A radio-frequency sheath model for complex waveforms

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Abstract

Plasma sheaths driven by radio-frequency voltages occur frequently, in contexts ranging from plasma processing applications to magnetically confined fusion experiments. These sheaths are crucial because they dominantly affect impedance, power absorption, ion acceleration and sometimes the stability of the nearby plasma. An analytical understanding of sheath behavior is therefore important, both intrinsically and as an element in more elaborate theoretical structures. In practice, these radio-frequency sheaths are commonly excited by highly anharmonic waveforms, but no analytical model exists for this general case. In this letter we present a mathematically simple sheath model that can be solved for essentially arbitrary excitation waveforms. We show that this model is in good agreement with earlier models for single frequency excitation, and we show by example how to develop a solution for a complex waveform. This solution is in good agreement with simulation data. This simple and accurate model is likely to have wide application.
In many radio-frequency discharges the sheath is the most important region, because impedance, power absorption and ion acceleration are dominated by sheath processes \cite{1, 2}. There are other contexts where radio-frequency sheath physics is a concern, for example when understanding the physics of heating in certain fusion plasmas \cite{3–5}. Consequently, models of the sheath are important, either in themselves or as elements in more complex situations, over a broad area of plasma physics. The problem has been considered on a number of occasions, \textit{e.g.} \cite{6–8}. Analytical models are particularly useful for developing physical insight and expressing the relationships between parameters in a clear way, but such models have proved elusive. Lieberman\cite{1, 9} supplied an analytical model for a radio-frequency sheath driven by a single frequency, but in practice much more complex waveforms frequently occur \cite{10–14}. There has been limited success in generalizing the Lieberman model to cover these cases, because of mathematical complexities \cite{15–17}. So there is essentially no sheath model available to describe many modern experiments. In this paper we present a new analytical sheath model, based on a simpler mathematical framework than that of Lieberman\cite{1, 9}. For the single frequency case, this model yields scaling laws that are identical in form to those of Lieberman\cite{1, 9}, differing only by numerical coefficients close to one. However, the new model may be straightforwardly solved for almost arbitrary current waveforms, and may be used to derive scaling laws for such cases.

Fig. 1 is a schematic representation of the charged particle densities and fields that occur in a radio-frequency sheath. For a sheath in this regime, the ion motion is determined by the time averaged field, while the electrons respond to the instantaneous field. A model describing such a sheath therefore has a time-averaged part and a time-dependent part, which must be consistent. We therefore insist on the same maximum sheath width, $s_m$, in both cases. The principal parameter determining $s_m$ in the time-averaged sense is the time-averaged sheath voltage, $\bar{V}$, while in the time-dependent model, $s_m$ is a function of $V_0$, the maximum sheath voltage. The simplest way to satisfy the constraint is to choose

$$\frac{\bar{V}}{V_0} = \frac{\bar{\rho}}{\rho_0} \equiv \xi, \quad (1)$$

where $\bar{\rho}$ is the time-averaged charge density, $\rho_0$ is the charge density when the sheath voltage is $V_0$, and $\xi$ emerges as a key parameter of our model. We note that $\rho_0 \neq \bar{\rho}$ because of the time dependence of the electron density in the sheath region. Since the ion density $n_i$ is time-independent, these relations imply $\bar{n}_e = (1 - \xi) n_i$, which is our central approximation.
We now consider specifically a sheath adjacent to a plasma of density \(n_0\) and electron temperature \(T_0\). Ions flow into the sheath at \(x = 0\) and are absorbed at an electrode at \(x = s_m\). The constant ion current density is \(J_i = en_0u_B\), where \(u_B = \sqrt{k_B T_0/M}\) and \(M\) is the ion mass. Now the governing equations for the time-averaged ion motion are

\[
n_i u_i = n_0 u_B \tag{2}
\]

\[
e\bar{\phi} + \frac{1}{2} Mu_i^2 = \frac{1}{2} Mu_B^2 \approx 0 \tag{3}
\]

\[
\frac{d^2\bar{\phi}}{dx^2} = \frac{e}{\epsilon_0} \frac{(\bar{n}_e - n_i)}{\epsilon_0} = -\frac{e\xi n_i}{\epsilon_0} \tag{4}
\]

where \(u_i\) is the (time independent) ion drift velocity and \(\bar{\phi}\) is the time-averaged potential, and we assume that \(e\bar{V} \gg k_B T_0\). These equations are those of the Child-Langmuir sheath model \([1, 2, 18, 19]\), with the addition of the parameter \(\xi\), and we can at once write down the solutions

\[
J_i = K_i \frac{\epsilon_0}{s_m} \left(\frac{2e}{M}\right)^{\frac{1}{2}} \left(-\bar{V}\right)^{\frac{3}{2}} \tag{5}
\]

\[
n_i(x) = -\frac{4}{9} \frac{\epsilon_0 \bar{V}}{\xi e s_m^2} \left(\frac{s_m}{x}\right)^{\frac{4}{3}} \tag{6}
\]

\[
\bar{\phi}(x) = \frac{\bar{V}}{s_m} \left(\frac{x}{s_m}\right)^{\frac{4}{3}} \tag{7}
\]

\[
\bar{E}(x) = -\frac{4}{3} \frac{\bar{V}}{s_m} \left(\frac{x}{s_m}\right)^{\frac{1}{3}} \tag{8}
\]

where the boundary condition \(\bar{E}(x = 0) = 0\) has been used, and where \(K_i = 4/(9\xi)\). The time-dependent field and potential can now be determined by integrating Poisson’s equation again with the assumption that

\[
n_e = \begin{cases} 0 & \text{if } s < x \leq s_m; \\ n_i & \text{otherwise,} \end{cases} \tag{9}
\]

where \(s(t)\) is the position of the sheath edge, at which point \(E = 0\) and \(\phi = 0\). We obtain for \(s < x \leq s_m\):

\[
\phi(x,t) = \frac{\bar{V}}{\xi} \left[\left(\frac{x}{s_m}\right)^{\frac{4}{3}} - \frac{4}{3} \left(\frac{s}{s_m}\right)^{\frac{1}{3}} \left(\frac{x}{s_m}\right)^{\frac{1}{3}} + \frac{1}{3} \left(\frac{s}{s_m}\right)^{\frac{4}{3}}\right] \tag{10}
\]

\[
E(x,t) = -\frac{4}{3} \frac{\bar{V}}{\xi s_m} \left[\left(\frac{x}{s_m}\right)^{\frac{1}{3}} - \left(\frac{s}{s_m}\right)^{\frac{1}{3}}\right], \tag{11}
\]

so that the time dependent sheath voltage is

\[
V(t) = V_0 \left[1 - \frac{4}{3} \left(\frac{s}{s_m}\right)^{\frac{1}{3}} + \frac{1}{3} \left(\frac{s}{s_m}\right)^{\frac{4}{3}}\right]. \tag{12}
\]
Now
\[ J = \epsilon_0 \frac{\partial E}{\partial t} \bigg|_{x=s_m} = \frac{4 \epsilon_0 V_0}{3 s_m} \frac{d}{dt} \left( \frac{s}{s_m} \right)^{\frac{1}{3}}, \] (13)
so that
\[ \frac{s}{s_m} = \left[ \frac{3 s_m}{4 \epsilon_0 V_0} \int_0^t J dt \right]^{3}. \] (14)
Since \( 0 \leq s/s_m \leq 1 \), once \( J(t) \) is chosen, \( s(t)/s_m \) is fully defined and we can express
\[ \xi = \left\langle \frac{V(t)}{V_0} \right\rangle = \left\langle 1 - \frac{4}{3} \left( \frac{s}{s_m} \right)^{\frac{1}{3}} + \frac{1}{3} \left( \frac{s}{s_m} \right)^{\frac{4}{3}} \right\rangle. \] (15)
Hence, once \( J(t) \) has been given, all the remaining quantities can be calculated without further assumption or approximation, as the following example shows.

For the single frequency case treated by Lieberman \[9\] we choose \( J(t) = -J_0 \sin \omega t \). From Eqs. (15) and (14) we find
\[ s(t) = \frac{s_m}{8} (1 - \cos \omega t)^3 \] (16)
\[ J_0 = -\frac{K_{\text{cap}} \omega \epsilon_0}{2} V_0 \] (17)
\[ \xi = \frac{163}{384} \] (18)
where \( K_{\text{cap}} = 4/3 \). The voltage waveform is obtained by inserting Eq. (16) into Eq. (12). Combining Eqs. (5) and (17) gives the sheath maximum expansion as a function of \( J_0 \),
\[ s_m = \frac{K_s J_0^3}{\epsilon_\epsilon_0 k_B T_0 \omega^3 n_0^2}, \] (19)
where \( K_s = 4\xi/3 \). These expressions are identical with those of Lieberman \[1, 9\], apart from numerical coefficients close to unity. Table \[\] compares \( \xi, K_i, K_{\text{cap}} \) and \( K_s \) for the two models and shows that they are not significantly different. Similarly, the voltage waveforms are almost identical in the two models. This may seem surprising, in view of the apparently bold approximation of Eq. (1). However, Brinkmann \[20\] has shown that the approximation of Eq. (9) is important, and because this approximation is integral to the Lieberman model, the accuracy of that model is not significantly better than the present one. However, the present model can be solved for a far greater range of waveforms. In particular, the current density can be expressed as an arbitrary Fourier series, leading, for example, to models for multiple-frequency excitation that are free of inconvenient restrictions on the component amplitudes (such as occur in dual-frequency generalizations of Lieberman’s model \[15-17\]).
For example, we can choose

$$J(t) = -J_0 \sin \omega_0 t - J_1 \sin \omega_1 t$$

(20)

and find at once

$$s(t) = \frac{s_m}{8} \left[ \frac{(J_0/\omega_0)(1 - \cos \omega_0 t) + (J_1/\omega_1)(1 - \cos \omega_1 t)}{J_0/\omega_0 + J_1/\omega_1} \right]^3$$

(21)

$$J_0 = -\frac{2}{3} \frac{\omega_0 V_0}{s_m} \left( 1 + \frac{J_1 \omega_0}{J_0 \omega_1} \right)$$

(22)

$$s_m = \frac{4}{3} \frac{\xi (J_0/\omega_0 + J_1/\omega_1)^3}{\epsilon_0 e n_0^2 k_B T_0}$$

(23)

$$\xi = \frac{1}{3} + \frac{35}{128} \left[ \frac{(J_0/\omega_0)^4 + (J_1/\omega_1)^4}{(J_0/\omega_0 + J_1/\omega_1)^4} \right] + \frac{5}{8} \left[ \frac{(J_0/\omega_0)^3}{J_0} + \frac{J_1 \omega_0}{J_0 \omega_1} \left( \frac{J_1}{\omega_1} \right)^3 \right] + \frac{27}{32} \left( \frac{J_0}{\omega_0} \right)^2 \left( \frac{J_1}{\omega_1} \right)^2$$

(24)

$$\approx \frac{163}{384},$$

(25)

where we note that eq. 24 yields a result never different by more than 10% from the single frequency result, which value can therefore be used for all practical purposes. These formulae are therefore more generally applicable, less cumbersome and obtained with less mathematical exertion than those previously given [15–17].

As a third example we consider a sheath excited by the pulsed waveform

$$J(t) = J_0 \left( \frac{t}{t_w} \right) \exp \left( \frac{1}{2} - \frac{1}{2} \frac{t^2}{t_w^2} \right),$$

(26)

which is representative of several topical experiments [10–12]. We assume that this pulse is repeated at intervals $t_p \ll t_w$, such that successive pulses do not appreciably overlap. In this case we find

$$s(t) = s_m \exp \left( -\frac{3}{2} \frac{t^2}{t_w^2} \right)$$

(27)

$$\xi = 1 - \frac{7}{3} \sqrt{\frac{\pi}{2}} \frac{t_w}{t_p}$$

(28)

$$J_0 = -\frac{4}{3} \frac{\epsilon_0 V_0}{s_m t_w \exp \left( \frac{1}{2} \right)}$$

(29)

$$s_m = \frac{\xi}{6} \exp \left( \frac{3}{2} \right) \frac{(J_0 t_w)^3}{\epsilon_0 e n_0^2 k_B T_0}$$

(30)

The Child law, and therefore the sheath width, are found by inserting Eq. (28) into Eq. (5). We have investigated the utility of this model by comparison with particle-in-cell simulation
These simulations treated a plasma formed in a space between two plane parallel electrodes separated by 6.7 cm, filled with argon gas at a pressure of 10 mTorr, and excited by a current density with the form of Eq. (26). The peak current density ranged from 5 to 70 A m$^{-2}$ and the pulse width from approximately 1 to 10 ns. These conditions lead to $T_0 \approx 1.5$ eV and $n_0 \approx 3 \times 10^{14} - 3 \times 10^{15}$ m$^{-3}$. In figs. 2, 3 and 4 we compare these simulation results with the predictions of the present model, and we find good agreement, both for time dependent currents and voltages, and scaling laws.

To summarize, in this paper we have developed a new sheath model that can be expressed in a small number of straightforward equations. For the single-frequency case, the model agrees well with the Lieberman model. The Lieberman model, in spite of its elegant construction, is mathematically complex and has proved resistant to generalization. The present model, however, is readily adaptable to a wide range of complex excitation waveforms, and leads to results in good agreement with simulations. Thus this model provides a valuable tool for designing and understanding experiments involving non-sinusoidal excitation of radio-frequency sheaths.

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| Present Lieberman | Value 1 | Value 2 |
|------------------|---------|---------|
| $\xi$            | 0.425   | 0.415   |
| $K_{cap}$        | 1.33    | 1.23    |
| $K_i$            | 1.05    | 0.82    |
| $K_s$            | 0.566   | 0.417   |

TABLE I: Comparison of numerical coefficients in eqs. \[19\], \[17\], and \[5\] determined from three different models.

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FIG. 1: Upper panel: Charged particle densities, showing the ion density, $n_i$ (solid line) the time averaged electron density, $\bar{n}_e$ (dotted line), and the electron density, $n_e$ at the instant when $s/s_m = 0.3$ (dashed line). Lower panel: Electrostatic potential, showing the time averaged potential, $\bar{\phi}$ (solid line) and the instantaneous potential when $s/s_m = 0.3$ (dashed line).
FIG. 2: Comparison of simulation results (solid lines) with the analytical theory of the text (dashed lines) for sheath voltage (upper panel) and sheath current density (lower panel). For this case $t_w = 5.2$ ns. The electrical control parameter for the sheath model is $\bar{V}$, the time averaged sheath voltage, which is here chosen to be the same as in the simulation.
FIG. 3: Comparison of the maximum radio-frequency current density found in simulation (horizontal axis) with the result computed from eq. [29] (vertical axis). The solid line denotes ideal agreement between theory and simulation.
FIG. 4: Comparison of the ion current density found in simulation (horizontal axis) with the result computed from eq. 5 and eq. 28 (vertical axis). The solid line denotes ideal agreement between theory and simulation.