Aust. J. Phys., 1979, **32**, 255–9

Comparison between the Boltzmann and Monte Carlo Simulation Methods for the Determination of Electron Swarm Transport Coefficients in Molecular Hydrogen

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Abstract

The transport properties of an electron swarm drifting and diffusing in hydrogen as determined from a numerical solution of Boltzmann's equation are compared with those derived previously from a Monte Carlo simulation. The same set of cross sections has been used with each method to calculate transport coefficients in the range $0{\cdot}5 \leqslant E/N \leqslant 200$ Td. The comparison shows that the Boltzmann analysis is valid in this case whenever ionization is not significant.

Introduction

In the preceding paper by Reid (1979; present issue pp. 231–54), the validity of numerical solutions of the Boltzmann equation for electron swarms in gases was investigated by studying several hypothetical model gases in order to establish under which conditions the two-term expansion of the energy distribution function will not give accurate transport coefficients. In the present paper a comparison is made between the results of a Monte Carlo simulation of electron transport in molecular hydrogen and those obtained from the conventional solution of the Boltzmann equation using a two-term spherical harmonic expansion for the velocity distribution function and approximations to the same order in the collision terms. The scattering cross sections and Monte Carlo results used in the comparison are those of Blevin *et al.* (1978*a*). In general these cross sections gave transport data that were consistent with experiment, although some significant differences ($>5\%$) were found even for values of $E/N \lesssim 20$ Td (E/N is the ratio of electric field strength to gas number density; $1\ \text{Td} \equiv 10^{-17}\ \text{V cm}^2$). These differences were not expected since the cross sections at low energies were derived from the same set of experimental data as that with which disagreement was then found. Thus, even though it seemed unlikely, the explanation of the observed differences at low E/N was assumed to be a breakdown of the validity of the Boltzmann analysis used to extract the cross sections, the breakdown occurring at lower values of E/N than had been anticipated. From the work described in this paper, it is now known that some but perhaps not all of these differences are due to the set of cross sections used by Blevin *et al.* (and also in this paper) rather than to an early (that is, low E/N) failure of the Boltzmann analysis. There remain some ranges of E/N where significant differences occur, particularly at high E/N where ionization is significant. The origin of these differences is discussed below.

Numerical and Simulation Methods

The numerical solution to the Boltzmann equation used in this work was originally obtained by Gibson (1970). Reid (1979) used the code developed by Gibson to compare the electron transport coefficients calculated for several model gases with those obtained from a Monte Carlo simulation. He showed that when the ratio of the total inelastic to elastic collision cross sections is not too large, and any anisotropy

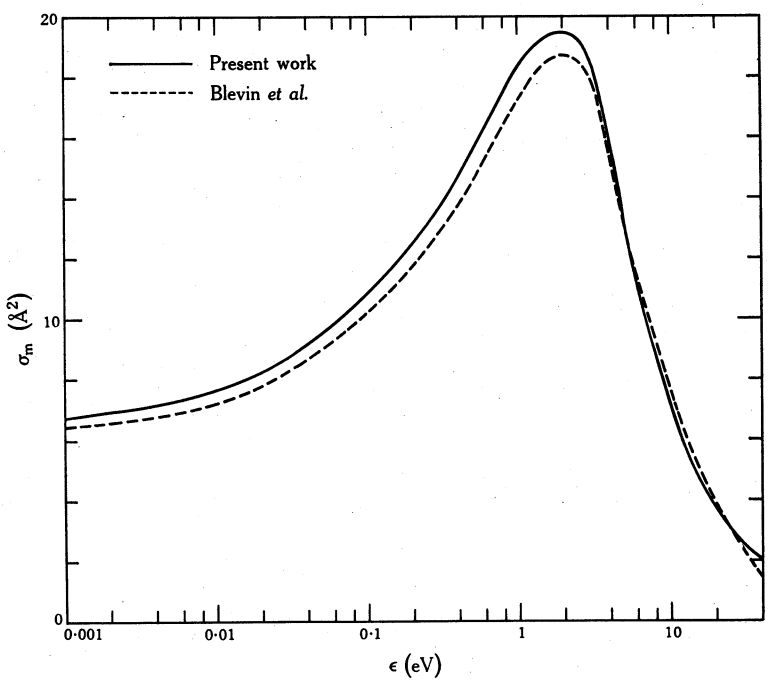

Fig. 1. Momentum transfer cross section σ_m used in the present work, which corresponds to the total cross section and angular distributions used by Blevin *et al.* (1978*a*). The cross section given in their Fig. 1 is shown for comparison. (Note also that the ordinate legend of Fig. 1 in the paper by Blevin *et al.* is incorrectly shown, and the cross section scales are actually in units of 10^{-16} cm^2, that is, Å^2.)

in the differential scattering cross sections is not severe, the Boltzmann approach can be used to derive accurate transport coefficients from a given set of collision cross sections. It was observed, however, that significant errors can arise when the above criteria are not met. Detailed modelling of real gases was not attempted due to the large amounts of computer time required to perform the Monte Carlo simulations which were used to check the Boltzmann calculations.

The Monte Carlo simulation technique used for the present comparison has been described by Hunter (1977) and Blevin *et al.* (1978*a*) and was used to determine the transport parameters of a drifting and diffusing electron swarm in molecular hydrogen over a wide E/N range using a detailed set of elastic and inelastic scattering cross sections based on presently available experimental and theoretical data. As pointed out in the Introduction, these cross sections would be expected to give transport data in close agreement with experiment at low values of E/N although not necessarily

at higher values, but significant discrepancies were found over the whole range of E/N. Most, if not all, of the discrepancy at low E/N is due to an error that was made in determining the total cross section used in the simulation from the assumed momentum transfer cross section and angular distributions. The total (and hence momentum transfer) cross sections actually used in the simulation were in fact larger than those given by Blevin *et al.* (1978*a*) and thus the simulated values of the drift velocity v_{dr} and transverse diffusion coefficient $D_\perp$ were too small. The difference in the cross sections is illustrated in Fig. 1. The same (larger) set of cross sections has been used in the present work as input for the calculations based on the numerical solution of Boltzmann's equation in order to make the results directly comparable with those from the Monte Carlo simulation of Blevin *et al.* The mean energy of the swarm $\langle\varepsilon\rangle$ as well as v_{dr} and $D_\perp$ have been calculated for comparison with the results from the simulation.

From the simulation it was possible to find v_{dr} and $D_\perp$ for the 'original' electron swarm as well as for the swarm as a whole. The original swarm is defined as the electron swarm which does not include the secondary electrons produced in ionizing collisions. When an ionizing collision occurs, the two electrons that are scattered from the gas molecule are indistinguishable. One electron is arbitrarily chosen to be the original electron, and its path followed to the end of the simulation or until a further ionizing event takes place, when a similar arbitrary choice is made. The original swarm is the ensemble chosen in this way, whereas the total swarm includes both primary and secondary electrons.

Results and Discussion

The electron swarm drift velocities obtained by the Boltzmann analysis and Monte Carlo simulations are compared in Fig. 2*a*, while the lateral diffusion coefficients are shown in Fig. 2*b*. The results for $\langle\varepsilon\rangle$ are not shown, as the values obtained by both methods were in very good agreement; values of $\langle\varepsilon\rangle$ have been published by Blevin *et al.* (1978*a*). The estimated uncertainties in the transport coefficients obtained by the Boltzmann analysis are $\pm 0{\cdot}2\%$. The Monte Carlo method, which followed a swarm of 1000 electrons through a total of approximately 10^6 collisions, gave uncertainties of $\pm 1\%$ in v_{dr} and $\pm 3\%$ in $D_\perp$ for the whole swarm.

The results for v_{dr} in Fig. 2*a* show a very good agreement between the Boltzmann analysis and the simulation over most of the values of E/N considered, and this agreement continues throughout the whole range of E/N for the original swarm results. Similar trends are apparent in the comparison of the $D_\perp$ results (Fig. 2*b*), despite the greater scatter in the simulation results. There are, however, some points at low E/N (<15 Td) where the discrepancies are slightly larger than the combined uncertainties, and these differences may be due to a breakdown of the standard Boltzmann analysis. Since there was some arbitrariness in the choice of the angular scattering distributions that have been used (Blevin *et al.* 1978*a*), confirmation of any breakdown in this region must await the outcome of further work.

Above $E/N \approx 100$ Td, ionization adds significantly to the total number of electrons in the swarm. However, in the Boltzmann analysis, no account is taken of the secondary electrons; the transport of the primary electrons alone is considered, an ionizing collision being treated simply as another excitation process with its associated energy loss. Thus it is to be expected that the Boltzmann results would follow more closely

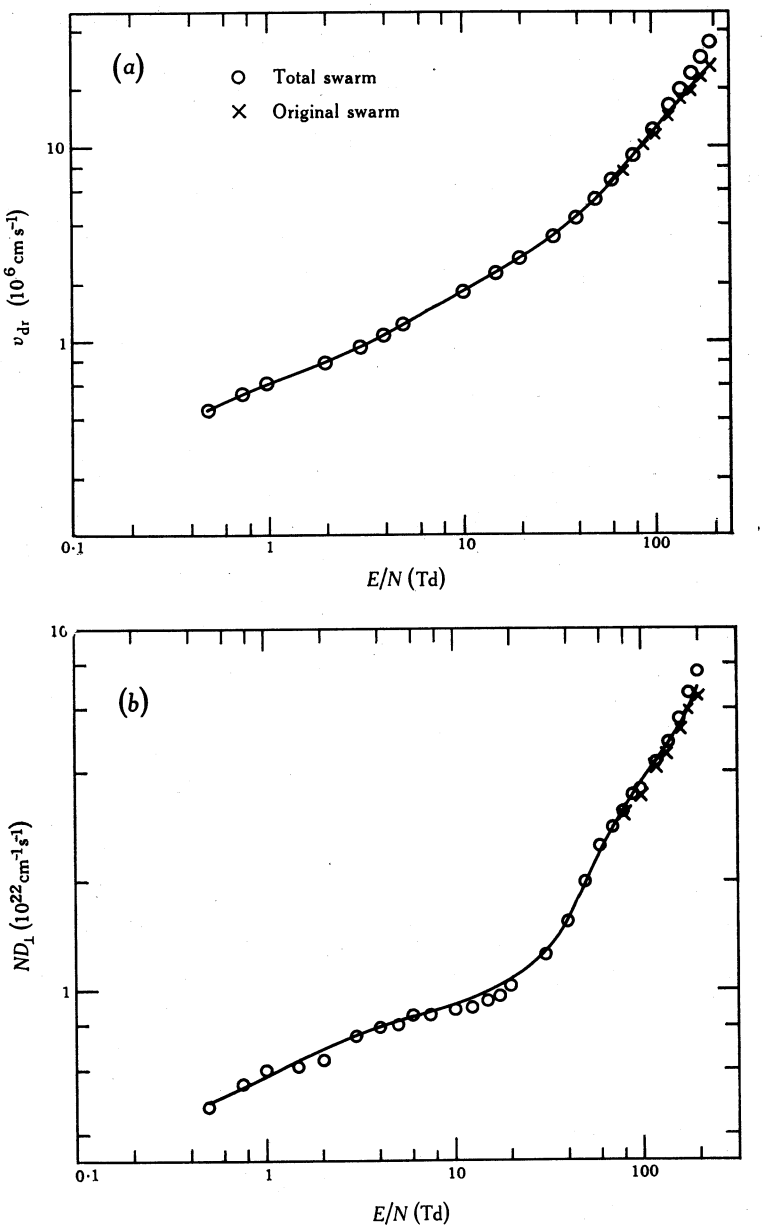

Fig. 2. Plots of (*a*) drift velocities v_{dr} and (*b*) transverse diffusion coefficients $D_\perp$ for an electron swarm in molecular hydrogen. The results calculated using the Boltzmann code (curves) are compared with those obtained from the Monte Carlo simulation (points) of Blevin *et al.* (1978*a*) for both the total swarm and the original swarm.

those for the original swarm. The discrepancy with the results for the swarm as a whole can be attributed almost entirely to the failure of the analysis to account for the production of further electrons in ionizing collisions.

The small discrepancies in $D_\perp$ between the Boltzmann results and those for the original swarm at high E/N probably arise from a combination of several factors.

Firstly, the Boltzmann analysis takes the energy of the scattered electron as the incident energy less the threshold energy for ionization, whereas in the simulation this energy is randomly shared between the two outgoing electrons. Secondly, the number of electrons in the original swarm decreases with increasing ionization, as the simulation was only carried out until 1000 electrons had been followed; at 200 Td only about 12% of these were original electrons. Decreasing the number of original electrons increases the statistical uncertainty in the calculation of their $D_{\perp}$. Finally, at higher energies (10–50 eV) the total inelastic cross section becomes a considerable fraction of the total scattering cross section, a situation which can cause a failure of the approximations inherent in the Boltzmann analysis (Reid 1979).

The differences in the transport coefficients for the original and total swarms are due to the large energy gradients that are present across the electron swarm (Blevin *et al.* 1978*b*). Since the average electron energy is larger at the front of the swarm than towards the rear, more electrons will be produced at the front, tending to move the centroid of the swarm to a forward position. This problem was discussed, for example, by Lucas (1970).

Conclusions

The results presented in this paper show that, where ionization is not significant, the conventional Boltzmann analysis applied to electron transport in hydrogen does not lead to large errors in the calculation of the transport coefficients. However, when ionizing collisions become significant, the Boltzmann method becomes invalid, and one must have recourse to other methods such as Monte Carlo simulations to obtain the transport coefficients.

Acknowledgments

The authors would like to thank Dr R. W. Crompton and Professor H. A. Blevin for their support and encouragement. One of us (I.D.R.) also thanks Professor Blevin for providing access to his simulation codes, and Dr G. N. Haddad for assistance with some of the computing. Both authors acknowledge receipt of Commonwealth Postgraduate Research Scholarships during part of this work.

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Manuscript received 11 January 1979