{f(x)\,dx}{(1 - x^2)^{1/2}} \tag{18}$$

where

$$f(x) = \left(\frac{1 - x^2}{1 - V(R_0/x)/E - b^2x^2/R_0^2}\right)^{1/2} \tag{19}$$

The integral can then be approximated by the series

$$\int_0^1 \frac{f(x)\,dx}{(1 - x^2)^{1/2}} = \frac{\pi}{n} \sum_{j=1}^{n/2} f(\cos[(2j - 1)\pi/2n]) \tag{20}$$

where n is an even integer; to take $n = 30$ is more than sufficient for convergence.

3.1. Pure Substances

Once the collision integrals have been calculated, the transport coefficients in any order of approximation can be evaluated. In first-order approximation, the self-diffusion coefficient D_1, viscosity η_1, and thermal conductivity λ_1 are given, respectively, by

$$\begin{aligned} D_1 &= \frac{3}{8}\left(\frac{2\pi K^3 T^3}{\mu}\right)^{1/2} \frac{1}{P\Omega^{(1,1)}} \\ \eta_1 &= \frac{5}{4}(2\pi\mu KT)^{1/2}\frac{1}{\Omega^{(2,2)}} \\ \lambda_1 &= \frac{75}{32}\left(\frac{2\pi KT}{\mu}\right)^{1/2}\frac{1}{\Omega^{(2,2)}} \end{aligned} \tag{21}$$

where $p = 1.013$ bar.

In second-order approximation, the self-diffusion coefficient, viscosity, and thermal conductivity are given, respectively, by

$$\begin{aligned} D_2 &= (1 + \delta)D_1 \\ \eta_2 &= \left(1 + \frac{3}{49}\delta'\right)\eta_1 \\ \lambda_2 &= \left(1 + \frac{2}{21}\delta'\right)\lambda_1 \end{aligned} \tag{22}$$

where

$$\begin{aligned} \delta &= \left[10 + 2\frac{\Omega^{(2,2)}}{\Omega^{(1,1)}}\right]^{-1}\left[\frac{\Omega^{(1,2)}}{\Omega^{(1,1)}} - \frac{5}{2}\right]^2 \\ \delta' &= \left[\frac{\Omega^{(2,3)}}{\Omega^{(2,2)}} - \frac{7}{2}\right]^2 \end{aligned}$$

3.2. Binary Mixture

Binary diffusion coefficient:

$$\begin{aligned} D_{12} &= \frac{3}{8}\left(\frac{2\pi K^3 T^3}{\mu}\right)^{1/2}\frac{1 + \Delta}{P\Omega_{12}^{(1,2)}} \\ \Delta &= \xi(6C_{12}^* - 5)^2 a x_1/(1 + b x_1) \end{aligned}$$

where

$$\begin{aligned} \xi &= 1.3 \\ C_{12}^* &= \Omega_{12}^{(1,2)}/3\Omega_{12}^{(1,1)} \\ a &= \frac{2^{1/2}}{8(1 + 1.8c)}\frac{\Omega_{12}^{(1,1)}}{\Omega_{22}^{(2,2)}} \\ b &= 10a(1 + 1.8c + 3c^2) - 1 \\ c &= \frac{m_2}{m_1} < 1 \end{aligned} \tag{23}$$

Binary viscosity η_{mix}:

$$\eta_{12} = \frac{5}{4}\,(2\pi\mu KT)^{1/2}\,\frac{1}{\Omega_{12}^{(2,2)}} \tag{24}$$

$$\eta_{\mathrm{mix}} = \frac{1 + Z_\eta}{X_\nu + Y_\eta}$$

where

$$X_\eta = \frac{x_1^2}{\eta_1} + \frac{2x_1x_2}{\eta_{12}} + \frac{x_2^2}{\eta_2}$$

$$Y_\eta = \frac{3}{5}\,A_{12}^*\left\{\frac{x_1^2}{\eta_1}\left(\frac{m_1}{m_2}\right) + \frac{2x_1x_2}{\eta_{12}}\,\frac{(m_1 + m_2)^2}{4m_1m_2}\left(\frac{\eta_{12}^2}{\eta_1\eta_2}\right) + \frac{x_2^2}{\eta_2}\,\frac{m_2}{m_1}\right)\right\}$$

$$Z_\eta = \frac{3}{5}\,A_{12}^*\left(x\left(\frac{m_2}{m_1}\right) + 2x_1x_2\left\{\left[\frac{(m_1 + m_2)^2}{4m_1m_2}\right]\left(\frac{\eta_{12}^2}{\eta_1} + \frac{\eta_{12}^2}{\eta_2}\right) - 1\right\} + x_2^2\left(\frac{m_2}{m_1}\right)\right)$$

Binary thermal conductivity λ_{mix}:

$$\lambda_{12} = \frac{75K}{32}\left(\frac{2\pi KT}{\mu}\right)^{1/2}\frac{(1 + \Delta)}{\Omega_{12}^{(2,2)}} \tag{25}$$

$$\lambda_{\mathrm{mix}} = \frac{1 + Z_\lambda}{X_\lambda + Y_\lambda}$$

where

$$X_\lambda = \frac{x_1^2}{\lambda_1} + \frac{2x_1x_2}{\lambda_{12}} + \frac{x_2^2}{\lambda_2}$$

$$Y_\lambda = \frac{x_1^2}{\lambda_1}\,U^{(1)} + \frac{2x_1x_2}{\lambda_{12}}\,U^{(Y)} + \frac{x_2^2}{\lambda_2}\,U^{(2)}$$

$$Z_\lambda = x_1^2U^{(1)} + 2x_1x_2U^{(Z)} + x_2^2U^{(2)}$$

and

$$U^{(1)} = \frac{4}{15}\,A_{12}^* - \frac{1}{12}\left(\frac{12}{5}\,B_{12}^* + 1\right)\frac{m_1}{m_2} + \frac{1}{2}\,\frac{(m_1 - m_2)^2}{m_1m_2}$$

$$U^{(2)} = \frac{4}{15}\,A_{12}^* - \frac{1}{12}\left(\frac{12}{5}\,B_{12}^* + 1\right)\frac{m_2}{m_1} + \frac{1}{2}\,\frac{(m_2 - m_1)^2}{m_1m_2}$$

$$U^{(Y)} = \frac{4}{15} A^*_{12} \left[\frac{(m_1 + m_2)^2}{4m_1 m_2}\right] \left(\frac{\lambda^2_{12}}{\lambda_1 \lambda_2}\right) - \frac{1}{12}\left(\frac{12}{5} B^*_{12} + 1\right)$$

$$- \frac{5}{32A^*_{12}} \left(\frac{12}{5} B^*_{12} - 5\right) \frac{(m_1 - m_2)^2}{m_1 m_2}$$

$$U^{(Z)} = \frac{4}{15} A^*_{12} \left\{\left[\frac{(m_1 + m_2)^2}{4m_1 m_2}\right] \left(\frac{\lambda_{12}}{\lambda_1} + \frac{\lambda_{12}}{\lambda_2}\right) - 1\right\} - \frac{1}{12}\left(\frac{12}{5} B^*_{12} + 1\right)$$

where

$$A^*_{12} = \frac{1}{2} \frac{\Omega^{(2,2)}_{12}}{\Omega^{(1,1)}_{12}} \tag{26}$$

$$B^*_{12} = (5\Omega^{(1,1)}_{12} - \Omega^{(1,3)}_{12})/(3\Omega^{(1,1)}_{12})$$

and x_1, x_2 are mole fractions and m_1, m_2 are the masses of the atoms, with subscript 1 denoting the heavier component and subscript 2 the lighter one.

4. RESULTS AND DISCUSSION

We have calculated the interaction potential between the noble gas atoms by employing the potential parameters in Table I and the Tang–Toennies model. We then calculated the transport properties of the two noble gases He and Ne: viscosity, thermal conductivity, self-diffusion, and binary diffusion coefficients. Our calculated transport properties are listed in Tables II–IV. In order to compare our results with others, we also list the best results given by Kestin *et al.*

It is well known that the different transport properties of gases are sensitive in different degrees to the different parts of the potential between gaseous atoms. So in order to check the accuracy of our calculated interaction potential, we have to calculate the viscosity, thermal conductivity, self-diffusion, and binary diffusion coefficients of the corresponding system at the same time. From the point of view of atomic and molecular physics, diffusion

Table I. Potential Parameters (a.u.) Used in the Tang–Toennies Model for Noble Gas Atoms He and Ne

System	R_m	ϵ	C_6	C_8	C_{10}	A	b
He–He	5.608	3.42E-5	1.462	4.11002	83.500	19.988	62.3751
Ne–Ne	5.834	1.34E-4	6.870	75.0000	1101.000	125.4183	2.3685
He–Ne	5.751	6.50E-4	3.1455	32.7279	443.865	50.3599	3.3698

Table II. Comparison of Present Results with Those of Kestin *et al.* (1984) for Transport Properties of Helium as a Function of Temperature

	η (upa · s)		λ (mW/mK)		D(1.013 bar) (cm^2/sec)	
T (K)	Kestin	Present	Kestin	Present	Kestin	Present
50.	6.04	6.02	47.17	47.11	0.0888	0.0822
100.	9.66	9.36	75.54	73.25	0.2874	0.2645
150.	12.61	12.20	98.63	95.44	0.5669	0.5217
200.	15.26	14.79	119.32	115.69	0.9188	0.8478
250.	17.72	17.25	138.53	134.86	1.3378	1.2389
300.	20.04	19.58	156.66	153.05	1.8200	1.6892
273.	18.81	18.33	147.04	143.32	1.5534	1.4385
293.	19.73	19.25	154.23	150.54	1.7503	1.6226
313.	20.63	20.16	161.29	157.65	1.9569	1.8158
333.	21.52	21.06	168.22	165.65	2.1731	2.0179
353.	22.40	21.95	175.04	171.55	2.3986	2.2289
373.	23.25	22.82	181.75	178.36	2.6333	2.4492
423.	25.35	24.96	198.11	195.08	3.2597	3.0386
473.	27.38	27.03	213.96	211.26	3.9411	3.6805
523.	29.35	31.02	229.37	227.03	4.6761	4.3737
573.	31.28	31.02	244.39	242.42	5.4632	5.1175
623.	33.16	32.95	259.07	257.28	6.3014	5.9108
673.	35.00	34.88	273.44	272.22	7.1895	6.7528
723.	36.80	36.69	287.54	286.70	8.1266	7.424
773.	38.58	38.51	301.39	300.90	9.1119	8.5789
873.	42.04	42.05	328.43	328.60	11.2242	10.5900
973.	45.41	45.49	354.70	355.45	13.5207	12.7816
1073.	48.69	48.83	380.30	381.57	15.9970	15.1508
1173.	51.90	52.09	405.33	407.01	18.6491	17.6913
1273.	55.04	55.28	429.84	431.92	21.4733	20.4006
1773.	69.96	70.30	546.30	549.26	38.0791	36.3932
2273.	83.94	84.24	655.33	658.13	58.6286	56.2840
2773.	97.24	97.45	759.14	761.29	82.9239	79.9009
3273.	110.04	110.14	859.01	860.354	110.8216	107.1223

coefficients are used to describe the statistical mean diffusive behavior when gaseous atoms are separated at a certain distance. Here the long-range attractive dispersion potential between gaseous atom plays a leading role because of less charge overlap. So to a great extent, what is good or bad in a calculated result for diffusion reflects directly the small or large deviation of the long-range attractive potential between the theoretical calculation and the real value below the ionization. However, viscosity and thermal conductivity describe statistical mean viscous and thermal conductive behavior when the gaseous atoms are close to each other. Here the short-range repulsive potential plays a leading role because of greater charge overlap. So what is good or bad in the calculated results for viscosity and thermal conductivity reflects

Table III. Comparison of Present Results with Those of Kestin *et al.* (1984) for Transport Properties of Neon as a Function of Temperature

	η (upa·s)		λ (mW/mK)		D(1.013 bar) (cm^2/sec)	
T (K)	Kestin	Present	Kestin	Present	Kestin	Present
50.	7.70	7.53	11.89	11.74	0.0206	0.0210
100.	14.39	15.01	22.25	23.47	0.0766	0.0793
150.	19.72	20.48	30.54	32.01	0.1589	0.1581
200.	24.29	24.98	37.63	39.08	0.2627	0.2658
250.	28.36	28.96	43.96	45.35	0.3851	0.3924
300.	32.10	32.53	49.77	50.95	0.5245	0.5348
273.	30.13	30.64	46.71	47.98	0.4476	0.4560
293.	31.60	32.06	49.00	50.19	0.5045	0.5140
313.	33.04	33.42	51.22	52.34	0.5639	0.5744
333.	34.43	34.75	53.39	54.42	0.6258	0.6374
353.	35.80	36.06	55.51	56.48	0.6901	0.7031
373.	37.13	37.33	57.58	58.45	0.7570	0.7714
423.	40.35	40.38	62.57	63.24	0.9345	0.9516
473.	43.42	43.33	67.34	67.85	1.1268	1.1469
523.	46.38	46.15	71.93	72.26	1.3328	1.3558
573.	49.25	48.91	76.38	76.58	1.5518	1.5795
623.	52.03	51.59	80.69	80.76	1.7835	1.8161
673.	54.74	54.19	84.90	84.83	2.0277	2.0661
723.	57.39	56.75	89.00	88.83	2.2842	2.3289
773.	59.99	59.25	93.02	92.75	2.5527	2.6045
873.	65.02	64.15	100.83	100.39	3.1256	3.1944
973.	69.89	68.90	108.36	107.81	3.7451	3.8342
1073.	74.60	73.53	115.67	115.05	4.4100	4.5228
1173.	79.19	78.05	122.78	122.11	5.1194	5.2563
1273.	83.67	82.47	129.72	129.00	5.8722	6.0354
1773.	104.72	103.50	162.33	161.82	10.2579	10.5812
2273.	124.15	123.16	192.41	192.53	15.6205	16.1571
2773.	142.44	141.81	220.73	221.66	21.8983	22.7045
3273.	159.85	159.69	247.69	249.58	29.0462	30.1799

directly the small or large deviation of the short-range repulsive potential between the theoretical calculation and the active value.

From the Tables II–IV we can see that our calculated transport properties are in good agreement with the results given by Kestin *et al.* within an acceptable tolerance. As we analyzed above, our calculated long-range attractive dispersion potential and short-range repulsive potential are both accurate, owing to the reasonableness of the Tang–Toennies potential model and the choice of potential parameters as well as the correctness of the method of computation. From Tables II–IV we also find that all our calculated transport properties increase with the increase of the temperature of the system. Our calculated diffusion coefficients decrease with the increase of gaseous mass

Table IV. Comparison of Present Results with Those of Kestin *et al.* (1984) for Transport Properties of a Binary Mixture of Helium and Neon with $X_{He} = 0.25$ and $X_{Ne} = 0.75$ as a Function of Temperature

	η (upa · s)		λ (mW/mK)		D(1.013 bar) (cm^2/sec)	
T (K)	Kestin	Present	Kestin	Present	Kestin	Present
50.	7.72	7.65	16.93	16.88	0.0510	0.0512
100.	14.00	14.43	29.79	30.45	0.1751	0.1739
150.	18.98	19.42	40.17	40.88	0.3500	0.3486
200.	23.27	23.59	49.16	49.71	0.5676	0.5647
250.	27.11	27.33	57.09	57.68	0.8252	0.8198
300.	30.66	30.73	64.69	65.01	1.1182	1.1136
273.	28.79	28.92	60.67	61.12	0.9567	0.9499
293.	30.19	30.26	63.68	64.01	1.0761	1.0686
313.	31.55	31.57	66.61	66.84	1.2007	1.1931
333.	32.88	32.84	69.47	69.60	1.3307	1.3231
353.	34.18	34.10	72.26	72.33	1.4658	1.4590
373.	35.45	35.32	74.99	75.00	1.6061	1.6002
423.	38.53	38.27	81.59	81.49	1.9790	1.9775
473.	41.49	41.14	87.92	87.79	2.3830	2.3891
423.	44.34	43.88	94.02	93.86	2.8174	2.8312
573.	47.10	46.57	99.95	99.78	3.2816	3.3031
623.	49.78	49.18	105.72	105.53	3.7747	3.8053
673.	52.40	51.72	111.35	111.17	4.2963	4.3369
723.	54.96	54.22	116.85	116.70	4.8458	4.8975
773.	57.49	56.67	122.25	122.12	5.4226	5.4864
873.	62.34	61.46	132.76	132.72	6.6465	6.7481
973.	67.05	66.11	142.93	142.99	7.9946	8.1183
1073.	71.63	70.65	152.82	153.03	9.4340	9.5948
1173.	76.08	75.08	162.16	162.83	10.9723	11.1772
1273.	80.42	79.40	171.97	172.42	12.6071	12.8601
1773.	100.89	99.99	216.33	217.93	22.1668	22.7340
2273.	119.82	119.22	257.58	260.46	33.9092	34.9363
2773.	137.66	137.43	296.55	300.80	47.7071	49.3331
3273.	154.67	154.86	333.81	339.48	63.4673	65.8327

(in the case of pure gases) or the reduced mass (in the case of binary gases). This is not different from what actually occurs. This shows that it is correct to proceed from the microscopic interaction potential to macroscopic transport properties by statistical principles. We can calculate all the transport properties over the full range of composition with our program.

In this paper, starting from the microscopic interaction Tang–Toennies potential model, we obtained transport properties by statistical principles. Then we investigated the reasonableness of the microscopic interaction potential model by combining our calculated results for the transport properties.

We have obtained a great deal of data on the behavior of gaseous matter under high temperatures.

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