Narrow gap electronegative capacitive discharges

E. Kawamura, a) M. A. Lieberman, and A. J. Lichtenberg

Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, California 94720, USA

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Narrow gap electronegative (EN) capacitive discharges are widely used in industry and have unique features not found in conventional discharges. In this paper, plasma parameters are determined over a range of decreasing gap length \(L\) from values for which an electropositive (EP) edge exists (2-region case) to smaller \(L\)-values for which the EN region connects directly to the sheath (1-region case). Parametric studies are performed at applied voltage \(V_{\text{rf}} = 500\) V for pressures of 10, 25, 50, and 100 mTorr, and additionally at 50 mTorr for 1000 and 2000 V. Numerical results are given for a parallel plate oxygen discharge using a planar 1D3v (1 spatial dimension, 3 velocity components) particle-in-cell (PIC) code. New interesting phenomena are found for the case in which an EP edge does not exist. This 1-region case has not previously been investigated in detail, either numerically or analytically. In particular, attachment in the sheaths is important, and the central electron density \(ne\) is depressed below the density \(n_{\text{eh}}\) at the sheath edge. The sheath oscillations also extend into the EN core, creating an edge region lying within the sheath and not characterized by the standard diffusion in an EN plasma. An analytical model is developed using minimal inputs from the PIC results, and compared to the PIC results for a base case at \(V_{\text{rf}} = 500\) V and 50 mTorr, showing good agreement. Selected comparisons are made at the other voltages and pressures. A self-consistent model is also developed and compared to the PIC results, giving reasonable agreement. © 2013 AIP Publishing LLC.

I. INTRODUCTION

We are very pleased to submit a paper to an issue honoring Lev Tsendin. His insight in an early paper1 that an electronegative (EN) plasma would separate into an EN core and an electropositive (EP) edge was fundamental to our various investigations of EN plasmas. Subsequently, we collaborated with him on an analytic and numerical study of the transition from parabolic to flat-topped negative ion density profiles with increasing pressure or size.2 In all our interactions with Lev, we considered ourselves fortunate to have access to his insights and his humor.

Our previous investigations of capacitively driven EN discharges divide into two categories. In the first category, we used oxygen as a feedstock gas, and assumed a fixed plasma width \(d\) at low-to-intermediate pressures \(p\) (e.g., 10 to 50 mTorr).3–5 We used a constant \(n_{e0}\) (central electron density in the EN core) as a known plasma parameter, representing the applied power or voltage. The sheaths were not considered in this formulation since their widths were small and fairly constant as parameters were varied. The electronegativity \(\alpha\) (ratio of negative ion to electron density) was not too large, such that an EP edge region usually existed. These conditions were generally consistent with the negative ions being in Boltzmann equilibrium, resulting in a parabolic negative ion density profile.3 However, as \(n_{e0}\) is decreased, the local ion sound velocity is reached within the EN core, which abruptly terminates the core.4 In the second category, we used a more attaching chlorine feedstock gas and higher pressures (e.g., 300 mTorr), and observed another transition,2,6 in which, with fixed \(n_{e0}\) and \(d\), the negative ion density profile changes from a parabolic to a flat-topped profile with increasing pressure.5 As in the first category, the sheaths were not considered in the equilibrium modeling.

The entire range of conditions can be theoretically explored for a given feedstock gas by varying a normalized \(p\) and \(n_{e0}\) using the plasma width \(d\) as the normalization factor. We have previously done this using oxygen,7 and applied the results to compare with experiments in larger devices, in both of the parameter ranges described above.8,9 In these larger devices, the sheaths widths were small compared to the system size so the sheath dynamics could be neglected in the modeling. Most of these EN equilibrium results have been summarized in Ref. 10.

Besides the previous work summarized above, there have been many developments in the study of EN equilibria. The approximation of an ambipolar diffusion coefficient assuming a Boltzmann equilibrium for negative ions was developed in Ref. 11, and a modified Bohm’s condition was investigated in Ref. 12. The abrupt termination of an EN plasma due to the ion drift is more complicated than in the simplest representation,4 leading to the possible existence of double layers or spatial positive ion oscillations.5,13–17 But these effects, while interesting theoretically, have only minor consequences for the overall equilibria.

Although comparisons of some plasma quantities are made between models and experiments (e.g., Refs. 6, 8, 13, and 16), it is difficult to compare a complete parameter set. Particle-in-cell (PIC) calculations allow more detailed comparisons, as we have partly done in a previous work1 and

References


a)kawamura@eecs.berkeley.edu
will do more completely in this paper. As in the previous works, both our numerical and theoretical calculations use a simplified oxygen cross-section set which does not include oxygen metastables. In this paper, we mainly explore lower electron densities which tend to give high x’s. In this regime, negative ion detachment due to oxygen atoms is weak compared to positive-negative ion recombination. If the x’s are low, then detachment can compete with recombination. This has been investigated analytically\(^{18,19}\) and using PIC.\(^{20}\)

Reference 20 emphasized the effect of non-Maxwellian electron energy distribution functions (EEDFs) when comparing models to experiments. The non-Maxwellian EEDFs found in our PIC simulations also complicate comparisons with models, as will be discussed.

Recent commercial interest in narrow gap capacitive discharges has increased the importance of examining some of the approximations made in the previous works on EN plasma equilibria. Since the plasma width \(d = L - 2s_m\), where \(L\) and \(s_m\) are the gap and maximum sheath width, respectively, the ratio \(d/L\) decreases rapidly with decreasing \(L\) for \(d/2s_m \approx 1\). The PIC results show that as \(L\) decreases, there is a transition from a “2-region” plasma with an EP edge to a “1-region” plasma in which the EN core connects directly to the sheath. Although the EP edge is usually thin when it exists, it is included in the modeling to take into account the drop in electron density from the value \(n_{0,0}\) at the core to the value \(n_{0,0}\) at the sheath edge. In the model, the core electron power flux \(S_{\text{core}}\) must be distinguished from the total power flux \(S_{\text{tot}}\), which is the power flux absorbed by the entire discharge. Determining the central electronegativity \(z_0\) in the model requires including attachment in the sheaths, which can be as important as attachment in the core for the 1-region plasmas.

In Sec. II, the results of PIC simulations of narrow gap EN discharges with varying gap spacing \(L\) are discussed. The gas pressure \(p\) and the applied rf voltage \(V_{\text{rf}}\) are parameters, and oxygen is used as the attaching gas. In Sec. III, two models of the narrow gap discharge are developed. A simplified model uses some plasma quantities from the PIC, as will be explained in the text. A self-consistent model uses only the input parameters of the discharge to determine the plasma equilibrium. The models are compared with the PIC results in Sec. IV. Conclusions and further comments are given in Sec. V.

II. 1D PIC SIMULATIONS

A. Description of the PIC code

We conducted PIC simulations of narrow gap parallel-plate capacitive oxygen discharges using the planar bounded plasma electrostatic 1 spatial dimension, 3 velocity components (1D3v) code PDP1.\(^{21,22}\) In a PIC code, each computer particle is actually a “superparticle” which represents a cluster of \(10^3\) to \(10^5\) real particles (electrons or ions). For each computer particle, PDP1 tracks the (1D) displacement in the axial \((x)\) direction and the three velocity components \((v)\) in the axial and perpendicular \((y)\) and \((z)\) directions. The simulation is run with a sufficient number of particles to minimize the discrete particle noise. The neutrals in PDP1 are assumed to form a constant and uniform background gas with a fixed temperature. PIC simulations obtain the fields, particle densities, and fluxes self-consistently from first principles, without making any assumptions about the particle temperatures or velocity distributions.

In a typical electrostatic PIC simulation, for each time-step \(\Delta t\), (i) particles are linearly weighted to the spatial grid to obtain the charge density \(p_j\) at the gridpoints, (ii) \(p_j\) is used in Poisson’s equation to solve for the electric field \(E_j\) at the gridpoints, (iii) \(E_j\) is linearly interpolated to each particle position \(x_i\) to determine the force \(F_i\) on each particle, (iv) the Newton-Lorenz equation of motion is used to advance the particles to new positions and velocities, (v) boundaries are checked and out of bound particles are removed, (vi) a Monte Carlo collision handler checks for collisions and adjusts the particle velocities and numbers accordingly.

Typically, in order to ensure stability and accuracy, the time-step \(\Delta t\) is chosen to resolve the electron plasma frequency \(\omega_p \equiv (e^2 n_e/\epsilon_0 m_e)^{1/2}\) while the grid spacing \(\Delta x\) is chosen to be of the same order as the electron Debye length \(\lambda_D \equiv (\epsilon_0 T_e/e n_e)^{1/2}\). The Monte-Carlo collision method and oxygen cross-section set used in PDP1 is described in detail in Ref. 22. For our oxygen discharge simulations, there are three charged particle species: electrons with density \(n_e\), \(O_2^+\) ions with density \(n_+\), and \(O^-\) ions with density \(n_-\). The net positive ion density is given by \(n_i \equiv n_+ - n_-\), and the central particle densities are \(n_{0,0}, n_{+0},\) and \(n_{-0}\), respectively.

The period-averaged electron power density profile \(p_e(x)\) is given by

\[
p_e(x) \equiv p_{\text{ohm}}(x) + p_{\text{ac}}(x) = (J_e(x,t) \cdot E(x,t)),
\]

with \(J_e(x,t)\) as the electron conduction current density, \(E(x,t)\) as the electric field, and the brackets denoting an average over a rf period. The electron power density profile \(p_e(x)\) has both ohmic \(p_{\text{ohm}}(x)\) and stochastic \(p_{\text{ac}}(x)\) heating components. In the left ion sheath region, where \(0 < x < s_m\), \(n_e(x) \approx n_i\) for \(x > x_{\text{sh1}}(t)\), and \(n_e(x) \approx 0\) for \(x < x_{\text{sh1}}(t)\), where \(x_{\text{sh1}}(t)\) is the instantaneous position of the left electron sheath edge. Similarly, for the right ion sheath region, where \(L - s_m < x < L\), \(n_e(x) \approx n_i\) for \(x < x_{\text{sh2}}(t)\), and \(n_e(x) \approx 0\) for \(x > x_{\text{sh2}}(t)\), where \(x_{\text{sh2}}(t)\) is the instantaneous position of the right electron sheath edge. Thus, the period-averaged ohmic heating profile is given by \(p_{\text{ohm}}(x) = \langle \Pi(x,t) \rangle\), where

\[
\Pi(x,t) = \frac{J_{\text{rf}}^2(t)}{\sigma_p + i\omega\epsilon_0} \text{ if } x_{\text{sh1}}(t) < x < x_{\text{sh2}}(t)
\]

and

\[
\Pi(x,t) = 0 \text{ otherwise. (2)}
\]

Here, \(J_{\text{rf}}(t)\) and \(\omega\) are the rf current density and radian frequency, respectively, and \(\sigma_p = \epsilon_0 \omega_p^2 (i\omega + \nu_{\text{coll}})\) is the plasma conductivity with \(\nu_{\text{coll}}\) the electron-neutral collision frequency. Note that

\[
\text{Re}\left(\frac{1}{\sigma_p + i\omega\epsilon_0}\right) = \frac{\nu_{\text{coll}} \omega_p^2}{\epsilon_0 (\omega^2 - \omega_p^2)^2 + \omega^2 \nu_{\text{coll}}^2},
\]

for \(\omega < \omega_p\).
Once $p_e(x)$ and $p_{\text{ohm}}(x)$ are calculated, $p_{\text{stoc}}(x)$ is obtained from $p_{\text{stoc}}(x) = p_e(x) - p_{\text{ohm}}(x)$.

**B. External parameters and plasma conditions**

We conducted PIC simulations over a range of decreasing $L$ from $L$-values for which an EP edge exists (2-region case) to smaller $L$-values for which the EN core connects directly to the sheath (1-region case). Parametric studies are carried out at (i) a relatively low applied voltage $V_{\text{rf}} = 500 \text{ V}$ for $p = 10, 25, 50,$ and $100 \text{ mTorr}$, and (ii) an intermediate pressure $p = 50 \text{ mTorr}$ for $V_{\text{rf}} = 500, 1000,$ and $2000 \text{ V}$. In all cases, the applied rf frequency $f = 13.56 \text{ MHz}$ and the plate area $A = 0.016 \text{ m}^2$. In the parameter space investigated, the negative ions are mainly in Boltzmann equilibrium, resulting in parabolic negative ion density profiles which may be truncated at the transition either to an EP edge or to a sheath.$^3,4$

For the cases we studied, we found that when an EP edge exists, it is thin compared to the core size, and the electron density is essentially a constant ($n_e \approx n_{e0}$) in the core, but may fall significantly (as much as a factor of five) in the thin EP transition to a sheath (see Figure 1(a)). With decreasing $L$, we observed a transition to a plasma in which the EN core connects directly to the sheaths, with lower $n_e$ in the core than at the sheath edge. This transition is an important consideration in our study.

**C. PIC results for the 50 mTorr, 500 V base case**

In Figures 1–3, we show PIC results for $L = 4.5, 3.25,$ and $2.5 \text{ cm}$, respectively, for our base case with $p = 50 \text{ mTorr}$ and $V_{\text{rf}} = 500 \text{ V}$. The figures show (1) a case with a distinct EP edge, (2) a transition case, and (3) a case with no EP region, respectively. The plasma quantities shown are period-averaged profiles of (a) densities, (b) current fluxes, (c) temperatures for positive ions (solid), negative ions (dash) and electrons (dot), and (d) period-averaged electron power density profiles $p_e(x)$ (solid), $p_{\text{ohm}}(x)$ (dash), and $p_{\text{stoc}}(x)$ (dot).

As $L$ decreases from 4.5 to 2.5 cm, we see from Figures 1(a)–3(a) that the positive and negative ion density maxima remain fairly constant, but the central core electron density $n_{e0}$ decreases sharply, resulting in central electronegativities $\alpha_0 = n_{e0}/n_{e0}$ of 9.7, 35.2, and 63.5, respectively. The sheath sizes do not vary much so that the ratio $dL/L$ decreases rapidly with decreasing $L$. For these narrow gap devices, the EP edge size is small compared to the size of the EN core.

From the current density profiles in Figures 1(b)–3(b), we see that roughly half the positive ion current density $eC_+\Gamma_+$ is generated outside of the core. Using the approximate relation,

$$S_e(x) = \int_{x_0}^{x} p_e(x')dx' = eE_c\Gamma_+(x),$$

FIG. 1. PIC results for a 50 mTorr, 500 V oxygen discharge with $L = 4.5 \text{ cm}$, showing period-averaged (a) densities, (b) current densities, and (c) temperatures for positive ions (solid), negative ions (dash), and electrons (dot), and (d) period-averaged electron power density profiles $p_e(x)$ (solid), $p_{\text{ohm}}(x)$ (dash), and $p_{\text{stoc}}(x)$ (dot).
where $S_e(x)$ is the period-averaged electron power per unit area from the core center at $x_0$ to any $x$, and $eE_e$ is the assumed constant energy necessary to generate an electron-ion pair. We have the rather surprising result that only about half the total electron power is absorbed in the EN core for all three cases.

The period-averaged electron temperature in Figure 1(c) for $L = 4.5$ cm is quite low compared to the other two cases shown in Figures 2(c) and 3(c). An obvious interpretation is that for larger $L$-values for which there is an EP edge, the EEDF is bi-Maxwellian while for smaller $L$-values for which there is no EP edge, the EEDF is nearly Maxwellian. This is
confirmed in Figure 4 which shows the EEDF in the central region for (a) $L = 4.5$ cm and (b) $L = 2.5$ cm.

In Figures 1(d)–3(d), we see the period-averaged electron power density profiles for the total electron power absorbed $p_e(x)$, as well as its ohmic and stochastic heating components, $p_{\text{ohm}}(x)$ and $p_{\text{stoc}}(x)$, respectively. For $L = 4.5$ cm, the electron power is almost all deposited outside of the EN core region due to the increased stochastic and ohmic heating in the low density edge regions. In this 2-region case, there is a potential barrier of the order of the cold electron temperature $T_{\text{ec}}$ in the EP edge region with respect to the EN core. Thus, electrons generated in the core do not easily traverse to the maximal heating regions at the edges. Theories describing the trapping of colder electrons in an EN core have been previously developed.23–25

For the transitional case of $L = 3.25$ cm, the ohmic heating increases since the driving current remains fairly constant while the plasma resistivity increases with the decreasing electron density. For the 1-region case of $L = 2.5$ cm, a new phenomena arises in which the stochastic heating is suppressed in the sheath, but also weakly occurs in the core. The suppression of the sheath stochastic heating can be qualitatively explained by the reduction of $n_{e0}$ with respect to $n_{esh}$. The reduced electron density also increases the ohmic heating, which becomes the dominant heating mechanism.

A further understanding of the difference between the 2-region and 1-region cases can be seen from Figure 5 which plots $n_e$ (dash) and $n_1 \equiv n_+ - n_-$ (solid) for (a) $L = 4.5$ cm and (b) $L = 2.5$ cm. The vertical lines occur at the positions where $n_0 \approx 0$ and at where the sheath region (net positive charge) begins. At $L = 4.5$ cm, we see that there is a small but significant EP edge, and that $n_e$ drops by more than a factor of two from $n_{e0}$ to $n_{esh}$. In this case, the number of electrons in the sheath is small compared to that in the bulk, which will be an important factor in the theory given in Sec. III. In contrast, at $L = 2.5$ cm, the sheath region begins where there is still significant $n_0$ ($\gg 1$). Interestingly, in contrast to usual sheath behavior, there is a small region where both $n_i$ and $n_e$ are increasing from the discharge midplane toward the sheath, with $n_i$ increasing much faster. A simple static picture would predict that the more mobile electrons would neutralize excess positive ionic charge. The resolution is seen in Figure 6 which gives eight snapshots of the electron cloud, equally spaced over a rf cycle. The electrons neutralize the ionic charge when they are present, but due to their finite inertia, the thinness of the core, and the consequent limited extent of the electron cloud, they uncover some of the ionic charge toward the end of each oscillation. Thus, the period-averaged $n_i$ does not neutralize the period-averaged $n_e$. This complex edge behavior for the 1-region case will be a factor when discussing the differences between the PIC results and the modeling in Sec. IV.

**D. Electron density versus gas density**

In Figure 7, we take all of the cases enumerated in Sec. II B and plot the normalized central core density $n_{e0}$ as a function of the normalized gas density $n_g$. The normalization factors use the bulk plasma size $d$ rather than the gap width $L$, and are described in Appendix B. The various PIC cases of pressures and voltages are given by symbols as shown in the figure caption. For each PIC case, the values of $L$ decrease from top to bottom in the figure, and the lowest values of $n_{e0}$ correspond to 1-region plasmas while the highest values correspond to 2-region plasmas. In between, the extreme values are the transitional cases.
The dashed-dotted curves labeled “500 V” and “2 kV” show the theoretical transitions between the upper $n_{eo}$ values corresponding to 2-region plasmas and the lower $n_{eo}$ values corresponding to 1-region plasmas for the applied voltages at 500 V and 2000 V, respectively. The lowest dashed-dotted curve labeled “No sheath attach,” corresponds to a limiting case in which no attachment occurs in the sheath. These transitions are generalized from the previous work\textsuperscript{7} to take into account the different applied voltages and are derived in Appendix B.

The solid curves enclose the regions of validity for the theory. On the three solid curves labeled “Recomb. = Endloss,” volume recombination loss is equal to positive ion wall loss for the specified applied voltages of “500 V” and “2 kV,” as well as for the case of no attachment in the sheaths. To the left of the three solid curves, the core size $d$ become smaller and the pressures lower, so that the theoretical model condition that positive ion flux to the sheaths exceeds bulk recombination loss is satisfied, resulting in a parabolic $n_-$ profile. To the right of these curves, this condition is no longer satisfied, resulting in a flat-topped $n_-$ profile. Below the solid line labeled “2 kV, $x_0 = 3$,” the central electronegativity $x_0 > 3$ for $V_{rf} \leq 2000$ V. This somewhat arbitrary condition satisfies the theoretical model assumption that $x_0$ is sufficiently large that the EP edges are small compared to the EN cores. At higher values of $n_{eo}$, $x_0$ decreases. The solid lines described above are derived in Appendix B using the model equations from Sec. III.

### III. ANALYTIC MODELING

#### A. Assumptions and equations

To analyze the variation of discharge parameters with gap width, power and pressure, we develop a simplified analytic model. We assume a high core electronegativity $x_0 = n_+0/n_{eo}$, such that $x_0 \gg 1$ in all formulae. We also assume that any electropositive edge region is thin compared to the electronegative core, setting $L = d + 2s_m$, where $L$ is the discharge gap width, $d$ is the core width, and $s_m$ is the sheath width. We assume $d$ is sufficiently thin that both negative species are Boltzmann with $T_+ \gg T_-$, such that the negative ion density is parabolic in the core, and the electron density is nearly uniform, $n_e = n_{eo}$. The core positive ion balance is

$$K_{+} n_{eo} n_0 d = \frac{8}{15} K_{rec} n_0^2 x_0^2 d + 2 \Gamma_+,$$  \hspace{1cm} (5)

where $K_+$ is the ionization coefficient, $n_+$ is the oxygen gas density, $K_{rec}$ is the positive-negative ion recombination coefficient, and $\Gamma_+$ is the positive ion flux leaving the core. The first and second terms on the right hand side give the positive ion loss in the core volume for $x_0 \gg 1$, and that flowing out of the core, respectively. The factor $8/15$ accounts for averaging the square of the parabolic negative ion profile over the core.

The positive ion flux is obtained from diffusion theory. For the 1-region model, with no EP edge, we assume, following the discussion of Figure 5, that the core positive ion density at the sheath edge drops rapidly to the core electron density $n_{eo}$ within a thin transition layer, in which the negative ion density drops to essentially zero and the positive ion velocity increases, from $u_{B+} = (eT_+/M_+)^{1/2}$ to the usual EP Bohm’s speed $u_{Be} = (eT_e/M_e)^{1/2}$

$$\Gamma_+ = n_{eo} u_{Be} \quad (1\text{-region}).$$  \hspace{1cm} (6)

For the 2-region model, the flux is

$$\Gamma_+ = h_l n_{eo} u_{B+} \quad (2\text{-region}).$$  \hspace{1cm} (7)

Here, $h_l \equiv x_s / x_0$, where $x_s$ is the electronegativity at the core edge. We use for $h_l$ the expression for $h_0$ given in Ref. 9 for a truncated parabolic negative ion density profile, with $T_+ = T_-$

$$h_l = \frac{1}{1 + \frac{d}{(8\pi)^{1/2} \lambda_+}},$$  \hspace{1cm} (8)

where $\lambda_+ = 1/n_e \sigma_+$ is the ion-neutral mean free path, with $\sigma_+$ as the ion-neutral cross section. In Eq. (7), the flux

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**FIG. 6.** PIC results for a 50 mTorr, 500 V oxygen discharge with $L = 2.5$ cm, showing snapshots of $n_e$ at eight equally spaced intervals of an rf cycle.

**FIG. 7.** Normalized $n_{eo}$ versus normalized $n_e$, space, showing the regime of interest in this work.
leaving the core is less than $n_{e0}u_{Be}$. This requires an EP transition region in which the ion velocity increases from $u_{Be}$ to $u_{sh}$, and the density drops from $n_{e0}$ to a sheath edge density $n_{sh}$, such that $\Gamma_{\pm} = n_{sh}u_{Be}$. Although $h_{i}$ is calculated for conditions of a truncated parabola for which the ion sound velocity is reached at the edge of the core and the electronegativity $\chi_{e}$ at the core edge is large, it gives approximately the correct flux even for a full parabola when there is no ion sound limitation in the core, provided $\chi_{0} \gg 1$. The transition from a 1-region to a 2-region model occurs at $\chi_{e} = h_{i}\chi_{0} = \gamma_{-}^{1/2}$, where $\gamma_{-} = T_{e}/T_{+}$. For the 2-region model with $h_{i}\chi_{0} < \gamma_{-}^{1/2}$, the electron density $n_{e}$ must drop in the electro-positive edge, which by flux continuity (assuming no generation in the thin EP edge region) requires that the electron density at the sheath edge $n_{sh}$ must satisfy $n_{sh}u_{Be} = \Gamma_{+}$, i.e., $n_{sh}/n_{e0} = h_{i}\chi_{0}/\gamma_{-}^{1/2}$. For the 1-region model, $n_{sh}/n_{e0} \equiv 1$, i.e., is the same value as at the transition.

The collisional Child law for the sheath is

$$\Gamma_{+} = \frac{1.68 \epsilon_{o} \rho_{e}}{e} \left( \frac{2 \epsilon_{o}}{M_{e}} \right)^{1/2} \left( \frac{\lambda_{+}}{s_{m}} \right)^{1/2} \frac{V_{dc}^{3/2}}{s_{m}}, \quad (9)$$

where $M_{e}$ is the positive ion mass, $\lambda_{+}$ is the positive ion mean free path, $V_{dc} = 0.78V_{f}$ is the dc voltage across the sheath, and $V_{f} = V_{rf}/2$ is the amplitude of the rf sheath voltage. As discussed above, we neglect flux generated in the electropositive edge, such that we can then equate the flux in Eq. (9) to the flux leaving the core, which gives a relation for $s_{m}$ in terms of the core flux.

An important feature of narrow gap discharges is that negative ions generated in the sheaths flow into the core and contribute to the balance between attachment and recombination there. For a collisional sheath, the time-average electron number/area within the two sheaths is obtained in Appendix A

$$N_{sh} = \frac{2J_{rf}}{e\epsilon_{0}}, \quad (10)$$

where

$$J_{rf} = 1.52\frac{\epsilon_{o}\chi_{0}}{s_{m}}V_{f}. \quad (11)$$

The number/area of core electrons is $N_{ecore} = n_{e0}d$. Therefore, we write the core negative ion balance as

$$K_{att}n_{e0}\left( n_{e0}d + \frac{2J_{rf}}{e\epsilon_{0}} \right) = \frac{8}{15}K_{me}n_{e0}^{2}\rho_{e}^{2}d, \quad (12)$$

where $K_{att}$ is the attachment rate coefficient.

The core electron energy balance is

$$S_{ecore} = e\mathcal{E}c_{e}K_{att}n_{e0}n_{e0}d + 2eT_{s}\Gamma_{+}, \quad (13)$$

where $S_{ecore}$ is the electron power/area deposited in the core, $e\mathcal{E}c_{e}$ is the collisional energy loss per electron-ion pair created, and $2eT_{s}$ is the kinetic energy carried by an electron out of the core. The first and second terms on the right hand side are the energies per unit area lost in the core and leaving the core, respectively. Substituting Eq. (5) into Eq. (13), we obtain

$$S_{ecore} = \frac{8}{15}K_{rec}n_{e0}^{2}\rho_{e}^{2}d \cdot e\mathcal{E}c_{e} + 2\Gamma_{+} \cdot e\mathcal{E}c_{e}, \quad (14)$$

where $\mathcal{E}c_{e} = \mathcal{E}_{e} + 2T_{s}$.

Although we will not use the equations for the ohmic and stochastic power generation in our first comparison of the theory to the PIC results, which we present in Sec. IV A, a self-consistent analytic theory needs this information, and the equations governing the power absorption are given below. The comparison with the PIC results, including calculated ohmic and stochastic heating, is presented in Sec. IV B.

The electron power absorbed by the core can be written as

$$S_{ecore} = f_{core}S_{riot} = f_{core}(S_{soc} + S_{ohmsh} + S_{ohmbulk}), \quad (15)$$

where $S_{soc}$, $S_{ohmsh}$, and $S_{ohmbulk}$ are the electron powers/area deposited in the discharge due to stochastic heating near the sheath edges, ohmic heating in the sheaths, and bulk ohmic heating, respectively, and $f_{core}$ is the fraction of the total electron power deposited in the core. For collisional sheaths, the stochastic heating is

$$S_{soc} = 1.22\epsilon_{o}^{1/2}m_{e}^{1/2}/\epsilon_{e}^{1/2}V_{f}, \quad (16)$$

and the ohmic heating in the sheaths is

$$S_{ohmsh} = 0.47\epsilon_{o}^{1/2}m_{e}^{1/2}V_{f}/V_{m}, \quad (17)$$

The ohmic heating in the bulk is

$$S_{ohmbulk} = \frac{1}{2}J_{rf}m_{e}^{1/2}n_{e0}d, \quad (18)$$

where $J_{rf}$ is given by Eq. (11). For the fraction $f_{core}$, we use the ratio of the number of core electrons $N_{ecore}$ to the number of total electrons $N_{etot} = N_{ecore} + N_{esh}$ in the discharge

$$f_{core} = \frac{N_{ecore}}{N_{esh} + N_{ecore}}, \quad (19)$$

where $N_{esh}$ is the number of core electrons and $N_{ecore}$ is given by Eq. (10). Typically, $S_{ecore}$ is of order half of the total electron power $S_{etot}$ absorbed by the discharge.

Equations (5)–(14) are solved to obtain the simplified model results. In addition to the input parameters $L$, $V_{rf}$, $\epsilon_{o}$, and $n_{e}$, we also use $K_{att}$, $\mathcal{E}c_{e}$, and $S_{ecore}$ obtained from the PIC results, as described in Sec. IV A. The procedure for obtaining the self-consistent model results also makes use of Eqs. (15)–(19) and does not use information from the PIC results, as described in Sec. IV B.

The scaling of ion flux and electron density with power is of interest for commercial applications. The electron density determines the flux of active species incident on the substrate surface. For simple scaling, we consider the main regime where recombination loss is much less than end loss,
the ion mean free path is small compared to the core size, and the electronegativity is much greater than unity. From Eq. (14), neglecting recombination
\[
\Gamma_+ = \frac{S_{\text{core}}}{2e\mathcal{E}_c'},
\]
yielding the usual result, for a fixed \(\mathcal{E}_c\), that \(\Gamma_+ \propto S_{\text{core}}\). For the 1-region model, the electron density is given from Eq. (6), and using Eq. (20), we obtain
\[
n_e^0 = \frac{S_{\text{core}}}{2e\mathcal{E}_c'\mu_{de}},
\]
showing the 1-region scaling \(n_e^0 \propto S_{\text{core}}\). For the 2-region model, the scaling of \(n_e^0\) is obtained from the fluxes (7) with (8) and from negative ion balance (12). From Eqs. (7) and (8) with \(h_l = (8\pi)^{1/2} \lambda_i/d\) for \(\lambda_i/d \ll 1\), we obtain
\[
n_e^0 = \frac{1}{(8\pi)^{1/2} \lambda_i/2e\mathcal{E}_c'\mu_{B+}}.
\]
From Eq. (12) neglecting attachment in the sheaths for \(L \gg s_{\text{sh}}\), we obtain
\[
n_e^0 = \frac{8}{15} \frac{K_{\text{rec}}}{K_{\text{att}} \mu_g} n_e^0. \tag{23}
\]
Substituting Eq. (22) into Eq. (23), we find
\[
n_e^0 = \frac{1}{15\pi} \frac{K_{\text{rec}}}{K_{\text{att}} \mu_g} \frac{d^2}{\lambda_i^2} \left( \frac{S_{\text{core}}}{2e\mathcal{E}_c'\mu_{B+}} \right)^2.
\]
This gives the 2-region scaling \(n_e^0 \propto n_e d^2 S_{\text{core}}^2\).

IV. COMPARISON OF MODEL CALCULATIONS WITH PIC RESULTS

As with the PIC calculations, the input parameters used in an analytic model include pressure \(p\), applied rf voltage \(V_{\text{rf}}\), radian frequency \(\omega\), and gap width \(L\). There can also be additional input parameters to the model which are determined from the PIC results.

A. Model employing PIC results

In previous work, we used the central core electron density \(n_{e^0}\) as an input. However, as observed from the PIC results, \(n_{e^0}\) is strongly varying in the transition from a 2-region to a 1-region plasma as \(L\) decreases. A more convenient parameter, which is fairly constant in this transition, is the electron power per unit area \(S_{\text{core}}\) deposited in the core. We note that a completely self-consistent analytical model does not need this additional input parameter since the driving voltage \(V_{\text{rf}}\) is specified. However, as seen in Figures 1(d), 2(d), and 3(d), the ohmic and stochastic heating profiles vary strongly with \(L\), and the transitions with decreasing \(L\) are not well understood. We treat the fully self-consistent analytic calculation in Subsection IV B.

There is an additional difficulty for 2-region cases which have bi-Maxwellian EEDFs as seen in Figure 4(a). The simple global model assumes a single Maxwellian, so we facilitate the comparison with PIC results by using the values of the collisional energy lost per ionization \(\mathcal{E}_c\) and the attachment rate coefficient \(K_{\text{att}}\) obtained from the PIC results in both the 1-region and 2-region cases. We note that this is not necessary for the 1-region cases which have single
Maxwellian distributions as seen in Figure 4(b), as the values of $E_c$ and $K_{att}$ can then be calculated from the literature.\textsuperscript{10}

For the base case of 50 mTorr and 500 V, Figure 8 shows the PIC results (symbols) versus $L$ for (a) $S_{core}$, (b) $E_c$, and (c) $K_{att}$, as well as the corresponding analytical parabolic fits for the 2-region (solid) and 1-region (dash) models. As seen in Figure 8(a), $S_{core}$ remains fairly constant at about 40 W/m$^2$ as $L$ is varied. Although not used, the dashed-dotted curves in Figs. 8(b) and 8(c) show the theoretical predictions for $E_c$ and $K_{att}$, respectively, when assuming a single Maxwellian EEDF. The dashed-dotted curves illustrate the difficulty posed due to the bi-Maxwellian EEDF in the 2-region plasmas. The Maxwellian $T_e$ is calculated from the determination of $K_{iz}$ which depends mostly on the high temperature component of the bi-Maxwellian EEDF, and is thus not the proper $T_e$ to use when calculating $E_c$ and $K_{att}$.

In Figure 8(d), one difficulty of a self-consistent analytical model is seen from the PIC results for the ohmic and stochastic heating fluxes, $S_{ohm}$ (squares) and $S_{stoc}$ (circles), respectively. The ohmic heating can be calculated in a straightforward manner from the current density $J_{rf}$ and the plasma conductivity $r_p$. The stochastic heating suffers a large decrease near the transition from a 2-region to a 1-region plasma due to the structure of the net heavy particle density $n_i$. For the 50 mTorr, 500 V base case results, the ohmic heating dominates at small $L$-values so that an approximate self-consistent calculation can be made.

In Figure 9, we compare the 50 mTorr, 500 V base case PIC results (symbols) for (a) $n_{t+0}$, (b) $n_{t0}$, (c) $d$, (e) $C_+$, core, and (f) $N_{ohm}/N_{core}$ with the analytical model results for the 2-region (solid) and 1-region (dash) models. Some of the analytical results have a slope discontinuity when transitioning from the 2-region to the 1-region model. Most of the comparisons give reasonably good agreement. The central positive ion density $n_{t+0}$ shown in Figure 9(a) increases faster for small $L$ in the analytical model versus the PIC simulations, differing by about a factor of two for the smallest $L$-value of 2.3 cm. For $L < 2.3$ cm, no PIC solution can be found for the

![Graph 1](image1)

**Figure 9.** PIC results (symbols) versus $L$ for 50 mTorr, 500 V base case and the analytical model results for the 2-region (solid) and 1-region (dash) models: (a) $n_{t+0}$, (b) $n_{t0}$, (c) $d = L - 2s_{m}$ (circles) and $d = L - 2s_{m}$ (squares) (d) $T_e$, (e) $C_+$, and (f) $N_{ohm}/N_{core}$. 
50 mTorr, 500 V base case. The core width $d$ shown in Figure 9(c) decreases faster for small $L$ in the analytical model compared to the PIC simulations. Note that there are two PIC values for $d$: (i) $d = L - 2s_m$ (circles) and (ii) $d = L - 2s$ (squares), where $s_-$ is the width of the edge regions where $n_- \approx 0$. From Figure 5, we saw that there is a cross-over of these two $d$-values with decreasing $L$. The simplified theory coalesces these two $d$-values into a single value. The too small values of $d = L - 2s_m$ in the analytical model due to the modification of the Child law (9) also lead to the too large values of $n_{+0}$ at the smallest $L$-values. This can be seen if we assume $n_{+0} \ll 2n_{-0}/e0$ in the core negative ion balance (12), giving

$$\frac{8}{15} K_{re} n_{-0}^2 d \approx K_{at} n_{+0}^2 \frac{2J_d}{e0} \approx \text{const},$$

such that $n_{-0} \approx n_{+0} \propto 1/\sqrt{d}$.

In Figure 10, we present the PIC results for $n_{+0}$ (circles) versus $L$ and the analytical model results for the 2-region (solid) and 1-region (dash) models for all the cases shown in Figure 7: (a) 10 mTorr, 500 V, (b) 25 mTorr, 500 V, (c) 50 mTorr, 500 V, (d) 100 mTorr, 500 V, (e) 50 mTorr, 1000 V, and (f) 50 mTorr, 2000 V. The transitions from the 2-region to the 1-region plasmas can be clearly seen by the sharp drops in $n_{+0}$ with decreasing $L$. The explicit transition in the theory at the $L$-value at which $s_+ = h/s_0 = \gamma^{1/2}$ is clear, joining the 2-region to the 1-region models. The transitions from 2-region to 1-region plasmas shift to smaller $L$-values at higher $p$. There is an accompanying shift to smaller $L$-values at higher $p$ for the smallest $L$-values at which a PIC solution is found. The largest PIC $n_{+0}$ values shown for each case, which correspond roughly to the crossing of the “Recomb. = Endloss” line in Figure 7, also shift to smaller $L$-values at higher $p$. 

FIG. 10. PIC results for $n_{+0}$ (circles) versus $L$ and the analytical model results for the 2-region (solid) and 1-region (dash) models for (a) 10 mTorr, 500 V, (b) 25 mTorr, 500 V, (c) 50 mTorr, 500 V, (d) 100 mTorr, 500 V, (e) 50 mTorr, 1000 V, and (f) 50 mTorr, 2000 V.
Comparing the $p = 50 \text{ mTorr}$ cases at differing $V_{\text{rf}}$ values of (c) 500 V, (e) 1000 V, and (f) 2000 V, we see the increase of $n_{e0}$ values with increasing $V_{\text{rf}}$, as expected since basic theory predicts $n_{e} \propto S_{\text{core}} \propto V_{\text{rf}}$. There are also shifts in the $L$-values of the various transitions described above. There is also poorer agreement between the PIC and theory at higher $V_{\text{rf}}$. This occurs because the size of the EP edge is larger for the higher $V_{\text{rf}}$ cases, which is not taken into account in the simplified theory. As seen from the ion balance in Eq. (12) and observing $n_{e0} \Gamma_{\text{att}} = n_{i0}$, then $n_{i0}$ increases more slowly than $n_{e0}$ with increasing $V_{\text{rf}}$ so that $x_{0}$ also decreases as $V_{\text{rf}}$ rises. For the highest voltages, the PIC simulations were halted for $L$-values at which $x_{0} < 3$, or, for the 100 mTorr, 500 V case, when recombination loss exceeds positive ion surface loss.

**B. Self-consistent model**

A completely self-consistent analytical model presents various difficulties, some of which have been mentioned in Secs. I–III. For this reason, the analytical model in Subsection IV A used an additional plasma parameter $S_{\text{core}}$ in addition to the given electrical and feedstock gas parameters (e.g., $V_{\text{rf}}$ and $p$). For the larger $L$-values for which an EP edge exists, the EEDF was bi-Maxwellian, but we used a Maxwellian approximation in the theory. Since this would lead to errors in calculating $K_{\text{att}}$ and $\mathcal{E}_{c}$ from the model, we instead used the PIC results for these quantities as input parameters to the analytical model when making comparisons to the PIC results. For a self-consistent theory, we need a different approach to finding acceptable plasma parameters. To do this, we use insights gained from the previous analysis and from the PIC results.

As in Sec. III, we use two expressions for $\Gamma_{\text{att}}$, the positive ion flux leaving the core, given by Eq. (6) for the 1-region model and Eq. (7) for the 2-region model. At the cross-over of the two theoretical $\Gamma_{\text{att}}$ values, the two models can be joined. This theoretical cross-over value does not correspond exactly to the PIC value of $L$ for which the EP edge disappears, but is within the PIC transition regions, as seen in the variations of $n_{e0}$ with $L$ in Figure 10. At the PIC cross-over point, the EEDF changes from bi-Maxwellian to Maxwellian as $L$ decreases, as explained by the disappearance of the EP potential which confines cold electrons to the EN core. Thus, at the transition, the quantities $K_{\text{att}}$ and $\mathcal{E}_{c}$ can be obtained from Maxwellian EEDFs. A simple model for our analytical calculations is to use these values for $K_{\text{att}}$ and $\mathcal{E}_{c}$ over the entire range of $L$-values. For the base case of 50 mTorr and 500 V, we obtain approximate values of $\mathcal{E}_{c} = 85 \text{ V}$ and $K_{\text{att}} = 2.9 \times 10^{-17} \text{ m}^{2} / \text{s}$. As seen in Figures 8(b) and 8(c), these values are reasonably close to the PIC results at the transition. The PIC results for these quantities are not constant as $L$ varies, but are sufficiently close to the transition values to be used in an approximate analysis.

Finally, a core electron power flux $S_{\text{core}}$ needs to be determined self-consistently. From the PIC results, we observed that $S_{\text{core}}$ was roughly constant, and somewhat surprisingly a little less than half of $S_{\text{tot}}$ except for the smallest $L$-values. One way to obtain a self-consistent analytical fraction of electron power deposited in the core is to use the intuitive relation as given in Eq. (19) that $f_{\text{core}} = S_{\text{core}} / S_{\text{tot}} = N_{\text{core}} / N_{\text{tot}}$. For the base case at 50 mTorr and 500 V, this yields $f_{\text{core}} = 0.54$ at the transition, which we use over the entire range of $L$’s. The powers used in the theory are the usual relations given by Eqs. (16)–(18).

In Figure 11, the self consistent theoretical result for $S_{\text{core}}$ for the 2-region (solid) and 1-region (dash) models are compared with the PIC results for $S_{\text{core}}$ (circles) for the base case of 50 mTorr and 500 V. The theoretical results are about 30% larger than the PIC results. This translates into a somewhat larger $\Gamma_{\text{att}}$ for the 2-region model, which, neglecting the recombination term in Eq. (14), is $\Gamma_{\text{att}} = S_{\text{core}} / (e\mathcal{E}_{c} + 2e\mathcal{E}_{r})$. Similarly, $n_{i0}$ is larger in the 2-region model, using Eq. (7) and making the substitution $x_{0}n_{e0} = n_{i0}$. Figure 12 shows the same plasma quantities as Figure 9 with the PIC results (symbols), the self-consistent model results (1-region (dash), 2-region (solid)), and the previous analytical results from Figure 9 (1-region (dot), 2-region (dash-dot)), all plotted together for ease of comparison. The self-consistent theory gives results similar to those found by the previous analytical theory which used PIC results, but as expected some results are not as close to the PIC results.

V. Conclusion and Further Discussion

We have studied narrow gap discharges over a range of decreasing gap lengths $L$, from larger $L$-values for which an EP edge exists to smaller $L$-values for which the EN core connects directly to the sheath. Parametric studies were carried out at pressures $p = 10, 25, 50, 100 \text{ mTorr}$ at an applied voltage $V_{\text{rf}} = 500 \text{ V}$, and additionally at $V_{\text{rf}} = 1000, 2000 \text{ V}$ at $p = 50 \text{ mTorr}$. Numerical results with an oxygen feedstock gas were obtained using PIC simulations from the largest $L$-values at which the center ion profiles begin to flatten, to the smallest $L$-values for which discharges could be sustained. New interesting phenomena have been found for the $L$-values in which the EP edge disappears, resulting in a 1-region plasma. This regime was not previously investigated in any detail, either analytically or numerically.

![FIG. 11. PIC results (circles) for $S_{\text{core}}$ versus $L$, and the self-consistent analytical model results for the 2-region (solid) and 1-region (dash) models for the base 50 mTorr, 500 V case.](image-url)
In particular, sheath attachment is important, the central electron density \( n_{e0} \) is depressed below the density \( n_{e\text{sh}} \) at the sheath edge, and the sheath oscillation extends into the EN core, creating an edge region that is not characterized by the standard diffusion in an EN plasma. The numerical PIC results include the effect of the varying sheath widths, which is usually not considered in the modeling, but becomes important for small L-values when the sheaths may be larger than the core EN plasma. Two types of theoretical models were developed, and unlike previous models, the sheath equations were explicitly included, as is necessary when treating narrow gaps. The first model used the PIC results for the power per unit area dissipated in the EN core \( S_{\text{core}} \), as input to the model equations. The second model is a self-consistent calculation for which \( S_{\text{core}} \) was obtained as a fraction of the total electron power flux \( S_{\text{rot}} \) delivered by ohmic and stochastic heating. Both models give reasonable agreement to the PIC results in the regime where they are expected to apply, shown in Figure 7 and calculated in Appendix B. As expected, the model which uses PIC results gives somewhat better agreement.

In addition to the depressed \( n_{e0} \) compared to \( n_{e\text{sh}} \), and the sheath penetration into the EN core for the smallest L-values, the PIC simulations showed how the plasma shuts itself off: the time-varying core electrons expose increasing fractions of the core to larger fields which modify and ultimately destroy the diffusive character of the core. The theory does not include this phenomenon, but shuts off the plasma by the related mechanism of a \( T_e \) asymptote (i.e., the plasma shuts off when \( T_e \) becomes very large). Another feature observed in the PIC results and from previous studies\(^{20,23,25} \) is that when an EP edge exists, it confines the cold electrons to the EN core, thus, creating a bi-Maxwellian EEDF. An additional feature that the EEDF becomes Maxwellian when the EP edge disappears was not previously considered. The bi-Maxwellian EEDF in the 2-region case and the Maxwellian distribution in the 1-region case are important in setting up the analytical models. For the smallest L-values,
the sheath widths become larger than the core size and errors in calculating the sheath width $s_m$ can lead to large errors in calculating the core width $d = L - 2s_m$. As described in the text, this can also lead to significant errors in other calculated quantities.

Some of the new effects, described above, are very difficult to incorporate into analytical models. This has required approximations of plasma quantities that can be either taken directly from the PIC results, as in the first simplified model, or developed from the understanding gained from the PIC, as in the second self-consistent model. The bi-Maxwellian EEDFs in 2-region plasmas have been calculated analytically in Refs. 20 and 26, but it would be difficult to incorporate this calculation into a completely self-consistent model including the sheaths. One useful observation from the PIC results is that the EP regions are much narrower than would be calculated from diffusion theory. This has allowed the EP region to be neglected as a source of ionization and attachment in the analytical models. However, this simplifying approximation also leads to increasing errors at low pressures and high rf voltages. The narrowing of the EP region can be understood by the existence of a small fraction of negative ions that remain there. A calculation of this fraction would lead to better understanding and better modeling.

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**APPENDIX A: AVERAGE NUMBER OF SHEATH ELECTRONS**

The dc electric field $E$ and time-average charge densities $n_+ $ and $\bar{n}_e$ in the sheath are related by

$$ \frac{d\bar{E}}{dx} = \frac{e}{\epsilon_0} (n_+(x) - \bar{n}_e(x)). $$  \hspace{1cm} (A1)

Integrating this equation over the entire sheath width and using $\bar{E}$ at the electrode surface from the collisional capacitive sheath solution in Ref. 27, we obtain

$$ N_+ - \bar{N}_e = \frac{J_{rf}}{\epsilon_0}, $$  \hspace{1cm} (A2)

where $J_{rf}$ is the rf current density flowing in the sheath. The sheath ion density, for a sheath with edge density $n_{esh}$, is

$$ n_+(x) = n_{esh} \beta E \left( \frac{nM_+}{2e^2\lambda_+ E} \right)^{1/2}. $$  \hspace{1cm} (A3)

Integrating this over the entire sheath width and using $\bar{E}(x)$ gives

$$ N_+ = \frac{2J_{rf}}{\epsilon_0}. $$  \hspace{1cm} (A4)

Subtracting Eq. (A2) from Eq. (A4) gives

$$ \bar{N}_e = \frac{J_{rf}}{\epsilon_0}. $$  \hspace{1cm} (A5)

where $N_e$ is the number of sheath electrons in a sheath with edge density $n_{esh}$. Referenced to the electron density $n_{e0}$ in the core, the number of electrons in the sheath is

$$ N_{esh} = \frac{n_{esh} J_{rf}}{n_{e0} \epsilon_0}. $$  \hspace{1cm} (A6)

**APPENDIX B: REGION OF MODEL VALIDITY**

As shown in Figure 7, the region of validity in the normalized variables is below the line $x_0 = 3$, taken, somewhat arbitrarily, as the high-$x_0$ condition, and to the left of the 1- and 2-region solid lines, where ion recombination loss and end loss are equal. To obtain the $x_0 = 3$ condition, we substitute Eq. (11) into Eq. (12) and solve for $\frac{8}{15} x_0^2$ to obtain

$$ \frac{8}{15} x_0^2 = K_{att} n_e \frac{E_{rec} n_{e0}^2}{\epsilon_0 n_{e0}} \left( 1 + \frac{3.04 e_0 V_1}{c_{esh} n_{e0} d} \right). $$  \hspace{1cm} (B1)

Introducing the normalized electron density $Y = K_{rec} n_{e0} d / \epsilon_0 n_{e0}$, and normalized gas density $X = d / \lambda_+$, into Eq. (B1), we find

$$ \frac{8}{15} x_0^2 = \frac{b}{a} \left( 1 + \frac{a}{Y} \right), $$  \hspace{1cm} (B2)

where

$$ a = \frac{3.04 e_0 V_1 K_{rec}}{c_{esh} \sigma B_+}, \quad b = \frac{K_{att}}{\sigma \mu B_+}. $$  \hspace{1cm} (B3)

For $\sigma_+ = 1 \times 10^{-18}$ m$^2$ and choosing nominal values $T_+ = 0.026$ V, $K_{att} = 1.6 \times 10^{-17}$ m$^3$/s, $s_m = 0.04$ m, and $x_0 = 3$, we plot the three $x_0 = 3$ curves of $Y$ versus $X$ for no attachment in the sheath, $V_{rf} = 2V_1 = 500$ V and 2000 V.

The condition that recombination loss and end loss are equal for the 2-region model is

$$ \frac{8}{15} K_{rec} n_{e0}^2 d = 2h_1 x_0 n_{e0} \mu B_+. $$  \hspace{1cm} (B4)

Introducing normalized variables and using Eq. (8) for $h_1$, which in normalized variables is

$$ h_1 = \frac{1}{\left( 1 + \frac{X}{\sqrt{8\pi}} \right)^2}, $$  \hspace{1cm} (B5)

we obtain

$$ \frac{2}{15} Y = \frac{1}{bX} \left( 1 + \frac{X}{\sqrt{8\pi}} \right)^2 - a. $$  \hspace{1cm} (B6)

These curves are plotted in Figure 7 for the three cases of no attachment in the sheath, $V_{rf} = 2V_1 = 500$ V and 2000 V. For the 1-region model, Eq. (B4) is replaced by

$$ \frac{8}{15} K_{rec} n_{e0}^2 d = 2n_{e0}^{1/2} \mu B_+. $$  \hspace{1cm} (B7)
Introducing normalized variables yields

\[ abX = (2\gamma_+^{1/2} - hX)Y. \quad (B8) \]

These curves are also plotted in Figure 7 for the three cases.

The transition from the 1-region to 2-region models occurs at \[ h_0 \gamma_0 = \gamma_+^{1/2} \]. Substituting \( \gamma_0 \) from Eq. (B2) and \( h_0 \) from Eq. (B5) into this condition, we obtain a quadratic equation for \( Y \)

\[ \frac{8}{15} \left(1 + \frac{X}{\sqrt{8\pi}}\right)Y^2 - bXY - abX = 0, \quad (B9) \]

which can be solved to obtain the dashed transition curves shown in Figure 7.

The Boltzmann condition for negative ions, required for validity of the parabolic model, is\(^2\)

\[ \frac{8}{15} K_{ne} n_0 \alpha_0 \sigma^2 = 8 D_, \quad (B10) \]

where \( D_ = (\pi/8)^{1/2} \tilde{\nu} \lambda_ \) is the negative ion diffusion coefficient, with \( \tilde{\nu}_ = (eT_ = M_)/2 \) and \( \lambda_ \) as the negative ion thermal velocity and mean free path. Accounting for the different masses \( M_ = M_+/2 \) and the different cross sections \( \sigma_ = \sigma_+/2 \) used in the simulation, and with \( T_ = T_+ \), from the simulation, we find \( D_ = 2 \sqrt{2} D_+ \).

Introducing normalized variables into Eq. (B10), we find the condition

\[ Y = \frac{7680\pi}{49bX} - a. \quad (B11) \]

This condition is not plotted in Figure 7, because the curves for the three cases are found to lie to the right of the 2-region recombination = endloss curves (B6); hence the Boltzmann condition is satisfied within the region of validity shown in the figure.