Interaction potential of K^+ in Ar: A Monte Carlo simulation mobility-comparison test

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A standarized Monte Carlo simulation (MCS) procedure is used as a routine test of the accuracy of any interaction potential of an ion-atom binary pair. By capitalizing on the performance of a supercomputer, the procedure achieves a highly realistic simulation of the ionic motion and calculates the resulting mobilities of the ions in the neutral gas. These values are then compared against accurate experimental values, assumed available. For cases where the same interaction potential has also been used as input for kinetic-theory calculations of mobilities, the procedure may be extended to check the accuracy of the theory itself. The interaction potentials of Lamm *et al.* [J. Chem. Phys. **74**, 3042 (1981)]; Budenholzer, Gislason, and Jorgensen [J. Chem. Phys. **78**, 5279 (1983)]; and Koutselos, Mason, and Viehland [J. Chem. Phys. **93**, 7125 (1990)] for the K^+-Ar pair as an illustrative case study are examined. The calculations indicate that the potential of Koutselos, Mason, and Viehland is the most accurate currently available. Furthermore, a comparison of the MCS calculations with the two-temperature theoretical mobilities of Lamm *et al.* and the three-temperature mobilities of Koutselos, Mason, and Viehland suggests that both theories are quite accurate at both the low- and high-ionic-drift-energy regions, but are up to about 2% too high at the intermediate-energy region.

INTRODUCTION

The accurate determination of the interaction potential of a binary atomic system is an endeavor necessary not only for the fundamental understanding of atomic forces but also in many applications such as plasma confinement, gas lasers, chemical kinetics, and the transport of heat and sound in a gas. The interatomic force between an alkali-metal ion and a monatomic rare-gas molecule represents a class of binary systems with three special advantages for its conducive theoretical and experimental investigations:

(1) Theoretically, they involve only fully closed spinless electronic shells with no fine-structure splitting so that the interaction is nonresonant, spherically symmetric, adiabatic and totally elastic up to fairly high collision energies, thus greatly reducing the complexity of the formidable computations required.

(2) Experimentally, the low ionization potential of the alkali-metal atoms makes their ions easy to produce as a purely ground-state species, such as by thermionic emission or uv photon impact. Furthermore, the electric charge on the ion makes its trajectory and energy easy to control electrically, thus simplifying the acquisition of accurate experimental data relevant to the interaction, such as scattering angle or ion swarm transport properties. At the same time, well-developed mass spectrometric methods afford a simple means for both the separation and the identification of different isotopic species.

(3) Unlike the case of atom-atom interactions, the first nonzero term in the long-range limit of ion-atom interaction is the well-established induced dipole polarization force which may be calculated from the neutral polarizability alone, so that this accurately known interaction serves as an authentic check for the asymptotic limit of any proposed interaction law.

For the above reasons, the alkali-metal-ion–rare-gas system offers the most idealized situations for a reliable test on theoretical interaction models. Among the possible procedures for a routine test, the Monte Carlo simulation (MCS) method which compares the MCS calculated mobility values derived from an assumed potential interaction with the available values obtainable from direct experimental measurements is both convenient and realistic, provided enough computing power is available. By making no *a priori* assumption other than the input interaction force between the colliding particles, the MCS offers a reliable and unbiased test for (a) the interaction force itself, and (b) any kinetic theory used to derive the theoretical mobility from this interaction. With the advent of supercomputing power today, the MCS can be readily stretched to achieve accuracies beyond the reach of currently available experimental data.

The K^+-Ar pair which typifies the interaction of two identical closed $^1S_0$ shells is used as an illustrative case in this paper.

THEORETICAL MODELS AND CALCULATIONS

Broadly speaking, four different approaches or their combinations have been used to calculate the interaction potential of the ion-atom pair. First, it is possible in principle to calculate *ab initio* the many-electron system wave function using different choices of primitive basis functions such as Slater-type orbitals (STO's), Gaussian-type orbitals (GTO's), elliptical orbitals (EO's), or some combinations of these [1]. The major problem with these calculations is the inordinate amount of computation time needed and the unpredictable dependence on the convergence of the iterations involved to arrive at sufficiently

accurate values. Consequently such calculations are only restricted to very simple ion-atom pairs and have not yet been successfully attempted for the K^+-Ar pair.

Second, there are various theoretical models or their variants which use appropriate localized approximation schemes to simplify the mathematics. Such methods are computationally more tractable, and potential information has been obtained, with fair success, using the coupled-electron-pair approximation (CEPA) with electron correlations [2], the self-consistent-field (SCF) and configuration-interaction (CI) techniques [3], and the statistical scaled electron-gas-cloud model [4]. Unfortunately most methods still do not yield results better than about 5%.

Third, a semiempirical functional form of the interaction potential is first assumed in accordance with physical understanding of the interaction force. Parameters of the analytic form are then adjusted to yield the best fit with experimental data. All the analytic functions describing the potential should necessarily yield the asymptotic long-range limit of an inverse fourth power attractive inductive potential, a sharp short-range electron core repulsion, and a medium-range combination of induction and dispersion forces. Of these, only the long-range potential is well established. The short-range region has been variously approximated to be either a Morse-type double exponential decay function, or more simply a Born-Mayer single exponential decay type, or just a central inverse nth power repulsive potential. The intermediate-range region has often been glossed over with a cubic spline fit, or with physically more meaningful inverse sixth and eighth power inductive and dispersive terms. In general, the resulting potential shape contains a broad spread around a single shallow potential minimum $V_{\min}$ at a certain internuclear distance $r_{\min}$.

Fourth, with the advent of the three-temperature kinetic theory [5] which is applicable for even large ion–to–neutral-species mass ratios and large E/N, the ratio of the electric field to the gas particle density, it is now possible to invert transport data even at high E/N to obtain interaction potentials of the alkali-metal-ion noble molecule pair in the repulsive range. This is partly because the interaction involves only monatomic particles with closed electronic configurations and hence the collision is adiabatic and totally elastic even at fairly large E/N. An alternative method more suitable for the repulsive region only is to derive the potential from single-collision studies of the differential scattering cross section of a monoenergetic ion beam by the neutral target gas. Between the two methods, there is an intermediate region of overlap in which $V(r)$ can be deduced by either approach, and thus they provide a mutual consistency test not only between the methods, but also for the ion transport theory employed in the inversion processes.

The classical formula for the ion-atom interactions due to Mason and Schamp [6] is of the 12-6-4 type, but the repulsive inverse-twelfth-power term has been found to be too hard [7]. Budenholzer, Gislason, and Jorgensen [8,9] replaced this potential with an n-6-4 (BGJ) function:

$$V(r)=C_n/r^n-C_6/r^6-C_4/r^4 \tag{1}$$

and adjusted the variable parameters to fit their experimental data for the angular scattering of a K^+ ion beam by Ar gas. They arrived at the best fit by setting $C_n=305\,806.7$, $n=10.62$, $C_6=69.302$, and $C_4=5.5300$, all quantities having been converted to atomic units. They also used a Morse-spline–van der Waals (MSV) form for the potential and found that both potential functions yielded approximately the same $V_{\min}$ and $r_{\min}$.

An example of a combined approach is the calculations by Lamm *et al.* [10] of the K^+-Ar potentials at various internuclear separations. Their experimentally obtained mobility values accurate to within 2% were used as a reference to compare theoretically obtained mobilities calculated by applying the Viehland-Mason two-temperature theory [11,12] on the theoretical potentials derived from the electron-gas Drude model of Waldman and Gordon. The theoretical potential values were then iteratively adjusted until they yielded a good match (denoted here as QL) to their experimental mobility values (denoted as LX). The final results were presented in pointwise form.

More recently, Koutselos, Mason and Viehland [13] applied a novel interaction universality and scaling law technique on the short-range exchange interaction and obtained a K^+-Ar potential (KMV) of the form

$$\begin{aligned}V(r)=&V_0[a_1\exp(-a_2r/\rho)-b_1\exp(-b_2r/\rho)]\\&-F(r)[(C_{8\text{ind}}+C_{8\text{dis}})/r^8+(C_{6\text{ind}}+C_{6\text{dis}})/r^6\\&+C_4/r^4]\,,\end{aligned} \tag{2}$$

where (in atomic units) $V_0=1.2020$, $a_1=146.98$, $a_2=1.5024$, $b_1=70.198$, $b_2=1.4041$, $\rho=0.9478$, $C_{8\text{ind}}=265.6$, $C_{8\text{dis}}=741.8$, $C_{6\text{ind}}=27.07$, $C_{6\text{dis}}=38.97$, $C_4=5.54$, and $F(r)$ is a damping parameter given by Ahlrichs, Penco, and Scoles [14],

$$F(r)=\begin{cases}1 & \text{for } r\geq 1.28r_{\min}\\ \exp[-(1-1.28r_{\min}/r)^2] & \text{otherwise}\,.\end{cases} \tag{3}$$

They further derived from this form, using the three-temperature theory, the resulting cross sections Q and hence the values of K_0 (denoted here by QKMV).

Regardless of the model used, the MCS procedure utilized here is a standardized routine which may be universally applied to test the model. In particular, the routine will be used to examine the suitability of the Lamm *et al.*, the BGJ, and KMV potentials by using them as input to our MCS calculations. Other potential data available in the literature do not contain enough information for their inclusion in these calculations.

MONTE CARLO CALCULATIONS AND RESULTS

The MCS calculations are based on the method developed by Skullerud [15], whose programs were adapted for an NEC SX1A supercomputer. The performance of the supercomputer is capitalized on to greatly enhance the speed and accuracy of the MCS calculations which necessitate high-volume computations. A detailed description of the procedure has been reported earlier [16] and will only be briefly mentioned here.

Essentially, the computation is divided into two parts. In part one, an interaction potential $V(r)$ is first assumed, and classical laws of momentum and energy conservation are applied to calculate the deflection angle $\chi(\varepsilon,b)$ of the ion in the centre-of-mass system as a function of the centre-of-mass collision energy ε and the impact parameter b. A classical treatment is appropriate because quantum-mechanical effects would only be appreciable in systems with much lower masses and at temperatures fairly close to absolute zero [17]. Small-angle scattering is handled by finding a correction to the total cross section which gives for a fixed $\chi_{\min}=0.15$ rad the same contribution to the momentum-transfer cross section as all collisions with $|\chi|<0.15$ rad. Varying $\chi_{\min}$ from 0.05 to 0.25 rad did not produce any appreciable change in the results of the calculations.

In part two, the scattering data obtained in part one with a specified interaction potential are used in a bulk simulation that keeps track of the ion trajectory (in the laboratory frame of reference) covering 2 500 000 collisions with different gas molecules for a given E/N. The mobility is computed as the ratio of the average velocity of the ion in the field direction, logged over all the free paths, to the applied electric field. All calculations are made at the chosen temperature of 295 K and computations of their standard errors are included.

Mobility values of K^+ in Ar and their standard errors calculated for the Lamm *et al.*, the BGJ, and the KMV potentials are listed in Tables I–III, respectively. The effective temperature $T_{\text{eff}}(T,E/N)$ at each pair of T and E/N values defined by the equation

$$T_{\text{eff}}(T,E/N)=T+\frac{1}{3k}MN_0^2[K_0(T,E/N)]^2(E/N)^2 \quad (4)$$

is also included as this value will be used in the subsequent comparison. Here, M is the neutral atom mass, N_0 is Loschmidt's number, $K_0(T,E/N)$ is the reduced mobility measured at absolute temperature T and at a specified E/N value, and k is Boltzmann's constant. Typically the standard error of the results is less than 3% at $E/N=4$ Td, 1% at 10 Td, 0.4% at 40 Td, 0.2% at 100 Td, and 0.1% at 500 Td (1 Td$=10^{-17}$ V cm^2). To test the effect of using different initial random number seeds on the results, repeated calculations starting with different seeds were made for the same potential at various selected E/N values. As an illustration of the results, the six values of K_0 for the BGJ potential at the less favorable E/N value of 10 Td range from 2.669 to 2.687 cm^2/V s and have a standard deviation of 0.23% which is much less than the error in the computation of the individual mobilities.

TABLE I. MCS calculated reduced mobility values of K^+ in Ar using the Lamm *et al.* potential as a function of T_{eff}.

E/N (Td)	T_{eff} (K)	K_0 (cm^2/V s)	Standard error (cm^2/V s)	(%)
5.0	297.1	2.680	0.041	1.5
10.0	303.2	2.664	0.019	0.7
15.0	313.3	2.656	0.013	0.5
20.0	327.7	2.666	0.010	0.4
25.0	346.9	2.686	0.009	0.3
30.0	371.7	2.721	0.008	0.3
35.0	403.0	2.769	0.008	0.3
35.0	403.0	2.768	0.007	0.3
42.0	458.8	2.840	0.006	0.2
50.0	540.9	2.924	0.006	0.2
65.0	755.4	3.077	0.006	0.2
80.0	1 043.5	3.188	0.005	0.2
100.0	1 513.7	3.254	0.005	0.1
100.0	1 512.6	3.253	0.005	0.1
120.0	2 053.9	3.258	0.004	0.1
140.0	2 653.0	3.234	0.004	0.1
170.0	3 601.6	3.153	0.004	0.1
200.0	4 600.2	3.058	0.004	0.1
230.0	5 681.3	2.975	0.003	0.1
260.0	6 816.4	2.896	0.004	0.1
300.0	8 394.4	2.797	0.003	0.1
360.0	10 937.2	2.671	0.003	0.1
420.0	13 607.7	2.561	0.003	0.1
500.0	17 431.3	2.441	0.002	0.1
600.0	22 617.8	2.321	0.002	0.1

TABLE II. MCS calculated reduced mobility values of K^+ in Ar using the BGJ potential as a function of T_{eff}.

E/N (Td)	T_{eff} (K)	K_0 (cm^2/V s)	Standard error (cm^2/V s)	(%)
4.0	296.3	2.659	0.071	2.7
4.0	296.3	2.652	0.082	3.1
4.0	296.3	2.645	0.052	2.0
5.0	297.0	2.653	0.045	1.7
5.0	297.1	2.696	0.041	1.5
7.0	299.0	2.662	0.041	1.5
7.0	299.1	2.689	0.029	1.1
10.0	303.2	2.669	0.029	1.1
10.0	303.2	2.673	0.023	0.9
10.0	303.3	2.687	0.020	0.8
10.0	303.2	2.676	0.033	1.2
10.0	303.2	2.673	0.023	0.9
10.0	303.3	2.679	0.018	0.7
15.0	313.6	2.683	0.020	0.7
15.0	313.4	2.666	0.012	0.4
15.0	313.2	2.649	0.010	0.4
25.0	347.3	2.696	0.009	0.3
25.0	347.4	2.700	0.008	0.3
40.0	439.1	2.798	0.008	0.3
40.0	440.3	2.809	0.005	0.2
40.0	441.3	2.819	0.008	0.3
65.0	759.1	3.090	0.006	0.2
80.0	1 067.2	3.238	0.005	0.2
100.0	1 586.7	3.351	0.006	0.2
100.0	1 589.3	3.354	0.005	0.1
130.0	2 517.5	3.381	0.005	0.2
160.0	3 514.2	3.306	0.004	0.1
200.0	4 895.2	3.161	0.005	0.2
250.0	6 702.9	2.985	0.003	0.1
320.0	9 330.1	2.769	0.003	0.1
400.0	12 462.1	2.571	0.003	0.1
500.0	16 602.3	2.381	0.002	0.1
600.0	20 891.3	2.230	0.002	0.1

TABLE III. MCS calculated reduced mobility values of K^+ in Ar using the KMV potential as a function of T_{eff}.

E/N (Td)	T_{eff} (K)	K_0 ($cm^2/V\,s$)	Standard error ($cm^2/V\,s$)	(%)
5.0	297.2	2.741	0.033	1.2
5.0	297.2	2.742	0.033	1.2
10.0	303.5	2.717	0.017	0.6
10.0	303.5	2.718	0.017	0.6
15.0	313.9	2.702	0.012	0.4
15.0	313.9	2.703	0.012	0.4
20.0	328.5	2.698	0.010	0.4
20.0	328.6	2.701	0.010	0.4
25.0	347.8	2.709	0.009	0.3
25.0	347.8	2.710	0.009	0.3
30.0	371.7	2.722	0.009	0.3
40.0	435.6	2.763	0.005	0.2
55.0	581.5	2.869	0.004	0.1
65.0	720.8	2.960	0.005	0.2
70.0	801.2	2.996	0.005	0.2
80.0	986.9	3.065	0.006	0.2
85.0	1 094.7	3.101	0.005	0.2
100.0	1 463.3	3.186	0.006	0.2
120.0	2 038.5	3.244	0.005	0.2
140.0	2 675.8	3.249	0.005	0.2
200.0	4 757.9	3.114	0.005	0.2
250.0	6 669.0	2.977	0.004	0.1
300.0	8 706.0	2.850	0.003	0.1
400.0	13 100.2	2.637	0.003	0.1
500.0	17 923.4	2.476	0.002	0.1
600.0	23 101.2	2.346	0.002	0.1

DISCUSSION

It is well known that the interaction potential of an ion-molecule system has a sensitive effect on the mobility of the ion in the neutral gas despite the statistical spread in impact parameter and energy of collision between the ion swarm and the gas. Thus a comparison of the theoretical mobility derivable from a given interaction with experimental values determined empirically should provide hard information on the accuracy of the interaction function and its likely deviation from the true function.

Figure 1 shows a comparison of the various reduced mobilities of K^+ drifting in Ar obtained by different means for E/N values up to 600 Td. Because the data have been obtained at different temperatures, it is not appropriate to compare them on the same E/N axis. Instead, they should be compared on the effective temperature, T_{eff}, axis. Support for using the T_{eff} scale combining the separate effects of the T and E/N parameters originates from the two-temperature kinetic theory whose results show that both K_0 and the collision integral $\Omega^{(1,1)}$ are functions of T_{eff} rather than of T or E/N separately [11].

In order to avoid cluttering the graph with too many data points, the calculated MCS data for each interaction potential is represented by a single smooth curve through the data points. In addition, for the closely spaced experimental points in the low T_{eff} region, only representative data points are selected. Furthermore, T_{eff} is plotted on

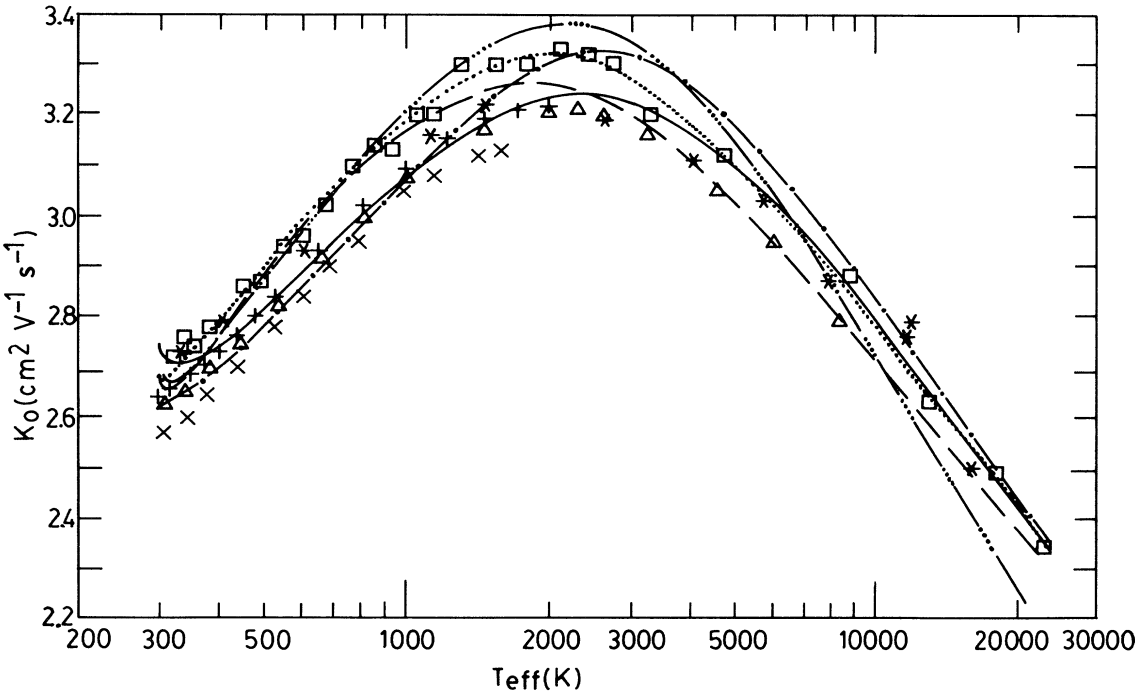

FIG. 1. Comparison between various theoretical and experimental mobility values. Lines trace calculated results and symbols show experimental measurements. —— represents MCS KMV results; — — — MCS Lamm *et al.* results; —· · · ·— MCS BGJ results; —·—·—·, QKMV results [13]; and ····· QL results [10]. The experimentally measured values are as follows: + for Cassidy and Elford [19], * for Skullerud [21]; △ for Takebe *et al* [20].; × for Creaser [18]; and □ for Lamm *et al.* (LX) [10].

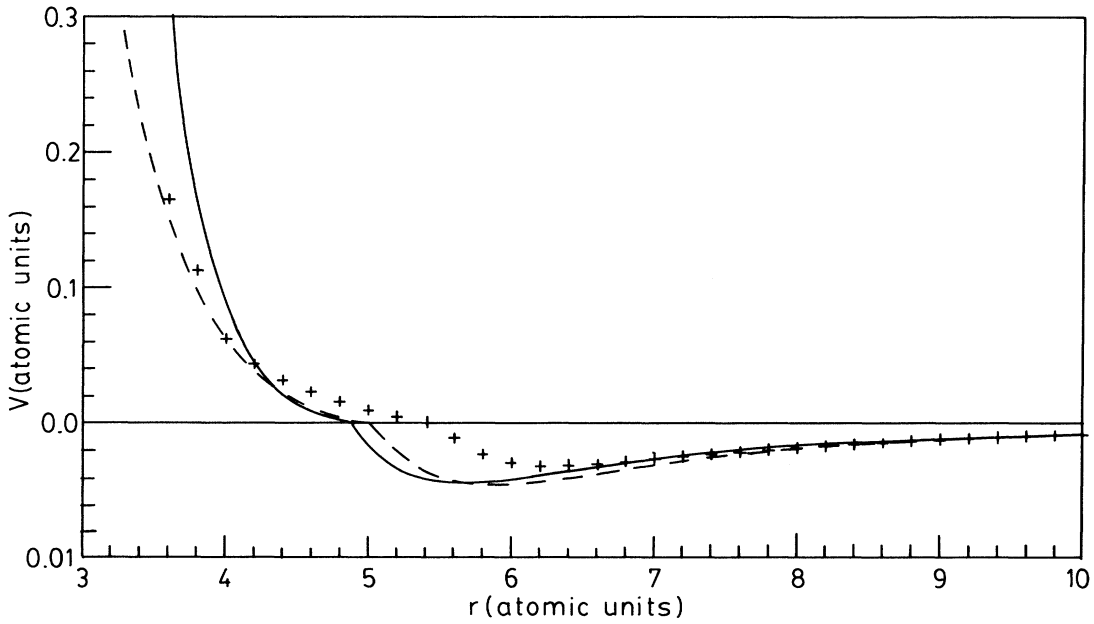

FIG. 2. Interaction potentials $V(r)$ in hartrees as a function of ion–neutral-species separation r in Bohr radius. + represents Lamm *et al.* [10] calculated points; — — —, BGJ [8,9] potential curve; and ——, KMV [13] potential curve. The V scale below the r axis is expanded ten times to show more clearly the negative potentials.

the logarithmic scale so as to space out the data points more evenly.

Among the experiment data, those of Creaser [18] are generally lower than the rest. As the discrepancy is believed to be due to systematic errors caused by the presence of charge layers on the Bradbury-Nielsen grids [19], Creaser's data are therefore disregarded. The difference between Cassidy and Elford's (CE) data [19] and Takebe *et al.*'s data [20] is very small over their common range, and they agree within the published experimental errors. Skullerud's early data [21] are somewhat higher up to about $T_{\text{eff}}=1500$ K, and overall are more scattered. At low T_{eff}, the Lamm *et al.* experimental data [10] (LX) are systematically higher than the other data sets. Similar discrepancies between the various experimental mobility data from the same system used by Lamm *et al.* and those from other laboratories for different alkali-metal ion and rare-gas atom combinations have been previously reported [22,23]. It therefore appears likely that a consistent systematic error in the LX data exists. Consistent with expectations based on the ion kinetics, the higher experimental mobility values of Lamm *et al.* have resulted in a larger repulsive potential at the important intermediate range of r between about 4.5 and 6 a.u. as shown in Fig. 2. In view of this discrepancy it would be interesting if the calculations of Lamm *et al.* for the interaction potential can be repeated with the accepted experimental mobility data as the new input.

In the high-T_{eff} ($>10\,000$ K) region, the only available experimental data are those of Skullerud and Lamm *et al.* In general, these data agree fairly well with the calculated values, but it is not possible to draw more definite conclusions on the accuracy of the data.

On the basis of the above comparison we adopt the published accuracy of CE's data (0.5%) for the range $T_{\text{eff}}<2000$ K, and Takebe's data (1.5%) for T_{eff} up to 6000 K. Within the respective accuracies specified, the experimental data are consistent with one another and are accepted for testing the input potential interaction function used in the MCS calculations.

Of the three input potentials used for the MCS calculations the KMV function gives the best match with the experimental data at T_{eff} between 320 and 2000 K. Above 2000 K the MCS KMV values are slightly higher than those of Skullerud and Takebe *et al.* but they still agree within the experimental accuracy. Based on the kinetics of the ions in the T_{eff} range studied, there are two important ranges of r which will have a significant effect on the resulting mobility calculated. Firstly, the region where r lies between about 3 to 5 a.u. is important because the net repulsive potential corresponds to the range of ion energies applicable in the drift tube. Secondly, the region of r between about 5 and 10 a.u. is where the net potential is appreciably negative and through which all ions must pass on their way to and from the shorter-range repulsive region. Since the agreement of the MCS KMV data with experiment is generally good it may be concluded that the KMV potential function represents quite well the true interaction potential especially in the energetically relevant regions. In the very low T_{eff} region the MCS KMV data exhibit an anomalous up-curving of K_0 as E/N tends towards zero. The up-curving seems also discernible in the other MCS data, but is much less pronounced. We suspect that this behavior is an artifact of the present simulation, possibly due to the fact that when the component of the ion energy due to the field-directed

motion is only a small fraction of the random component, the error in computing the ratio of the time-averaged z component of velocity to the electric-field strength becomes large. Evidence of this effect is shown in the rapid increase in the standard error of the calculated K_0 as $E/N \rightarrow 0$ (Tables I–III).

At low T_{eff} the Lamm *et al.* potential yields MCS calculated values of K_0 that match closely the Lamm *et al.* calculated mobilities (QL) using the same Lamm *et al.* potential. Remembering that this potential was obtained by iterative adjustments of the Waldman-Gordon potential until it yielded K_0 values calculated by the two-temperature theory that match their experimental values, the good agreement between the MCS Lamm *et al.* and the QL mobility data provides evidence of the accuracy of both the present MCS procedure and the two-temperature theory [11,12] used by them.

At higher T_{eff}, the Lamm *et al.* potential yields MCS data that fit well the experimental values of Takebe *et al.* However, the MCS Lamm *et al.* data are systematically slightly lower than the two-temperature QL values calculated from the same potential. In the worst case around the peak K_0 value the two sets of data differ by up to 2% but they appear to be converging again at high T_{eff}. It may thus be surmised that the two-temperature theory is accurate at both low and high E/N but predicts mobility values which are slightly too high at E/N around the peak K_0.

The BGJ potential yields systematically higher K_0 values in the range of T_{eff} between 0 and about 10 000 K and thereafter systematically lower values as T_{eff} tends towards higher values. The discrepancy in the low-T_{eff} region may be due to the larger inaccuracy inherent in low-energy ion-beam measurements from which the BGJ potential was derived [24,25]. For the high-T_{eff} region, in approximating the entire repulsive range with a single inverse power term, the BJG potential over-emphasizes the shorter-range repulsion and underestimates the longer-range portion of the repulsive region (see Fig. 2). Similarly, it overestimates the near-end region of the intermediate term but counters it with an underestimation at the far end of this region. As shown in Fig. 2 the $V(r)$ plots for the three potentials studied confirm that the BGJ potential has the hardest repulsive term but also the largest negative potential between the zero-potential position and r_{min}. Although the BGJ potential is an improvement over Mason and Schamp's potential, there are obviously still not enough adjustable parameters to represent accurately both the short-range and intermediate-range potentials simultaneously.

The comparison of QKMV mobility values with the corresponding MCS calculated values is very similar to that between the QL values with the MCS Lamm *et al.* data. The QKMV values agree well with the MCS KMV values in the low- and high-T_{eff} ranges but tend to become systematically higher by up to 2% in the intermediate collision energy region. This trend seems to indicate similar deviations of the three-temperature theory used in the QKMV calculations as was earlier suggested for the two-temperature theory from the comparison of the QL and MCS Lamm *et al.* data.

CONCLUSION

It is hoped that we have demonstrated the effectiveness of the MCS method in testing the accuracy of the various potential representations for the interaction of K^+ and Ar. Provided that accurate experimental data on the mobility of an ion–neutral-species pair is available, the method provides a general means for routine testing of any proposed interaction of any ion–neutral-species system. In the case where both the mobility data and the interaction potential of the ion-atom pair are accurately known, the MCS procedure also provides a reliable test of the kinetic transport theory used in deriving the theoretical mobility values from the interaction potential.

Based on the illustrative calculations and comparisons presented here, it appears that the KMV potential is the most accurate currently available. This conclusion lends support to the applicability of the universal scaling scheme of KMV to other closed-shell interaction potentials.

With the continuous, but gradual, parallel improvement in the accuracy of experimental mobility data and the newer kinetic theory, as well as the development of more powerful computers, the MCS method should have a long life span of usefulness to serve as an important linkage combining all three advancements to yield steady improvements in testing the accuracy of the potential interaction between any atomic pair. In the long term we expect that the proposed MCS test would continue to be a reliable test for both new interaction potentials as well as any new kinetic theory of ions drifting in a gas. One hopes with continued improvement in both the accuracy of available experimental data as well as computer performance, the present procedure can be further developed into a benchmark test.

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