Double layer formation in a two-region electronegative plasma

M.A. Lieberman¹, E. Kawamura¹, A.J. Lichtenberg¹ and J.P. Verboncoeur²

¹Department of Electrical Engineering and Computer Sciences
²Department of Nuclear Engineering
University of California, Berkeley CA 94720, USA

Abstract: A two-dimensional particle-in-cell (PIC) code is used to study the double layer that forms in an electronegative gas near the transition between a small diameter source chamber connected to a larger diameter processing chamber.

Keywords: double layer, electronegative discharge

1. Introduction

We describe the formation of a double layer (DL) in a two-dimensional (2D) electronegative plasma with a source (heating) section connected to a larger diameter downstream section. A 2D particle-in-cell (PIC) code is used to exhibit the DL, which appears near the transition between the source and downstream chambers, over a range of pressures and electronegativities (ratios of negative ion to electron density). Diagnostics of the PIC code allow the calculation of various plasma parameters, not easily measured in experiments, to be compared to an analytic theory. The theory, modifying a previous calculation [1, 2] to conform to the simulation, consists of a collisionless one-dimensional model of a DL separating 2D source and downstream globally-modeled regions. In the global models the conditions of positive and negative ion balance upstream and downstream, and the downstream energy balance, are used to determine the double layer potential, electron temperatures, and other plasma parameters. Because of computational limitations of the PIC simulation, a rescaled oxygen reaction set is used both for the simulation and for the analytic comparison, to accommodate lower densities and smaller sizes than those of a typical experiment. The two-region configuration is shown in Fig. 1. A small “diameter” source chamber in which electrons are heated by a uniform rf electric field is connected to a larger diffusion chamber. Besides small geometric factors, there is little difference between rectangular and cylindrical coordinates, so we work in the simpler rectangular form.

2. Results

In contrast to experimentally observed electron distributions [2, 3], the PIC simulations exhibit a Maxwellian electron distribution in the source region at temperature $T_{e2}$ and a bi-Maxwellian distribution downstream, with a low energy population at a lower temperature $T_{e1} < T_{e2}$ and with a hotter tail also having temperature $T_{e2}$. Using these results in the model, a DL is found in reasonable agreement with that obtained in the simulation. We have also investigated numerically and analytically the range of pressures over which a DL can exist.

Figure 2 shows the on-axis dc potential and the on-axis charge density versus axial position $x$ at 6 mTorr pressure, with $w_1 = l_1 = l_2 = 5$ cm and $w_2 = 1.5$ cm. We see that a double layer with a potential drop of approximately 11 volts forms at the junction between the source and downstream chambers. The charge density is positive at the upstream edge and negative at the downstream edge, a structure characteristic of DL formation.

In the analytic model, we use six groups of particles to describe the charge balance within the double layer: Maxwellian positive ions, Maxwellian negative ions, accelerated positive ions flowing downstream, accelerated electrons flowing upstream, accelerated negative ions flowing upstream, and thermal electrons. For the acceler-
ated species, we use a half-Maxwellian group of positive ions formed upstream and accelerated downstream through the double layer. We use half-Maxwellian groups of negative ions and electrons, formed downstream and accelerated upstream through the double layer. We use a Maxwellian population of thermal electrons created upstream that is truncated (no electrons) for upstream-directed energies exceeding the double layer potential. With these choices, the electrons at the downstream edge of the double layer have a bi-Maxwellian distribution. At the upstream edge, the electron distribution consists of an accelerated group of electrons and a truncated Maxwellian group of electrons. We assume that the accelerated electrons thermalize within the upstream region, leading to the single Maxwellian distribution observed in the simulations.

Summing the contributions of the six groups, we obtain the total charge density within the double layer. The boundary conditions at the downstream and upstream edges are that the total charge densities at the upstream and downstream double layer edges must vanish, and that the space-derivatives of the total positive and negative charge densities must be equal at the upstream and downstream edges. An additional condition is that the sum of positive and negative charge in the double layer must vanish, or, equivalently, that the total force acting on the double layer must vanish. This determines the density ratios of all the species at the upstream and downstream edges as a function of $V_s / T_{e2}$, the ratio of the double layer potential to the upstream electron temperature.

Although a double layer can, in principle, form over a wide range of values of $V_s / T_{e2}$, the net flow of electron current through the double layer is constrained by either the downstream or upstream loss of positive ions to the walls. To separately obtain the double layer voltage, we impose a final condition that the upstream- and downstream-directed electron fluxes passing through the double layer are nearly equal. This sets a condition on the ratio of $V_s / T_{e2}$; if $V_s / T_{e2}$ is too small, then too many upstream electrons flow downstream. Under typical conditions the double layer potential is 1–1.5 times the electron temperature $T_{e2}$.

To determine the double layer voltage $V_s$, the upstream electron temperature $T_{e2}$, and the downstream temperature bi-Maxwellian components $T_{e2}$ and $T_{e1}$ (as well as other equilibrium parameters), we use the particle balance relations in the upstream and downstream regions, and we use the downstream energy balance. The upstream energy balance, which determines the value of the upstream electron density, depends on the input power which is outside the scope of this study. The upstream particle balance relations for positive and negative ions are written assuming that downstream accelerated electrons entering the upstream region thermalize, joining the upstream population of hotter thermal electrons. We use global (volume-averaged) particle balance models and assume constant electron densities in the upstream region equal to those at the upstream double layer edge. In the downstream region, we use similar global particle balances for the positive and negative ions.

![Figure 3](image-url)

**Figure 3.** (a) Upstream and (b) downstream particle balance: Iz (ionization), Att (attachment), Gam- (negative ion upstream flow), Gam+ (positive ion downstream flow), Wall (wall losses); (c) downstream energy balance: edn (electron power flowing downstream), eup (electron power flowing upstream), idn (positive ion power flowing downstream), nup (negative ion power flowing upstream), coll (power lost to collisions), wall (power lost to the walls).

Finally, we use a global downstream energy balance relation. The energy input at the downstream double layer edge is mainly driven by the difference between the energy flux carried by the hotter upstream electrons into the downstream region, and the energy flux carried out of the downstream region by the cooler electrons flowing upstream. Equating this difference to the volume and surface losses of energy yields the energy balance relation.
Figure 3 shows the balances determined from the PIC simulation (black bars) and the comparison to the double layer and global model calculation of the balances (white bars), for a system at 6 mTorr that is twice as large as the system for which the data in Figure 2 is shown \( (w_1 = l_1 = L_2 = 10 \text{ cm and } w_2 = 3 \text{ cm}) \). For this system a 6.5 volt double layer is found to form. The larger size makes the PIC double layer more one-dimensional, corresponding more closely to the 1D model. There is a reasonable agreement between the 2D PIC simulations and the double layer and equilibrium global model calculations.

2D PIC simulations have been made over a wide range of pressures from 0.5 to 12 mTorr in the system shown in Figure 1 with \( w_1 = l_1 = L_2 = 10 \text{ cm and } w_2 = 3 \text{ cm} \). At 0.5 mTorr, the double layer does not appear to exist. At 1 and 1.5 mTorr a stable double layer is formed. At 2 and 3 mTorr, a double layer is formed that co-exists with an unstable slow wave that originates downstream at low amplitude and propagates upstream into the double layer as it grows. The wave frequency is 50–100 kHz and the wavelength is of order of 1 cm. This wave produces small (~20%) fluctuations in the double layer potential and in the position of the double layer within the system. We believe this is the unstable slow wave downstream instability predicted and observed by Tuszewski and Gary [4]. It is driven by the counter-streaming flows of the positive and negative ions in the downstream region near the double layer. At higher pressures of 4.5, 6, and 12 mTorr, a double layer is formed that co-exists both with the unstable slow wave and with an additional fast wave having a wave frequency of order 1 MHz and a wavelength of order of 1 cm. This fast wave also originates in the downstream region and propagates upstream into the double layer as it grows in amplitude, but its stability is uncertain.

The smaller-dimensioned device resulted in results similar to those described above, at correspondingly larger pressures, except that the wave activity was less evident.

3. Conclusions

Two-dimensional particle-in-cell simulations have been found to be powerful tools to study the physics of double layer formation in a two-dimensional electronegative plasma formed in a source heating chamber that is connected to a larger downstream chamber. The PIC simulations allow non-perturbing “measurements” to be made within the double layer itself, which would be very difficult, if not impossible, to do in a laboratory experiment. For example, in Figure 2 we determined the charge density within the double layer itself; this charge density, and its decomposition into the three charged species (positive ions, negative ions and electrons) in the simulation, will allow us to make detailed comparisons with analytic models of double layer structure. The simulations also suggest that a double layer having a given "strength" (double layer potential \( V_d \)) forms between the upstream source region and the downstream region in order that the equilibrium particle and energy balance relations within the two regions can be satisfied. A global model of particle and energy balances for the two regions, as shown in Figure 3, has been found to capture the essential physics leading to double layer formation in this system.

References