Spatio-temporal analysis of the electron power absorption in electropositive capacitive RF plasmas based on moments of the Boltzmann equation

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Abstract
Power absorption by electrons from the space- and time-dependent electric field represents the basic sustaining mechanism of all radio-frequency driven plasmas. This complex phenomenon has attracted significant attention. However, most theories and models are, so far, only able to account for part of the relevant mechanisms. The aim of this work is to present an in-depth analysis of the power absorption by electrons, via the use of a moment analysis of the Boltzmann equation without any ad-hoc assumptions. This analysis, for which the input quantities are taken from kinetic, particle based simulations, allows the identification of all physical mechanisms involved and an accurate quantification of their contributions. The perfect agreement between the sum of these contributions and the simulation results verifies the completeness of the model. We study the relative importance of these mechanisms as a function of pressure, with high spatial and temporal resolution, in an electropositive argon discharge. In contrast to some widely accepted previous models we find that high space- and time-dependent ambipolar electric fields outside the sheaths play a key role for electron power absorption. This ambipolar field is time-dependent within the RF period and temporally asymmetric, i.e., the sheath expansion is not a ‘mirror image’ of the sheath collapse. We demonstrate that this time-dependence is mainly caused by a time modulation of the electron temperature resulting from the energy transfer to electrons by the ambipolar field itself during sheath expansion. We provide a theoretical proof that this ambipolar electron power absorption would vanish completely, if the electron temperature was constant in time. This mechanism of electron power absorption is based on a time modulated electron temperature, markedly different from the Hard Wall Model, of key importance for energy transfer to electrons on time average and, thus, essential for the generation of capacitively coupled plasmas.

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1. Introduction

Capacitively coupled radio frequency (RF) plasma sources exhibit a rich variety of physical effects, some of which are only now being uncovered and understood in detail. One of the most important issues is the field-particle energy transfer mechanism that provides the basis for plasma formation and sustainment [1–4]. This energy or power transfer mechanism has traditionally been called ‘electron heating’. One has to realize, however, that the electric field modifies the electron velocity distribution function in an anisotropic manner and collisions are necessary to redistribute the energy between the different velocity components. Heating can, actually, only be said to occur, when and where this redistribution is complete, at a spatial position and time, which may differ from the position and time of the energy transfer. Therefore, ‘electron power absorption’ is a more appropriate expression than ‘electron heating’ for the actual energy transfer. Thus, we will use the latter expression only in our review of previous works, while in the context of the present study we use the terminology ‘electron power absorption’.

Periodically varying electric fields can only deposit energy to a charged particle provided that some processes break the phase coherence between the field and the particle motion. Such processes can be the collisions between the electrons and gas atoms/molecules. This collisional mechanism is typically modeled as ohmic heating, based on a simplified version of the first velocity moment of the Boltzmann equation, i.e., the electron momentum conservation equation, with the terms representing electron inertia and the pressure gradient being neglected, and adopting the assumption of a harmonic time dependence of the electric field [1, 2].

Godyak et al. [5, 6] were the first to show that this description of electron heating is incomplete and that there must be additional ‘collisionless’ heating mechanisms that sustain capacitively coupled plasmas (CCPs) at low gas pressures. A separate theory, initially based on the Hard Wall Model, was developed to describe this collisionless (also referred to as stochastic) electron heating [7–10]. In the framework of this model, the electron density, is assumed to be zero in the sheath and increase abruptly at the sheath edge, which oscillates at the RF frequency and is symmetric in time. During sheath expansion electrons are accelerated by the space- and time-dependent sheath electric field, which is assumed to be high inside the sheath and zero outside the sheath. For the Hard Wall Model the shape of the electron energy distribution function at the sheath edge plays an important role, but it is not obtained self-consistently from the Boltzmann equation.

In this sense it is viewed as being separate and distinct from the theory of ohmic heating. Nevertheless, the total power absorbed by the electrons is often calculated as the sum of the heating obtained from both these models and the result is found to agree with experiments in some cases [5, 6].

A variety of experimental, computational, and theoretical investigations of the spatio-temporal dynamics of collisionless electron heating has since been performed based on these original pioneering works [11–23]. Additional insights were obtained such as the conclusions that sheath expansion results in the formation of energetic electron beams, that propagate from the sheath edge into the plasma bulk and can cause bounce resonance heating, and that resonance phenomena (nonlinear electron resonance heating—NERH) as well as plasma-surface interactions such as the emission of secondary electrons can play an important role. These fundamental insights into electron power absorption are linked to different modes of discharge operation such as the α-, γ-, drift-ambipolar-, or striation mode [23–32].

During the past years several limitations and inconsistencies of the electron heating models in CCPs were identified. For example, particle in cell (PIC) simulations revealed that the electric field does not vanish outside the sheath and is not a harmonic function of time in electro-positive single frequency low-pressure CCPs [33]. Based on a simplified moment analysis of the Boltzmann equation, where, e.g., the electron temperature gradient was neglected, a strong ambipolar electric field was observed outside the sheaths due to the ion density gradient and shown to contribute significantly to electron heating. This ambipolar field was found to be time modulated due to a time modulated mean electron energy, implying that the sheath expansion phase is generally not a mirror image of the sheath collapse and the electric field is not harmonic in time. Experimental electric field measurements have verified this computational result [11, 12, 25] originally called ‘low field tail’ during sheath expansion (see Czarnetzki et al. [25]). In the original work on ambipolar electron heating in CCPs [33], the ambipolar electric field was defined according to its classical derivation based on the electric and ion momentum balance equations in drift-diffusion and isothermal approximation, i.e. neglecting all inertia terms and any spatial changes of the electron temperature [1]. Here, this classical definition of the ambipolar electric field is followed, i.e. \( E_{\text{amb}} = \frac{\partial T_e}{\partial x} - \frac{\partial p_e}{\partial x} \), where \( T_e \) is the (parallel) electron temperature (with respect to the \( x \)-direction that is parallel to the direction of the electric field), \( n_e \) is the electron density, and \( e \) is the elementary charge. However, the electron temperature is taken from PIC simulations and, thus, is space dependent. Moreover, the isothermic approximation is relaxed, and the full electron momentum balance equation is considered without any assumptions. This results in the fact that the power dissipated to electrons via the ambipolar electric field—defined as ambipolar electron heating—is different from pressure heating [10, 34, 35], which also includes the contribution from the electron temperature gradient term in the momentum balance equation.

Surendra and Dalvie were the first to develop a consistent and complete description of electron heating in CCPs based on a moment analysis of the Boltzmann equation and PIC simulations [36]. In their study, in contrast to the original theory of ohmic heating, all terms and, therefore, all electron heating mechanisms were included self-consistently. Using input parameters such as the electron and current densities from PIC simulations they could calculate the power dissipated to electrons and could distinguish between contributions originating from different terms in the electron heating.
momentum balance equation and, thus, from different physical mechanisms. They found that the electron pressure term—originally neglected in the theory of ohmic heating—contributes strongly to collisionless heating. While they mainly analyzed the electron heating on time average without temporal resolution within the RF period, they concluded that collisionless electron heating will vanish on time average, if the electron temperature is constant, and that, therefore, any space and time dependence of the mean electron energy in CCPs is crucially important to obtain a non-zero collisionless heating of electrons on time average. Turner and Gozdinos developed their theory of electron pressure heating in CCPs to describe the true nature of collisionless electron heating, which is based on similar arguments and inherently includes ambipolar electron heating, which results from the electron pressure gradient [10, 34, 35]. Lafleur et al [37] revisited electron heating in CCPs based on a similar approach as Surendra and Dalvie [36]. They have found that only ohmic and pressure heating contribute significantly to the power dissipation to electrons on time average. They also pointed out the importance of the space and time dependence of the mean electron energy for a non-zero heating on time average. More recently, Liu et al [38] repeated this analysis using a two dimensional PIC simulation of a CCP, and again confirmed that only ohmic and pressure heating give important contributions to the electron power absorption. This work also demonstrated that ohmic heating can be enhanced near the side walls of a CCP due to the lower plasma density, and hence reduced conductivity, in this region. Based on his Smooth Step Model to calculate the electric field, including the field on the bulk side of the oscillating sheath edge, Brinkmann derived a unified description of electron heating in CCPs [39, 40]. He showed that the total electron heating on time average is the sum of four terms, each one corresponding to one of the heating mechanisms known from separate previous theories, i.e. NERH, stochastic heating (Hard Wall Model), ambipolar/pressure heating, and ohmic heating. Brinkmann also demonstrated that a time dependence of the electron temperature is necessary to obtain a non-zero collisionless electron heating on time average [39, 40]. Grapperhaus and Kushner developed a semianalytic RF sheath model and included it in a two-dimensional discharge model to describe electron heating in CCPs [41]. This model is intermediate in complexity between hard wall and ab initio calculations. Finally, Kaganovich et al developed a non-local theory of electron heating, which strongly contributed to a more detailed understanding of this phenomenon [42].

In summary, previous work on electron heating in CCPs has shown that the original models of ohmic and stochastic heating (Hard Wall Model) are inconsistent and incomplete. Although they describe experimental results correctly under some conditions, they do not explain the physical mechanisms of electron heating completely and correctly. Instead, a complete analysis of the first moments of the Boltzmann equation is required without ab initio assumptions. Such investigations have so far focused on the time-averaged electron heating and have concluded that a time modulation of the mean electron energy is crucially important to obtain a non-zero collisionless heating of electrons on time average. However, the exact reasons why such temporal asymmetries exist, how the electric field generated by different physical mechanisms and the mean electron energy depend on time and space within the RF period, and how these asymmetries cause power absorption on time average are still unknown. Therefore, in this work we perform a detailed space- and time-resolved analysis of the electron power dissipation dynamics in electropositive single frequency CCPs at pressures ranging from 1 to 50 Pa in argon. Our investigation is based on a rigorous moment analysis of the Boltzmann equation and we take input parameters for this moment analysis directly from PIC simulations. In this way we divide the electric field into 7 terms—each one corresponding to a distinct physical mechanism. Then, with nanosecond time resolution within the RF period and high spatial resolution perpendicular to the electrodes, we calculate the power dissipated to electrons based on these electric field terms and the electron conduction current density obtained from the simulations. We demonstrate that the electric field is high outside the sheaths, mainly due to the ambipolar field, and asymmetric in time, i.e., at a given electrode the sheath expansion phase is not a mirror image of the collapse phase. We explain this temporal asymmetry by a time-dependence of the ambipolar field due to a time-modulation of the mean electron energy caused by energy transfer to electrons upon sheath expansion by the ambipolar field itself and the presence of collisions. We show that this space- and time-dependent ambipolar electric field outside the sheaths strongly contributes to electron heating and that its time-dependence within the RF period is essential for the operation of CCPs. We provide theoretical evidence that this ambipolar electron power absorption would vanish completely, if the electron temperature was constant in time. We conclude that this time dependence is indirectly linked to collisions, since collisions prevent energetic electrons generated at one electrode during sheath expansion to arrive at the opposite electrode during sheath collapse. Moreover, collisions lead to an increase of the electron temperature during sheath expansion. Thus, ‘collisionless’ electron heating is not truly collisionless as previous models have assumed, but is indirectly linked to collisions. We also demonstrate that spatial gradients of the mean electron energy influence the electron power absorption dynamics. Both effects result from the electric pressure term in the momentum balance equation, are linked to each other, and are understood in this work. Finally, we show that collisional ohmic heating increases as a function of pressure, while ambipolar heating remains significant under all conditions investigated, but is partially compensated by the electron temperature gradient term so that the sum of these two terms, i.e., pressure heating remains approximately constant as a function of pressure at high pressures. This is the first space- and time-resolved analysis of electron power absorption in CCPs based on a model with no major assumptions, which, therefore, yields a clear and complete understanding of this complex phenomenon, which is not only of significant fundamental relevance, but is also the basis for optimization of
any applications of CCPs based on a scientific understanding of their generation.

The paper is structured in the following way: in section 2, the theoretical background of the analysis of electron power absorption based on the moments of the Boltzmann equation is explained. Section 3 contains a description of the PIC simulation used to obtain input parameters for the moment analysis. In section 4, the results are presented and discussed. Finally, conclusions are drawn in section 5.

2. Theoretical background

The starting point of our analysis is the pair of the first two moment equations of the electron Boltzmann equation (see e.g. [37]), i.e. the continuity and momentum balance equations, which, in the case of a one-dimensional system setting, read as

\[\frac{\partial n_e}{\partial t} + \frac{\partial}{\partial x}(n_e u_e) = G, \tag{1}\]

\[m_e n_e \left( \frac{\partial u_e}{\partial t} + u_e \frac{\partial u_e}{\partial x} \right) = -n_e e E - \nabla p_{xx} - m_e u_e G - \Pi_e. \tag{2}\]

Here, \(n_e\) and \(u_e\) are the electron density and mean velocity, respectively, \(p_{xx} = m_e n_e (v_e^2 - u_e^2)\) is the diagonal element of the pressure tensor, where \(v_e\) is the velocity in the x-direction of an individual electron, \(G\) is the ionization rate, \(E\) is the electric field, and \(\Pi_e\) is the change of momentum due to collisions, \(m_e\) is the electron mass and \(e\) is the elementary charge. We proceed by expressing the electric field as a sum of several space and time dependent terms based on the combination of equations (1) and (2) as follows, i.e. \(E_{\text{tot}} = \sum_{i=1}^{7} E_i\).

\[E_1(x, t) = -\frac{m_e}{e} \frac{\partial n_e}{\partial t}, \]

\[E_2(x, t) = \frac{m_e u_e^2}{n_e} \frac{\partial n_e}{\partial x}, \]

\[E_3(x, t) = \frac{m_e u_e}{n_e} \frac{\partial u_e}{\partial t}, \]

\[E_4(x, t) = -\frac{1}{e} \frac{\partial T_{xx}}{\partial x}, \]

\[E_5(x, t) = \Pi_e(x, t), \]

\[E_6(x, t) = \frac{2m_e u_e}{n_e} G(x, t). \tag{3}\]

Here, \(T_{xx}\) is the parallel electron temperature in eV (with respect to the x-direction—simply called ‘temperature’ in the following) derived from the pressure tensor element as \(T_{xx}(x, t) = \frac{p_{xx}(x, t)}{n_e(x, t)}\).

Each electric field term, \(E_i(x, t)\), in equation (3) has a distinct origin, i.e., it corresponds to a particular physical mechanism that causes the generation of an electric field. The first three terms in equations (3), \(E_1...E_3\), originate from electron inertia. \(E_4\) and \(E_5\) are electric fields needed to balance the change in electron momentum, when that momentum changes due to a temporal change in the local drift velocity and electron density, respectively. \(E_6\) is the electric field required to balance the electron momentum flux gradient associated with the electron drift momentum. It is related to the mean electron velocity, while \(E_7\) has a similar nature, but is related to the thermal electron velocity. Terms \(E_4\) and \(E_5\) originate from the pressure gradient, which is, however, decomposed here in order to be able to study the separate effects of the electron density and temperature gradients. \(E_4\) is an electric field needed to balance the electron momentum flux gradient associated with the electron thermal momentum, and in particular, the density gradient of this thermal momentum. It corresponds to the classical ambipolar electric field as derived from the electron and ion momentum balance equations using the drift-diffusion and isothermal approximation to couple the electron and ion motion [1]. In our model, however, we allow a temporal and spatial variation of \(T_{xx}\) in this term, in contrast with the traditional definition that assumes an isothermal system. \(E_6\) is an electric field needed to balance the electron momentum flux gradient associated with the electron thermal momentum, and in particular, the temperature gradient of this thermal momentum. The sixth term represents the electric field needed to balance the electron-neutral collisional drag force, while the last term, \(E_7\), accounts for ionization. This is an electric field needed to balance the additional ‘effective’ drag force caused by ionization. Electrons created by ionization initially have a zero drift velocity. Thus, to accelerate these electrons to the local drift velocity this electric field is required.

The electric field terms are calculated based on space- and time-resolved data for \(u_e\), \(n_e\), \(T_{xx}\), \(\Pi_e\), and \(G\) obtained from PIC simulations. Based on these electric field terms and the electron conduction current density, \(j_e(x, t)\), which is also taken from PIC simulations, the total power absorbed by the electrons, \(P_{\text{tot}}(x, t)\), is calculated space- and time-resolved within the RF period:

\[P_{\text{tot}}(x, t) = \sum_{i=1}^{7} P_i(x, t) = \sum_{i=1}^{7} j_e(x, t) E_i(x, t). \tag{4}\]

This approach allows us to explicitly identify the physical mechanisms of electric field generation and electron power absorption with high spatial and temporal resolution within the RF period by distinguishing between contributions resulting from different terms of the electron momentum balance equation. As no ad-hoc assumptions are made, this analysis includes all mechanisms of electron power absorption and yields a complete understanding of this complex phenomenon. The results are exact within the domain of conditions where the PIC simulations (which assume, e.g., a one-dimensional geometry, neglect electromagnetic effects, and use a simple model for surface processes) are valid. These limitations can be relaxed by extending the simulations (which is, however, not the aim of the present study).
completeness of the present model is proven by the fact that in every scenario studied in this work, the sum of all electric field terms and of all power absorption terms agrees very well with the total electric field and the total power dissipated to electrons, which are directly obtained from the PIC simulation, at every position and time within the RF period, respectively.

3. Computational method

The numerical calculations are based on our 1d3v PIC/Monte Carlo collision simulation code, described elsewhere [43]. The code traces electrons and Ar$^+$ ions in a uniformly distributed background of neutral atoms, at $T_{\text{gas}} = 350$ K temperature. For the electrons, elastic collisions, as well as excitation and ionization processes are considered. In the computation of the collision probabilities (collision frequency) we adopt the cold gas approximation. For the elastic scattering of electrons we use the momentum transfer cross section and assume isotropic angular scattering. The electron energy loss during these collisions is accounted for in the implementation. In inelastic collisions the threshold energy is first subtracted from the energy of the incoming electron. In excitations, the direction of the new velocity vector of the electron is sampled from an isotropic distribution. In ionizations, the remaining kinetic energy is partitioned equally between the two electrons, for which the directions are also sampled from an isotropic distribution. For Ar$^+$ ionic–atom scattering, collision partners are sampled randomly from the background gas (having a Maxwell–Boltzmann distribution, corresponding to the gas temperature) at every time step, for each of the ions, in order to compute the collision probability (collision frequency) properly. In the description of ionic–atom collisions Phelps’s approach [44] is followed: two collision channels are distinguished, one of which results in isotropic scattering, while the other one results in backward scattering (corresponding to charge exchange), in the center of mass frame. The source of cross sections is [44]. To simplify the analysis, secondary electron emission from the electrode surfaces is omitted in the model, only the reflection of the impinging electrons is taken into account with a probability of 20% [45]. In order to fulfill all relevant stability criteria and to provide high resolution data we use 1200 grid points in the electrode gap of $L = 5$ cm and 4000 time steps within the RF period $T = 1/f$, where $f = 13.56$ MHz. The driving voltage waveform is $\phi = \phi_0 \cos(2\pi ft)$ with $\phi_0 = 400$ V. A neutral gas pressure range of 1–50 Pa is studied covering a wide range of collisionality.

The computation of the different terms contributing to the formation of the electric field and the absorbed electron power are incorporated into the code. To obtain high quality data for these quantities we use $\sim 3 \times 10^5$ particles of each species (electrons and Ar$^+$ ions) and acquire data during $10^7$ RF cycles (after full convergence) with high spatial and temporal resolution. We note that $H_x$ is directly obtained in the code from collision events and that the parallel temperature $T_{xx}$ is computed from the particles’ thermal velocities (excluding the mean velocity).

4. Results

The results will be presented for the pressure range between 1 and 50 Pa, covering largely differing degrees of collisionality, for a driving voltage amplitude of $\phi_0 = 400$ V. First, we present results for the spatial distribution of the time-averaged power absorbed by the electrons, $P_{\text{tot}}(x, t)$, and subsequently discuss the spatio-temporal distribution of each term contributing to the total electric field, $E_{\text{ed}}(x, t)$, according to equations (3) and the total electron power absorption, $P_{\text{ed}}(x, t)$, according to equation (4) at different pressures.

Figure 1 shows the time average of the total power absorbed by the electrons, $P_{\text{ed}}(x, t)$, and of all individual terms $P(x, t)$ as a function of distance from the powered electrode in the sheath region adjacent to this electrode, for selected values of the gas pressure, i.e., 50 Pa, 20 Pa, 5 Pa, and 1 Pa (panels (a), (b), (c), and (d), respectively). As the discharge is perfectly symmetric, the corresponding plot adjacent to the grounded electrode is identical and, thus, is not shown.

We start the analysis with the case of the highest pressure, $p = 50$ Pa, which appears to exhibit the most simple patterns. In this case only terms 4, 5, and 6 play important roles. Term 4 is related to the ambipolar field [33] originating from the electron density gradient. As it results from the electron pressure term of the electron momentum balance equation, it is part of ‘pressure heating’ [34]. The maximum of the time-averaged power absorption due to this term occurs close to the position of maximum sheath width, $s_{\text{max}}$ where the normalized electron density gradient, $(1/n_e)(\partial n_e/\partial x)$, is high. The maximum sheath width is indicated by a vertical dashed line in figure 1 for each pressure, respectively. Term 4 is positive over almost the whole spatial domain except in the immediate vicinity of the electrode. Term 5, related to the electron temperature gradient, causes significant electron power loss on time average with a local extremum around the position of maximum sheath width. It partially compensates term 4. The collisional term 6, which represents ohmic heating, acquires its highest value near the position of the maximum sheath width and remains at a constant positive value within the whole bulk region of the plasma. As the pressure is decreased, the contribution of term 6 decreases due to the increased conductivity of the plasma caused by the lower collisionality, while the characteristics of terms 4 and 5 do not change until the pressure reaches very low values, such as 1 Pa in figure 1(d). At low pressures the magnitude of the ohmic term is much lower than terms 4 and 5, which determine the distribution of the total power absorption to a large extent. At 1 Pa the discharge is operated in a mode described by Wilczek et al [16], where the electron mean free path is longer than the electrode gap, so that energetic electrons generated during sheath expansion reach the opposite electrode. In this mode, kinetic resonance effects are self-excited and multiple energetic electron beams are generated at a given
electrode per sheath expansion phase due to a poor confinement quality of energetic electrons [16]. Under these conditions the time average of term 5 of the power absorbed by electrons changes sign multiple times as a function of position due to the complex spatio-temporal dynamics of the electron temperature caused by the impingement of energetic electrons originating from one electrode at the opposite sheath during sheath collapse (see figure 8 later). We note that the contributions of the inertia terms, $P_1$–$P_3$, are small and nearly compensate each other. The contribution of the ionization source term, $P_7$, is negligible on time average at all conditions considered.

The physical origin of these observations can only be revealed by a time resolved analysis of each of the terms of equations (3) and (4) in combination with the spatio-temporally resolved electron conduction current density, $j_e(x, t)$. Therefore, in the following we analyze the spatio-temporal distributions of all individual terms contributing to the electric field and to the electron power absorption as well as the electron conduction current density. Data for the terms of equation (3) (electric field) and equation (4) (power absorption) are presented for the highest pressure, 50 Pa, case in figure 2, as well as for the lowest pressure, 1 Pa, case in figure 3. Figure 4 shows spatio-temporal plots of $j_e$ at both pressures. These figures provide a unique and complete understanding of the electron power absorption dynamics. To convey more quantitative information, spatial profiles of all electric field and power terms at $t/T = 0.25$ and 0.75 (where $T$ is the RF period) are displayed in figures 5 and 6, in the vicinity of the powered electrode. These selected times are symmetrical around the middle of the RF period, and correspond, respectively, to sheath expansion and sheath collapse periods for the specific, cosine, excitation voltage waveform. The corresponding data for all times within the RF period can be found as animations in stacks.iop.org/psst/27/055010/mmedia.

Again, we start with the analysis of the high pressure, $p = 50$ Pa, case. At 50 Pa the contributions of the inertia terms 1–3 to the total electric field in the vicinity of the instantaneous sheath edge, i.e. in regions of high electron density, as well as to the total power absorption are low. The strongest fields adjacent to the instantaneous sheath edge and power contributions are generated by terms 4 (ambipolar field) and 5 (electron temperature gradient). The corresponding panels of figure 2 make it very clear that strong electric fields are found well outside the sheath regions and these fields (mainly terms 4 and 5) have a major effect on the electron power absorption dynamics. $P_4$ exhibits two extrema as a function of spatial position, one close to the position of the instantaneous sheath edge and another one close to the position of maximum sheath width according to the corresponding maxima of the ambipolar field. $P_5$, which is
Figure 2. Spatio-temporal distribution of the electric field terms (left) and the electron power density terms (right) at the powered electrode during one RF period at 50 Pa.
Figure 3. Spatio-temporal distribution of the electric field terms (left) and the electron power density terms (right) at the powered electrode during one RF period at 1 Pa.
related to the electron temperature gradient, exhibits a complex structure due to the spatio-temporal dynamics of the electron temperature (discussed later). While the contribution of the ohmic term, $E_6$, to the overall electric field is minor in the sheath region (see figure 2(k)), it extends into the bulk plasma, where the conduction current density is high. Thus, a significant power absorption is induced by this term. Term 6 is necessarily antisymmetric in time, since $\Pi_c$ changes its sign within the RF period as electrons move towards the grounded electrode during the first half of the RF period and towards the powered electrode during the second half. If multiplied by the electron conduction current density, the ohmic power dissipation is approximately proportional to $j_e^2$ and, therefore, always yields a non-zero electron power absorption on time average. The magnitude of this ohmic heating depends on the collision frequency and, thus, is important at higher pressure and is low at low pressure, as shown in figure 1. Finally, the contributions of $E_7$ and $P_7$ to the overall electric field and total power absorption are vanishingly small.

At $p = 1$ Pa, figure 3 reveals that the spatio-temporal distributions of the electric field and power components are much more complex compared to the 50 Pa case. Also, the electron conduction current density (shown in figure 4(b)) exhibits a complicated time-dependence and contains significant higher
harmonic contributions [16]. These high frequency oscillations are self-excited due to kinetic effects related to the electron inertia that lead to the formation of multiple beams of energetic electrons during the sheath expansion phase at a given electrode such as described previously by Wilczek et al [20]. All electric field terms that are related to the mean velocity and, thus, to $j_e$, i.e., $E_1$–$E_5$, show these high frequency oscillations as well. In order to obtain the power density, each electric field term is multiplied by $j_e$. Consequently, all power absorption terms show high frequency oscillations at low pressure, but not at high pressure, where these oscillations are strongly damped by collisions (see figure 4). A prominent feature of the spatio-temporal plots of all electric field and power absorption terms at 1 Pa is the presence of a strong extremum at $t \approx 58$ ns located approximately at the position of the instantaneous sheath edge. These extrema are caused by the impingement of an energetic electron beam at the sheath adjacent to the powered electrode. This beam is generated during sheath expansion at the grounded electrode [13]. When this electron beam hits the collapsing sheath edge at the powered electrode, the conduction current density and the electron temperature are enhanced locally with consequences on each electric field and power absorption term according to equations (3) and (4). This effect vanishes at higher pressure (recall figure 2), for which the electron mean free path is shorter than the electrode gap and essentially no energetic beam electrons reach the opposite sheath. In contrast to the high pressure scenario, at low pressure the inertia terms, $E_2$ and $E_3$, of the electric field are no longer negligible inside the sheaths (see figure 5). However, they compensate each other approximately and are high only in regions, where essentially no electrons are present. Thus, they hardly contribute to the power absorption (see figure 6) and are not discussed in detail. The ionization source term, $E_7$, is generally negligible.

The spatio-temporal plots of each electric field and power absorption term show complex dynamics and spatial profiles. They clearly show that there is no sheath edge in the sense of the Hard Wall model, which moves harmonically in time and separates a region of high electric field from a region of no electric field. Nevertheless, a sheath edge position, $s(t)$, can be found according to Brinkmann’s criterion [46]. Its time dependence is shown in figure 7(a) for different pressures. The important point, however, is that there are high electric fields outside the sheaths in regions of high electron density. These fields are essential for a non-zero power dissipation to electrons on time average and have been completely neglected in many previous models. Figure 7(b) shows that the sheath oscillation is asymmetric in time, i.e., the sheath expansion phase is not a mirror image of the collapse phase, since $s(t) - s(T - t) \neq 0$ during the phases of sheath expansion and collapse. This is again in strong contradiction to many models of electron power absorption in CCPs, which assume a harmonic and, thus, temporally symmetric motion of the sheath edge. Similarly, the spatio-temporal plots of all electric field and power absorption terms are asymmetric in time, i.e., a region of higher electric field and stronger power absorption extends further into the plasma during sheath expansion compared to sheath collapse (see figures 5 and 6). These findings agree with experimental observations [11, 12, 25].
The temporal asymmetries of the most important electric field terms 4 and 5 are further analyzed based on figures 5 and 6. These terms exhibit significant temporal asymmetries outside the sheath at a large distance from the electrode in a region of high electron density. For instance, the ambipolar (and the total) electric field at a distance of about 11 mm from the powered electrode is much higher during sheath expansion compared to sheath collapse at 1 Pa. Therefore, the contributions of these electric field terms to electron power absorption on time average are strong (see figures 2, 3, 5, and 6).

The time modulation of the ambipolar electric field (term 4) is strong, since the electron temperature is much higher on the bulk side of the instantaneous sheath edge during the sheath expansion phase compared to the sheath collapse phase, whereas the normalized density gradient is similar during sheath expansion and collapse in this spatial region (see figure 8). The time modulation of the electron temperature is caused by the presence of energetic electrons generated via acceleration by the spatio-temporal electric field distribution around the position of the instantaneous sheath edge only during sheath expansion, but not during sheath collapse. This electric field is predominantly the ambipolar field itself. When the sheath starts to expand, cold electrons are initially accelerated towards the plasma bulk by the ambipolar electric field, which is determined by the ion density gradient. Consequently, the electron temperature increases and causes the ambipolar field itself to increase during sheath expansion. This effect is visible in figures 2(g) and 3(g), where the ambipolar field increases as a function of time during sheath expansion at the position of maximum sheath width. The self-amplification stops, when the sheath is fully expanded and no electrons are present in this region of high electric field adjacent to the electrode. This mechanism does not work during sheath collapse since cold bulk electrons enter the sheath region. It is indirectly caused by the presence of collisions, which prevent energetic electrons generated during sheath expansion at the grounded electrode from arriving at the powered electrode during sheath collapse. Thus, the ambipolar field is lower during sheath collapse compared to the sheath expansion phase. Moreover, the electron conduction current density has reversed its sign compared to the sheath expansion phase, while the sign of the ambipolar electric field does not change, since it is determined by the ion density gradient. Therefore, electrons are “cooled” during
sheath collapse by the ambipolar field, but this ‘cooling’ is weaker compared to the ambipolar power absorption during sheath expansion. This explains the strong contribution of ambipolar electron power absorption to the power dissipation to electrons on time average. The instantaneous profiles of the ambipolar electron power absorption rate show two peaks at different positions (see figure 6). One peak occurs close to the instantaneous sheath edge and the second peak occurs around the position of the maximum sheath width according to the positions of the extrema of $T_e$ and $(1/\rho_e)(\partial n_e/\partial x)$ shown in figure 8. This mechanism is quite different from the concept of stochastic heating used in the Hard Wall Model. The ambipolar electron power absorption generates electrons with energies above the ionization threshold. Thus, it is essential for the operation of CCPs.

Obviously the temporal modulation of the electron temperature is essential for a non-zero ambipolar electron power absorption and for a non-zero total electron power absorption at low pressures on time average. As shown in the appendix for conditions, where ambipolar power absorption dominates, the time averaged power absorbed by electrons per area, $S_e$, is zero in the presence of a temporally constant electron temperature in typical CCPs according to:

$$\langle S_{e,T=\text{const}} \rangle = 0.$$  \hfill (5)

Thus, there would be no ambipolar electron power absorption on time average without a time modulated electron temperature and temporally asymmetric dynamic. At low pressure, where the ambipolar power absorption is dominant, there would be essentially no electron power absorption on time average at all. Therefore, the dynamics and temporal asymmetries discussed in this work are absolutely essential for the operation of CCPs.

The fifth electric field term is proportional to the gradient of the electron temperature and causes significant electron power loss on time average at positions, where strong ambipolar electron power absorption occurs (see figure 1). The time resolved data (figures 3–6) show that this term causes strong electron power loss at the position of maximum sheath width during sheath expansion at all pressures investigated in this work. During this fraction of the RF period the electron temperature decreases towards the bulk and, thus, results in electron power loss on time average at positions, where strong ambipolar power absorption is dominant, there would be essentially no electron power absorption on time average at all. Therefore, the dynamics and temporal asymmetries discussed in this work are absolutely essential for the operation of CCPs.

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Figure 9. Space and time averaged electron power density corresponding to each electric field term, the sum of terms 4 and 5 (‘pressure heating’), and the total power dissipated to electrons as a function of pressure.

The impingement of these energetic beam electrons at the collapsing sheath edge leads to a local increase of the mean electron energy. Consequently, the electron temperature decreases towards the bulk during sheath collapse, while it increases towards the bulk at high pressure. Therefore, term 5 causes power loss during sheath collapse at high pressure, while it causes power absorption at low pressure.

Figure 9 shows the space- and time-averaged absorbed electron power density corresponding to each electric field term, the sum of terms 4 and 5, which corresponds to pressure heating, and the total power dissipated to electrons as a function of pressure. The plot of the total power dissipated to electrons is similar to figure 2 in [5], but is now based on a fully self-consistent theory without any assumptions. Based on our analysis its interpretation is quite different, since there is no ‘stochastic heating’, which historically is a result of the Hard Wall Model, which is inconsistent with the moments of the Boltzmann equation. Instead, ambipolar electron power absorption, $P_a$, is found to be important at all pressures investigated here. This power absorption mechanism is very different from the classical concept of stochastic heating, since it depends on strong and time dependent electric fields outside the sheaths. The electric field generated by the electron temperature gradient, $P_a$, yields significant electron power loss. The sum of terms 4 and 5 corresponds to pressure heating and is dominant at low pressures, remains approximately constant, and is significantly smaller than the ohmic term, $P_{\text{ne}}$, at higher pressures. The relative contribution of ohmic heating to the total power dissipated to electrons increases as a function of pressure. All other terms play a minor role. The strong decrease of the total power absorption of electrons as the pressure is reduced from 2 to 1 Pa is caused by a transition of the mode of discharge operation from the classical α–mode at 2 Pa, where one electron beam is generated at each electrode per sheath expansion phase, to a mode described previously by Wilczek et al [16], where the confinement of energetic electrons is poor and multiple beams
are generated at each electrode during sheath expansion due to kinetic resonance effects.

The observed changes of the relative contributions of different power absorption mechanisms on space and time average as a function of pressure are understood in detail based on the previous space- and time-resolved analysis. Thus, this space- and time-resolved analysis of the power dissipation to electrons based on a moment analysis of the Boltzmann equation provides an in-depth understanding of electron power absorption in electropositive low pressure CCPs.

5. Conclusions

The electron power absorption dynamics in electropositive low pressure capacitive RF plasmas operated in argon at 13.56 MHz were studied space- and time-resolved within the RF period based on the first two moment equations of the Boltzmann equation using input parameters from 1d3v electrostatic PIC/MCC simulations. In contrast to a variety of previous models, this approach makes no assumptions (other than those already inherently present in the simulations themselves), but is fully self-consistent and, therefore, yields an in depth understanding of this complex phenomenon.

By combining the first two velocity moments, the electric field and the power absorbed by electrons is found to be the sum of seven terms, respectively, each one corresponding to a distinct physical mechanism of electron power absorption. By analyzing the spatio-temporal distributions of each term individually as a function of the neutral gas pressure, the dominant electron power absorption mechanisms have been identified space- and time-resolved within the RF period.

In contrast to previous models, strong electric fields are observed outside the sheaths, i.e., there is no Hard Wall, and the sheath dynamics are found to be asymmetric in time, i.e., the sheath expansion phase is not a mirror image of the sheath collapse. Both these insights are found to play a key role for electron power absorption in CCPs. The electric field outside the sheaths is predominantly an ambipolar field caused by the electron density gradient and the non-zero electron temperature. It was found to be maximum around the position of maximum sheath width as well as at the instantaneous sheath edge and to be time modulated within the RF period due to a time modulation of the electron mean energy. The latter effect is caused by an acceleration of electrons by the ambipolar field itself during the sheath expansion phase. This is a self-amplifying mechanism that leads to an increase of the instantaneous ambipolar electric field and an even stronger acceleration of electrons during sheath expansion. It stops, when the sheath is fully expanded, due to the absence of electrons in the region of steep normalized plasma density profile adjacent to the electrode. This mechanism does not work during the collapse phase of the sheath, since the direction of the electron current is reversed, but the sign of the ambipolar field remains the same, because it is determined by the ions, which cannot react on the timescale of one RF period. This has been identified as the dominant source for the temporal asymmetry of the electric field and for a non-zero electron power absorption on time average at low pressures. A theoretical argument was derived that demonstrates that the ambipolar electron power absorption would vanish completely on time average in the absence of a time modulation of the electron temperature. Thus, this time modulation and the temporal asymmetry of the sheath dynamics within the RF period are absolutely essential for the generation of CCPs at low pressures. The gradient of the electron temperature was found to cause electron power loss on time average. This ‘cooling’ mechanism was explained at the kinetic level and found to partly compensate the ambipolar electron power absorption. Both effects are inherently linked to each other. The collisional ohmic power absorption was found to increase as a function of pressure in agreement to previous findings.

On space and time average, the power dissipated to electrons was found to increase as a function of the neutral gas pressure. These results are in qualitative agreement with the original findings of Godyak et al [5], but their interpretation is quite different. While two inconsistent theories of ohmic and stochastic heating based on strong simplifications, e.g., the negligence of the pressure term in the electron momentum balance equation, were used originally, we used a fully self-consistent approach, which identified the electron pressure term and temporal asymmetries to play a key role via ambipolar electron power absorption.

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Appendix

We derive equation (5) that states that the time-averaged electron power absorption \( \langle S_e \rangle \) will vanish, if the ambipolar electric field dominates and the electron temperature, \( T_e \), is constant. We consider a spatial region \([x_L, x_R]\), where \( x_L \) denotes the position of the electrode and \( x_R \) a point on the bulk side of the sheath edge where quasi-neutrality is fulfilled at all times. The considered equations are electron continuity and the electron momentum balance equation. We neglect ionization sources and assume that the ambipolar electric field is the dominant contribution to the total electric field \( (E \approx E_a) \). This is well justified by the results presented in this work (e.g., in figure 5). This is equivalent to assuming the electrons to be in Boltzmann equilibrium:

\[
\frac{\partial n_e}{\partial t} - \frac{1}{e} \frac{\partial j_e}{\partial x} = 0, \tag{A.1}
\]

\[
T_e \frac{\partial n_e}{\partial x} = -en_e E. \tag{A.2}
\]

The motion of the ions is not modulated at the RF frequency, hence \( n_i = n_i(x) \), and the ion current density, \( j_i \), is constant.
Finally, there is Poisson’s equation
\[ \varepsilon_0 \frac{\partial E}{\partial x} = \epsilon (n_l - n_e). \]  
(A.3)
The total current density—the sum of displacement, electron, and ion current densities—is a spatial constant. It is assumed to be periodic and average free:
\[ J(t) = \varepsilon_0 \frac{\partial E}{\partial t} + J_i + J_e. \]  
(A.4)
The sheath charge per area, \( Q \), in the domain \([x_e, x_B]\) is as follows, where the second identity stems from substituting Poisson’s equation (A.3):
\[ Q(t) = \epsilon \int_{x_e}^{x_B} (n_l - n_e) \, dx = \varepsilon_0 (E(x_B, t) - E(x_e, t)). \]  
(A.5)
Assuming that the electric field at \( x_B \), or at least its time derivative, is negligible, we get
\[ \frac{dQ}{dt} = -\varepsilon_0 \frac{\partial E}{\partial t} \bigg|_{x_e}, \]  
which allows to evaluate the total current at the electrode as
\[ J(t) = \frac{dQ}{dt} + J_i + J_e(x_e, t). \]  
(A.7)
By combining equations (A.4) and (A.7), the electron conduction current density at a given position \( x \) is
\[ J_e(x, t) = -\frac{dQ}{dt} - \varepsilon_0 \frac{\partial E}{\partial t} + J_e(x_e, t). \]  
(A.8)
Multiplying this equation with the electric field and integrating over the sheath \([x_e, x_B]\) reveals the electron energy balance. Introducing the sheath voltage drop \( V(t) \) and the electric energy \( W(t) \) stored in the sheath,
\[ V(t) = -\int_{x_e}^{x_B} E(x, t) \, dx, \]  
(A.9)
\[ W(t) = \int_{x_e}^{x_B} \frac{1}{2} \varepsilon_0 E^2 \, dx, \]  
(A.10)
we obtain the following expressions for the time-resolved electron power per area:
\[ \langle S_e(t) \rangle = \int_{x_e}^{x_B} E(x, t) J_e(x, t) \, dx = V(t) \frac{dQ}{dt} - \frac{dW}{dt} - V(t) J_e(x_e, t). \]  
(A.11)
Performing the phase average, and making use of the fact that \( W(t) \) is periodic, we find
\[ \langle S_e \rangle = \frac{1}{T} \int_0^T V(t) \frac{dQ}{dt} \, dt - \frac{1}{T} \int_0^T V(t) J_e(x_e, t) \, dt. \]  
(A.12)
So far, the Boltzmann relation (A.2) was not used. Making use of it now, we realize that (A.2) and the Poisson equation (A.3) constitute a system of two differential equations of first order which was extensively discussed in [46]. The system has two degrees of freedom and requires two boundary conditions or constraints. One suitable condition is quasi-neutrality at \( x_B \); as the other, we prescribe the value of \( Q \). The system (A.2) and (A.3) can then be solved uniquely.

For a given ion density \( n_i(x) \), the solution depends on \( Q(t) \) and \( T_e \). This holds in particular for the electric field, which is a space charge field in the depletion region and of ambipolar character in the quasineutral zone:
\[ E(x, t) = E(x, Q(t), T_e). \]  
(A.13)

Also the sheath voltage depends on the parameters \( Q(t) \) and \( T_e \):
\[ V(t) = -\int_{x_e}^{x_B} E(x, Q(t), T_e) \, dx = V(x, Q(t), T_e). \]  
(A.14)

Let us now focus on the first term of expression (A.12). Define some function, \( f \), such that \( \frac{dQ}{dt} = V = \frac{df}{dt} \).
\[ \frac{dQ}{dt} = \frac{dQ}{dt} \frac{df}{dt} = \frac{df}{dt}. \]  
(A.15)
Inserting this into expression (A.12), one realizes that the first term will vanish, if the electrode temperature is constant, since \( f \) is a periodic function, i.e. \( f(t = 0) = f(T) \):
\[ \frac{1}{T} \int_0^T V(x, Q(t), T_e) \frac{dQ}{dt} \, dt = \frac{1}{T} \int_0^T \frac{df}{dt} \, dt = 0. \]  
(A.16)
The remaining contribution to the phase-averaged absorbed power per area \( \langle S_e \rangle \) is, thus, the second term, which describes the work done by the electron flow through the sheath. In the absence of secondary electron emission from the electrodes this term is small and negative. It involves the electron current density at the electrode, which vanishes for most of the time, except for the moment of the sheath collapse. During sheath collapse electrons must overcome the floating potential to get to the electrode in order to compensate the ion current to the electrode on time average. As this potential acts to impede the flow of electrons towards the electrode, the second term on the right hand side of equation (A.12), and thus, \( \langle S_e \rangle \) are typically negative. If we neglect this term, this implies that, if \( T_e \) is constant, the average power absorbed by electrons per area is zero.
\[ \langle S_e \rangle = \frac{1}{T} \int_0^T V(t) J_e(x_e, t) \, dt \approx 0, \]
\[ \langle S_e \rangle = \langle S_{a,T_e=const} \rangle \approx 0. \]  
(A.17)
Therefore, for a positive power absorption by the ambipolar field a time-dependent \( T_e \) is required.

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