3 ECR discharge modeling

3.1 Motivation

Low-temperature methane plasmas have been intensively studied already for several decades. The interest in such plasmas was mainly due to their wide application in various fields of plasma-surface technologies, such as film deposition, surface etching, and surface modification [Lieberman, 1994]. In particular, there is a wide application for deposition of diamond-like carbon films using hydrocarbon plasmas created by electron-cyclotron resonance (ECR) [Jacob, 1998].

Recently, interest in such plasmas has strongly increased in the fusion community. In fusion devices with carbon plasma-facing components (PFC) (limiters and divertors tiles) neutral hydrocarbons can appear due to chemical erosion of carbon by the flux of hydrogen ions [Federici, 2001a]. Chemical sputtering of carbon, contrary to physical sputtering, has low energy threshold [Salonen, 2002], thus the total erosion rate is quite high even for low energies of impinging hydrogen ions. In a real fusion device it would decrease the lifetime of carbon components and make the long-term operation of the device impossible. Measurements on the JET tokamak with the MkI divertor give a peak net carbon erosion rate of 24 nm·s⁻¹ (75 cm/burn-yr) [Guo, 1997]. According to calculations of [Federici, 2001b] the peak net erosion rate of carbon PFC in the coming ITER-FEAT tokamak will be 6.4 nm·s⁻¹ (i.e. 2.6 μm/400 s pulse or 20 cm/burn-yr) and will occur almost entirely due to chemical sputtering. Hydrocarbon species produced due to chemical erosion can be further ionized by electron impact-ionization in the scrape-of-layer (SOL), producing a low-density plasma, which then diffuses all around the peripheral region of the fusion device (see Fig. 3.1). The particle fluxes from such low-density, low-temperature hydrocarbon plasmas result in the deposition of C-H films on the vessel walls, the inner side of the divertor, the pumping system, and especially on cold surfaces, even those far away from the plasma. Such depositions
were discovered in many fusion experiments where carbon was used in the PFC’s. In Fig 3.2 we present photos of such C-H depositions taken at the JET and ASDEX Upgrade tokamaks. In a commercial fusion reactor Tritium, a radioactive isotope of hydrogen, will be used as a fuel, and will be captured with carbon in such depositions. This will result in the dilution of expensive thermonuclear fuel from the reaction region and make difficult to control the Tritium cycle in reactor. It will also raise issue of radiation safety. There are strict limits on the amount of radioactive Tritium allowed in the reactors. For example, the maximum amount of Tritium permitted for the JET tokamak

![Figure 3.1 Schematics of carbon erosion and Tritium co-deposition in a fusion device.](image)

![Figure 3.2 Tritium, trapped in co-depositions with carbon in JET (left) and ASDEX UPGRADE (right).](image)
is 90 g and for the TFTR tokamak - only 2 g [Federici, 2001a]. Upon reaching this limit, the reactor should be immediately shut down and the Tritium depositions cleaned out. According to [Skinner, 2001], during the DTE1 campaign on the JET tokamak in 1997 35 g of the Tritium was injected into the system, 11.5 g of which was retained inside the torus in co-deposited layers. After purging procedures following the campaign, the distribution of deposited Tritium in the vessel was measured [Coad, 2001]. Depositions occurred mostly on the pumping louvers, far away from the plasma. Figure 3.3 shows the distribution of Tritium inside the JET vessel after the DTE1 campaign [Coad, 2001].

![Figure 3.3](image)

**Figure 3.3** Distribution of Tritium in the JET vessel in the shutdown following the DTE1 campaign. The amounts at each location are integrated around the torus [Coad, 2001].

The simulations made by [Federici, 2001b] for the ITER-FEAT tokamak give ~1-2 g of tritium, co-deposited with carbon for one 400 s pulse. Considering a safety limit of the total amount of Tritium inside the ITER vessel of 450-1000 g, only 180-450 discharges will be possible before a cleaning procedure is necessary [Janeschitz, 2001].
These two issues connected with chemical erosion and Tritium co-deposition are the most serious drawbacks of carbon as a plasma facing material. Without resolving these problems the application of otherwise favorable carbon PFC’s in fusion devices becomes questionable. For this purpose an understanding of the physical and chemical processes in low-temperature hydrocarbon plasmas and their interaction with surfaces is necessary in order to make predictions and extrapolations for future fusion reactors, e.g. ITER.

Figure 3.4 Schematic drawing of the PLATO ECR microwave deposition device.

An ideal test system for understanding these physics issues is a low-temperature hydrocarbon plasma created in a small and simple laboratory device. Such devices are also widely used for carbon-film deposition. Figure 3.4 shows a schematic of such a device, an electron-cyclotron resonance (ECR) plasma reactor, which was used in the Material Science Department of IPP in Garching for deposition of hydrogenated carbon films (a-C:H-layers) [Jacob, 1993], [Rohde, 2002]. The name of this device is PLATO and because of its small size and simple geometry we have chosen it as a reference system for our modeling work. In brief, the PLATO device consists of a cylindrical stainless steel chamber 27 cm in diameter and 15 l volume. It is surrounded by two sets of solenoids (A and B) to
provide the magnetic field, necessary to fulfill the ECR condition (see Fig. 3.4). Solenoid B can be also used to change the magnetic field configuration in the reactor chamber (more homogeneous or more diverging field). Microwave power with frequency $f_{HF} = 2.45$ GHz is fed axially into the chamber as a circularly polarized electromagnetic wave through a fundamental mode rectangular waveguide equipped with a stub tuner, followed by a circular polarizer and a quartz window. In order to allow for the propagation of the wave through the magnetized plasma towards the electron-cyclotron resonance zone, the microwave approaches the resonance from a region of high magnetic field. The electron cyclotron resonance takes place when electron gyro-frequency $f_{ce} = \frac{eB}{2\pi m_e c}$ equals the microwave frequency. For microwave frequency $f_{HF} = 2.45$ GHz this corresponds to a resonant magnetic field of $B_{res} = 875$ Gauss. The chamber is pumped to a base pressure of $10^{-5}$ Pa by a turbo-molecular pump. The working gas (usually methane) is fed into the system through flow mass controllers while the pressure is independently controlled by means of an automatic throttle valve between the chamber and the turbo-molecular pump. When microwave power is applied, the ECR discharge lights up [Lieberman, 1994], breaking down the working gas. A plasma with a low ionization factor (typically $f = 10^{-5} - 10^{-3}$) is formed, which contains a large amount of reactive hydrocarbon radicals. The plasma streams along the magnetic field lines toward the substrate holder, where the film deposition takes place. Typical plasma parameters produced in the PLATO device are electron temperature $T_e \sim 2 - 4$ eV, neutrals temperature $T_n \sim 500$ K, electron density $n_e \sim 10^{10} - 10^{11}$ cm$^{-3}$, and neutral gas pressure $p \sim 0.1 - 20$ Pa [Pecher, 1998]. The typical flow rate of the working gas is $\Gamma = 2 - 20$ sccm. The gas flux is measured in cubic centimeters of gas per minute at normal conditions (sccm), 1 sccm = $4.48 \cdot 10^{17}$ s$^{-1}$.

### 3.2 Rate equations model

In order to get some insight into the complexity of a multi-species hydrocarbon plasma in the PLATO device, we set up a zero-dimensional particle-balance model. In this model we omit the whole plasma physics part. We assume that the plasma is uniform, electrons and ions are Maxwellian, and electron temperature and density and ion temperature are constant. What we are aiming for with this model
are the neutral and ion species densities. We assume that they change only due to volume chemical reactions, external sources and pumping. In this case, all species densities are governed by the system of particle-balance equations:

\[
\frac{dn_a}{dt} = \sum_{\beta, \gamma} R_{\beta \gamma}^a n_\beta n_\gamma - n_a \sum_{\beta, \gamma} R_{\alpha \gamma}^a n_\gamma + S_a - P_a, \tag{3.1}
\]

where

\[
R_{\beta \gamma}^a = \int \sigma_{\beta \gamma}^a (E_{\beta \gamma}) \tilde{u}_{\beta \gamma} f_\beta (\tilde{v}_\beta) f_\gamma (\tilde{v}_\gamma) d^3v_\beta d^3v_\gamma \tag{3.2}
\]

is the rate coefficient for volume reaction between species \(\beta\) and \(\gamma\) leading to the creation of species \(a\), \(\sigma_{\beta \gamma}^a (E_{\beta \gamma})\) is the cross-section of this process, which depends on the center-of-mass energy \(E_{\beta \gamma} = \mu_{\beta \gamma} u_{\beta \gamma}^2 / 2\) of colliding particles, \(\tilde{u}_{\beta \gamma} = \tilde{v}_\beta - \tilde{v}_\gamma\) is the relative velocity, \(\mu_{\beta \gamma} = m_\beta m_\gamma / (m_\beta + m_\gamma)\) is the effective mass of the particles, \(f_\beta (\tilde{v}_\beta)\) is the distribution function of particle \(\beta\), \(n_\alpha\) is the density of species \(\alpha\), \(S_a\) is the volume source and \(P_a\) is the volume pumping rate of species \(a\). We also assume that the total pumping rate is equal to the source gas influx (methane) and that the pumping rate of each species is proportional to its density. As we consider the electron density to be constant, in order to keep quasi-neutrality we multiply ion densities by a factor of \(n_e / \sum_k n_{i_k}\) at every time step.

In our model we account for 175 volume reactions involving 14 neutral and 13 charged species: \(\text{C}_2\text{H}_6, \text{C}_2\text{H}_5, \text{C}_2\text{H}_4, \text{C}_2\text{H}_3, \text{C}_2\text{H}_2, \text{C}_2, \text{CH}_4, \text{CH}_3, \text{CH}_2, \text{CH}, \text{C}, \text{H}_2, \text{H}\) and \(\text{C}_2\text{H}_5^+, \text{C}_2\text{H}_4^+, \text{C}_2\text{H}_3^+, \text{C}_2\text{H}_2^+, \text{C}_2\text{H}^+, \text{CH}_4^+, \text{CH}_3^+, \text{CH}_2^+, \text{CH}^+, \text{C}^+, \text{H}_2^+, \text{H}^+\).

The number of reactions considered was determined by the available data for reaction rate coefficients. For reaction rate coefficients of electron and proton induced methane break-up, we used well-known Ehrhardt-Langer analytical fits from [Ehrhardt, 1988]. For ion-neutral, neutral-neutral hydrocarbon reactions and electron-impact reactions for hydrocarbons higher then \(\text{CH}_4\), we used constant rate coefficient from datasets used in [Riccardi, 2000; Herrebout, 2001].

In Fig. 3.5 we present the evolution of neutral species calculated for the PLATO device \(T_e = 3.2\) eV, \(T_{ln} = 450\) K, \(n_e = 10^{10}\) cm\(^{-3}\), \(p = 1.25\) Pa, constant influx of
methane $\Gamma_{CH_4} = 2.3 \cdot 10^{15} \text{ s}^{-1}\text{cm}^{-3}$) and densities measured in [Pecher, 1998]. In Fig. 3.6 corresponding calculations for the case of ECR discharge from [Fantz, 2002] ($T_e = 2.2$ eV, $T_{in} = 450$ K, $n_e = 10^{11} \text{ cm}^{-3}$, $p = 10$ Pa, constant influx of methane $\Gamma_{CH_4} = 10^{18} \text{ s}^{-1}\text{cm}^{-3}$) are presented together with experimental points.

**Figure 3.5** Evolution of neutral species densities calculated for the case of $T_e = 3.2$ eV, $T_{in} = 450$ K, $n_e = 10^{10} \text{ cm}^{-3}$, $p = 1.25$ Pa, constant influx of methane $\Gamma_{CH_4} = 2.3 \cdot 10^{15} \text{ s}^{-1}\text{cm}^{-3}$ (lines) and densities measured in PLATO device [Pecher, 1998] (points).
Figure 3.6 Evolution of neutral species densities calculated for the case of $T_e = 2.2$ eV, $T_{ln} = 450$ K, $n_e = 10^{11}$ cm$^{-3}$, $p = 10$ Pa, constant influx of methane $\Gamma_{CH_4} = 10^{18}$ s$^{-1}$cm$^{-3}$ (lines) and densities measured in [Fantz, 2002] (points).

The most important result is that among the most abundant neutral species, besides methane and products of its direct dissociation, we can also see the higher hydrocarbon molecules $C_2H_2$, $C_2H_4$ and $C_2H_6$. This reveals the important branch of hydrocarbon reactions in our system: electron impact dissociation of methane yields highly reactive neutral radicals $CH_3$, $CH_2$, $CH$, which then lead to a formation
of higher hydrocarbon molecules and radicals. This is in quite good agreement with experimental results from [Fantz, 2002; Pecher, 1998; Jacob, 1998; Jacob, 1997] and simulations in [Riccardi, 2000; Herrebout, 2001]. These stable higher hydrocarbons with high sticking coefficient can be dominant in the formation of Tritium co-depositions far from the plasma striking zone [von Keudell, 1999].

When comparing the model results with experimental measurements of the neutral densities in ECR methane discharges with similar conditions (Fig. 3.5 and Fig. 3.6), we can see that overall agreement is quite good. The only exception is for atomic hydrogen, in which case our model gives almost two orders of magnitude higher density than the experimental value from [Fantz, 2002]. This indicates that the hydrogen balance is somewhat overestimated, a problem which has to be checked in future.

This simple particle balance model shows the complexity of multi-species hydrocarbon plasmas. This is seen in the high chemical activity of hydrocarbon radicals, starting from pure methane as the background gas, and ending with a variety of hydrocarbon species. It is possible to make quite realistic estimations of hydrocarbon densities in devices similar to PLATO with this model. However, to get the full picture of such systems it is necessary to include in our model a self-consistent description of the plasma together with plasma-wall interaction. This is basically the next step of our modeling work.

### 3.3 Application of fluid model (B2- EIRENE code)

A standard tool for studying edge plasmas in fusion devices is the B2-EIRENE coupled code package. This package was successfully applied for modeling transport phenomena in the edge plasma of various fusion machines [Schneider, 2000; Rozhansky, 2002].

B2 [Braams, 1986; Braams, 1987] is a 2D multi-fluid plasma code which treats the motion of charged particles parallel to the magnetic field as a hydrodynamic flow, and the motion perpendicular to magnetic field lines as a diffusion process. Basically it solves the set of Braginskii equations [Braginskii, 1965], assuming plasma quasi-neutrality. The resulting set of equations [Braams, 1987] consists of continuity and momentum equations for ion species, and two energy equations, one for the ions and one for the electrons.
The EIRENE code [Reiter, 1992; Reiter, 1995] is a 3D Monte-Carlo code for neutrals transport. It resolves the real geometry of a device, taking into account the interaction of neutral particles with the plasma and the surface.

![Schematic of the B2 code computational domain inside the PLATO device.](image)

**Figure 3.7** Schematic of the B2 code computational domain inside the PLATO device.

We applied the B2-EIRENE package to the low-temperature plasma in the PLATO device. We studied the case of a pure hydrogen plasma with e, H⁺, H₂ and H only. In Fig 3.7 we present the geometry of the computational domain. The coordinate system is defined by the magnetic field produced by the coils. Longitudinal (axial) coordinate lines are chosen along magnetic flux surfaces and the perpendicular coordinate along their orthogonals. The domain in the axial direction is limited by the target wall (Y = 0 cm) from below and the plane Y = 22 cm from above. In the radial direction it is limited by last magnetic surface, intersecting the target wall as the outer boundary and the symmetry axis from the inner side. Due to the axial symmetry only half of the domain was covered. Zero-gradient boundary conditions were applied at the symmetry axis. At the outer boundary, decaying plasma boundary conditions were applied with decay length $\lambda_{\text{decay}} = 10 \text{ cm}$. In the axial direction, at the position of the target wall, the recycling wall boundary...
conditions were applied: gradients of charged particles densities were set to zero, ion velocity was set to sound velocity, and the H$^+$ flux was returned from the wall as molecular hydrogen. At the upper boundary the zero-gradient boundary condition was applied. The ECR heating was included in the simulation by applying uniformly distributed energy source for electrons in area shown on Fig. 3.8.

![Figure 3.8](image.png)

**Figure 3.8** Electron (left) and ion (right) temperature profiles, calculated with B2-EIRENE.

The simulations were performed for neutral gas pressure $p = 1$Pa, initial electron density $n_e = 10^{11}$ cm$^{-3}$, and input power $P=100$ W.

In the Fig.3.8 we present calculated electron and ion temperature profiles. The electron temperature in the heating zone reaches unrealistically high 200 eV, due to overestimation of localized heating sources. The electron temperatures observed in the experiments are typically about 3 eV [von Keudell, 1999; Fantz, 2002], which is obtained in the fluid simulation in the target region beyond the source gradient zone. The simulated ion temperature is in good agreement with the experimental values of 500 K – 1000 K only in an intermediate region between the source and the target plate.
Figure 3.9 H⁺ (left) and H (right) densities resulting from B2-EIRENE calculations.

Figure 3.10 Trajectory of test H₂ particle inside the PLATO device simulated with EIRENE.

Fig. 3.9 shows the calculated H⁺ density profile (due to quasineutrality \( n_e = n_{H^+} \)). The charged particle density is rather flat in most of the domain, having a minimum
in the region of the heating source, which is conditioned by the pressure gradient, expelling electrons from the hot zone. The atomic hydrogen density is presented in Fig. 3.9. The H density builds up near the target wall due to dissociation of molecular hydrogen and then is depleted upstream by electron impact ionization.

The trajectory of a hydrogen molecule as modeled with EIRENE is shown in Fig. 3.10. We can see how, after multiple reflections from the walls, it sputters the carbon atom from surface.

Analyzing obtained results in terms of the mean free path for electron Coulomb collisions we can see that its maximum value, \( \lambda_e = 10^6 \) cm reached in the heating zone, is much larger than the system length of \( L_e = 22 \) cm and can not create the steep gradients of electron temperature, with a gradient length about \( \lambda_{gr} = 2 \) cm, observed in this region. It is obvious that we are far beyond the applicability of the fluid model formalism, which relies on the local thermodynamic equilibrium conditions, when plasma particles have Maxwellian velocity distribution, and plasma parameters are not changing on the mean free path scale. In order to understand the physics in PLATO properly we have to use the fully kinetic model, making no assumptions about the particle distribution functions and collisional scale length.

### 3.4 Application of PIC-MCC model

In order to get a fully kinetic description of our system we applied the 2D3V electrostatic PIC MCC model described in Chapter 2. In this model electrons and ions are treated as particles, moving in self-consistent electric and externally applied magnetic fields. 2 spatial and 3 velocity components are used, and a binary Monte-Carlo Coulomb collision model for electron-electron, electron-ion and ion-ion collisions is applied. Inter-species reactions are included by application of the binary inelastic collision model (Chapter 2.7). This enabled us to include in the model all reactions from the Ehrhardt-Langer list [Ehrhardt, 1988]: electron-impact ionization, dissociation, dissociative ionization and recombinative dissociation as well as charge exchange proton-neutral reactions. Inclusion of other types of elastic and inelastic collisions in the model is now rather straightforward and is only a question of available cross-section data for the collision of interest. Due to the lack
of reliable data for reaction cross-sections our model is limited to methane break-up reactions from [Ehrhardt, 1988] and hydrogen dissociation and ionization reactions from [Janev, 1987]. In total, we take into account 7 neutral and 7 charged species: CH$_4$, CH$_3$, CH$_2$, CH, C, H$_2$, H and CH$_4^+$, CH$_3^+$, CH$_2^+$, CH$^+$, C$^+$, H$_2^+$, H$^+$, participating in 34 reactions. The full set of reactions included in the model is presented in Appendix A.

We also included in the model a simplified surface interaction model in which we assumed that all electrons get absorbed by the target wall, and all carbon-containing species are either deposited on the target wall or pumped out. To balance these losses an equal amount of CH$_4$ is injected into the system from the source side. All hydrogen species (H$_2$, H, H$_2^+$, H$^+$) return from the wall as H$_2$, except for a small amount (~5%), which gets pumped out.

In order to trace the densities of neutral species, which may rise to values several orders of magnitude higher than the electron density, we use a Russian-roulette algorithm, which reduces particle numbers in cells, increasing their weights instead to keep the number of neutral particles below a certain limit. This algorithm is described in Chapter 2.8.

In order to model a closed system, in which all charged particles are generated by ionization inside the volume, we added a simplified ECR heating model, applying an external right-hand circularly-polarized HF electric field with prescribed spatial distribution:

\[
E_x(x,y) = E_0(x,y) \cos(\omega_{HF}t + \phi_0) \\
E_y(x,y) = -E_0(x,y) \sin(\omega_{HF}t + \phi_0) \quad (3.3)
\]

In this case, we get a steady state solution by applying a feedback control loop, which adjusts the amplitude of the applied HF electric field to keep the electron density within a desired range.

Below we present results of calculations for the case of an ECR methane plasma with parameters \(n_e \sim 10^{10} \text{ cm}^{-3}\), \(p \sim 0.4 \text{ Pa}\), ECR power density \(P_{HF} \sim 0.01 \text{ W/cm}^3\), which are similar to those in [Reinke, 1992; Pecher, 1998]. The computation domain is shown on the Figure 3.11. The length of the system modeled is \(d = Y_{\text{max}} = 12 \text{ cm}\) and the width \(-X_{\text{max}} = 0.37 \text{ cm}\), which corresponds to a thin slab along the plasma core in the real PLATO device. The periodic boundary conditions are applied at the boundaries in the X direction. In the Y direction at \(Y = 0\), zero-gradient and zero-flux boundary conditions are applied. Target wall boundary conditions with
potential $\phi = 0$ are applied at $Y = Y_{\text{max}}$. The applied microwave electric field is located only in the thin strip along the system axis (red strip on the Figure 3.11, where its amplitude is constant:

$$E_0(x, y) = \begin{cases} E_{HF} & |x - X_{\text{max}}/2| \leq x_{ECR} \\ 0 & \text{else} \end{cases}$$ (3.4)

with strip width $x_{ECR} = 0.0472$ cm.

\[ \text{Figure 3.11 Potential profile, calculated with PIC MCC for the PLATO device.} \]

In order to avoid decreasing the time step to fulfill the stability criterion for oscillatory motion of electrons in the HF field [Birdsall, 1985], we instead reduced the frequency of the microwave field as compared to the experiment to $\omega_{HF} = 3.38$ GHz. This microwave frequency corresponds to a resonant magnetic field $B_{res} = 192.1$ Gauss. The applied external magnetic field is directed along the Y axis. Its
distribution was calculated for the case when only solenoids of set A were operating (see Figure 3.4). The distribution of the magnetic field along the system is shown at Figure 3.12. The conditions for electron-cyclotron resonance are satisfied near the position $Y_{\text{res}} = 0.5 \text{ cm}$. In calculations the grid size $\Delta x = \lambda_D/2 = 0.0117 \text{ cm}$ and time step $\Delta t = 0.2/\omega_{pe} = 3.55 \times 10^{-11} \text{ s}$ were used. The number of computational particles per Debye cell was $N_d = 100$, totally about $5 \times 10^6$ computational particles were used. The calculations were done on 32 processor Linux cluster in about 10 days.

![Figure 3.12](image) Distribution of the axial magnetic field along the system.

In Fig. 3.13 we plot parallel and perpendicular electron temperatures $T_{ey}$ and $T_{ex}$. In these pictures we can distinguish maxima, which correspond to the profile of absorbed HF power, as well as a pronounced temperature anisotropy, caused by the applied ECR heating. On Fig. 3.14 the densities of the electrons and CH$_4^+$ ions are presented. We can see the effect of strong spatial non-uniformity of the applied ECR heating on the electron density profile. The pressure gradient force expels electrons from the high temperature region to the periphery, trying to flatten the pressure profile. This results in breaking up the quasi-neutrality condition in this area and building up the strong radial electric field (see potential maximum at the heating source on the Figure 3.11). This in turn accelerates the ions and creates the ambipolar plasma outflow from the heating source to the periphery, so that the ion density profile closely follows the electron density. At the equilibrium, this ambipolar outflow is balanced by the plasma, created by electron impact ionization in the hot source region.
Figure 3.13 Profiles of longitudinal (top) and perpendicular (bottom) electron temperature, calculated with PIC MCC for the PLATO device.
Figure 3.14  Profiles of electron (top) and CH4+ (bottom) density, calculated with PIC MCC for the PLATO device.

The strong radial electric field at the heating source creates the strong \( E \times B \) drift in the z direction with drift velocity \( \vec{v}_d = \frac{\vec{E} \times \vec{B}}{B^2} \). In Fig. 3.15 we present the plot of the z-component of electron average velocity, where such drifts can be seen. The maximum drift velocity corresponds to the maximum of the ambipolar
electric field, at the radial boundaries of the heating source. In the cylindrical geometry such drift would correspond to an azimuthal rotation of a hollow structure on the system axis.

![Figure 3.15 z-component of the electron drift velocity.](image)

Such hollow structures ('plasma holes'), rotating with supersonic velocities, were observed in laboratory experiments with strongly heated ECR plasmas. In Fig. 3.16 we present experimental results from the HYPER-I device at the National Institute for Fusion Science, Toki, Japan [Nagaoka, 2001]. In this experiment plasma with \( n_e \sim 10^{13} \text{ cm}^{-3} \) and \( T_e \sim 20 \text{ eV} \) was created by ECR discharge in argon with microwave power \( P_{HF} \sim 4-15 \text{ kW} \). The density profile in the experiment was measured with a Langmuir probe, the potential was measured with an emissive probe and the plasma flow velocity was measured with a directional Langmuir probe (DLP) [Nagaoka, 2001]. In Fig. 16a we present a photo of a plasma in the HYPER-I device, made by CCD camera. The 'plasma hole' can be seen on the system axis as a dark axi-symmetric structure. The plasma density profile (Fig. 16b) indicates that the density in the region of the hollow structure on the axis is almost an order of magnitude smaller than in the bulk plasma. The measured potential profile (Fig. 16c) has a maximum at the axis such that the resulting ambipolar electric field expels plasma from the center to the periphery. The azimuthal plasma
flow velocity at Fig. 16d reveals, that the plasma rotates with supersonic velocity in the direction corresponding to $\vec{E} \times \vec{B}$ drift. We can see that results obtained within our model are in good agreement with experiments [Nagaoka, 2001].

![Figure 3.16](image)

**Figure 3.16** CCD image of the ‘plasma hole’ (a), the plasma density contour at $z = 110$ cm, showing the hollow structure in the center of the plasma column (b), radial profile of plasma potential at $z = 110$ cm, the azimuthal velocity profile at $z = 110$ cm, revealing the rotation of the ‘plasma hole’ in the direction corresponding to $\vec{E} \times \vec{B}$ drift. (Figures from [Nagaoka, 2001]).
Figure 3.17 Profiles of neutral CH$_4$ (top) and H$_2$ (bottom) density, calculated with PIC MCC for the PLATO device.

In Fig. 3.17 the densities of CH$_4$ and H$_2$ neutral species, obtained with our PIC MCC model, are plotted. Both densities are determined by applied injection and
recycling schemes. The methane is fed into system from the open side ($Y = 0$) with Maxwellian distribution, so that its density decreases strongly toward the target wall. The molecular hydrogen is launched from the opposite side of the system due to recycling of hydrogen species on the target wall, so its density has a maximum at the target wall and decays fast toward the open side of the system. The density of $\text{CH}_3$ - the most abundant hydrocarbon radical in this model is presented at Fig. 3.18. All $\text{CH}_3$ is produced inside the system, mostly due to electron impact dissociation, so its density shows a flatter profile, decreasing slowly toward the absorbing wall.

Figure 3.18 Profiles of neutral $\text{CH}_3$ radical density, calculated with PIC MCC for the PLATO device

The behavior of the plasma in front of the absorbing wall is one of the oldest problems in plasma physics. This is one of the major issues for bounded plasmas, to a large extent determining their properties, and so, it is of particular importance for plasma technology and fusion. The pioneering work on plasma-wall interaction, revealing the basic mechanism of space-charge region (sheath) formation in the plasma near the absorbing wall, was done by Langmuir in 1929 [Langmuir, 1929].
Since then the plasma-wall interaction was studied intensively, a number of models of different complexity being created (see [Riemann, 1991]) and references). But still this problem remains not completely understood, attracting unceasing interest in the plasma physics community.

**Figure 3.19** Schematic view of the plasma potential in front of the wall (top). The relevant length scales are shown: Debye-length $\lambda_D$, sheath edge position $x_s$ and ionization length for neutrals $\lambda_{ion}$ (Figure from [Schneider, 2001]). In the bottom, the velocity distribution functions for ions and electrons are shown at the sheath edge, in the sheath and at the wall. The electrons have a cut-off Maxwellian distribution (with a cut-off velocity $v_{cs}$). At the wall no electrons are going back (half-Maxwellian distribution). The ions have already at the sheath edge a non-Maxwellian distribution function, as they are accelerated to $c_s$ or larger because of the Bohm criterion. (Figure from [Chodura, 1986a]).

The mechanism of the space-charge sheath formation in the plasma in front of the absorbing wall can be illustrated with a simplified fluid model. The electrons
due to higher mobility escape from the plasma to the boundary faster than ions, which depletes the electron density near the surface. Thus, the quasi-neutrality breaks down in the layer adjacent to the wall and a sheath potential drop with the length scale of a few Debye length \( L_{sh} \sim \lambda_D \) is developing. This potential drop near the wall repulses the electrons and accelerates the ions, such that at equilibrium the flux of the electrons toward the wall is compensated by the ion flux. If we consider cold ions, the ion temperature \( T_i \ll T_e \) and electron density, governed by the Boltzmann distribution \( n_e \sim \exp\left(-\frac{e\phi}{kT_e}\right) \), then we can determine that in order to have a stable solution for the potential in front of the wall, ions should enter the sheath region with velocity equal to or greater than the ion sound velocity:

\[
v_s \geq \sqrt{\frac{kT_e}{m_i}} \quad (3.4)
\]

(Bohm criterion [Bohm, 1949]). In other words, ions should be fast enough to be able to screen the wall from quasi-neutral bulk plasma. In order to accelerate ions to this velocity, in front of the sheath the so-called pre-sheath region with potential drop \( \Delta\phi_{psh} \geq -\frac{kT_e}{2e} \) should exist. The characteristic length scale of the pre-sheath is determined by the process which dominates the ion transport in the system: collisional ion friction, ionization, geometrical current concentration, magnetic ion deflection, etc [Riemann, 1991]. The sheath potential drop then can be derived from the zero net current on the wall condition and is:

\[
\varphi_{sh} = -\frac{kT_e}{e} \ln\left(\sqrt{\frac{m_i}{2\pi m_e}}\right). \quad (3.5)
\]

For hydrogen plasma \( \varphi_{sh} = -2.8 \frac{kT_e}{e} \).

The process of the sheath potential formation, its characteristic lengths and its influence on the electron and ion velocity distributions is shown in Fig.3.19.
Figure 3.20 Distribution function for the perpendicular (top) and parallel (bottom) component of electron velocity, calculated with MCC for the PLATO device.
In Fig. 3.11 we present the calculated potential profile. The total potential drop along the device axis consists of an ambipolar drop at the hot source region $U_a \sim 3$ V, pre-sheath with characteristic length of about the electron-neutral ionization collision mean free path $L_{psh} \sim \lambda_{eni} = \frac{1}{n_i \sigma_i} \sim 10 \text{ cm}$ and the sheath drop of a few Debye lengths in front of the target wall. The sheath potential drop value $U_{sh} \sim 5.2$ V calculated with our model agrees quite well with the value $U_{sh} = 5.8$ V, given by the Bohm theory. (3.5), taking into account calculated temperature $T_y \sim 2.1$ eV and mass ratio $\frac{m_{CH_i}}{m_e} = 1600$ used in calculations.

![Figure 3.21](image)

**Figure 3.21** Distribution function for the parallel component of CH$_4^+$ velocity, calculated with MCC for the PLATO device.

The perpendicular and longitudinal electron velocity component distribution functions, calculated along the system axis, are plotted in Fig. 3.20. The electron velocity distribution is anisotropic, with perpendicular temperature being higher (see also Figure 3.13), reflecting the anisotropy of the applied heating source. We can see that the electron velocity distribution strongly deviates from Maxwellian for
both velocity components. The perpendicular velocity distribution, in particular, has high-energy tails, pronounced in the ECR heating zone. Due to a retarding electric field at the sheath region, near the target wall, the distribution of the parallel electron velocity component becomes asymmetrical, showing a pattern similar to that in [Chodura, 1986a].

The longitudinal velocity distribution function for \( \text{CH}_4^+ \) ions is presented in Fig. 3.21. Here we can see how ions are accelerated along the system in the longitudinal electric field of the pre-sheath and sheath regions, their longitudinal velocity following the profile of the potential from Fig. 3.11.

![Figure 3.21](image)

**Figure 3.21** Comparison of the ion energy distribution function, calculated with PIC MCC (left) and measured in [Pecher, 1998] (right).

The measurements of the longitudinal ion energy distribution were done in the PLATO device for different species of ions in [Pecher, 1998], [Jacob, 1997]. In Fig. 3.22 we compare the parallel energy distributions for the most abundant ions \( \text{CH}_4^+ \), \( \text{CH}_3^+ \) and \( \text{CH}_2^+ \) calculated at the target surface with our PIC MCC model with the corresponding data from [Pecher, 1998], [Jacob, 1997]. We can see that in both cases all ions have the same energy distribution, which shows that ion energy distribution at the target wall in our system is fully determined by the established ambipolar potential profile. The influence of ion-neutral collisions is negligible, as the mean free path for these collisions is more than the system length: \( \lambda_{\text{gi}} \approx 50 \text{cm} \geq L \). We can see that in our calculations for all ion species the mean
energy of random motion $T_{ij} \approx 0.04$ eV is much less than the energy of directed motion $E_{ij0} \approx 6.9$ eV, which qualitatively agrees with the experimental results from [Pecher, 1998], [Jacob, 1997].

In Fig. 3.23 we can see how the feedback control described in Chapter 2.9 is working. Here we present the time history of the run in terms of the averaged electron density, electron temperature and the amplitude of the applied HF electric field. The HF field amplitude was adjusted automatically during the simulation in order to get a stable solution. At time $t = 1.8 \cdot 10^6 \cdot \Delta t$ the feedback parameters were adjusted, which improved the stability of the solution considerably.

3.5 Principal results

Low-temperature methane plasmas heated by electron cyclotron resonance in the PLATO device were studied. These plasmas are important for plasma technology (thin film deposition, surface modification) and are also ideal model systems for the
edge plasma in front of carbon divertors in magnetic fusion devices. To gain insight into the complexity of the multi-species hydrocarbon plasma a simple zero dimensional rate equations model was used. In total, 27 species were included in this model, participating in 175 reactions. In agreement with experiment a large number of higher hydrocarbons were formed. The necessity for kinetic modeling was demonstrated by analyzing results of a fluid simulation (B2-EIRENE).

The PIC modeling of PLATO showed the dominance of kinetic effects in such plasmas. The electron energy distribution is highly non-isotropic due to the applied heating mechanism, which heats the electrons mainly in the perpendicular direction. The model reproduces the experimental observations: a rotating plasma hole due to the effect of strong spatial non-uniformity of the applied ECR heating on the electron density profile. This results in breaking up the quasi-neutrality condition in this area and building up the strong radial electric field. This in turn accelerates the ions and creates the ambipolar plasma outflow from the heating source to the periphery, so that the ion density profile closely follows the electron density. At equilibrium, this ambipolar outflow is balanced by the plasma, created by electron impact ionization in the hot source region. The strong radial electric field at the heating source creates a large drift velocity at the radial boundaries of the heating source. In the cylindrical geometry such drift would correspond to an azimuthal rotation of a hollow structure on the system axis as observed experimentally.

Ions are accelerated along the system in the longitudinal electric field of the presheath and sheath regions, their longitudinal velocity following the profile of the potential. All ions have the same energy distribution, which shows that ion energy distribution at the target wall in our system is fully determined by the established ambipolar potential profile. The influence of ion-neutral collisions is negligible, as the mean free path for these collisions is more than the system length. All ion species at the wall have the same mean energy of random motion which is much less than the energy of directed motion. This is in agreement with experiment.