Chapter 6

Diffusion during Plasma Formation

Interesting processes occur in the plasma formation stage of the Basil discharge. This early stage has particular interest because the highest plasma densities are obtained during this time. The higher densities allow applications such as the argon ion laser [113], which operated during the plasma formation stage. The initial stage evolves on the time scale of milliseconds, with the final equilibrium sometimes not being reached until after 20msec or longer. This chapter will discuss some of the processes which occur during the plasma formation and stabilisation stage. Results are compared to a 1-D diffusion model to support the theory that neutral densities are important in establishing the longitudinal discharge profiles.

6.1 Time Evolution of the Discharge

Figure 6.1 shows the diffusion of the plasma along the axis of the experiment away from the antenna region (the edge of the antenna is at 10cm). At the edge of an expanding
plasma, where the density is low, electrons and ions diffuse independently, under conditions known as free diffusion. As the density increases and sufficient space charge is produced, free diffusion changes to ambipolar diffusion. Under ambipolar conditions separation of the more mobile electrons from the ions produces a charge imbalance and consequently an electric field. This field acts to retard the diffusion of electrons, and drag the ions along with the electrons, in order to maintain flux balance. Ambipolar diffusion is important for densities above \( n_{\text{ion}} \approx n_e = 10^{14}\text{m}^{-3} \) [23]. The overall speed at which the main body of the plasma diffuses longitudinally is limited by the inertia of the ions, while the profile of the leading edge of the discharge is determined by ambipolar and free diffusion.

The speed of the discharge diffusing longitudinally was measured for 6 argon plasmas with a range of magnetic fields and was found to have an average value of \(350\pm20\text{m sec}^{-1} \). For a Maxwellian distribution the average velocity is given by

\[
<v> = \left( \frac{3kT}{m} \right)^{\frac{1}{2}}
\]

(6.1)

However, the tail of the Maxwellian has the effect of skewing the average velocity to a higher value than the bulk of the particles. Most of the particles will travel slower than this, with the most probable velocity [85], \(v_p\), given by

\[
v_p = \left( \frac{2kT}{m} \right)^{\frac{1}{2}}
\]

(6.2)

For ions at room temperature, \(T_i \approx 0.025\text{eV}\), and the most probable velocity is \(v_{pi} \approx 350\text{m}\)
Figure 6.1: Time evolution of the ion saturation current as a function of longitudinal position for argon with a double saddle coil antenna at a static field of 1024 gauss and filling pressure of 7mTorr. The times are with respect to the start of the discharge. The vertical dotted lines indicate the edge of the antenna at 13cm and the last field coil at 70cm.
sec$^{-1}$, which is in good agreement with the measured speed.

Once the plasma reaches the end of the uniform static field region (at 70cm) a density hump develops at the end of the discharge (see figures 6.2 and 6.1). After approximately 6msec this density hump collapses very rapidly and the discharge density to a lower value, which is uniform along its length. While the time scales of this phenomenon are not the same for all conditions, most discharges show an increase in density near the end of the static field before dropping to the equilibrium value. Similar behaviour is observed in the radial density profiles, at a position 30cm from the antenna, as shown in figure 6.3. This phenomenon has also been observed by Chen [32]. For the Basil discharge it is shown that the increased density near the end of the field coils can be explained by a higher ionisation rate in this region due to neutrals diffusing back into the plasma from the end of the tube. Once this neutral reservoir is depleted the density drops and an equilibrium is established. To investigate the role of neutrals in the evolution of the discharge a 1 dimensional model has been developed. The details of this model and results are given in section 6.2.

The final equilibrium of the plasma will be determined by the energy balance. For standard conditions the numerical model determined that the radiation resistance initially increases with increasing density, reaches a maximum and then decreases with further increase in density. At equilibrium the plasma loss rate will equal the ionisation rate. Assuming the ionisation rate is proportional to the absorbed rf power, then under equilibrium conditions the loss rate will also be proportional to the absorbed rf power. However, as the density increases so does the loss rate of plasma from the system. Initially when the plasma is formed the density increases, which increases the radiation resistance, so more power is coupled into the plasma and consequently the density continues to grow.
Figure 6.2: Ion saturation current as a function of time and longitudinal position for argon with a double saddle coil antenna at a static field of 1024 gauss and filling pressure of 7mTorr. The antenna extends between 0cm and 13cm and the end of the field coils is at 70cm
Figure 6.3: Evolution of the radial density profile 30cm from the antenna versus time for argon using a double saddle coil antenna at a static field of 896 gauss and filling pressure of 30mTorr.
Equilibrium is reached when the radiation resistance starts decreasing, and any further increase/decrease in the density will result in a decrease/increase in the power coupled to the plasma producing a stabilising effect. This is an important consideration for the design of helicon plasma sources as higher densities will not necessarily be reached by increasing applied rf power.

### 6.2 Discharge Model

The longitudinal on axis discharge of Basil is modelled using a Monte Carlo code with 1 spatial dimension. The model explicitly simulates ions and “fast” neutrals as individual particles, which move according to Newton’s Laws. Background “thermalised” neutrals are modelled as a spatially varying density along the axis of the discharge. Electrons are modelled implicitly assuming a density proportional to the ion density, in order to determine ionising collision rates. They are not included explicitly in the model since following the electron dynamics would require very small time steps (of the order of $10^{-9}$ sec), which would preclude modelling the long time scale phenomena of interest.

It would be computationally impossible to follow each particle in the model, there-
fore the model uses scaled particles which represent large number of actual plasma particles. This technique is extensively employed in well known modelling methods such as Particle-in-Cell [8]. Whenever the number of scaled particles becomes larger than a specified value (in this case 50 000) then particles are systematically removed from the system and the scale factor increased proportionately.

Ions, neutrals, and electrons are all modelled as having finite temperatures, and assumed to have the appropriate Maxwell-Boltzmann distributions. Ions and neutrals are assumed to be at “room” temperature, $T_{iV} \sim 0.025\text{eV}$, while electrons have a temperature of 3-4eV. The density distributions of ions and electrons are used to determine average collision statistics, assuming locally dependant collision properties. Ions can make charge exchange collisions with the background “thermal” neutral density. When this occurs the charge exchange neutrals are transferred to the particle neutral array and followed explicitly. The electrons can make ionisation collisions, with the collision frequency being dependant on the local density.

The collision frequencies per unit volume, $\nu_{\text{coll}}$, is given by

$$\nu_{\text{coll}} = N_{\text{neut}} \times K_{\text{coll}} \times n_{\text{chgd}}$$  \hspace{1cm} (6.3)

where $N_{\text{neut}}$ is the neutral species density, $K_{\text{coll}}$ is the collision rate constant, and $n_{\text{chgd}}$ is the charged species density.

Only collisions between charged species and neutrals are considered in this model. Although Coulomb (electron-ion) collision rates are approximately equal to electron-neutral collision rates, electron-ion collisions are not explicitly included in the model, since they
will have little effect on diffusion along the field lines and consequently on the longitudinal expansion of the plasma. However, Coulomb collisions will be important for cross field diffusion and are considered later in the radial loss calculations.

The ionisation collision rate constant can be determined from experimental cross-section data. An Arrhenius fit is used to obtain an expression of the form [80]

\[ K_{\text{ion}} = K_{\text{ion}0}e^{-\varepsilon_{\text{ion}}/kT_e} \]  

(6.4)

where \( K_{\text{ion}0} = 6.0 \times 10^{-14}\text{m}^3\text{sec}^{-1} \) and \( \varepsilon_{\text{ion}} = 15.76\text{eV} \). For \( kT_e = 3\text{eV} \) the collision constant is \( K_{\text{ion}} = 3.1 \times 10^{-16}\text{m}^3\text{sec}^{-1} \). Charge exchange cross-sections are assumed to be relatively independent of temperature and \( K_{\text{chx}} = 2.5 \times 10^{-17}\text{m}^3\text{sec}^{-1} \) is used.

The code explicitly models the length of the discharge from the end of the antenna (the source region) to the end of the magnetic field coils, a distance of approximately 0.5m. A tube radius of 25mm is used and the applied magnetic field is assumed to be uniform and parallel to the tube axis. The simulation commences with a given source density of ions which are then allowed to diffuse along the length of the tube through the background neutral density. Ions are lost through radial and longitudinal diffusion. Particles can diffuse freely in the longitudinal direction along the field lines. The longitudinal motion is given by

\[ \frac{dv_\|}{dt} = \frac{q}{m}E_\| \]  

(6.5)

\[ \frac{dx}{dt} = v_\| \]  

(6.6)
These equations can be expressed in finite difference form as

\[
\frac{v^{t+\frac{1}{2}}}{v^t} = v^{t-\frac{1}{2}} + \Delta t \frac{q}{m} E_i^t\tag{6.7}
\]

\[
x^{t+1} = x^t + \Delta t v^{t + \frac{1}{2}}\tag{6.8}
\]

Note that positions are evaluated at integral time-steps and velocities at \(\frac{1}{2}\) time-steps. This is a standard numerical technique known as the leapfrog method [8] and is important for maintaining stable integration.

Ions are continually fed into the discharge at the source end as though the plasma existed with a density \(n_s\) outside the modelled region. The number of ions added at each time step, \(N_{add}\) depends on the flux, \(\Gamma_s\), the cross sectional area, \(A\), and time step duration, \(\Delta t\). The flux will depend on the density of the source and the thermal velocity of the source particles. New ions are given a random velocity with a Gaussian distribution. The number of particles added at each time step is given by

\[
N_{add} = \Gamma_s A \Delta t = \frac{1}{3} n_s v_{th} A \Delta t\tag{6.9}
\]

The presence of the static magnetic field substantially inhibits radial diffusion. The mechanism by which plasma diffuses radially in Basil is classical cross-field diffusion, since even at the lowest fields the ion cyclotron radius is less than the tube diameter. The classical diffusion coefficient \(D_c\) is given by [30]

\[
D_c = \eta n_0 (kT_e V + kT_i V) / B^2\tag{6.10}
\]
where $\eta$ is the resistivity, $T_{eV}$ and $T_{iV}$ are electron and ion temperatures (in eV), $B$ is the magnetic field (in Tesla), and $n_0$ is the plasma density on axis. The resistivity can be calculated from the electric field and the ion current [23]

$$E = \eta j = m <v> \nu/e$$  \hspace{1cm} (6.11)

and

$$j = en <v>$$ \hspace{1cm} (6.12)

where $<v>$ is the average velocity and $\nu$ is a collision frequency. Therefore

$$\eta = \frac{mv}{e^2 n}$$ \hspace{1cm} (6.13)

When considering ions diffusing across magnetic field lines, for the conditions in Basil the electron-ion collision rate is orders of magnitude larger than ion-neutral collision rate and therefore is most important in inducing cross-field diffusion. From Chen [31]

$$\nu_{ei} = \frac{2 \times 10^{-12} n_e}{T^{3/2}_{eV}} \ln \Lambda$$ \hspace{1cm} (6.14)

where $\ln \Lambda = 10$ for the plasma conditions of interest. The radial flux of ions is therefore [80]

$$\Gamma_r = \mu n(r) E_r - D_c \nabla n(r)$$ \hspace{1cm} (6.15)

where $\mu$ is the ion mobility, and $E_r$ is the radial electric field. Assuming a cosine radial
density distribution:

\[ n(r) = n_0 \cos \left( \frac{\pi r}{2R} \right) \]  

(6.16)

where \( n_0 \) is the density on axis, and \( R \) is the tube radius. The density becomes very small approaching the walls, while the gradient of the density is very large. The electric field component of the flux in equation 6.15 can be neglected and the flux to the walls is therefore

\[ \Gamma_r|_{wall} = \frac{D_c n_0 \pi}{2R} \]  

(6.17)

The diffusion and mobility coefficients are anisotropic when there is a magnetic field. If the field lines terminate on conducting surfaces, then the transverse electric fields set up to aid electron diffusion perpendicular to the magnetic field can be “short circuited” by electrons travelling along these field lines. However, in the case of Basil the tube length is much larger than the radius, and the boundary walls are non-conducting and so the perpendicular flux of ions and electrons must be equal to avoid charge build-up.

The number of ions lost radially, \( N_{\text{lost}} \), from a single cell of width \( \Delta x \), during a time step \( \Delta t \) long is given by

\[ N_{\text{lost}} = \Gamma_r 2\pi R \Delta x \Delta t = D_c n_0 \pi^2 \Delta x \Delta t \]  

(6.18)

A percentage of the ions which diffuse radially to the walls are assumed to be neutralised and reflected back into the plasma. These are re-incorporated into the background neutral density.

At the end of the uniform field region radial diffusion is assumed to become domi-
nant so that particles are rapidly lost to the walls. The tube extends approximately 20cm beyond the uniform field region. In the model this is assumed to provide a reservoir of neutrals which can diffuse back into the simulation region.

The neutral density of the end reservoir is increased by the flux of “fast” neutrals and ions into this region and decreased by neutrals which diffuse back into the discharge. Neutrals are added back into the discharge in a similar fashion to the addition of ions at the source end of the tube. The background neutrals in the discharge region are assumed to diffuse in such a manner as to equalise the pressure along the length of the tube. Charge exchange collisions produce neutrals with a velocity in the direction of the ion flux. As the plasma moves down the tube it acts as a plunger “pushing” neutrals into the end reservoir.

6.3 Diffusion Model Results

Figures 6.6 and 6.7 shows the time evolution of the diffusion model results. The solid line shows the ion density, while the dashed and dotted lines display the background and particle neutral densities respectively. The background neutral density is divided by 10 so that it can be plotted on the same scale as the ion and particle neutral densities. The ions are seen to diffuse longitudinally in a very similar fashion to the experimental measurements, and on the same time scale.

As the ions diffuse downstream a peak of fast neutrals can be seen to develop at the leading edge of the ion density. This occurs due to charge exchange collisions between the ions and background “thermal” neutrals, which transfers a directed velocity to these neutrals. These “fast” neutrals travel downstream with the same velocity as the ions.
Calculate initial ion positions and velocities at time $t = 0$ and load a uniform background neutral density based on the gas pressure.

Calculate initial densities

Start time-step loop

Move ions and fast neutrals one time step

Check for particles that have left the system

Rescale if there are too many simulation particles

Determine ionising collisions

If ionising collisions occur then the calculated number of ions are created, given random positions within the cells that the collisions took place, and random velocities with a thermal distribution

Determine charge exchange collisions

If charge exchange collisions occur then fast neutral particles are created with the velocity and position of the colliding ion and the ion is given a random velocity with thermal distribution

Load ions from source region

Calculate ion density profile along the tube

Determine radial losses and remove ions

Add neutrals from the walls (proportional to radial ion losses)

Add neutrals from end reservoir

Diffuse background neutral density

Restart loop

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Figure 6.5: Flow diagram of the diffusion model.
Figure 6.6: Time evolution of the ion density (solid line), neutral density divided by 10 (dotted line), and “fast” neutral density (dashed line) calculated by the model as a function of longitudinal position for argon at a static field of 1024 gauss and filling pressure of 7mTorr.
Figure 6.7: Ion density calculated by the model as a function of time and longitudinal position for argon at a static field of 1024 gauss and filling pressure of 7mTorr.
When they reach the end of the diffusion region they accumulate in the end reservoir producing an increased density here. Ions which diffuse into this region are assumed to be neutralised at the walls and further contribute to the neutral density increase. The higher density causes neutrals to diffuse back into the plasma, producing an increase in neutral density at the end of the tube, resulting in higher ionisation and producing the observed density hump at the end of the discharge.

Figure 6.2 shows that in the experiment the drop in density occurs very rapidly and results in a longitudinally uniform plasma density. In the model this occurs more gradually and is caused by the slow depletion of neutrals from the reservoir, as they diffuse back into the plasma. In the experiment as the neutral density decreases at the end of the tube, the drop in ionisation rate produces a density drop. This changes how power is coupled to the plasma, which consequently affects the electron temperature, further reducing the ionisation. A feedback effect is produced which causes the rapid decrease in density observed, until an equilibrium condition is achieved at a lower density. In the model power deposition is assumed to be constant and consequently the electron temperature cannot change. Furthermore the source density in the model is assumed to be constant, whereas in the experiment the density in the antenna region will also drop as the power coupling changes.

6.4 Effects of Increased Magnetic Field and Power

The applied static field can be considered high if the Larmor radius, $r_L$, is smaller than the radius of the discharge. For electrons this is always the case, but for the ions the Larmor
radius is closer to the discharge radius at the lowest fields used in Basil.

\[ r_L = \frac{mv_\perp}{|q|B} \]  

(6.19)

At a static field of 500 gauss, the ion Larmor radius for Basil conditions is approximately 2mm while the tube radius is 25mm. Along with the high collisionality and low temperature of the Basil discharge it would be expected that the main source of cross-field diffusion would be classical diffusion [80]. The classical diffusion coefficient \( D_c \) is given by equation 6.10.

Figure 6.8 demonstrates the effects of increased static field on the ion saturation current of an axially located Langmuir probe 60cm from the antenna. This clearly shows that for magnetic fields in the range 450-800 gauss the plasma density increases with increasing field. However, the density remains constant after 800 gauss. From equation 6.10, the radial losses will decrease with the square of the increasing field. To understand how this effects the plasma density, the power balance of the system must be considered.

At equilibrium the power deposited into the plasma by the antenna must equal the power losses. Power losses will be due to a variety of mechanisms including inelastic collisions by electrons and ions, and particle losses to the boundaries. In the case of Basil the longitudinal losses to the ends of the tube will be small in comparison to radial losses, even though radial diffusion is inhibited by the magnetic field, simply due to the relative sizes of the areas. The radial loss rates to the wall depends on the diffusion time constant, \( \tau_r \). In cylindrical geometry

\[ \frac{1}{\tau_r} = \frac{D_c \times 5.76}{R^2} \]  

(6.20)

141
where \( R \) is the tube radius. The power lost to the walls per electron ion pair is therefore

\[
P_{\text{wall}} = \frac{n ne\eta_{\text{ion}} V}{\tau_r}
\]  \hfill (6.21)

where \( n \) is the plasma density, \( \eta_{\text{ion}} \) is the threshold energy for ionisation (i.e. each particle “takes out” the ionisation energy required to create it) and \( V \) is the volume, \( V = \pi R^2 L \).

Therefore from equations 6.20 and 6.10

\[
P_{\text{wall}} = C \left( \frac{n e}{B} \right)^2
\]  \hfill (6.22)

where the constant \( C \) is given by

\[
C = \frac{2 \times 10^{-11} \eta_{\text{ion}} m_e V}{T_{eV}^{1/2} R^2}
\]  \hfill (6.23)

At low fields the plasma radial confinement is relatively weak and the density is relatively low. The radial loss term is important and gives the dependence \( n \propto \sqrt{PB} \). Assuming that the power into the plasma remains fairly constant or increases slowly as the density increases then \( n \propto B \), as seen in the low field cases in figure 6.8. As a critical field is reached the radial confinement becomes sufficiently large that losses to the walls are negligible and most power will be dissipated through collisions, or losses to the ends of the tube. Power lost through collisions is given by

\[
P_{\text{coll}} = n \Sigma \nu_{\text{coll}} n_{\text{lost}} V
\]  \hfill (6.24)
where $\nu_{\text{coll}}$ is the frequency for given collision and $\eta_{\text{lost}}$ is the energy lost per particle in the collision. In this case $n \propto P$, and so if the power is relatively constant, the density will also be constant. At these higher fields the plasma is operating in the regime of decreasing radiation resistance with increasing density.

### 6.5 Summary

The time evolution of the Basil discharge consists of two stages. The initial stage is characterised by higher densities, and often a density hump downstream from the antenna. The density hump is due to higher ionisation rates caused by an increased neutral density, close to the end of the discharge. This relatively higher neutral density is caused by a directed flux of neutrals, created through charge exchange collisions, which is pushed into this region by the expanding plasma.

As the neutral density equalises along the length the discharge, through diffusion of neutrals back out of the end region of the discharge tube, the density starts to decrease altering the power coupling to the plasma. This results in a sudden decrease in density with a final equilibrium state being reached at approximately 20msec.
Figure 6.8: Applied field scan with a helical antenna, axial Langmuir probe at 60cm from antenna feeders, pressure=30 mTorr.