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Transport coefficients and cross sections for electrons in water vapour: Comparison of cross section sets using an improved Boltzmann equation solution

K. F. Ness,[1] R. E. Robson,[1] M. J. Brunger,[2,3] and R. D. White[1,a)]

[1]*ARC Centre for Antimatter-Matter Studies, School of Engineering and Physical Sciences, James Cook University, Townsville 4810, Australia*
[2]*ARC Centre for Antimatter-Matter Studies, School of Chemical and Physical Sciences, Flinders University, GPO Box 2100, Adelaide, South Australia 5001, Australia*
[3]*Institute of Mathematical Sciences, University of Malaya, Kuala Lumpur 50603, Malaysia*

This paper revisits the issues surrounding computation of electron transport properties in water vapour as a function of E/n_0 (the ratio of the applied electric field to the water vapour number density) up to 1200 Td. We solve the Boltzmann equation using an improved version of the code of Ness and Robson [Phys. Rev. A **38**, 1446 (1988)], facilitating the calculation of transport coefficients to a considerably higher degree of accuracy. This allows a correspondingly more discriminating test of the various electron–water vapour cross section sets proposed by a number of authors, which has become an important issue as such sets are now being applied to study electron driven processes in atmospheric phenomena [P. Thorn, L. Campbell, and M. Brunger, PMC Physics B **2**, 1 (2009)] and in modeling charged particle tracks in matter [A. Munoz, F. Blanco, G. Garcia, P. A. Thorn, M. J. Brunger, J. P. Sullivan, and S. J. Buckman, Int. J. Mass Spectrom. **277**, 175 (2008)]. © *2012 American Institute of Physics*. [doi:10.1063/1.3675921]

I. INTRODUCTION

The determination of a comprehensive set of electron–water vapour cross sections is fundamental to understanding electron induced processes involving H_2O, e.g. in astrophysics, planetary, terrestrial and cometary atmospheres, and associated phenomena.[2] From a technological standpoint, plasma treatments in waste water, pollution, and medicine also demand a knowledge of electron transport and reactions in stock gas mixtures involving water vapour under non-equilibrium conditions.[4]

Ionizing radiation based imaging and therapeutic procedures are important for diagnosing and treating a wide range of medical conditions.[5] Water vapour is currently used as a surrogate for biological material in the modeling of radiolysis tracks, etc.[3,6,7] Low-energy secondary electrons resulting from this radiation have been shown to be one of the major sources of damage to cells and DNA.[8] Optimal accuracy and selectivity of these technologies require an understanding and quantification of the underpinning fundamental physical processes, enabling accurate theoretical models to be developed with a firm physical basis. Recently, a procedure was outlined to adapt gas-phase data in the study of soft-condensed matter appropriate for dealing with biological matter.[9,10] At present, however, current simulations implement approximate and/or effective cross sections and assume a gas phase environment.[3,5,6]

Quite recently a survey of electron scattering cross sections in water vapour was conducted,[11] and a complete set of cross sections was recommended (where possible) based on a critical assessment of the available experimental and theoretical data. One of the major findings of that review was the almost complete lack of available cross section data, both differential and integral, for electron impact excitation of the electronic states in water. As a result of this, groups at Sophia University and Flinders University began a series of studies[12–15] to try and rectify this situation. Both groups made independent cross check measurements and, to within the uncertainties of their measurements, found good agreement. All these cross sections, at the integral level, were later summarized in Thorn *et al.*[2] However, while the measured cross sections of both groups were consistent with one another, there has been no further validation of those cross sections, through a comparison of independently measured swarm transport coefficients with those calculated using these cross sections. This validation, therefore, forms part of the present investigation. The only other major advance in terms of cross section data has been a study of Khakoo *et al.*[15] on electron impact vibrational excitation of the bending and symmetric and asymmetric stretch modes. That work extended but also confirmed (to within experimental uncertainties) the data of El-Zein *et al.*,[16,17] which are rather different from those recommended by Itikawa and Mason[11] but largely consistent with those of Seng and Linder.[18]

One of the key discriminating tests on the completeness and accuracy of any given cross section set is provided through electron swarm experiments.[19–21] In swarm experiments, electrons are passed through a gas at known pressure and temperature under the influence of a uniform electric field. Currents are interpreted in terms of drift and

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a)Author to whom correspondence should be addressed. Electronic mail: ronald.white@jcu.edu.au.

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diffusion and other transport coefficients. By varying the electric field one can modify the distribution of velocities of the electrons, and thus one can sample various energy ranges of the cross sections. In general, the variation of the transport coefficients with E/n_0 (the ratio of the applied electric field E to the target number density n_0) is a macroscopic reflection of the way microscopic cross sections depend upon energy, and indeed this provides the rationale for the so-called "swarm method" for inverting transport data to obtain cross sections.[19] However, we emphasize at the outset that we are *not* involved with any such inversion scheme in this paper. Unlike beam experiments, swarm experiments are "many/multiple scattering" experiments. They require particle number, momentum, and energy (and higher order) balance relations on the entire ensemble of electrons to be met. While the issue of cross section degeneracy (i.e., different cross section sets capable of reproducing the measured transport coefficients) has limited their use in deriving cross sections,[22, 23] swarm experiments do provide a test on the completeness and consistency of any cross section set proposed.[21, 22]

This paper revisits the issues surrounding computation of electron transport properties in water vapour as a function of E/n_0 in the range 0.01–1200 Td (1 Td = 1 townsend = 10^{-21} V m^2). Various cross sections are incorporated into the Boltzmann equation and solved using similar procedures as described in Ref. 1, but taking advantage of modern computing power to calculate transport coefficients to a considerably higher degree of accuracy than was previously possible. This allows a correspondingly more discriminating test of the various electron–water vapour cross section sets proposed,[1, 2, 11, 24–26] by establishing which among them furnishes the transport coefficients agreeing best with those from swarm experiments.

The discussion starts with a brief review of the peculiar way in which electron transport properties in water vapour vary with E/n_0, something which is of interest in its own right. There are three distinct regions of E/n_0 as can be seen from Figures 1 and 2, with the intermediate range providing special analytic and computational challenges. We then move on to examine in depth how transport properties calculated on the basis of the various proposed sets compare with the corresponding experimentally measured properties.

II. THE DISTINCTIVE VARIATION OF TRANSPORT COEFFICIENTS WITH E/n_0 AND ASSOCIATED COMPUTATIONAL ISSUES

In Figures 1 and 2, we present the variation with E/n_0 of the drift velocities and diffusion coefficients respectively for electrons in water vapour. These plots were calculated based on the original set of cross sections proposed in Ref. 1 (see Sec. III A for a discussion of that cross section set). The results are also compared with the available experimental swarm data. In what follows we highlight the distinctive regions of E/n_0, discuss the physical origins of the behaviour, and outline the computational challenges that are present in those regions. We should note that when nonconservative processes, such as attachment and ionization, become operative, the definition of transport coefficients (bulk and flux coef-
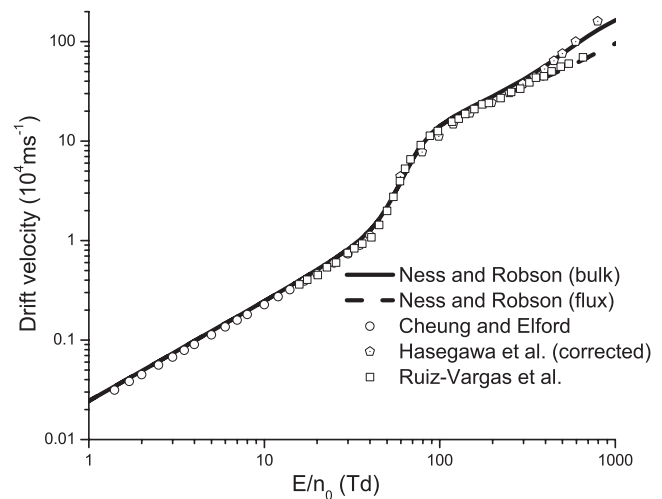

FIG. 1. Comparison of the bulk and flux drift velocities calculated using the cross section set proposed by Ness and Robson[1] with the available experimental measurements of Cheung and Elford,[27] Hasegawa *et al.*,[28, 29] and Ruiz-Vargas *et al.*[24] See text for a discussion of the differences between the bulk and flux drift velocities.

ficients) becomes an issue along with the interpretation of transport coefficients/properties arising from the various experimental swarm configurations. This will be discussed further in Sec. II C.

A. Low energies and low fields ($0 \lesssim E/n_0 \lesssim 35$ Td) – the need for a comprehensive set of rotational cross sections

The very accurate measurements for the drift velocity W and transverse diffusion coefficient to mobility ratio (D_T/μ) of Cheung and Elford[27] and Elford,[30, 31] with associated errors of 0.5% and 2%, respectively, still provide the most stringent test for the low energy threshold rotational cross sections. Here,
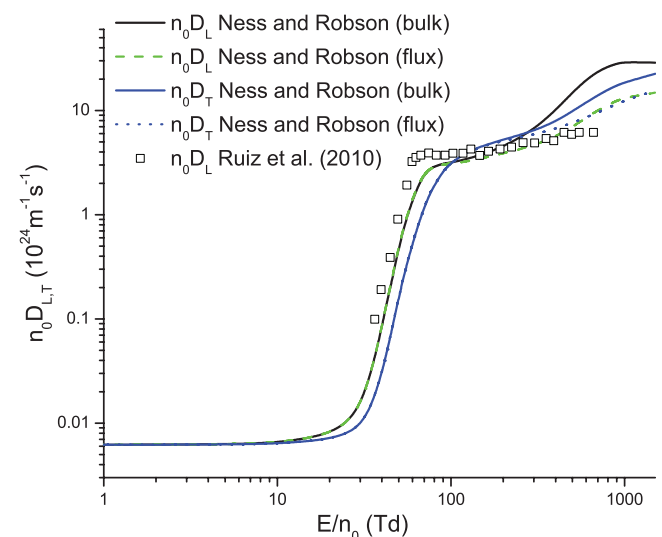

FIG. 2. Comparison of the bulk and flux longitudinal (n_0D_L) and transverse (n_0D_T) diffusion coefficients calculated using the cross section set proposed by Ness and Robson[1] with the experimental measurements of Ruiz-Vargas *et al.*[24] See text for a discussion of the differences between the bulk and flux quantities.

the large number of open rotational channels act to suppress any significant deviations from thermal equilibrium, and in particular D_L and D_T (and indeed D_T/μ and D_L/μ) vary only slowly with E/n_0 up to around 30 Td. As Ness and Robson[1] pointed out, using Itikawa's rotational cross sections[32] calculated on the basis of the Born approximation, it is possible to obtain agreement between theory and *both* D_T/μ and W experimental data *to within experimental accuracy*, if and only if the cross sections for a large number ($\lesssim$100) of rotational processes are included *separately* in the solution of Boltzmann's equation. This issue will be addressed further below. Note at this time, however, that the basis for the validity of the Born approximation is that the energy of the electrons is much greater than the excitation energy for the inelastic process in question, which would appear to be reasonable for the rotational processes. Nonetheless, we caution that the Born approximation is not a very sophisticated approach and that as a result of this scaling procedures are often employed in conjunction with its use.[33,34]

B. Intermediate fields (30 Td $\lesssim E/n_0 \lesssim$ 90 Td) – a computational challenge

Although the thermal equilibrium "deadlock" is finally broken above 30 Td, a quasi-runaway situation soon develops due to the rapidly falling nature of the momentum transfer and rotational cross sections, and consequently D_L/μ and D_T/μ increase very rapidly until "quenched" by the opening of vibrational channels. The difficulties originally reported in the solution of Boltzmann's equation in this region have been eliminated by application of modern day computing power. Namely, up to an order of 240 in Sonine polynomials have now been included in the Burnett function expansion to generate Figures 1 and 2 and the required accuracy of a few parts in a thousand or better for the drift velocity, and better than 1% for the diffusion coefficients is thereby obtained. With this implementation, the numerical instability originally encountered was avoided.

C. High fields ($E/n_0 \gtrsim$ 90 Td), nonconservative collisions, transport coefficient definition

At higher fields, above the runaway region, transport properties once again vary only relatively slowly with E/n_0 as ionization becomes an increasingly important factor. In this regime numerical solution of Boltzmann's equation presents no particular difficulty. Nevertheless, this region needs special attention from a different perspective, in view of the continued confusion[28] surrounding transport coefficient definition in the presence of nonconservative collisions (ionization and attachment).[29,35,36] Thus names are sometimes assigned to drift velocities according to the experiment in which they are measured, e.g., time-of-flight, arrival time spectra, steady state Townsend, and pulsed Townsend drift velocities, although as has been pointed out a number of times, this is neither desirable nor necessary, given that there are just two fundamental types of transport properties, which can be defined independently of any experimental arrangement. The measurable and universal transport coefficients (independent

of experiment) are the "bulk" transport coefficients[35] which appear in the diffusion equation. The "flux" transport coefficients are the proportionality constants in a density gradient expansion (Fick's law) of the electron flux. The flux drift velocity is the swarm averaged velocity, while the bulk drift velocity is the rate of change of the swarm's centre of mass. Physically, they differ only when nonconservative processes are present, with nonconservative processes modifying the swarm's centre of mass. The distinctions between the two sets of coefficients can be generalised to diffusion coefficients.

The connection between the bulk drift velocity W, as measured by Elford and co-workers in their time-of-flight experiment[27,30,31] and calculated by Ness and Robson,[1] and the "arrival time spectra" drift velocity W_m, as measured by Hasegawa *et al.*,[28] is provided by Eq. (40b) of Kondo and Tagashira,[37] and Eq. (16) of Ref. 29,

$$W = W_m + 2\alpha D_L. \tag{1}$$

The Townsend ionization coefficient α has been measured by Hasegawa *et al.*,[28] but it can also be found as an eigenvalue of the Boltzmann collision operator as discussed in Ref. 29. The longitudinal diffusion coefficient D_L is calculated theoretically using the original cross section set of Ness and Robson[1] and shown in Figure 2, allowing the "correction factor" $2\alpha D_L$ to be estimated over the required range of fields. Figure 1 illustrates that there is excellent agreement between the theoretically derived bulk drift velocities W and the experimental data of Hasegawa *et al.*,[28] after the correction factor has been applied to their W_m.[29] While the relationship between drift velocities as measured in arrival time spectra and time-of-flight experiments, W_m and W, respectively, is now clear,[29] there still remains after many years and much discussion some uncertainty as to what is actually measured in a pulsed Townsend experiment. Thus, we observe that the pulsed Townsend drift velocity measurements of Ref. 24 are close to our theoretical flux drift velocity calculations, as expected from Tagashira *et al.*,[38] however, Fletcher[39] argues that it is W which is actually measured in his own pulsed Townsend experiments. In other words, while we can calculate both flux and bulk transport properties theoretically, for any set of cross sections, further information is required from the experimentalists before we can make a legitimate comparison with their data. We emphasize that the distinction between different types of transport coefficients becomes important at higher E/n_0 only, when nonconservative collisions are significant, so that the data of Ref. 24 can still be used unambiguously in the intermediate range of E/n_0.

III. RESULTS

We now report on our calculations using a number of different sets of cross sections, including the cross sections used in our original work on this problem[1] and, as in that original analysis, employing a multiterm analysis in all cases to achieve the required accuracy in solving Boltzmann's equation. We compare with the experimental data of the Cheung and Elford,[27,30,31] Hasegawa *et al.*[28] and the de Urquijo group.[24] The latter provides an important contribution in the intermediate E/n_0, quasi-runaway region and

allows a stringent test in regard to the combined influence of the rotational, vibrational, electronic-state excitation, and ionization cross sections.

A. The original cross section set of Ness and Robson

The benchmark we will use to assess the importance and impact of the various cross sections is the set proposed originally in Ref. 1. The details of this cross section set are described below:

- A combination of the total momentum-transfer cross sections of Pack *et al.*[40] and Gianturco and Thompson[41] was used to cover the whole energy range of interest in this paper.
- Analytic expressions for rotational differential cross sections, furnished by the Born approximation assuming a charge-dipole interaction, as described by Itikawa.[32] It is important to note that these expressions allow us to account for anisotropic scattering.[1]
- For vibrational processes, the cross section set of Seng and Linder,[18] represented by two cross sections corresponding to the fundamental stretching and bending modes, was implemented.
- Five electronic-state excitation cross sections from Cohen and Phelps[42] were considered, while the dissociative attachment and ionization processes were also taken from Cohen and Phelps.[42]

It is important to note that the elastic momentum-transfer cross section required for the Boltzmann code was determined by appropriate subtraction of the inelastic momentum transfer cross sections from the total momentum-transfer cross section.

Using modern computing power, the accuracy of the present calculations has been substantially improved over those in Ref. 1, particularly in the quasi-runaway region between 30 and 90 Td. Thus, by employing very high orders (up to 240) of Sonine polynomials, we have typically achieved overall accuracies of better than 0.01% and 0.05% for bulk drift velocity and longitudinal and transverse diffusion coefficients, respectively, for the curves shown in Figures 1 and 2, although it is somewhat less accurate (0.5% and 1.5%, respectively) in the quasi-runaway region. These results are compared with the available experimental measurements of Cheung and Elford,[27, 30, 31] Hasegawa *et al.*,[28, 29] and Ruiz-Vargas *et al.*[24] in Figures 1 and 2.

B. The low-field regime: an assessment of the rotational cross sections

Figures 3 and 4 illustrate the importance of including an accurate representation for the rotational cross sections in our Boltzmann equation analysis. In the literature, rotational cross sections are often incorporated with the elastic cross sections so that "quasi-elastic" cross sections are presented.[11, 43] From a transport theory perspective this is in general not satisfactory. In Figure 3, we illustrate this through calculations of the transport properties where the original elastic and rotational cross sections in Ref. 1 are replaced with the quasi-elastic
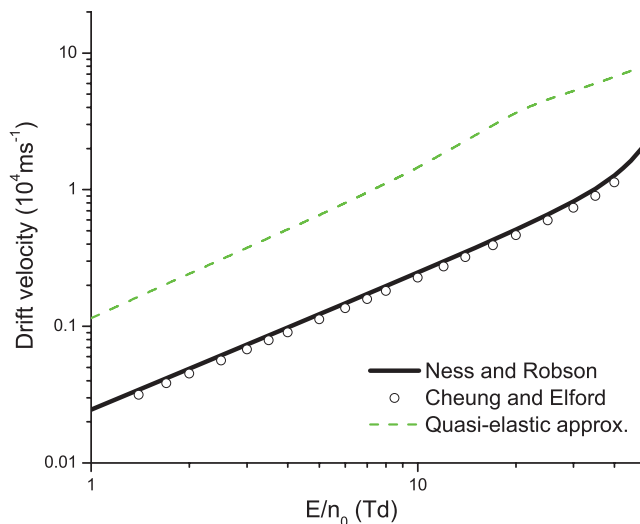

FIG. 3. Calculations of the electron drift velocity that are based on an assumed quasi-elastic cross-section set as proposed by Itikawa and Mason.[11, 26] These results are also compared with the original drift velocity calculations, using the cross section set proposed by Ness and Robson,[1] and with the available experimental measurements of Cheung and Elford[27] in the low-field regime.

momentum transfer cross sections of Itikawa and Mason.[11, 43] The disagreements of approximately an order of magnitude highlight the importance of providing separate elastic and rotational cross sections.

As detailed previously in Sec. II, it is also important to assess the number of rotational cross sections required to obtain transport coefficients within the experimental error of the results of Elford and co-workers,[27, 30] and to also be consistent with the recent results of de Urquijo *et al.*[24] In the original cross section set, 100 rotational cross-sections (with anisotropy[32]) were required. In the set of Itikawa and Mason[11] only the first three rotational cross sections are recommended
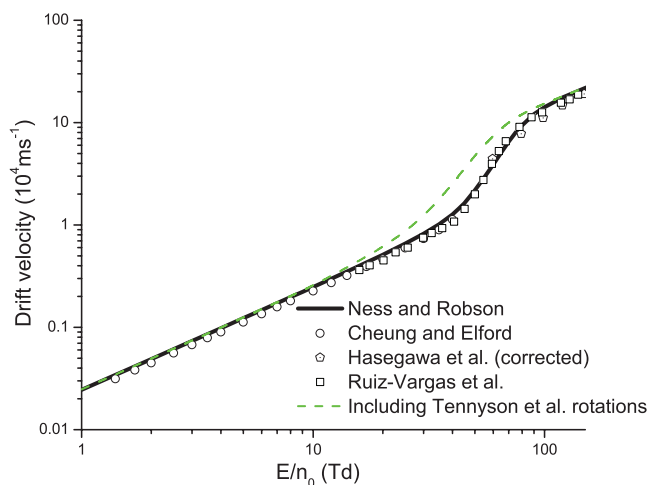

FIG. 4. Calculations of the electron drift velocity that are based on the available rotational cross section set from Tennyson *et al.*[26] These results are compared with the original drift velocity calculations using the cross section set proposed by Ness and Robson,[1] and with the available experimental measurements of Cheung and Elford[27] in the low-field regime. Also shown are the corrected measurements of Hasegawa *et al.*[28, 29] and data from Ruiz-Vargas *et al.*[24]

with no anisotropy prescribed. Replacing the rotational cross sections of Ref. 1 with the recommended set of rotational cross sections from Ref. 11, leaving all other cross sections as given by Ref. 1 yields the drift velocity profiles displayed in Figure 4. Considering now Figure 4 in more detail, in the low-field regime the results for the drift velocity calculations remain consistent with experiment; however, the differences between calculation and experiment are as high as 1000% in the E/n_0 region from 5 to 70 Td under this approximation. These calculations illustrate that any analysis which considers such processes must, therefore, both incorporate them separately from the elastic channel, and must include a sufficient number of them to have any chance of reproducing the measured transport coefficients. Furthermore, since there are insufficient rotational cross sections in the proposed set of Itikawa and Mason,[11] they cannot be comprehensively tested for accuracy against the transport coefficient measurements as they are incomplete. Note that rotational cross sections calculated by the methods of Faure *et al.*[44] and Gianturco *et al.*[45] are more accurate than those from Itikawa.[32] However, once again, their results[44, 45] are not available over the entire energy range we require or for the number of channels we need. Therefore, at this time, we have not been able to test them with our approach.In view of this dilemma, we have chosen for the moment to abide by the rotational cross sections used by Ness and Robson,[1] which after all reproduce the measured transport data. We hope that the present results serve to motivate others to provide further higher order rotational cross-sections.

C. The intermediate-field regime: An assessment of the vibrational cross sections

In Figure 5, we isolate the impact of the vibrational cross section sets on the drift velocity. We do this by replacing the vibrational cross sections of the original set[1] (namely, those from Seng and Linder[18]) with those of Ref. 25 (prescribed in the recommended set[11]), keeping all other cross

sections the same. Vibrational excitations become manifest in the field regime of ∼25–70 Td, with discrepancies as high as 80% being found in this regime. Clearly, the results of Figure 5 indicate some limitations in the vibrational cross-section data from Ref. 25 and thus with the recommended vibrational cross sections of Itikawa and Mason.[11] The new and more detailed transport data of de Urquijo *et al.*,[24] in this region provide useful information for assessing the accuracy and completeness of the vibrational cross section sets. As the vibrational cross sections of Seng and Linder[18] are largely consistent with those from the more recent studies of El-Zein *et al.*[16, 17] and Khakoo *et al.*,[15, 46] the results in Figure 5 clearly validate the choice of Ness and Robson[1] in this respect.

D. The high-field regime: an assessment of the electronic-state and ionization cross sections

The final component of this investigation is to assess the impact of recent measurements of the electronic-state, dissociative attachment, and ionization cross sections from Refs. 2, 14, and 47 on the calculated drift velocity. These results are thus shown in Figure 6 and compared with those from the original drift velocity calculations, using the cross section set proposed by Ness and Robson,[1] and the available experimental swarm measurements of Hasegawa *et al.*[28] and Ruiz-Vargas *et al.*[24] We have included both the calculated bulk and flux drift velocities in this plot in order to compare with both the Hasegawa *et al.*[28] and Ruiz-Vargas *et al.*[24] data. As pointed out above, the drift velocities measured with the arrival time spectra and pulsed Townsend techniques yield different results at higher fields, when non-particle-conserving processes, such as ionization, are significant. This is clearly seen in this figure. One of the problems in drawing quantitative conclusions is that while the uncertainty estimates on the measured swarm data are quoted typically as 1%–1.5% in the
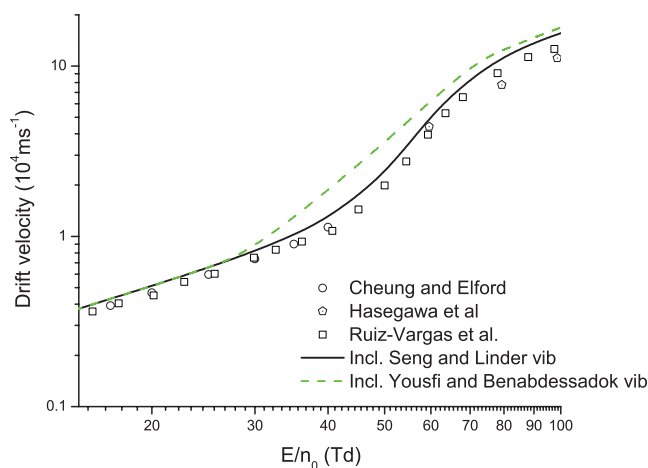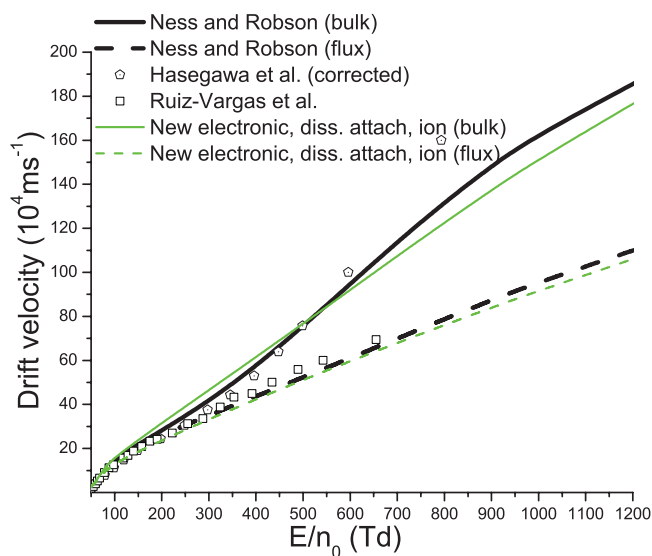

FIG. 5. Comparison of the current drift velocity calculations using two of the available sets of vibrational cross sections: Seng and Linder[18] and Yousfi and Benadbessadok,[25] with the available experimental measurements of Cheung and Elford,[27] corrected measurements of Hasegawa *et al.*,[28, 29] and Ruiz-Vargas *et al.*[24]

FIG. 6. Comparison of the current drift velocity calculations using newly available electronic-state excitation,[2] dissociative attachment,[11] and ionization[47] cross sections, with calculated drift velocities using the set proposed by Ness and Robson,[1] and with the available experimental measurements from Hasegawa *et al.*[28, 29] and Ruiz-Vargas *et al.*[24]
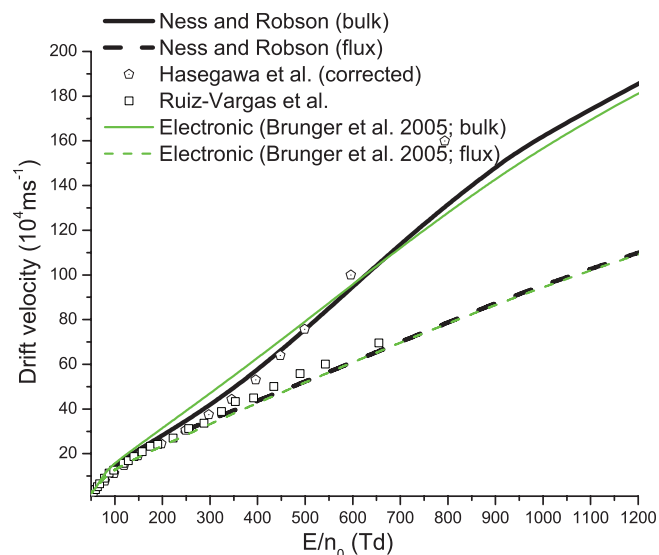
FIG. 7. Comparison of the drift velocity calculations using newly available electronic-state excitation[2] with those from the Ness and Robson set.[1,42] Results are compared with the available experimental measurements of Hasegawa *et al.*[28,29] and Ruiz-Vargas *et al.*[24]

crucial E/n_0 range from $\sim$100–500 Td,[24] we feel that these may only represent the statistical uncertainties. Nevertheless it appears here that the drift velocities calculated with the new cross sections lead to a small (note that it is now a linear scale in Figure 6) but systematic overestimation compared to the measured swarm data.

In Figure 7, we now isolate the consistency of the new electronic-state excitation cross sections of Thorn *et al.*[2] with experiment. This is particularly important as they are currently the only complete set available for atmospherical modeling[2] and charged-particle track simulations.[3,7] To this end, the drift velocities calculated from the original cross section set[1] are also compared with those calculated using the new electronic cross sections of Ref. 2 (keeping all other cross sections the same as in the original study). We observe here that drift velocities arising from including the new electronic-state cross sections are largely consistent with the broad features observed with the old cross section set, even though their form is somewhat different. This is really quite a remarkable result as the new electronic-state cross section set incorporates in excess of 25 such cross sections, while that of Ness and Robson[1] include only five cross sections. Physically, there is of course an infinite number of electronic-states below the ionization threshold.[12] Thus while we have not captured all of them in this study, we have still included a significant number of the electronic-state cross sections and we believe they are the most important of those cross sections. We can, therefore, only reconcile the results in Figure 7 by suggesting that electronic-state processes are not playing a pivotal role in electron transport phenomena in water. Note again that we cannot be more definitive here given the possible underestimation in the true uncertainties in the measurements,[24] although given the linear vertical axis the differences between the calculated and measured transport data are really quite modest. While the cross section set proposed for Figure 6 approximates the experimental swarm data slightly better than

that in Figure 7, in summary we find that the original set still appears the most consistent with the measured swarm data in this field region, in spite of the fact that questions relating to how physical some elements of the original cross section set are remain open.

IV. CONCLUDING REMARKS

In this study, we have revisited the issue of assessing the completeness, accuracy, and consistency of electron water vapour cross section sets through comparisons of calculated transport coefficients with those measured in swarm experiments. We have used an improved Boltzmann equation solution code to facilitate higher accuracy and have also included the recent swarm measurements of Hasegawa *et al.*[28,29] and Ruiz-Vargas *et al.*[24] as part of this investigation. Our results clearly demonstrate the sensitivity of the calculated transport coefficients to variations in the cross sections in the various E/n_0 regions. They also highlight some inadequacies in the recommended cross section set for electron-water scattering interactions from Itikawa and Mason[11] and indicate possibilities for improvements to this set and motivation for further cross section calculations and/or measurements for various scattering processes. The results also suggested that the recent electronic-state cross sections reported by Refs. 2 and 12–14, given the uncertainties on those cross sections and the possible under-estimation of uncertainties on the measured transport coefficients, appear to be a reasonable set to use in atmospheric and charged-particle track modeling. This study highlights an important role for swarm experiments (and associated analysis) as a complementary technique for assessing the completeness and accuracy of cross section sets.

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