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Chapter 9

Spatial relaxation of electron swarm in dc electric and magnetic fields crossed at arbitrary angle

9.1 Introduction

In this chapter, the non-hydrodynamic kinetic theory and SST Monte Carlo simulation code discussed in previous chapters are employed to investigate the spatial relaxation of electron swarms under the influence of dc electric and magnetic fields crossed at arbitrary angle when non-conservative collisions are operative. Similar studies for conservative model and real gases in a crossed field configuration have been recently published by Winkler et al. (2000), Li et al. (2006) and White et al. (2006). In this thesis, we extend these previous contributions to include a magnetic field at arbitrary angle with respect to the electric field and to consider the explicit effects of non-conservative collisions on the spatial relaxation process of electron swarms. Therefore, this work represents the first systematic treatment of the effect of non-conservative processes on the spatial relaxation of electron swarms in dc electric and magnetic fields crossed at arbitrary angle. Another important point concerning the calculation of transport properties under conditions when non-conservative collisions are present, should be emphasized from the outset: When nonconservative processes are operative, the SST transport properties are different from those determined from hydrodynamic calculations often calculated in TOF (time-of-flight) and PT (pulsed-Townsend) analysis (Tagashira et al. (1977); Sakai et al. (1977); Robson (1991); Dujko et al. (2008a)). In this chapter we have considered the convergence of the density gradient expansion often used in the hydrodynamic analysis of swarm experiments. In other words, the SST transport properties are represented in terms of general quantities calculated under hydrodynamic conditions. One of the primary purposes of this chapter is to use Monte Carlo simulations to test these hydrodynamic expansions under SST conditions, their convergence and range of applicability. Once more we would like to emphasize that we are not advocating the use of labels to assign different transport properties to different experiments. However, for emphasis
in this thesis we shall use the subscript SST to designate that the properties have relaxed to their spatially independent values, e.g. “SST average energy” $\bar{\varepsilon}_{\text{SST}}$ and “SST average velocity” $\bar{v}_{\text{SST}}$.

Another important aspect of the present chapter is to investigate the effects of magnetic field crossed at arbitrary angle with respect to the electric field on the spatial relaxation of electrons and corresponding evolution of the transport properties. The study has been performed for an appropriate range of magnetic and electric field strengths and angles between the fields. In this Chapter we present results of a Monte Carlo simulation and Boltzmann equation analysis of spatial relaxation of electrons in the presence of a magnetic field, applied at arbitrary angles to the electric field, extending the previous Boltzmann studies for orthogonal fields referred to above. We also generalize these earlier results by including non-conservative collisional processes, and believe that modeling of magnetrons and inductively coupled plasma discharges may benefit from this study.

9.2 Spatial relaxation of electron swarms in dc electric fields

9.2.1 Inelastic system: Step model

To understand the role of elastic and inelastic collisions on spatial relaxation profiles of the electron transport properties, we study here electrons in a model gas, using an inelastic step function model. This model was employed previously when studying eigenvalue spectra in the case of electric field only (Robson et al., 2000) and when magnetic field is present (Li et al., 2006). The details of this model are

$$\sigma_m = 6 \, \text{Å}^2, \quad \sigma_i = 0.1 \, \text{Å}^2, \quad \epsilon_i = 2 \, \text{eV}, \quad m_0 = 4 \, \text{amu}, \quad T_0 = 0 \, \text{K}, \quad (9.1)$$

where the inelastic collisions are characterized by a cross section $\sigma_i$ and a threshold $\epsilon_i$ while $\sigma_m$ is the cross section for elastic collisions. $m_0$ is the mass of the background neutral particles while $T_0$ is the temperature of the background gas. Here the electric field strength of interest varies between 1 Td and 25 Td. Initially, electrons have energy of 1 eV and are released isotropically from the cathode surface into the half space. Spatial relaxation can be characterized by a spatial relaxation length and a relaxation period if oscillatory behavior exists. In what follows these properties are examined for the step model.

Figures 9.1 and 9.2 show how mean energy and average velocity vary with the position as $E/n_0$ changes. A ‘window’ of electric field strengths (Winkler et al. (1996; 1997); Petrov and Winkler (1997); Robson et al. (2000); Li et al. (2002)) is clearly evident for which both the mean energy and average velocity exhibit oscillatory behavior as they relax to the equilibrium state far downstream from the cathode. Between 3 and 15 Td, spatial relaxation is slow and for the distances between the electrodes considered in this work, the spatially uniform values...
are not reached. The periods of oscillations for the reduced electric field in the range 2-15 Td are consistent with those calculated theoretically through $P_{th} = \epsilon_i/eE$, where $\epsilon_i$ is the threshold of the cross section for inelastic collisions. All these results are consistent with experimental observations of Hayashi (1982) and Fletcher (1985), and theoretical calculations of Winkler and co-workers (Winkler et al. (1996; 1997); Petrov and Winkler (1997) and Robson and co-workers (Robson et al. (2000); Li et al. (2002))).
From figures 9.1 and 9.2 we observe that the spatial relaxation length, period and amplitude of oscillations are strongly controlled by competition between elastic and inelastic collisional energy losses, which play distinctively different roles. For $E/n_0$ of 1 Td the elastic collisions play the predominant role and the relaxation is monotonic. In general, elastic collisions always produce monotonic relaxation to a spatially uniform state, by virtue of continuous energy losses in such processes. However, as $E/n_0$ increases, inelastic collisions start to play significant role and we observe that both the mean energy and average velocity relax toward a spatially uniform state via oscillatory decay. In contrast to elastic collisional processes, inelastic collisional processes are discrete energy loss processes. In the absence of elastic collisions, electrons would experience energy accumulation from the field followed by a discrete energy loss due to an inelastic collision. This would result in a periodic spatial profile with a period of oscillations inversely proportional to the field strength and proportional to the energy threshold for the process. In figure 9.3 we show what happens when the cross section for elastic collisions $\sigma_m$ is reduced by a factor of 2, 3 and 10, respectively at $E/n_0$ of 6 Td. As can be observed, the amplitude of oscillations is markedly increased and the damping is significantly reduced. On the other hand, the period of oscillations is essentially unaltered. Two important conclusions follow from this discussion. First, elastic collisions are always present and tend to damp the oscillatory behavior and broaden the peaks. Second, since the Franck-Hertz experiment is focused solely on examination of the quantization of atomic levels, the neglect of elastic collisions in a traditional description of this experiment seems to be acceptable. On the other hand, the full understanding of the oscillatory phenomena, experimentally observed by Hayashi (1982) and Fletcher (1985) and others in low-pressure, low-current discharges, requires a rigorous kinetic treatment of electron kinetics.

Figure 9.3: Spatial relaxation of the mean energy for the step model at $E/n_0$ of 6 Td for different magnitudes of the cross section for elastic collisions.
In summary we may identify two distinctively different physical situations: (i) if the collisional energy loss is governed essentially by ‘continuous’ energy loss processes then we have monotonic decay (e.g. when the mean swarm energy is much less than the lowest energy threshold and elastic collisional processes are dominant, or when mean swarm energies are much greater than the lowest threshold); (ii) if the collisional energy loss is dominated by ‘discrete’ energy loss processes then we have damped periodic decay (e.g. when the mean swarm energy is less than the lowest energy threshold). This suggests that certain gases only exhibit oscillatory spatial relaxation over a limited range of $E/n_0$.

Another issue that is highly relevant for understanding the mechanism of spatial relaxation processes is the influence of initial conditions. For a particular value of $E/n_0$, the spatial relaxation for a given transport property will be different if the initial conditions are different. However, the spatially independent values of that transport property must be the same, independent of the initial conditions. As an illustrative example, figure 9.4 shows spatial relaxation of the mean energy for the step model at $E/n_0$ of 25 Td as a function of different initial conditions. Four different electron swarms, each with an initial beam velocity distribution function, with the average electron energies of 0.5, 5, 10 and 20 eV are considered. It is clearly evident from this figure that the spatial relaxation of the mean energy is different, even though the spatially independent value is not affected by the average energy of the initial velocity distribution function. We observe that different initial conditions alter the relaxation profiles, including the modulation amplitude, relaxation length and period of oscillations of the mean energy. From this figure, it can be seen that, among all considered initial average energies, the modulation amplitude, relaxation length and period of oscillations are significantly diminished for the highest initial average energy. In such a case, the initial average swarm energy is much greater than the threshold for inelastic collisions and both the elastic and inelastic collisional losses are essentially ‘continuous’ energy loss processes. Thus the monotonic relaxation towards the spatially independent state follows.

9.2.2 The ionization model of Lucas and Saelee

To understand the fundamental effects of ionization on spatial relaxation profiles of the electron transport properties we consider electrons in the ionization Lucas-Saelee model (6.2). As remarked previously, there are some interesting aspects associated with this model. Firstly, the sum of the inelastic and ionization cross sections is independent of the parameter $F$, while secondly the threshold energies are the same for both processes. Thus, this model can be used to isolate and separate effects of inelastic and ionization collisions, respectively. This can be done through the variation of a parameter $F$. However, it is common in the literature on electron swarms to find ionization processes simply as another inelastic process (Kortshagen et al. (1991) and Petrov and Winkler (1997)). If this scenario was used in our considerations there would be no variation in the calculated transport properties with respect to variation in the parameter $F$. In other words, there would be no differences between the transport properties obtained under the SST conditions and flux transport coefficients calculated under hydrodynamic conditions.
Figure 9.4: Spatial relaxation of the mean energy for the step model at $E/n_0$ of 25 Td starting from the beam initial velocity distribution function with the average electron energies of 0.5, 5, 10 and 20 eV.

Figure 9.5: Spatial relaxation of the (a) mean energy, (b) average velocity and (c) ionization rate coefficient for the ionization model of Lucas and Saelee at $E/n_0 = 10$ Td. The initial electron energy is 1.5 eV.

In figure 9.5, we display spatial relaxation of the mean energy, average velocity and ionization...
rate coefficient, respectively, for different values of \( F \). We observe periodic relaxation profiles for all the conditions considered and this behavior is consistent with previous results published by Li et al. (2002). The average energy does not depend on \( F \) near the cathode region, reflecting the distance required for electrons emitted at the initial energy to obtain sufficient energy to initiate ionization collisional processes. Figure 9.5 (b) shows the relaxation of the average velocity. The positions of the extremes in average velocity are found to correspond to those of the mean energy. Figure 9.5 (c) shows spatial relaxation of the ionization rate. 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 a distance sufficient for their energy to be higher than the ionization threshold. The ionization rate peaks at the positions which correspond to the peaks of the mean energy. The explanation for this is associated with the fact that the ionization collision frequency increases with energy for this model and consequently electrons undergo more ionization collisions at higher energy.

As emphasized in the previous section, spatial relaxation can be characterized by a spatial relaxation length and a relaxation period if oscillatory behavior exists. The detailed calculations of the positions of the extremes in transport properties for the Lucas-Saelee model revealed a small increase in the periods of oscillations of the various transport properties when increasing \( F \). In addition, it has been observed that the relaxation periods are approximately one and a half times longer than the theoretical value calculated through \( \Delta z = \varepsilon_i/eE \), where \( \varepsilon_i \) is the threshold for inelastic cross section, \( e \) is the electron charge and \( E \) is the magnitude of the electric field. Figures 9.5 (a)(c) also demonstrate that the relaxation lengths of all transport properties increase with the parameter \( F \). These results independently confirm the previous calculations of Li et al. (2002).

Table 9.1: Comparison between the SST and mean energies, as well as accuracy of the low-order truncations of the density gradient expansion for the ionization model of Lucas and Saelee.

<table>
<thead>
<tr>
<th>( F )</th>
<th>( F = 0 )</th>
<th>( F = 0.25 )</th>
<th>( F = 0.5 )</th>
<th>( F = 0.75 )</th>
<th>( F = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tilde{\varepsilon} ) (eV)</td>
<td>5.57</td>
<td>5.39</td>
<td>5.22</td>
<td>5.09</td>
<td>4.97</td>
</tr>
<tr>
<td>( \varepsilon_{SST} ) (eV)</td>
<td>5.57</td>
<td>5.30</td>
<td>5.11</td>
<td>4.95</td>
<td>4.82</td>
</tr>
<tr>
<td>( \alpha \gamma ) (eV)</td>
<td>0.00</td>
<td>-0.07</td>
<td>-0.11</td>
<td>-0.13</td>
<td>-0.13</td>
</tr>
<tr>
<td>( \tilde{\varepsilon} + \alpha \gamma ) (eV)</td>
<td>5.57</td>
<td>5.32</td>
<td>5.11</td>
<td>4.96</td>
<td>4.84</td>
</tr>
<tr>
<td>( \Delta ) (%)</td>
<td>0.0</td>
<td>0.4</td>
<td>0.0</td>
<td>0.2</td>
<td>0.4</td>
</tr>
</tbody>
</table>

In what follows we restrict our discussion to the stage of evolution in the SST experiment where the average energy and average velocity have relaxed to their spatially independent values \( \varepsilon_{SST} \) and \( v_{SST} \). We can see immediately from tables 9.1 and 9.2 that the SST values disagree with the mean energy and flux drift velocities traditionally determined in hydrodynamic calculations. As expected, from tables 9.1 and 9.2 we observe that for \( F = 0 \), when conservative collisions are operative only, \( \varepsilon_{SST} \) and \( v_{SST} \) reduce to \( \tilde{\varepsilon} \) and \( W^{(\ast)} \) respectively. While there are no/minimal variations in \( W^{(\ast)} \) with increasing \( F \), the \( \tilde{\varepsilon} \) decreases with increasing \( F \) (Nolan et al., 1997). For SST conditions, both the \( \varepsilon_{SST} \) and \( v_{SST} \) decrease with \( F \). This is illustrated in figure 9.5 (a).
Table 9.2: Comparison between the SST and flux drift velocities, as well as accuracy of the low-order truncations of the density gradient expansion for the ionization model of Lucas and Saelee.

<table>
<thead>
<tr>
<th></th>
<th>$F = 0$</th>
<th>$F = 0.25$</th>
<th>$F = 0.5$</th>
<th>$F = 0.75$</th>
<th>$F = 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W^{(s)}$ (10^4 m/s)</td>
<td>7.32</td>
<td>7.32</td>
<td>7.32</td>
<td>7.32</td>
<td>7.32</td>
</tr>
<tr>
<td>$v_{SST}$ (10^4 m/s)</td>
<td>7.32</td>
<td>7.08</td>
<td>6.92</td>
<td>6.79</td>
<td>6.68</td>
</tr>
<tr>
<td>$\Delta$ (%)</td>
<td>0.0</td>
<td>3.3</td>
<td>5.5</td>
<td>7.2</td>
<td>8.7</td>
</tr>
<tr>
<td>$D_L^* \alpha$ (10^3 m/s)</td>
<td>0.00</td>
<td>2.32</td>
<td>4.05</td>
<td>5.40</td>
<td>6.53</td>
</tr>
<tr>
<td>$W^{(s)} - D_L^* \alpha$ (10^4 m/s)</td>
<td>7.32</td>
<td>7.09</td>
<td>6.92</td>
<td>6.78</td>
<td>6.67</td>
</tr>
<tr>
<td>$\Delta$ (%)</td>
<td>0.0</td>
<td>0.1</td>
<td>0.0</td>
<td>0.1</td>
<td>0.1</td>
</tr>
</tbody>
</table>

A striking feature of the data presented in the tables 9.1 and 9.2 is a small but noticeable discrepancy between $\varepsilon_{SST}$ and $\tilde{\varepsilon}$, and $v_{SST}$ with $W^{(s)}$ as $F$ increases. In addition, it is clearly evident that the differences between $v_{SST}$ with $W^{(s)}$ are more affected by a parameter $F$ (the degree of ionization) than the differences between the $\varepsilon_{SST}$ and $\tilde{\varepsilon}$. For the highest ionization degree of $F = 1$, the differences between $v_{SST}$ with $W^{(s)}$ approaches to 10%. These properties are quite general when ionization is involved, i.e.

- The SST average velocity is always less than the flux drift velocity, and
- The SST average energy is always less than the mean energy.

One can immediately see that these are general properties by referring to the relations (5.49) and (5.50). For example, from (5.50) and using the fact that both $D_L$ and $\alpha$ are positive it follows immediately that $v_{SST} < W^{(s)}$. Likewise, from (5.49) since $\gamma$ (or $\varepsilon_1$) is always negative (White et al., 1995) and $\alpha$ is positive for ionization, it then follows that $\varepsilon_{SST} < \tilde{\varepsilon}$.

Physically, (to first order in density gradients) the flux of electrons in the SST experiment is a combination of the drift due to the electric field force ($n W^{(s)}$) and a diffusive flux due to gradients in the electron density profile ($-D_L dn/dz$). When ionization processes are dominant in the SST experiment, the density profile increases exponentially with distance in the direction of the electric field force. Hence, the diffusive flux arising from this gradient in the electron number density is then in opposite direction to the drifted flux due to the electric field. It then follows that the diffusive flux acts to reduce the field flux and hence $v_{SST} < W^{(s)}$.

Likewise, (to first order in density gradients) the average energy of electrons is a combination of the mean energy $\bar{\varepsilon}$ and a contribution associated with the energy losses/gains due to diffusive processes ($\gamma dn/dz$). The mean energy of electrons far from the source is a balance of energy deposited by the field and that dissipated in collisions. As electrons move away from the source they fall through a greater potential and hence have more energy deposited by field. Now considering the contribution to the average energy associated with the diffusive flux electrons: since this diffusive flux is against the electric field force (due to the increasing electron density profile) these electrons are going against the field force and this contribution is acting to reduce the average energy. It then follows that $\varepsilon_{SST} < \bar{\varepsilon}$.
To investigate spatial relaxation in the presence of the electron attachment, the modified Ness-Robson attachment model has been considered. The details of this gas model are given by (6.4). This thesis considers zero attachment model (MA0: \(a = 0, p = 0\)) and the case studies where the attachment cross section is proportional to the electron velocity (MA1: \(a = 5 \times 10^{-4}, p = 0.5\)), inversely proportional to the electron velocity (MA2: \(a = 2 \times 10^{-3}, p = -0.5\)) and inversely proportional to the electron energy (MA3: \(a = 8 \times 10^{-3}, p = -1.0\)), where parameters \(a\) and \(p\) determine the magnitude and energy dependence of the attachment cross section, respectively.

Figure 9.6: Spatial relaxation of the (a) mean energy, (b) average velocity and (c) ionization rate coefficient for modified attachment model of Ness and Robson at \(E/n_0 = 10\) Td. The initial electron energy is 1.5 eV.

In figure 9.6 we demonstrate the spatial relaxation of the average energy, average velocity and attachment rate coefficient. They display the same general behavior in the relaxation profiles as those for ionization. The only noticeable differences arise from the difference in the thresholds for the ionization and attachment models. For the attachment model, the threshold is zero and hence the average energy and average velocity deviate from the conservative case in close vicinity of the cathode. In the regime where the transport properties have relaxed to spatially-independent values, the following important general properties for attachment in SST are observed:

- The SST drift velocity is always greater than the flux drift velocity, and
- The SST average energy is always greater than the mean energy.
Table 9.3: Comparison between the SST and mean energies, as well as accuracy of the low-order truncations of the density gradient expansion for the modified attachment model of Ness and Robson.

<table>
<thead>
<tr>
<th>MA0</th>
<th>MA1</th>
<th>MA2</th>
<th>MA3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tilde{\varepsilon}$ (eV)</td>
<td>5.57</td>
<td>5.45</td>
<td>5.57</td>
</tr>
<tr>
<td>$\varepsilon_{\text{SST}}$ (eV)</td>
<td>5.57</td>
<td>5.66</td>
<td>5.71</td>
</tr>
<tr>
<td>$\Delta$ (%)</td>
<td>0.0</td>
<td>3.7</td>
<td>2.5</td>
</tr>
<tr>
<td>$\alpha\gamma$ (eV)</td>
<td>0.00</td>
<td>0.21</td>
<td>0.14</td>
</tr>
<tr>
<td>$\tilde{\varepsilon} + \alpha\gamma$ (eV)</td>
<td>5.57</td>
<td>5.66</td>
<td>5.71</td>
</tr>
<tr>
<td>$\Delta$ (%)</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table 9.4: Comparison between the SST and flux drift velocities, as well as accuracy of the low-order truncations of the density gradient expansion for the ionization model of Lucas and Saelee.

<table>
<thead>
<tr>
<th>MA0</th>
<th>MA1</th>
<th>MA2</th>
<th>MA3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W^{(\star)}$ ($10^4$ m/s)</td>
<td>7.32</td>
<td>7.32</td>
<td>7.32</td>
</tr>
<tr>
<td>$v_{\text{SST}}$ ($10^4$ m/s)</td>
<td>7.32</td>
<td>7.89</td>
<td>7.72</td>
</tr>
<tr>
<td>$\Delta$ (%)</td>
<td>0.0</td>
<td>7.2</td>
<td>5.2</td>
</tr>
<tr>
<td>$D^{(\star)}\alpha$ ($10^3$ m/s)</td>
<td>0.00</td>
<td>5.27</td>
<td>3.82</td>
</tr>
<tr>
<td>$W^{(\star)} - D^{(\star)}\alpha$ ($10^4$ m/s)</td>
<td>7.32</td>
<td>7.85</td>
<td>7.70</td>
</tr>
<tr>
<td>$\Delta$ (%)</td>
<td>0.0</td>
<td>0.5</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Using similar arguments to that outlined for ionization, but with our arguments modified with $\alpha$ now being negative, these general properties can be inferred from relations (5.49) and (5.50). Physically, when attachment is the dominant non-conservative process, the diffusive flux contribution to the average velocity of the electrons is now in the direction of the directed flux $nW^{(\star)}$ since the density profile decreases exponentially with distance from the source. It then follows that the diffusive flux acts to enhance the field flux and hence $v_{\text{SST}} > W^{(\star)}$. Likewise, since the diffusive flux is in the direction of the field force, the contribution to the average energy associated with diffusive processes is now positive, and it follows that $\varepsilon_{\text{SST}} > \tilde{\varepsilon}$.

9.2.4 Real gases: argon, CF$_4$ and argon-CF$_4$ mixture

To illustrate a spatial relaxation process in real gases, we consider electrons in argon, CF$_4$ and its mixture for a range of $E/n_0$. The primary electrons are isotropically released, one by one, from the cathode surface into the half space with an initial energy of 1 eV. Figures 9.7 and 9.8 illustrate the spatial relaxation of the mean energy and average velocity in pure argon. The cross sections for electrons in argon are displayed and detailed in Chapter 7 (see figure 7.32 (b)) while the cross sections for CF$_4$ are displayed and detailed in Chapter 8 (see figure 8.1). The figures emphasize that the spatial relaxation of the mean energy and average velocity is considerably different at different field strengths. Qualitatively, the spatial relaxation profiles exhibit similar behavior to that demonstrated for model gases of the previous section.
In figure 9.9 (a) and (b) we show spatial relaxation of the mean energy and average velocity in CF$_4$. We observe that as the field increases, the mean energy monotonically increases throughout the space. However, the average velocity shown in figure 9.9 (b) exhibits quite different behavior. First, during the early stage of the relaxation process, the average velocity increases
with an increasing field. For $E/n_0 \geq 20$ Td, however, as the relaxation process proceeds further throughout the space, the average velocity reduces. The spatially independent value for $E/n_0$ of 70 Td is less than those of 10, 20, 30 and 40 Td away from the immediate vicinity of the cathode. This effect may be viewed as a non-hydrodynamic counterpart of hydrodynamic negative differential conductivity (NDC). A comprehensive investigation of NDC for model gases in pure dc electric fields under hydrodynamic conditions was performed by Petrović et al. (1984) and Robson (1984). As pointed out in these studies, NDC arises for certain combinations of elastic and inelastic cross sections in which, on increasing the electric field, there is a rapid transition in the dominant energy loss mechanism from inelastic to elastic. The determining factor is how rapidly the ratio of the inelastic to elastic cross sections falls with the increasing mean energy/applied field. As can be observed from figure 9.9 (b), this effect carries over directly to the case where non-hydrodynamic conditions dominate.

Figure 9.9: Spatial relaxation of the mean energy (a) and average velocity for electrons in CF$_4$ for a range of reduced electric fields.

Comparison of the relaxation behavior of electrons in CF$_4$ and that in argon indicates that a very different spatial evolution of electrons in CF$_4$ takes place. While in argon the spatial relaxation profiles of various transport properties are weakly damped, in CF$_4$ the spatial profiles are heavily damped due to the presence of other inelastic channels such as rotational, vibrational and electronic excitations which usually have threshold energies over a wide range. As a consequence of these inelastic channels, already after a distance of about 1 cm (at the gas pressure of 1 Torr) the mean energy and average velocity are reached the steady-state values whilst a distance of more than 30 cm is necessary in argon at the same $E/n_0$. This is a clear sign that the spatial relaxation process of electrons in atomic and molecular gases differs considerably. In what follows we consider the spatial relaxation processes of electrons in argon-CF$_4$ mixture. As remarked previously, this mixture plays an important role in many plasma devices used in plasma processing technology. Experimentally, on the basis of the photon-flux technique, Fletcher (1985) showed that by introducing a small amount of molecular gas
admixture, luminous layers can be quenched. Therefore, we have been motivated to check this important experimental observation. In figure 9.10 we show the spatial relaxation of the mean energy in pure argon and argon-CF₄ mixture at \( E/n_0 \) of 15 Td. We observe that the mean energy in pure argon exhibits a damped oscillatory relaxation along a decaying profile. However, by introducing a small amount of molecular admixture (e.g. CF₄) the oscillations are firstly suppressed and then entirely quenched in the limit of higher concentration of CF₄. By introducing a molecular admixture other collision processes, preferentially lower threshold vibrational excitations are introduced. These new collision processes lead to more efficient damping than elastic collisions, by virtue of larger and different energy loss mechanisms.

![Figure 9.10: Spatial relaxation of the mean energy for electrons in argon-CF₄ mixture.](image)

Generally speaking, monoatomic gases are much better candidates than the molecular gases for observing the luminous layers. As an illustrative example, the threshold energies of different excitation processes for noble gases are concentrated in a relatively narrow region. This favors the development of luminous layers. In molecular gases, rotational, vibrational and lower electronic excitation loss diminishes the periodic structure of the electron energy in space. However, periodic behavior of the transport properties is observable for molecular gases as well (see for example Segur et al. (1995)). As pointed out by Li et al. (2002), this can happen as long as the field strengths are concentrated in the ‘window’ range pertinent to the specific excitation of interest.
9.3 The effects of magnetic field on the spatial relaxation profiles

9.3.1 Inelastic systems: Step and conservative Lucas-Saelee ionization models

A. The effects of the magnetic field strength on the spatial relaxation processes

To understand the fundamental effects of the magnetic field on relaxation characteristics when inelastic collisions are present, we study here electrons in model gases, using both the step inelastic model (9.1) and conservative Lucas-Saelee model. The step inelastic model has been recently investigated by Li et al. (2006) in a crossed field configuration. In order to test the present Monte Carlo method and see how it compares with the work of Li et al. (2006), we calculate the spatial relaxation profiles of various transport properties under the same conditions.

Figure 9.11: Spatial relaxation of the mean energy (first row) and average velocities \( v_z \) (second row) and \( v_x \) (third row) for the step model at \( E/n_0 = 6 \) Td for a range of magnetic fields: \( B/n_0 = 0 \) (first column), 100 Hx (second column), 500 Hx (third column), and 1000 Hx (fourth column).

Figure 9.11 displays the spatial relaxation of transport properties at \( E/n_0 = 6 \) Td for varying \( B/n_0 \). In the absence of a magnetic field both the mean energy and the average velocity relax...
toward a spatially uniform state via oscillatory decay. The relaxation of these quantities is very slow and as can be observed the steady-state is not reached for the spatial region shown. For \( B/n_0 = 100 \) Hx, we observe from figure 9.11 that both the maximal and spatially independent (steady-state) values of the mean energy and average velocity are lower than those for \( B/n_0 = 0 \) Hx. The reason for this is the well-known cooling effects of an orthogonal magnetic field. In addition, due to electron gyrations the \( E \times B \) average velocity component \( v_x \) is now non-zero. Both the relaxation length and period of oscillations are not significantly affected by the application of magnetic field of 100 Hx. However, when the magnetic field strength is further increased to 500 Hx, a distinctively different spatial evolution of all transport properties can be observed. First, both \( \varepsilon \) and \( v_z \) are significantly lower than for the case \( B/n_0 = 100 \) Hx, while \( v_x \) is enhanced in both the maximal and spatially uniform values. In this case, the spatial relaxation occurs in an almost aperiodic manner with a much stronger damping. In addition, the relaxation length is markedly shorter. Finally, in the limit of the highest \( B/n_0 \) of 1000 Hx, all the quantities are much less than the magnetic field-free case. The spatial relaxation profiles of all transport properties show very weak irregular oscillations which are quickly damped.

Generally speaking, under conditions considered in this example, the application of an orthogonal magnetic field cools the swarm reducing the discrete nature of energy loss processes. This is verified at the figure 9.12 where the spatial relaxation of the collisional rates for elastic and inelastic collisions is shown. Further enhancement of the magnetic field cools the swarm to a state such that continuous energy loss elastic collisional processes are dominant and relaxation is monotonic. The behavior of rate coefficients shown in figure 9.12 supports this physical picture. As can be observed, the rate coefficient for elastic collisions is increased for an order of magnitude while the rate coefficient for inelastic collisions is significantly reduced in the limit of the highest \( B/n_0 \) of 1000 Hx. This is a clear indication that magnetic field can be used to control the spatial relaxation.

B. The effects of the angle between the fields on the spatial relaxation processes

In this section we consider the influence of the angle between the electric and magnetic fields on the spatial relaxation processes of electrons. In figure 9.13 we demonstrate the impact of angle between the fields on the spatial relaxation of the mean energy and rate coefficients for elastic and inelastic collisions. Figure 9.14 displays the spatial relaxation of the average velocity components as a function of the angle between the fields. The profiles are presented for \( B/n_0 \) of 200 Hx.

For parallel fields \( (\psi = 0^\circ) \), the spatial relaxation profiles of the mean energy and average velocity \( v_z \) are in excellent agreement with those associated with a pure electric field. This follows from the symmetry property outlined by White et al. (1999a). These properties were demonstrated under hydrodynamic conditions but as can be observed from above figures, they carry over to the case where non-hydrodynamic conditions prevail. The same symmetry properties impose the following (see figure 9.14): \( v_x = v_y \) for \( \psi = 0^\circ \) and \( v_y = 0 \) for \( \psi = 90^\circ \). For parallel fields, on average the electrons are traveling in the direction of the electric and magnetic field and hence the magnetic field has no explicit effect. Under the same field orientation, we observe
that both $\varepsilon$ and $v_z$ exhibit a damped oscillatory relaxation along a decaying profile for a chosen set of conditions. However, as the angle between the fields increases, both the maximal and spatially independent (steady-state) values of $\varepsilon$ and $v_z$ are lower than those for parallel fields. The physical mechanism for the cooling action of a magnetic field when electric and magnetic fields are crossed at arbitrary angle is given in Chapter 6 of this thesis and in previous papers of White et al. (1999a; 1999d). In brief, the cooling mechanism is enhanced as the component of the magnetic field perpendicular to the electric field (and hence the angle between the fields) is increased. This means that the cooling mechanism is the strongest in the limit of a crossed field configuration.

From figure 9.14 we see that the steady-state values of both $v_x$ and $v_y$ monotonically increases with an increasing $\psi$ for a chosen $B/n_0$ of 200 Hx. It is interesting to note that the modulation amplitude of $v_x$ first increases for $\psi = 60^\circ$ and then decreases for $\psi = 90^\circ$. One may expect different trends if different values of $B/n_0$ are chosen. These two transport quantities have the worst statistics in our simulations. Despite this, it can be seen that $v_y$ is comparable with $v_x$ and $v_z$ but yet it is common in the literature for plasma modelers to fail to include this quantity in their models. An extension of standard plasma models to include the $(E \times B) \times B$ effects on electron transport may led to a better understanding of the power transfer to magnetically assisted/enhanced plasma reactors.

In general, under the conditions considered in this example, as the angle between the fields increases the magnetic field cools the swarm and lowers its mean energy. In addition, both
Figure 9.13: Spatial relaxation of the mean energy (first row) and rate coefficients for elastic (second row) and inelastic (third row) collisions for the step model at $E/n_0 = 6$ Td for various field orientations: $\psi = 0^\circ$ (first column), $\psi = 30^\circ$ (second column), $\psi = 60^\circ$ (third column), and $\psi = 90^\circ$ (fourth column).

the relaxation length and period of oscillations are significantly reduced. This is indicative of reducing the discrete nature of energy loss processes. The spatial relaxation profiles of the rate coefficients for elastic and inelastic collisions shown in figure 9.13 supports these physical arguments. We observe that as the angle between the fields increases, the continuous energy losses in elastic collisions are enhanced while the discrete energy loss processes in inelastic collisions are weakened. These results suggest that in addition to the magnetic field strength, the angle between the fields has an ability to control the spatial relaxation of electrons in an idealized SST experiment.

In what follows, the non-hydrodynamic theory for solving the spatially-dependent Boltzmann equation discussed in the previous chapters is applied to calculate the spatial profiles of the average velocity components for electrons. In figure 9.15 we show the spatial relaxation of $v_z$ and $v_x$ at $E/n_0 = 10$ Td for varying $B/n_0$ in a crossed field configuration for the conservative Lucas-Saelee model (the parameter $F$ is set to 0). The parameters of the source drifted Maxwellian distribution are $T_i = 8 \times 10^3$ K and $v_i = 8 \times 10^3$ m/s. For this choice of $E/n_0$, in the absence of a magnetic field, our Monte Carlo method (see section 9.2.2) showed that the average velocity relaxes toward a spatially uniform state via oscillatory decay. By virtue of different initial conditions, the relaxation profiles obtained by a Monte Carlo simulation technique and Boltzmann equation do not coincide. However, the excellent agreement for the spatially uniform values of the average velocity obtained by these two independent techniques is found.
Figure 9.14: Spatial relaxation of the average velocity components: $v_x$ (first row), $v_y$ (second row) and $v_z$ (third row) for the step model at $E/n_0 = 6$ Td for various field orientations: $\psi = 0^\circ$ (first column), $\psi = 30^\circ$ (second column), $\psi = 60^\circ$ (third column), and $\psi = 90^\circ$ (fourth column).

In obtaining the spatial profiles in figure 9.14, it was found that the two-term approximation is sufficient for three-figure accuracy.

When magnetic field is applied, we observe from figure 9.14 that the oscillations are heavily damped. As a consequence, the relaxation proceeds much faster than the magnetic-field-free case. As for the step inelastic model, this occurs due to a decrease of the mean energy as $B/n_0$ increases, enhancing the continuous energy losses in elastic collisions. Hence as $B/n_0$ increases, the peaks are more broaden and the period of oscillations becomes longer. In the limit of 500 Hx, the profiles of both $v_z$ and $v_x$ are monotonic.

9.3.2 The Lucas-Saelee ionization model and Ness-Robson modified attachment model

In this section we consider the explicit effects of non-conservative collisions (ionization and/or attachment) on spatial relaxation of electrons when electric and magnetic fields are crossed at arbitrary angle. We employ the ionization model of Lucas and Saelee (6.2) and modified attachment model of Ness and Robson (6.4).

Figures 9.16 display the spatial relaxation of the mean energy, average velocity component along the z-direction and ionization model for the Lucas-Saelee ionization model ($F = 0.5$) as a function of $B/n_0$ in a crossed field configuration. In the absence of the magnetic field, the characteristic features of the relaxation process as relaxation length and period of oscillations...
Figure 9.15: Spatial relaxation of the average velocity components: $v_z$ (first column) and $v_x$ (second column) for the conservative Lucas-Saelee ionization model ($F = 0$) as a function of $B/n_0$.

Figure 9.16: Spatial relaxation of the mean energy, $z$-components of the average velocity and ionization rate as a function of $B/n_0$ for the Lucas-Saelee ionization model.

are analyzed in section 9.2.2 and in paper of Li et al. (2002). The application of a magnetic field leads to significant changes in the relaxation profiles. When $B/n_0 = 100$ Hx, we observe that both the maximal and spatially uniform values of $e$, $v_z$ and $\alpha$ are lower than the case
when $B/n_0 = 0$ Hx. This is caused by magnetic cooling effects associated with gyrations of the electrons. When $B/n_0$ is increased further to 200 Hx, we see that the mean energy is much less than the threshold energy of both inelastic and ionization collision processes, energy losses via these collisions are reduced, and elastic collisions are enhanced. The relaxation profiles show weak irregular oscillations which are damped in the early stage of the relaxation process. At the highest $B/n_0$ of 500 Hx, the effects of inelastic and ionization collisions are suppressed and the relaxation process is dominated by elastic collisions. Consequently $\varepsilon$ and $v_z$ relax towards a spatially uniform state monotonically.

Figure 9.17: Spatial relaxation of the mean energy as a function of the angle between the fields for the Lucas-Saelee ionization model.

Figure 9.18: Spatial relaxation of the average velocity component along the $z$-direction as a function of the angle between the fields for the Lucas-Saelee ionization model.
Figures 9.17 and 9.18 show spatial relaxation of transport properties for different field orientations as a function of the parameter $F$. The magnetic field strength is set to 200 Hx. In figure 9.18, we observe that the mean energy decreases when increasing $F$ for all field orientations, except in region near the cathode (about less than 0.05 Torr m). In region near the origin, the mean energy is directly affected by the source. We observe that as $\psi$ increases both the maximal and steady-state values of the mean energy are lower than those for parallel field orientation. $v_z$ shows similar relaxation behavior. We see that the positions of the peaks in $v_z$ correspond to those of the mean energy. However, the steady state values of $\varepsilon$ and $v_z$ do not correspond to those obtained under hydrodynamic conditions as detailed in sections 9.2.3 and 9.2.4. These phenomena can be understood using similar arguments to those used in section 9.2.2 with appropriate modification due to the presence of a magnetic field. The identification of the relations for the conversion of hydrodynamic transport properties to those found in the SST experiment when both the electric and magnetic fields are present is deferred to a future work.

![Figure 9.19: Spatial relaxation of the ionization rate as a function of the angle between the fields for the Lucas-Saelee ionization model.](image)

In figure 9.19 we show spatial relaxation of the ionization rate. As expected, the ionization rate decreases with $\psi$ throughout the entire region. Figure 9.20 displays the spatial profile of the number of electrons. We observe that for a chosen set of conditions and for all field orientations, the number of electrons exponentially grows. This is a clear sign that in the presence of ionization no spatially homogeneous state for number density is possible. On the other hand, in the absence of ionization, the profile of the number density simply relaxes to a spatially independent value. The number density also decreases with increasing $\psi$ throughout the entire region, reflecting reduced electron production by ionization.

Figures 9.17-9.19 demonstrate that as $\psi$ increases, the relaxation to steady-state proceeds quicker while the period of oscillation becomes larger. This change is caused by the alteration of the dominant relaxation mechanism with increasing angle between the fields. As $\psi$ increases,
the magnetic field perpendicular to the electric field is increased cooling the swarm to a state such that continuous energy loss elastic collisional processes are dominant. As a consequence, the oscillations are heavily damped and one may expect monotonic relaxation profiles for more higher values of $B/n_0$. In addition, as $\psi$ increases for higher values of $B/n_0$ than that of 200 Hx considered in this work, one may expect significant reduction of the effects of the ionization processes. In other words, for high $B/n_0$ there would be no variation in the calculated transport properties with respect to variation in the parameter $F$.

Figures 9.21 (a) and (b) displays the spatial relaxation of the mean energy for the modified attachment model of Ness and Robson as a function of $B/n_0$. Both the so-called attachment cooling and attachment heating models are considered. When attachment plays an important role, such as in the case studied here, an extremely large number of initial electrons must be followed in order to retain the good statistics for transport properties at long distances from the cathode. The fluctuations imprinted on the relaxation profile of $\varepsilon$ and $v_z$ at long distances from the cathode are statistical in nature only. In figures 9.21 (a) and (b) we observe that the spatial profiles of $\varepsilon$ and $v_z$ undergo similar variations with $B/n_0$ as all model and real gases considered previously: both the maximal and spatially independent values are lower than the case when $B/n_0 = 0$ Hx. However, it is important to note that the spatially independent value of $\varepsilon$ is not the same as that under hydrodynamic conditions. Likewise, the spatially independent value of $v_z$ is not the same as the flux drift velocity obtained under hydrodynamic conditions. Using similar arguments to that outlined for the magnetic-field-free case with appropriate modifications due to the presence of a magnetic field, these general properties follows.

The spatial profiles of the number of electrons for the so-called attachment cooling model are shown in figures 9.22 (a) and (b). In figure 9.22 (a) these profiles are shown as a function of $B/n_0$ in a crossed field configuration while in figure 9.22 (b) the profiles are shown as a function of $\psi$ when $B/n_0$ is set to 200 Hx. In both cases, the spatial profiles of the number of
Figure 9.21: Spatial relaxation of the mean energy (a) and \( z \)-component of the average velocity (b) as a function of \( B/n_0 \) for the modified attachment model of Ness and Robson.

Figure 9.22: Spatial profile of the number of electrons as a function of \( B/n_0 \) (a) and \( \psi \) (b) for the modified attachment model of Ness and Robson.

electrons exhibits some interesting features. Apart from oscillations developed near the source, in the region far downstream the profile decreases exponentially. This means that in contrast to conservative cases where the number density relaxes to a spatially uniform value, in the presence of attachment no spatially homogeneous state is possible. We observe that as \( B/n_0 \) and/or \( \psi \) is increased the number of electrons is decreased at the fixed position except in the immediate vicinity of the cathode.
Chapter 10

Concluding remarks

Advancements in modern day technology associated with non-equilibrium low-temperature magnetized plasma discharges demand the most accurate modeling of the underlying transport processes involved. In order to meet this demand, in this thesis we have undertaken a program to understand the kinetic behavior of charged particle swarms under the combined action of electric and magnetic fields in neutral gases. The scope of this program has covered a variety of hydrodynamic and non-hydrodynamic studies of charged particle transport processes in varying configurations of electric and magnetic fields when non-conservative collisions (attachment/ionization) are operative. A time-dependent multi-term solution of the spatially inhomogeneous Boltzmann’s equation has been developed to investigate the transport properties of charged particle swarms under hydrodynamic conditions in time-dependent electric and magnetic fields crossed at arbitrary angle. Among many critical issues relevant for such studies, the following important points are of particular note. First, we highlight the rigorous treatment of non-conservative collisions on the electron transport properties by going to second order in the density gradient expansion. Second, no restrictions are placed on the number of spherical harmonics so our formalism is of “multi-term” nature. Lastly, the present formalism and associated code is equally valid for both electrons and ions, and as such this work is quite general in its applications. The presented hydrodynamic kinetic theory is generally independent of geometry and applicable for swarms moving in an unbounded gases where spatial dependence of the phase space distribution function is expressible in terms of the instantaneous number density and its spatial derivatives. This stands in contrast with demands for a rigorous non-hydrodynamic theory required for modeling the steady-state Townsend discharges. As a first step towards this direction, we have developed non-hydrodynamic kinetic theory for charged particle swarms under the influence of electric and magnetic fields crossed at arbitrary angle in an idealized steady-state Townsend experiment. An existing Monte Carlo simulation technique for a treatment of electron swarms under hydrodynamic conditions in an infinite neutral gas has been redesigned and implemented, as to extend its applicability to the simulation of an idealized steady-state Townsend experiment.

Under hydrodynamic conditions, the emphasis is placed on electron kinetics in time-dependent spatially uniform electric and magnetic fields crossed at arbitrary angle. Calculation of the trans-
port coefficients for a variety of model and real gases over a wide range of electric and magnetic field strengths, field frequencies, angles and phases between the fields unearthed numerous interesting and sometimes unexpected kinetic phenomena, generally inexplicable through the use of dc steady-state results. Phenomena of significant note include the existence of transient negative diffusivity, time-resolved negative differential conductivity and anomalous behavior of certain diagonal elements of the diffusion tensor in ac electric and magnetic fields. Perhaps most notably, a new mechanism for collisional heating of electrons in inductively coupled plasmas was proposed. In order to fully appreciate the structure and sometimes paradoxical variation of the temporal profiles a comprehensive investigation of the temporal relaxation of the electron swarm transport properties was required. The explicit influence of a magnetic field and non-conservative collisions on the hydrodynamic temporal relaxation has been investigated. To illustrate the wide spectrum of the temporal relaxation phenomena and to indicate significant differences between the temporal relaxation of the bulk and flux transport coefficients, a consequent kinetic study of the temporal transient processes of the electrons was carried out using appropriate relaxation models. The magnetic field was found to induce damped oscillatory temporal relaxation profiles for the drift velocity components and diffusion tensor elements. In contrast, the mean energy exhibits exclusively monotonic relaxation profiles independently of the field configuration. Most strikingly, the negative diffusion was observed in the profiles of both the bulk and flux diagonal elements of the diffusion tensor and physical arguments were used to explain the origin of this phenomenon. To our knowledge, this work represent the first rigorous treatment of non-conservative collisions on the temporal relaxation profiles in dc electric and magnetic fields crossed at arbitrary angle. Steady-state transport coefficients and properties have been also calculated for charged particle swarms in certain model gases over a range of angles between the fields and electric and magnetic field strengths. It was shown that some of the well established phenomena previously observed in dc electric fields in model and real gases such as ionization and attachment cooling and/or attachment heating are directly carried over to the dc electric and magnetic fields crossed at arbitrary angle. It was found that these phenomena can be controlled either by the variation of the magnetic field strengths or by the angles between the fields. The errors associated with the two term approximation and inadequacies of Legendre polynomial expansions were highlighted. These errors have been discussed and the need for a genuine multi-term technique was illustrated. An existing Monte Carlo technique for swarms under hydrodynamic conditions has been extended to arbitrary angles between the electric and magnetic fields. The results of simulations are compared with those obtained by a multi-term solution of Boltzmann’s equation. The comparison clearly validates the theoretical basis and support the numerical integrity of both techniques.

An investigation of the non-hydrodynamic phenomena associated with an idealized steady-state Townsend experiment for swarms in electric and magnetic field crossed at arbitrary angle has been described. The study has included a theoretical investigation in parallel with Monte Carlo simulations using certain model and real gases. It should be noted that one of the primary motivation factors for this study was to consider the spatial relaxation of electrons for an idealized SST experiment. The study has focused on the explicit influence of non-conservative
collisional processes on the relaxation behavior, and some important and quite general properties associated with the impact of attachment/ionization have emerged from this study. Also in this thesis we have considered the convergence of the density gradient expansion often used in the hydrodynamic analysis of swarm experiments. To do this, we have developed a technique that allows us to accurately calculate expansion coefficients in the density gradient expansion using the Monte Carlo technique. We were able to demonstrate for the cases considered that when hydrodynamic conditions prevailed the density gradient expansion converged rapidly. Convergence to within 1.0% was achieved in the SST properties using only the first two terms in the expansion. Another motivation factor for this study was to consider the explicit influence of a magnetic field on spatial relaxation of electron swarms. The influence of a magnetic field on the spatial relaxation characteristics is examined for certain model gases by numerical solutions of the Boltzmann equation and Monte Carlo simulation. It was shown that magnetic field strength and/or angle between the electric and magnetic fields has an ability to suppress or enhance the oscillatory feature in the spatial relaxation profiles as well as to modify the spatial relaxation distance.

There are several possible directions of future work suggested by the results of this thesis. First, since the measurements of the positron transport properties are rare, future work could extend this database with the goal of improving and optimizing the positron collisional traps. This would almost certainly require a rigorous treatment of non-conservative collisions (positron annihilation and/or positronium formation) on the positron transport properties in electric and magnetic fields crossed at arbitrary angle. Second, particularly attractive is the prospect of modeling the radiation detectors. These detectors are usually operated under various configurations of electric and magnetic fields with specific requirements on the transport properties of the swarm needed to achieve the desired spatial and temporal resolution for detection, big and fast signals, good energy deposition per unit length, etc. Third, the presented theory is equally valid for both electrons and ions and hence the computer code is easily extendable to the examination of the time-dependent behavior of ion swarms in electric and magnetic fields. Thus the theory and mathematical machinery in this thesis could be applied to the space and time kinetic modeling of plasma discharges, incorporating the effects of space-charge through a multi-term solution of Boltzmanns equation for both the electron and ion species in the discharge.