FACTA UNIVERSITATIS
Series: **Physics, Chemistry and Technology** Vol. 6, Nº 1, 2008, pp. 57 - 69
DOI: 10.2298/FUPCT0801057D

THE DETERMINATION OF LOW ENERGY ELECTRON-MOLECULE CROSS SECTIONS VIA SWARM ANALYSIS

UDC 539.196

S. Dujko[1,2], R.D. White[2], Z.Lj. Petrović[1]

[1]Institute of Physics, University of Belgrade, Pregrevica 118, Zemun, Serbia
[2]ARC Centre for Antimatter-Matter Studies, School of Mathematics, Physics and IT, James Cook University, Townsville 4811, QLD, Australia

Abstract. *In this paper we discuss the swarm physics based techniques including the Boltzmann equation analysis and Monte Carlo simulation technique for determination of low energy electron-molecule cross sections. A multi term theory for solving the Boltzmann equation and Monte Carlo simulation code have been developed and used to investigate some critical aspects of electron transport in neutral gases under the varying configurations of electric and magnetic fields when non-conservative collisions are operative. These aspects include the validity of the two term approximation and the Legendre polynomial expansion procedure for solving the Boltzmann equation, treatment of non-conservative collisions, the effects of a magnetic field on the electron transport and nature and difference between transport data obtained under various experimental arrangements. It was found that these issues must be carefully considered before unfolding the cross sections from swarms transport data.*

Key words: *Boltzmann equation, electron swarms, cross sections, transport data*

INTRODUCTION

One of the primary motivating factors behind transport theory of charged particle swarms in neutral gases is the determination of low energy electron-molecule cross sections. The swarm method falls into the category of the 'inverse' problems in physics, where the cross sections are adjusted until some preset agreement is obtained between experimentally measured and theoretically calculated transport coefficients. Perhaps the first use of transport theory to obtain the collision cross sections was that of Townsend and Ramsauer in the early 1920s. These early methods were based on measuring the drift velocity in a gas as a function of E/p (electric field strength divided by a gas pressure), and inverting the integral relating the drift velocity and momentum transfer cross section using an approximate expression for the energy distribution of the electrons. In the 1960s Phelps and many other collaborators developed algorithms for solving the Boltzmann equation for transport of electrons in gases to obtain the electron transport coefficients

Received August 2, 2008

and distribution functions valid for higher fields and in the presence of inelastic collisions (see for example Phelps (1968) and references therein). At the same time, the swarm experiments of the drift velocity and transverse diffusion coefficient in an electric field increased in accuracy and hence it became possible to make comparisons between cross sections obtained by the swarm method and beam experiments. The swarm methods of deriving cross sections developed by Phelps and collaborators became accepted as competitive and complementary to other established techniques, such as crossed-beam or total attenuation experiments, particularly in low energy range where these experimental techniques were faced with a wide range of systematic problems if absolute values of integral cross sections are required. The gas laser modeling community was the first to benefit from very accurate momentum transfer and lower energy (rotational and vibrational) inelastic cross sections that have been derived from measurements of the drift and diffusion of electron swarms in gases.

The swarm technique of deriving cross sections has increased in sophistication over the years. The review papers of Crompton (1994) and Petrović *et al.* (2007) outlines the current status in the field. One of the most critical aspects associated with the swarm method is the accuracy of calculation of the electron transport coefficients from a given set of cross sections. The common thread among early and more recent swarm methods for determination of the cross sections is the use of the two term theory (representation of the electron velocity distribution by the first two terms of an expansion in spherical harmonics in velocity space) for solving the Boltzmann equation. Originally the two term approximation was used to unfold the transport data, but subsequent multi term calculations of Ness and Robson (1986), Petrović (1984) and Yousfi and Benabdessadok (1996) revealed large discrepancies between the cross sections obtained with these two techniques, particularly for molecular gases. In spite of these and many other well-known examples which illustrate the inadequacies of a two term theory, there are many public domain Boltzmann solvers based on the two term approximation and specifically developed for the cross section adjustments. Even the fully automated numerical optimization procedures to manipulate the input cross sections was based on a two term theory and have been developed and extensively used for a wide range of gases (Taniguchi *et al.* (1987); Morgan (1991)). One important aspect of the present work concerns the adequacy of the two term approximation for inversion of swarm data to obtain electron-molecule cross sections. The investigation is carried out for electron swarms under the influence of varying configurations of electric and magnetic fields. Similar studies have been published previously for both model and real gases (White *et al.* (1999,2003)) but we extend these studies by: (i) highlighting the explicit effects of non-conservative collisions on the electron transport properties and (ii) addressing the temporal relaxation of spatial inhomogeneities through a study of the diffusion tensor. It is important to note that the application of an orthogonal configuration of electric and magnetic fields gives rise to an additional number of transport coefficients and thus one is able to exploit this in the inversion procedure. Thus by varying the magnitude of a magnetic field an additional check on the validity of a cross section set may be made through comparison with such measured electron swarm data (Schmidt *et al.* (1994)). For an arbitrary configuration of electric and magnetic fields, the degrees of freedom are further increased by varying the angle between the fields. In such cases the number of independent transport coefficients is even greater. With these remarks as background, we have been motivated to investigate

the accuracy of the two term approximation for solving the Boltzmann equation when both electric and magnetic fields are present.

The next point of confusion has arisen in connection with identification of transport coefficients in the presence of non-conservative collisions. Under hydrodynamic conditions, two distinctively different types of transport coefficients can be distinguished: the bulk and flux. Both of these transport coefficients are often calculated in the analysis of time-of-flight (TOF) swarm experiments. Physically, the bulk transport coefficients are associated with the swarm's centre of mass transport and should be used for comparisons with experimentally measured transport data. However, when non-conservative processes are operative, the average energy and average velocity under steady-state Townsend (SST) conditions are different from those determined from hydrodynamic calculations of the mean energy and flux (or bulk) drift velocities respectively (traditionally calculated in time-of-flight TOF analyses). These differences can be quite large and may induce large errors in cross sections if one applies the SST transport properties as input data of the inversion procedure. In order to avoid these difficulties, we identify the relations for the conversion of hydrodynamic transport properties to those found in the steady-state Townsend (SST) experiment. Our Monte Carlo simulation code and sampling techniques appropriate to these experiments has provided us with a way to test these conversion formulae and their convergence.

In section 2 the multi term theory for solving the Boltzmann equation and Monte Carlo simulation technique valid for an arbitrary field configuration when non-conservative collisions are operative are discussed in more detail. In section 3 we give numerical examples for various cases of special interest for the swarm method and determination of the cross sections.

THEORETICAL METHODS

Multi Term Theory for Solving the Boltzmann Equation

The behavior of charged particles in neutral gases under the influence of electric and magnetic fields is described by the phase-space distribution function $f(\mathbf{r}, \mathbf{c}, t)$ representing the solution of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{q}{m}\left[\mathbf{E} + \mathbf{v} \times \mathbf{B}\right]\frac{\partial f}{\partial \mathbf{c}} = -J(f, f_0) \tag{1}$$

where **r** and **c** denote the position and velocity co-ordinates, e and m are the charge and mass of the swarm particle and t is time. The electric and magnetic fields are assumed to be spatially homogeneous and time-dependent. In what follows, we employ a co-ordinate system in which **E** defines the z-axis while **B** lies in the y-z plane, making an angle ψ with respect to the **E**. Swarm conditions are assumed to apply where the charged particle number density is much less than number density of neutral species and mutual interactions between swarm particles are negligible compared with swarm particle-neutral particle interactions. The right-hand side of Eq. (1) denotes the linear charged particle-neutral molecule collision operator, accounting for elastic, inelastic and non-conservative (e.g. ionizing and attaching) collisions.

In the present approach equation (1) is solved by decomposing $f(\mathbf{r}, \mathbf{c}, t)$ in terms of spherical harmonics in velocity space and powers of the gradient operation acting on the number density $n(\mathbf{r}, t)$ in configuration space, i.e.

$$f(\mathbf{r},\mathbf{c},t)=\sum_{l=0}^{l_{\max}}\sum_{m=-l}^{l}\sum_{s=0}^{\infty}\sum_{\lambda=0}^{s}\sum_{\mu=-\lambda}^{\lambda} f(lm\,|\,s\lambda\mu;c,t)Y_m^{[l]}(\hat{\mathbf{c}})G_\mu^{(s\lambda)}n(\mathbf{r},t)\,, \tag{2}$$

where $Y_m^{[l]}(\hat{\mathbf{c}})$ denotes the spherical harmonics and $G_\mu^{(s\lambda)}$ denotes the sth application of the gradient operator in irreducible tensor notation. The value of $l_{\max}$ is incremented until some predefined accuracy criterion is satisfied. This value indicates the deviation of the velocity distribution function from isotropy. The two term approximation is based upon the setting of the upper bound on the summation to $l_{\max} = 1$. Truncation at $s = 2$ is necessary to determine transport coefficients up to and including diffusion when non-conservative collisions are operative.

The speed dependence of the coefficients in Eq. (2) is represented by an expansion about a Maxwellian at an internally determined time-dependent temperature $T_b(t)$, in terms of Sonine polynomials

$$f(lm\,|\,s\lambda\mu;c,t)=\omega(\alpha(t),c)\sum_{\nu=0}^{\infty}F(\nu lm\,|\,s\lambda\mu;\alpha(t),t)R_{\nu l}(\alpha(t)c))\,, \tag{3}$$

where $\alpha(t)^2 = m/kT_b(t)$ and $\omega(\alpha(t),c)$ is a Maxwellian,

$$R_{\nu l}(\alpha(t)c)=N_{\nu l}\left[\frac{\alpha c}{\sqrt{2}}\right]^l S_{l+1/2}^{(\nu)}(\alpha(t)^2c^2/2)\,, \tag{4}$$

$$N_{\nu l}{}^2=\frac{2\pi^{3/2}\nu!}{\Gamma(\nu+l+3/2)}\,, \tag{5}$$

and $S_{l+1/2}^{(\nu)}$ is a Sonine polynomial. Using the appropriate orthogonality relations of the spherical harmonics and modified Sonine polynomials the following system of coupled differential equations for the moments $F(\nu lm\,|\,s\lambda\mu;\,\alpha(t),\,t)$ is generated

$$\sum_{\nu'=0}^{\infty}\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'}[\partial_t\delta_{\nu\nu'}\delta_{ll'}\delta_{mm'}+n_0J_{\nu\nu'}^{l}\delta_{ll'}\delta_{mm'}+\omega(000)\delta_{\nu\nu'}\delta_{ll'}\delta_{mm'}$$

$$+i\frac{q}{m}E(lm\,|\,l'm10)\alpha_t\left\langle\nu l\left\|K^{[1]}\right\|\nu'l'\right\rangle\delta_{mm'}$$

$$+\frac{qB}{m}\left\{\frac{\sin\psi}{\sqrt{2}}\left[\sqrt{(l-m)(l+m+1)}\delta_{m'm+1}-\sqrt{(l+m)(l-m+1)}\delta_{m'm-1}\right]-im\cos\psi\delta_{m'm}\right\}\delta_{\nu\nu'}\delta_{ll'}$$

$$-n_0J_{0\nu'}^{0}F(\nu lm\,|\,000)(1-\delta_{s0}\delta_{\lambda0}\delta_{\mu0})\delta_{l'0}\delta_{m'0}]F(\nu'l'm'\,|\,s\lambda\mu)=X(\nu lm\,|\,s\lambda\mu)\,, \tag{6}$$

where $J_{\nu\nu'}^{l}$ and $\langle\nu l\,\|\,K^{[1]}\,\|\,\nu'l'\rangle$ are reduced matrix elements, $\omega(000)$ represents the net

creation rate and ($lm \mid l' m10$) is a Clebsch-Gordan coefficient. The explicit expressions for the RHS are given in Ness (1994) for the case of crossed dc electric and magnetic fields. These expressions are modified in this paper in order to consider the time-dependent fields crossed at arbitrary angles in the presence of non-conservative collisions. Discretising in time using an implicit finite difference scheme converts the system of coupled differential equations into a hierarchy of coupled matrix equations. To establish the transport coefficients of interest we are required to solve the following members of the hierarchy (s,λ,μ) = (0,0,0), (1,1,0), (1,1,1), (2,0,0), (2,2,0), (2,2,2).

Monte Carlo Simulation Technique

Another independent method for investigating the charged-particle transport in dc electric and magnetic fields is a Monte Carlo simulation technique. In the context of hydrodynamic studies, it is assumed that the charged-particle swarm develops in an infinite space. At time $t = 0$, electrons are initially released from the origin according to Maxwellian velocity distribution with the mean starting energy of 1 eV under the influence of electric and magnetic fields.

Spatial relaxation of the electrons has been studied by our steady-state Townsend Monte Carlo simulation code. The primary electrons are isotropically released one by one from the cathode surface into the half space with an initial energy ε_o. When an ionization collision occurs, a set of all dynamic properties (the moment of an ionization collision, the position of new electron, the starting energy and velocity) of secondary electron are established and placed at the stack. When primary electron reaches the anode surface or disappears in an attachment collision event, the first available electron from the stack is followed. These secondary electrons from the stack are released isotropically. In an attachment collision the electron is consumed and hence not followed further. If the stack is empty, the next primary electron is released and the whole procedure repeats. Thermal motion of the background neutral particles and electron-electron interactions are neglected. The electrodes are considered to be perfectly absorbing.

In both the hydrodynamic and non-hydrodynamic versions of Monte Carlo codes, we follow the spatiotemporal evolution of each electron through time steps governed by the minimum of two relevant time constants: mean collision time and cyclotron period for **E**×**B** field. These finite time steps are used to solve the integral equation for the collision probability in order to determine the time of the next collision. Once the moment of the next collision is established, the nature of the collision is determined by using the relative probabilities of the various collision types. All electron scattering is assumed to be isotropic regardless of the collision nature.

The way of sampling of transport properties depends upon the manner of swarm observation. The definitions and corresponding formulae for the electron transport coefficients under the hydrodynamic conditions were given in our previous publications (Dujko *et al.* 2005,2006). The spatially resolved electron transport properties have been obtained using the following formula:

$$\langle \xi \rangle_j = \frac{\frac{1}{\Delta z}\int_{z_j-\Delta z/2}^{z_j+\Delta z/2} \xi f_{SST}(z,\mathbf{v}) dz dv}{\frac{1}{\Delta z}\int_{z_j-\Delta z/2}^{z_j+\Delta z/2} f_{SST}(z,\mathbf{v}) dz dv} \approx \frac{\sum_{k=1}^{N} \xi_k^j \Delta t_k^j}{\sum_{k=1}^{N} \Delta t_k^j}, \tag{7}$$

where $f_{SST}(z, \mathbf{v})$ is the steady state distribution function, ξ_k^j is the value of the quantity to be sampled when kth electron is contained in jth box, Δt_k^j is the residence time of the electron in that box and N is the total number of electrons which appear there. Electrons moving towards both the cathode and anode must be considered and sampled.

RESULTS AND DISCUSSION

The two term approximation versus multi term theory

In this section the two term approximation is tested using an accurate multi term solution of the Boltzmann equation and Monte Carlo simulation code. First we employ the Reid ramp model (Reid 1979). The Reid ramp model has been extensively used as a benchmark for a variety of field configurations due to its well known illustration of the failure of the two term approximation (White et al. 1999). In this work we extend the previous works by illustrating how large errors in the determination of the cross sections can be if one applies the two term approximation. The Reid ramp model is defined as follows:

$$\begin{aligned}
&\sigma_{el}(\varepsilon) = 6\cdot 10^{-20} \quad \mathrm{m}^2 \\
&\sigma_{ne}(\varepsilon) = \begin{cases} 10(\varepsilon - 0.2)\cdot 10^{-20} \quad m^2 & \varepsilon \geq 0.2 \ \mathrm{eV} \\ 0 \qquad\qquad\quad\ \ \varepsilon \leq 0.2 \ \mathrm{eV} \end{cases} \\
&m_o = 4 \ \ amu \\
&N = 3.54\cdot 10^{22} \quad \mathrm{m}^{-3} \\
&T_0 = 0 \ \ \mathrm{K}
\end{aligned} \tag{8}$$

where $\sigma_{el}(\varepsilon)$ is the cross section for elastic collisions, $\sigma_{in}(\varepsilon)$ is the cross section for inelastic collisions, ε is the electron energy, m is the electron mass, N is the gas number density and T_0 is its temperature.

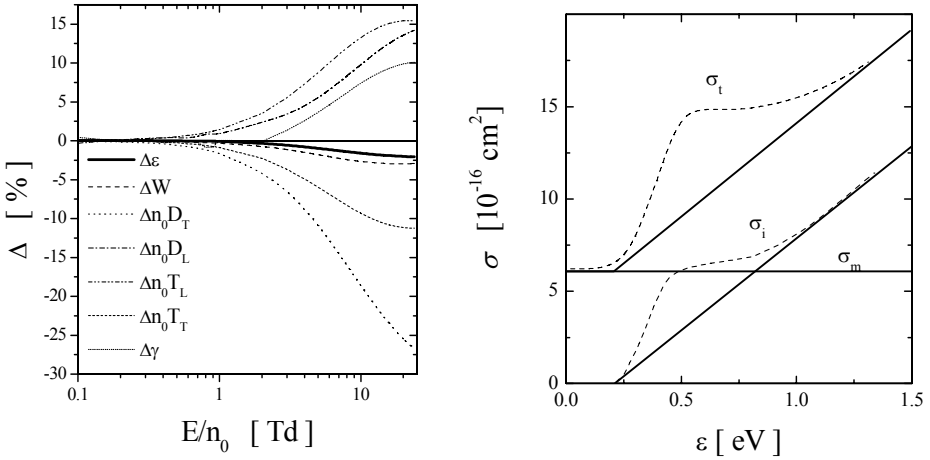

Fig. 1. (a) Percentage difference between the two term and multi term solution of Boltzmann equation in various transport properties for electrons and (b) Reid's ramp model (full line) and the cross sections that can be derived from the "exact" values of the transport coefficients (in a limited E/n_0 range) if one uses the two term theory (dashed line).

In Figure 1 (a) we display the percentage difference between the two term and multi term values for the mean energy (ε), drift velocity (W), diffusion tensor components (n_0D_L, n_0D_T), temperature tensor components (T_L, T_T) and gradient energy parameter (γ). The inadequacy of the two-term approximation for all transport coefficients and properties for this model is clearly evident. The l_{max} = 6 is required to achieve 0.1% accuracy for all transport coefficients and properties. We observe that as E/n_0 increases, the percentage difference between the two term and multi term values of various transport properties is increased. The largest errors are associated with the diffusion coefficients and are of the order of 30% in the limit of the highest E/n_0 considered in this work. These data were then analyzed using the two term approximation in an attempt to determine the cross sections that would best fit the data. The result of this procedure, shown in Figure 1 (b), clearly indicates that large errors can result from the use of inaccurate methods for calculating the transport coefficients.

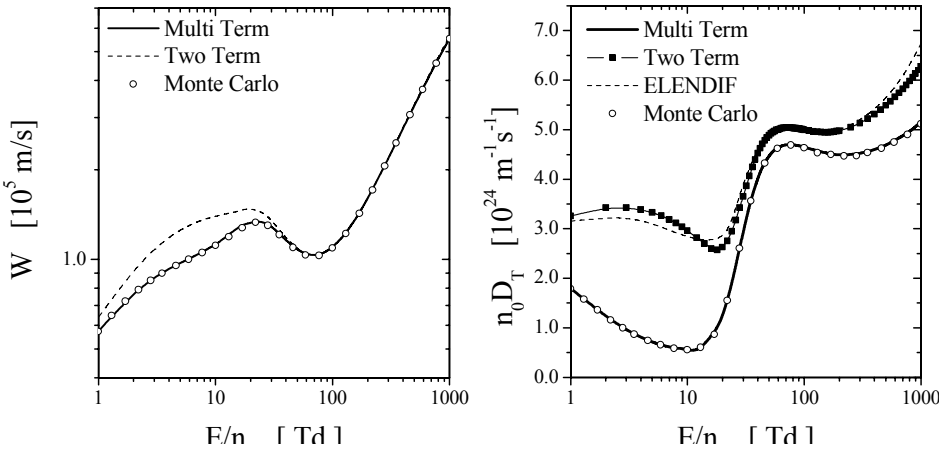

Fig. 2. (a) Drift velocity and (b) transverse diffusion coefficient as a function of E/n_0.

Similar calculations have been done for CF_4 (carbon tetrafluoride). The momentum transfer and 15 inelastic cross sections of Kurihara *et al.* (2000) are used. Isotropic scattering is assumed. Although CF_4 has numerous technological applications, we consider it here more for illustrative purposes, particularly as we expect significant anisotropy of the velocity distribution function for average energies in the vicinity of the Ramsauer-Townsend minimum. Electron transport in CF_4 is examined for E/n_0 in the range 1-1000 Td. The results of calculations for the drift velocity and transverse diffusion coefficient obtained by both the two term and multi term theories for solving the Boltzmann equation and Monte Carlo simulation techniques are compared and shown in Figures 2 (a) and (b). In order to check our two term results for n_0D_T, the well-known Boltzmann solver ELENDIF developed by Morgan (1990) was used to calculate this transport coefficient. The l_{max} = 7 within the multi term calculations was required to achieve 0.5% accuracy for all transport coefficients and properties. From the plot of the drift velocity it is seen that electrons in CF_4 exhibit negative differential conductivity, i.e.,

over a range of E/n_0 values the drift velocity decreases as the field is increased. Conditions leading to this phenomenon have been discussed by Robson (1984) and Petrović *et al.* (1984). The agreement between a multi term theory and Monte Carlo simulation is excellent. The comparison validates the basis of transport theory and numerical integrity of both approaches.

Comparing two term and multi theory, however, we see that the maximum error in the two term approximation for both W and n_0D_T occurs for the low values of E/n_0. As E/n_0 increases, the two term results for W increase in accuracy while for n_0D_T there still exist large disagreements with respect to the multi term results. For the low values of E/n_0, disagreements up to 30% in W and 400% in n_0D_T exist. This large deviation between the two term and multi term results is a clear sign of large asymmetry in velocity space which makes the two term approximation inadequate for the analysis of transport data and determination of the cross sections. Another interesting point is associated with the fact that it is sometimes claimed that the two term approximation becomes increasingly difficult to satisfy at higher fields. This example clearly shows that this is not the case; Figures 2 (a) and (b) indicate that the two term results are worst for the low E/n_0 values.

The effects of non-conservative collisions

Another issue that is highly relevant for determination of the cross sections is nature of the hydrodynamic transport coefficients. Care must be taken when non-conservative collisions are operative to ensure the calculated quantities correspond to those which are measured. In this context, it is the bulk and flux transport coefficients upon which we focus attention. At this point we wish to sound a warning to those who use swarm transport data for determination of the cross sections, to be aware in the differences between these two sets of transport data. The most appropriate procedure is to use the bulk values of transport coefficients for comparisons with experimentally measured transport coefficients and then to calculate the flux quantities which are necessary as input data in fluid modeling of plasma discharges.

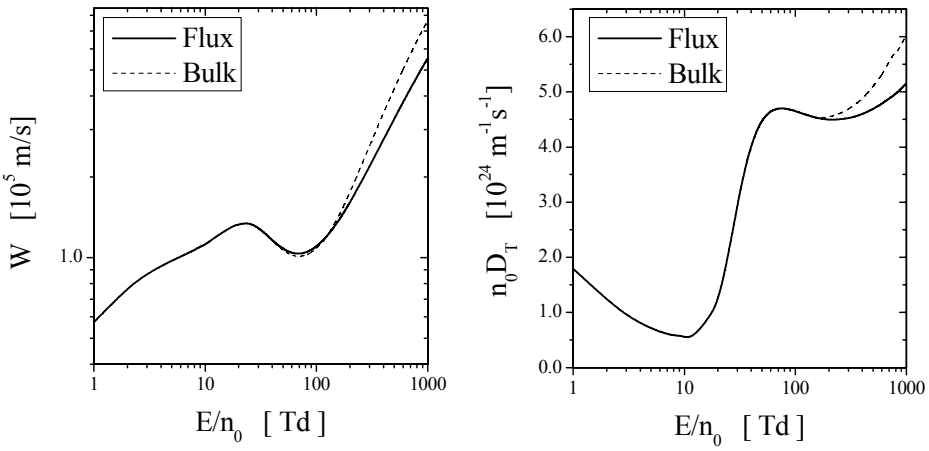

Fig. 3. Variation of the bulk and flux values of the drift velocity and transverse diffusion coefficient as a function of E/n_0.

In Figure 3 (a) and (b) we show the bulk and flux values of the drift velocity and transverse diffusion coefficients as a function of E/n_0 in CF_4. The effects of the ionization processes for the high values of E/n_0 are clearly evident. The differences between the bulk and flux values are of the order of 30%. On the other hand, the effects of the electron attachment are significantly smaller. These effects can be observed in the profile of the drift velocity at intermediate field strengths, between 40 and 100 Td where the flux dominate the bulk values. In contrast, the electron attachment has no visible influence on the transverse diffusion coefficient. One may expect these small effects associated with the electron attachment due to the weak electronegative nature of the CF_4 molecule.

Transport in varying configurations of electric and magnetic fields

One of the biggest disadvantages of the swarm technique for determination of low energy electron molecule cross section is non-uniqueness – various combinations of cross sections can generate the same set of transport data. This means that if we modify one inelastic cross section it is still possible to achieve a good energy balance by modifying another inelastic cross section. This problem can be avoided by seeking for some additional information about the relative magnitude of the cross sections either from electron scattering theory or from electron beam experiments or through the use of gas mixtures. As already remarked, when magnetic field is added to the electric field, the number of transport coefficients more than doubles and these additional transport coefficients can be used for the inversion procedure. In other words, the application of a magnetic field can be used to overcome the problem of non-uniqueness. This was the program of Schmidt and co-workers at Heidelberg who initiated a series of electron swarm experiments in crossed electric and magnetic fields (Schmidt *et al.* 1994). Thus it is important to check the validity of the two term approximation when the electron swarms are acted upon by both the electric and magnetic fields. In what follows, the two term approximation is tested within our studies of the temporal relaxation processes of the electrons in electric and magnetic fields crossed at arbitrary angle.

Figure 4 displays the temporal relaxation profiles of the diagonal elements of the diffusion tensor as a function of B/n_0 and angle between the fields. The results obtained by the multi-term theory are compared with those obtained by the two-term approximation for solving the Boltzmann equation. The inadequacy of the two-term approximation is clearly evident. In particular, significant deviations between temporal profiles in the early and intermediate stages of the relaxation process can be observed. This is a clear indication that the initial distribution function and its initial evolution deviates substantially from isotropy in velocity space (we should note that the initial distribution is the steady-state **E**-only case). In general, however, as magnetic field and the angle between the fields increase, the deviations between the results obtained by the two-term approximation and multi-term theory are significantly diminished. This suggests that the magnetic field acts to destroy the anisotropy of the velocity distribution function, consequently inducing enhanced convergence in the *l*-index.

Other approximations have found their ways into mainstream Boltzmann public domain codes. Some of these codes/approximations avoid the mathematical complexity associated with an accurate solution of Boltzmann's equation, but because of assumptions of symmetry and/or near isotropy in velocity space they may be incorrect. Typical example is the use of Legendre polynomial expansion procedure for solving the

Boltzmann equation. For electron swarms in electric fields only, transverse spatial gradients can destroy rotational symmetry in velocity space and Legendre polynomial expansions are thus invalid for spatially inhomogeneous swarms. For electron swarms in electric and magnetic fields even under spatially homogeneous conditions, there exist no axis of symmetry in velocity space and the use of Legendre polynomials is entirely invalid (White *et al.* 2002).

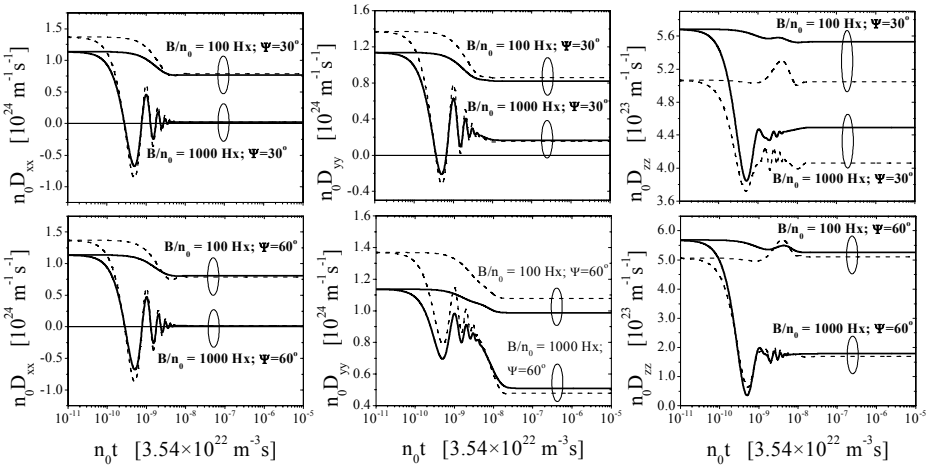

Fig. 4. Temporal relaxation of the diagonal elements of the diffusion tensor for B/n_0 of 100 and 1000Hx and ψ of 30^o and 60^o for Reid ramp model (dashed lines: two term approximation; full lines: multi term theory).

Nature and differences between transport data observed under different experimental conditions

Another issue that is highly relevant for determination of the cross sections via swarm analysis concerns the nature and difference between transport data obtained under different experimental arrangements and conditions. In this section we discuss the spatial relaxation of electrons under SST conditions when non-conservative collisions are operative. The distinction between transport properties obtained under different experimental conditions has been ignored in the majority of previous works in both the swarm and plasma modeling communities. In particular, the majority of experiments deal with SST conditions and hence it is of great importance to be able to represent the SST transport properties in terms of general quantities calculated under hydrodynamic conditions.

We investigate the spatial relaxation of electrons for the ionization model of Lucas and Saelee (Lucas and Saelee 1975). This model is defined as follows:

$$
\begin{aligned}
&\sigma_e = \frac{4}{\sqrt{\varepsilon}}\ 10^{-20}\ \mathrm{m}^2 \\
&\sigma_{ex} = \begin{cases} 0.1\cdot(1-F)\cdot(\varepsilon-\varepsilon_i)\ 10^{-20}\ \mathrm{m}^2, & \varepsilon \geq \varepsilon_{\mathrm{i}} \\ 0, & \varepsilon \leq \varepsilon \end{cases} \\
&\sigma_i = \begin{cases} 0.1\cdot F\cdot(\varepsilon-\varepsilon_i)\ 10^{-20}\ \mathrm{m}^2, & \varepsilon \geq \varepsilon_{\mathrm{i}} \\ 0, & \varepsilon \leq \varepsilon \end{cases} \\
&\frac{m}{m_0} = 0.001 \\
&N = 3.54\times 10^{23}\ \ \mathrm{m}^{-3} \\
&T_0 = 0\ \ \mathrm{K}
\end{aligned}
\tag{9}
$$

where σ_e, σ_{ex} and σ_i are the cross sections for elastic, inelastic and ionization collisions, respectively. Other details of the model include $\varepsilon_i = 15.6$ eV, $T_0 = 0$ K, $E/n_0 = 10$ Td (1 Td = 10^{-21} Vm^2), m/M = 10^{-3} where m and M denote the electron and molecular mass, respectively

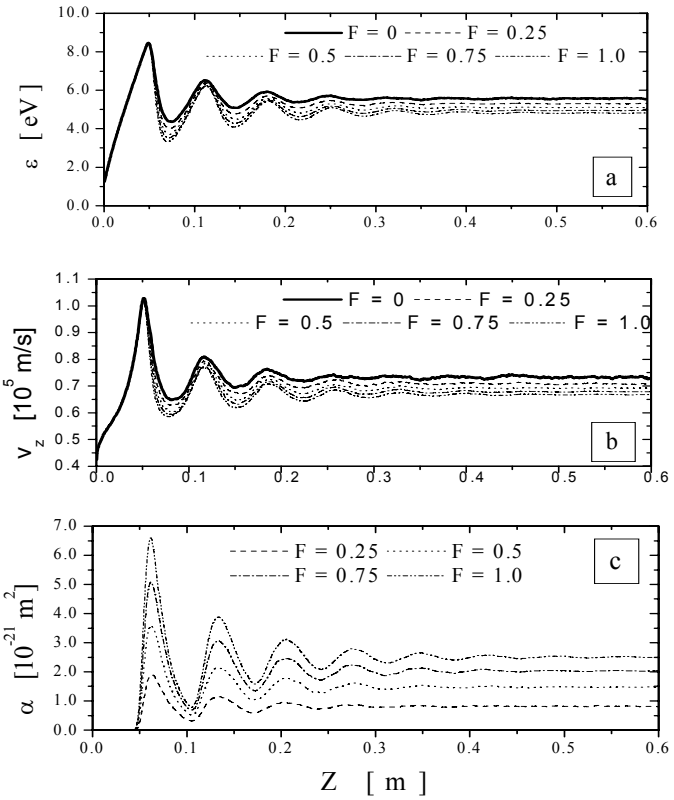

Fig. 5. Spatial relaxation of the (a) mean energy, (b) average velocity and (c) ionization rate coefficient as a function of the parameter F for Lucas-Saelee ionization model at $E/n_0 = 10$ Td.

In Figure 5 we show the spatial relaxation of the mean energy, average velocity and first Townsend's ionization coefficient as a function of the parameter *F*. The mean energy and average velocity do not depend on *F* near the cathode region reflecting the fact that these transport properties are directly influenced by the cathode. However, the steady-state values of both the mean energy and average velocity decrease for an increasing ionization degree. As expected, the ionization rate increases when increasing the parameter F. In the region near the cathode the ionization rate is significantly reduced and it begins rapidly to grow after electrons travel enough long distance sufficient for their energy to be higher that the ionization threshold. The ionization rate peaks at the positions which correspond to the peaks of the mean energy.

We identify the following relations for the conversion of hydrodynamic transport properties to those found in the SST experiment:

$$\varepsilon_{SST} = \sum_{s=0}^{\infty} \varepsilon_s (-\alpha)^s = \varepsilon - \gamma\alpha + \ldots \tag{10}$$

$$v_{SST} = \sum_{s=0}^{\infty} \Gamma_s (-\alpha)^s = W^{flux} - \alpha D_L^{flux} + \alpha^2 \Gamma^{(3)} + \ldots \tag{11}$$

$$k_{ion} = \sum_{s=0}^{\infty} \omega_s (-\alpha)^s = \alpha W^{bulk} - \alpha^2 D_L^{bulk} + \alpha^2 \omega^{(3)} + \ldots \tag{12}$$

Problems of convergence of these series can arise if α is not sufficiently small. Our preliminary calculations for the ionization model of Lucas and Saelee revealed that the truncation at $s = 2$ in the above equations is required to accurately calculate steady-state SST transport data from hydrodynamic flux transport coefficients including the mean energy. On the other hand, the expansion (12) requires truncation at $s = 3$ in order to achieve the accuracy criterion of 0.5%. Another interesting aspect lies with the fact that if the ionization processes are the dominant non-conservative processes, the SST average energy and SST average velocity are always less than the corresponding flux transport data under hydrodynamic conditions, regardless of the energy dependence of the cross sections. If the electron attachment dominates the ionization processes, the opposite situation holds (Dujko *et al.* 2008).

CONCLUSION

Using a multi term theory for solving the Boltzmann equation and Monte Carlo simulation technique we have tried to sound a warning to the potential users of computer codes for electron transport in gases in electric and magnetic fields that

1. a multi term expansion in full spherical harmonics for solving the Boltzmann equation is generally required;
2. care must be taken when non-conservative collisions are operative and it is the bulk values of the electron transport coefficients which should be used for the inversion procedure;
3. the problem of non-uniqueness of the cross sections associated with the swarm analysis can be reduced by developing both the accurate experiments in **E×B** experiments and theories for solving the Boltzmann equation and/or Monte Carlo codes;

4. correct implementation of swarm data under SST conditions when non-conservative collisions are operative requires their representation in terms of general quantities calculated under hydrodynamic conditions.

Acknowledgments: *The authors wish to thank to Dr R.E. Robson and Dr K.F. Ness for their helpful discussions and suggestions. This work has been supported by MNZZSRS Grant 141025 and the Australian Research Council– Centre of Excellence program.*

REFERENCES

1. A.V. Phelps, *Rev. Mod. Phys.* **40** 399-410 (1968).
2. B. Schmidt, K. Berkhan, B. Gotz and M. Muller, *Phys. Scripta* **T53** 30-42 (1994).
3. J. Lucas and H T Saelee, *J. Phys. D: Appl. Phys.* **8** 640-650 (1975).
4. I.D. Reid, *Aust. J. Phys.* **32** 231-254 (1979).
5. K.F. Ness and R.E. Robson, *Phys. Rev. A* **34** 2185-2209 (1986).
6. M. Kurihara, Z.Lj. Petrović and T. Makabe, *J. Phys. D: Appl. Phys.* **33** 2146-2153 (2000).
7. M. Yousfi and M.D. Benabdessadok, *J. Appl. Phys.* **80** 6619-6630 (1996).
8. R.D. White, K.F. Ness, R.E. Robson and B Li, *Phys. Rev. E* **60** 2231-2249 (1999).
9. R.D. White, K.F. Ness and R.E. Robson, *Appl. Surf. Sci.* **192** 26-49 (2002).
10. R.D. White, R.E. Robson, B. Schmidt and M.A. Morrison, *J. Phys. D: Appl. Phys.* **36** 3125-3131 (2003).
11. R.W. Crompton, *Adv. At. Mol. Opt. Phys.* **32** 97 (1994).
12. R.E. Robson, *Aust. J. Phys.* **37** 34 (1984).
13. S. Dujko, Z.M. Raspopović and Z.Lj. Petrović, *J. Phys. D: Appl. Phys.* **38** 2952-2966 (2005).
14. S. Dujko, R.D. White, K.F. Ness, Z.Lj. Petrović and R.E. Robson, *J. Phys. D: Appl. Phys.* **39** 4788-4798 (2006).
15. S.Dujko, R.D. White and Z.Lj. Petrović, to be published (2008).
16. T. Taniguchi, M. Suzuki, K. Kawamura, F. Noto and H. Tagashira, *J.Phys.D: Appl. Phys.* **20** 1085-1087 (1987).
17. W.L. Morgan, *Comp. Phys. Comunn.* **58** 127-152 (1990).
18. W.L. Morgan, *Phys. Rev. A* **44** 1677-1681 (1991).
19. Z.Lj. Petrović, PhD Thesis, Australian National University (1984).
20. Z.Lj. Petrović, M. Šuvakov, Ž. Nikitović, S. Dujko, O. Šašić, J. Jovanović, G. Malović and V. Stojanović, *Plasma Source Sci. Technol.* **16** S1-S12 (2007).
21. Z.Lj. Petrović, R.W. Crompton and G.N. Haddad, *Aust. J. Phys.* **37** 23 (1984).

ODREĐIVANJE PRESEKA ZA SUDARE ELEKTRONA I MOLEKULA NA NISKIM ENERGIJAMA ANALIZOM TRANSPORTNIH OSOBINA ROJEVA ELEKTRONA

S. Dujko, R.D. White, Z.Lj. Petrović

U ovom radu diskutovane su tehnike razvijene u okviru fizike rojeva elektrona koje uključuju rešavanje Boltzmannove jednačine i Monte Carlo simulaciju za određivanje preseka za sudare elektrona i molekula na niskim energijama. Razvijena je metoda za rešavanje Boltzmannove jednačine, bazirana na razvoju funkcije raspodele u red sa proizvoljnim brojem članova kao i Monte Carlo kod, koji su korišćeni za proučavanje važnih aspekata u transportu elektrona u neutralnim gasovima u uslovima promenljivih konfiguracija električnih i magnetskih polja kada nekonzervativni sudari jako utiču na transportne osobine elektrona. Ovi aspekti podrazumevaju proveru validnosti tehnike za rešavanje Boltzmannove jednačine bazirane na razvoju funkcije raspodele u red do dva člana po Legendreovim polinomima, tretman nekonzervativnih sudara, uticaj magnetskog polja na transport elektrona kao i prirodu i razlike između transportnih osobina dobijenih u različitim eksperimentalnim uslovima. Pokazano je da ovi aspekti transporta elektrona moraju biti pažljivo razmotreni prilikom konstrukcije skupova preseka za rasejanje elektrona na molekulima.