On the applicability of Sato’s equation to Capacitative RF Sheaths

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Abstract

We show that the time dependent version of Sato’s equation, when applied to capacitative rf sheaths is no longer independent of the electric field of the space charge, and discuss the use of the equation for a specific sheath model.
1. Introduction

A few years ago, Sato derived an expression for the current flowing in the external circuit due to the motion of charged particles in the gap within a discharge tube [1], for a constant voltage applied to the gap. Very recently, this work was generalised by Morrow & Sato [2] to include time-dependent applied voltages. They used an energy balance equation to obtain their results, which in both cases were independent of the space charge effects.

While their methods and inferences drawn thereby are striking in their elegance and simplicity, one must exercise caution while applying them, for in certain situations, these can lead to results which are quite the reverse of the inferences drawn in their papers, as we show here.

In a high voltage radio frequency discharge tube, there is a high concentration of positive ions at the electron-depleted dark space region adjoining the electrode, and a consequent build-up of field distortion, so that one expects a time and frequency dependence of the conduction process. The build-up of field distortion can therefore be modelled by a two-layer capacitor of the Maxwell-Wagner type [3].

The plasma state is characterised by equal numbers of positive and negative charges, but because of diffusion effects and recombinations on boundary surfaces in the discharge tube, there is charge depletion in the adjoining gas phase, resulting in the formation of a thin sheath. Electrons diffuse fastest, since they are lightest and have high energies, and they leave behind them a surplus of positive charge and a plasma potential which is positive relative to the walls. Since there is a larger number of charged particles in the central plasma regions of the tube, and hence better conductivity there, almost all of the potential drop occurs across the sheath. The clear difference in the magnitudes of the potential at the plasma and at the sheath, leads one to describe the plasma-sheath system in a discharge tube by a two-layered capacitor, with a dielectric coefficient $\epsilon_{sh}$ for the sheath region.

It is shown in this work that such a representation of the plasma-sheath system leads to terms in Sato’s equation, which depend upon the sheath potential and field. We calculate the non-zero contributions to the current in the external circuit from the space charge field and the sheath capacitance for a symmetric RF discharge for a simplified electrode geometry, in the case of the Godyak-Lieberman (GL) theory [4,5] for RF sheaths, using this energy balance method.
2. The energy balance method of Sato & Morrow

The continuity equations which describe the development in time $t$ of the space charge in a gap in air are [6]:

\[
\begin{align*}
\frac{\partial n_e}{\partial t} &= n_e \alpha v_e - n_e \eta v_e - n_e n_p \beta_1 - \nabla \cdot (n_e v_e - D_e \nabla n_e) \\
\frac{\partial n_p}{\partial t} &= n_e \alpha v_e - n_e n_p \beta_1 - n_n n_p \beta_2 - \nabla \cdot (n_p v_p - D_p \nabla n_p) \\
\frac{\partial n_n}{\partial t} &= n_e \eta v_e - n_n n_p \beta_2 - \nabla \cdot (n_n v_n - D_n \nabla n_n)
\end{align*}
\] (1)

where $n_e, n_p$, and $n_n$ denote the electron, positive ion and negative ion densities respectively, $v_e, v_p$, and $v_n$ denote the drift velocity vectors of the electrons, positive ions & negative ions respectively, $\alpha$ is the electron ionization coefficient, $\eta$ the attachment coefficient, and $\beta_1$ and $\beta_2$ are the electron-positive ion and negative ion-positive ion recombination coefficients respectively. $D_e, D_p$ and $D_n$ are the diffusion coefficients for the electron, positive ion and negative ion respectively.

Combining these, one obtains the equation for the net space charge density $\rho$:

\[
\frac{\partial \rho}{\partial t} = e \frac{\partial (n_p - n_e - n_n)}{\partial t} = -e \nabla \cdot \Gamma
\] (2)

where $e$ is the electron charge, and the total particle flux $\Gamma$ is given by

\[
\Gamma = n_p v_p - n_n v_n - n_e v_e - D_p \nabla n_p + D_n \nabla n_n + D_e \nabla n_e
\] (3)

One starts with these basic equations to study the electrodynamics of the charged particles in a discharge tube. In an RF discharge tube, since most of the potential drop in the gap occurs across the sheath, we treat the plasma-sheath system as a two-layer capacitor, with a dielectric constant $\epsilon_{sh}$ for the sheath and the dielectric constant of free space $\epsilon_0$ for the plasma region.

The total current density $J$ in the gap is

\[
J = e \Gamma + \frac{\partial D}{\partial t}
\] (4)

where the electric displacement $D$ relates to the local field $E$ through the effective complex dielectric constant $\epsilon$ of the gap:

\[
D = \epsilon E
\] (5)

This can be separated into a part $D_{sh}$ describing the sheath, and a plasma part $D_p$:

\[
D = \epsilon_0 E_p + \epsilon_{sh} E_{sh} = D_p + D_{sh}
\] (6)

$D$ obeys Poisson’s equation:

\[
\nabla \cdot D = \rho = \epsilon_0 \nabla \cdot E_p + \nabla \cdot (\epsilon_{sh} E_{sh})
\] (7)
while \( E_p \) satisfies Laplace’s equation:
\[
\nabla \cdot E_p = 0
\] (8)

The plasma and sheath electric fields \( E_p \) and \( E_{sh} \) are related to their respective potential distributions through
\[
E_p = -\nabla \psi_p \quad \text{and} \quad E_{sh} = -\nabla \psi_{sh}.
\] (9)

The energy balance equation can be used to relate the applied potential \( V_a \) and the current \( I \) in the external circuit, to the current density and the local field in the gap through the volume integral \( \int_V dV \) over the discharge space:
\[
V_a I = \int_V J.E dV
\] (10)

Separating out the plasma and the sheath electric fields as:
\[
E = E_p + E_{sh}
\] (11)

and making use of (4), one obtains:

\[

V_a I = \int_V [\epsilon \Gamma + \epsilon_0 \frac{\partial D}{\partial t} \cdot E_p] dV + \int_V [\epsilon \Gamma + \epsilon_0 \frac{\partial D}{\partial t} \cdot E_{sh}] dV
\]

\[
= \int_V [\epsilon \Gamma + \epsilon_0 \frac{\partial D}{\partial t}] \cdot E_p dV - \int_V \psi_{sh}(x,t) \frac{\partial P(x,t)}{\partial t} dV - \int_S [\epsilon \Gamma \psi_{sh}(x,t) \cdot dS
\]

\[
+ \int_V \epsilon_0 \frac{\partial D}{\partial t} \cdot E_{sh} dV
\] (12)

where we have made use of the second of equations (9), performed an integration by parts, \( \int_S dS \) representing a surface integration over the closed surface of the discharge space, and then used (2).

The second term in the right hand side of (12) can be rewritten using (7), and after again performing an integration by parts, this term can be written as:

\[
\int_V \psi_{sh}(x,t) \frac{\partial P(x,t)}{\partial t} dV = \int_V \frac{\partial D}{\partial t} E_{sh} dV + \int_S \psi_{sh}(x,t) \frac{\partial D(x,t)}{\partial t} dS
\] (13)

Next, we substitute (13) and (6) back into (12) to obtain:

\[
V_a I = \int_V [\epsilon \Gamma + \epsilon_0 \frac{\partial E_p}{\partial t}] \cdot E_p dV + \int_V \frac{\partial D_{sh}}{\partial t} E_p dV - \int_S (\epsilon \Gamma + \epsilon_0 \frac{\partial D}{\partial t}) \psi_{sh} dS
\] (14)

The first two terms within the first volume integral on the right hand side of (14) constituted the final form of Sato’s equation derived in [2] for a time-dependent applied voltage. The boundary condition chosen in [2] was, that \( \psi_{sh} \) was set to zero on both electrodes, and \( \psi_p \) was set to zero on one electrode and to the applied voltage \( V_a \) on the other. The authors in [2] obtained the gap capacitance for a simple system from the second of the two terms in the first volume integral.
On the other hand, by ascribing a non-trivial dielectric constant to the sheath, we have obtained terms additional to those obtained in [2], and these extra terms depend upon the sheath field and potential.

3. Capacitative RF discharges

Low pressure plasma chambers are widely used in the material processing industry, such as in the fabrication of semiconductor wafers, and in reactive ion etching. Many applications need high ion energies which are generated by biasing the substrate with a radio frequency (RF) current source [7,8]. Proper understanding of the electrodynamics involved in the sheath and near the plasma-sheath boundary is thus highly desirable.

We consider a low density, low pressure plasma where a single power supply generates both the discharge and the RF sheath. In this high frequency regime, the sheaths are primarily capacitative in nature. The sheath is assumed to be collisionless. As is well known [4,5,9,10], the analysis of sheath models depends on the ratio of the applied RF frequency $\omega$ to the ion plasma frequency $\omega_{pi}$: when $\omega << \omega_{pi}$, the ions cross the sheath quickly and can instantaneously adjust to the applied field, and the properties of the sheath at different times of the RF cycle are identical to those of a dc sheath having a potential given by its instantaneous value (RF plus dc). However, when $\omega >> \omega_{pi}$, the inertia of the ions prevents them from adjusting to the applied field, and they cannot respond to its time variation. Then the ions cross the sheath in many RF periods and they respond only to the dc field – their dynamics is governed by the time-averaged field in the sheath.

In the Godyak-Lieberman (GL) theory [4,5] (which we consider now), valid in the low density, high frequency, high current regime [11], the ions are assumed to react only to the dc fields and not to the RF fields. Also it is assumed that the transit time for the ions across the sheath is large compared to the oscillation time. These assumptions lead the GL theory to predict monoenergetic ions impinging on the substrate.

The ions are assumed to enter the sheath with a Bohm presheath velocity [12]

$$v_B = \frac{eT_e}{m_i}$$

where $e$ is the ion charge, $T_e$ denotes the electron temperature in volts and $m_i$ is the ion mass. The ion sheath-plasma boundary is taken to be stationary, and it is assumed that the electrons being inertialess, respond to the instantaneous field.

The GL theory holds in the regime in which the applied RF voltage is very large compared to $T_e$, so that one can assume that the electron Debye length $\lambda_D$ everywhere within the sheath is much smaller than the thickness of the ion sheath $s_m$, implying that the electron density drops sharply from $n_e = n_i$ at the boundary with the plasma to $n_e = 0$ in the sheath (at the electrode side).
The electron sheath penetrates into the ion sheath for a distance \( s(t) \) from the plasma-ion sheath boundary at \( x = 0 \), and oscillates between a maximum thickness of \( s_m \) and a minimum thickness which is a few Debye lengths distant from the electrode, so that the electron sheath thickness is effectively \( s_m - s(t) \).

We follow here, the analysis given in [4,5], but modified to include a finite dielectric constant \( \epsilon_{sh} \) for the sheath.

The ion flux is conserved at the plasma-ion sheath boundary. This is expressed by:

\[
    n_i v_i = n_0 v_B \quad (15)
\]

where we denote the ion density \( n_i(x) \) at the plasma-ion sheath boundary by \( n_0 \), and \( v_i \) is the ion velocity. From energy conservation, one obtains:

\[
    \frac{1}{2} m_i v_i^2 = \frac{1}{2} m_i v_B^2 - e\bar{\psi}_{sh}(x) \quad (16)
\]

where \( \bar{\psi}_{sh}(x) \) is the time averaged potential within the sheath. Combining (15) and (16), one obtains for the ion density:

\[
    n_i(x) = n_0 \left( 1 - \frac{2}{T_e} \bar{\psi}_{sh}(x) \right)^{-1/2} \quad (17)
\]

In the GL theory, a spatially uniform, sinusoidal RF current density is assumed to pass through the sheath:

\[
    J_{RF}(t) = -J_0 \sin \omega t \quad (18)
\]

This current is carried by the electrons: \( J = -ne \frac{d\bar{D}_{sh}}{dt} \), \( n \) being the electron density in the bulk plasma at the sheath edge. As these electrons oscillate away from the electrode, they leave behind a positive space charge space, pulling the positive ions there. At the electron sheath boundary, the displacement current given by (18) must be equated to the conduction current, for continuity:

\[
    -en_i(s) \frac{ds}{dt} = -J_0 \sin \omega t \quad (19)
\]

The instantaneous electric displacement \( D_{sh}(x,t) \) within the sheath is then given by:

\[
    \frac{\partial D_{sh}}{\partial x} = \begin{cases} 
    en_i(x), & x > s(t) \\
    0, & x < s(t)
    \end{cases} \quad (20)
\]

where \( D_{sh}(x,t) = \epsilon_{sh}(x,t)E_{sh}(x,t) \).

The time-averaged electric displacement and potential are given by:

\[
    \frac{d\bar{D}_{sh}}{dx} = \epsilon(n_i(x) - \bar{n}_e(x)) \\
    \frac{d\bar{\psi}_{sh}}{dx} = -\bar{E}_{sh} \quad (21)
\]
\(\bar{n}_e(x)\) being the time averaged electron density within the sheath.

The electric displacement field within the sheath can be found by integrating (20):

\[
D_{sh} = e \int_{s(t)}^x n_i(\xi) d\xi
\] (22)

This is done with the help of eqn.(19). Integrating its left hand side between the limits 0 and \(s\), and the right hand side between the limits 0 and \(\omega t\), one gets:

\[
e \int_0^s n_i(\xi) d\xi = \frac{J_0}{\omega}(1 - \cos \omega t)
\] (23)

Using (23) in (22), one obtains

\[
D_{sh}(x, \omega t) = e \int_{s(t)}^x n_i(\xi) d\xi = e \int_0^x n_i(\xi) d\xi - e \int_0^{s(t)} n_i(\xi) d\xi , \quad x > s(t)
\]

\[
= 0 , \quad x < s(t)
\] (24)

Since the GL theory is valid for the high frequency regime, one is interested in the time-averaged quantities. These can be found from \(s(t)\). Lieberman denotes by \(2\phi\), the phase during which \(x > s(t)\): then for \(x \approx 0, \quad 2\phi \approx 0\), and for \(x \approx s_m, \quad 2\phi \approx 2\pi\). Because \(n_e(x, t) = 0\) during the part of the RF cycle when \(x > s(t)\), he writes:

\[
\bar{n}_e(x) = \left(1 - \frac{2\phi}{2\pi}\right)n_i(x)
\] (25)

so that \(-\phi < \omega t < \phi\), for \(x > s(t)\), and \(\omega t = \pm\phi\) for \(x = s(t)\).

Then, from (23) and (24), one obtains:

\[
\bar{D}_{sh}(x) = \frac{1}{2\pi} \int_{-\phi}^{+\phi} D_{sh}(x, \omega t) d(\omega t)
\]

\[
= \frac{J_0}{\omega \pi}(\sin \phi - \phi \cos \phi)
\] (26)

From the second of eqns.(21) and the definition of \(D_{sh}\), we have:

\[
\epsilon_{sh} \frac{d\bar{\psi}_{sh}}{dx} = -\frac{J_0}{\omega \pi}(\sin \phi - \phi \cos \phi)
\] (27)

where we have assumed that the time averaging procedure allows us to factor out \(\epsilon_{sh}\) outside the spatial derivative. From (19) and (17), we get

\[
\frac{d\phi}{dx} = \frac{(1 - \frac{2\phi}{s_0})^{-1/2}}{s_0 \sin \phi}
\] (28)

where \(\omega t\) was set equal to \(\phi\) in (19), \(s\) to \(x\), and \(s_0 = \frac{J_0}{\epsilon_{sh} n_i}\).

Combining eqns.(27) and (28) we find

\[
\epsilon_{sh} \frac{d\bar{\psi}_{sh}}{d\phi} = \frac{J_0 s_0}{2\omega \pi}(1 + \cos 2\phi - \phi \sin 2\phi)(1 - \frac{2}{T_e} \bar{\psi}_{sh}(x))^{1/2}
\] (29)
which upon integration leads to
\[
(1 - \frac{2}{T_c} \bar{\psi}_{sh}(x))^ {1/2} = 1 - \frac{L}{\epsilon_{sh}} \left(\frac{3}{8} \sin 2\phi - \frac{\phi}{4} \cos 2\phi - \frac{\phi}{2}\right)
\]  
(30)
where
\[
L = \frac{J_0^2}{\epsilon \pi T_c \epsilon^2 n_0}
\]
and we have assumed that \(\epsilon_{sh}\) is independent of \(\phi\). Substituting (30) in (17), one finds the following expression for the ion density:
\[
n_i = n_0 \left(1 - \frac{L}{\epsilon_{sh}} \left(\frac{3}{8} \sin 2\phi - \frac{\phi}{4} \cos 2\phi - \frac{\phi}{2}\right)\right)^{-1}
\]  
(32)

Differentiating (26) with respect to \(x\) gives us
\[
\nabla \cdot \bar{D}_{sh} = \frac{J_0}{\omega \pi} \sin \phi \frac{d\phi}{dx} = \frac{J_0 \phi}{\omega \pi s_0} \left(1 - \frac{L}{\epsilon_{sh}} \left(\frac{3}{8} \sin 2\phi - \frac{\phi}{4} \cos 2\phi - \frac{\phi}{2}\right)\right)^{-1}
\]  
(33)

Since the net charge density in the sheath \(\rho_{sh}\) is given by
\[
\nabla \cdot \bar{D}_{sh} = \rho_{sh}
\]  
(34)
on one obtains
\[
\rho_{sh} = \frac{e \phi n_i}{\pi}
\]  
(35)

In order to calculate the sheath capacitance, one must consider the instantaneous values.

From (23) and (24), the instantaneous displacement field in the sheath is
\[
D_{sh} = e \int_0^x n_i(\xi) d\xi - \frac{J_0}{\omega} (1 - \cos \omega t)
\]
\[
= \frac{J_0}{\omega} (\cos \omega t - \cos \phi) \quad , \quad x > s(t)
\]
\[
= 0 \quad , \quad x < s(t)
\]  
(36)

Integrating both sides of (36) with respect to \(x\), we get
\[
D_{sh}(t) = \int_{s(t)}^{s_m} D_{sh}(x, t) dx = \int_{s(t)}^{s_m} \epsilon_{sh} E_{sh}(x, t) dx
\]
\[
= \frac{J_0 s_0}{\omega} \int_0^{\pi} (\cos \omega t - \cos \phi) \sin \phi \left[1 - \frac{L}{\epsilon_{sh}} \left(\frac{3}{8} \sin 2\phi - \frac{\phi}{4} \cos 2\phi - \frac{\phi}{2}\right)\right] d\phi
\]  
(37)
\[
= \frac{\pi T_c}{4} (3 + 4 \cos \omega t + \cos 2\omega t) - \frac{\pi L^2 T_c}{\epsilon_{sh}} \left(\frac{15}{16} \pi + \frac{3}{8} \omega t + \frac{5}{3} \pi \cos \omega t + \frac{1}{48} \omega t \cos 4\omega t - \frac{5}{18} \sin 2\omega t - \frac{25}{576} \sin 4\omega t\right)
\]  
(38)

where a change of variables from \(x\) to \(\phi\) has been made in (37). We now use these results of the GL theory modified to include a finite sheath dielectric constant \(\epsilon_{sh}\), to the correct form of Sato’s
equation (14) for an RF discharge.

The contribution to the current in the external circuit from the last integral in (14) then is:

\[
\frac{1}{V_a} \int_S \frac{\partial D}{\partial t} \psi_{sh} dS = \epsilon_0 \frac{1}{V_a} \int_S \frac{\partial E_p}{\partial t} \psi_{sh} dS + \frac{1}{V_a} \int_S \frac{\partial D_{sh}}{\partial t} \psi_{sh} dS
\]  

(39)

If it is assumed that the plasma is a good conductor, then the electric field in the plasma can be taken as vanishing. Then it is the last term of (39) whose contribution is relevant to the discharge current.

We consider again, the GL theory. For simplicity, we consider a symmetric discharge, and circular electrodes of area \( A \) separated a distance \( d \) apart. Since the electric displacement and the potential in the sheath are assumed to vary only in the axial direction and are assumed to be uniform in the radial direction (implicit in the assumption that the charge density is uniform across the radius and varies in the axial direction only), therefore, the area can be factored out of the surface integral. If we make also the further assumption that \( \epsilon_{sh}(x,t) \approx \epsilon_{sh}(t) \), that is, that the spatial variation of the sheath dielectric constant can be neglected, then one deduces, making use of (9) and (6) in (39), that the contribution of the term:

\[
\frac{1}{V_a} \int_S \frac{\partial D_{sh}}{\partial t} \psi_{sh} dS
\]

in (40) coming from the RF sheath to the gap capacitance is given by \( C_{sh} \), where:

\[
C_{sh} = -\frac{A}{V_a} \int D_{sh}(x,t) dx = -\frac{A}{V_a} D_{sh}(t)
\]

(40)

where \( D_{sh} \) is given in (38). Notice, that as expected, this contribution is independent of the distance \( d \) separating the electrodes and depends only upon the RF frequency, the electron temperature, the area of the electrodes, \( n_0 \), the amplitude of the current density, and the sheath dielectric constant \( \epsilon_{sh} \).

In the case of RF discharges, the contribution to the total particle flux \( \Gamma \) from diffusion of the particles can be taken to be vanishing because the ions and electrons would be expected to react faster to the rapidly changing applied RF voltage, than be influenced by the diffusion gradients in a significant way. Thus in these cases, only the \( n_l v_l \), \( (l = i, e) \) terms in (3) would contribute to \( \Gamma \).

The dc contribution to the voltage across the sheath comes from the dc ion current \( J_i \). This contributes to the \( \Gamma \) term in (14), for the current \( I \) in the external circuit:

\[
J_i = e n_0 v_B = K \frac{2e}{m_i} \left( \frac{\bar{\psi}_{sh}^{3/2}}{s_{sh}^2} \right)^{1/2}
\]

(41)

where \( K = \frac{200}{43} \) in Lieberman’s theory, while \( K = \frac{4}{9} \) for Child’s law. \( \bar{\psi}_{sh} \) is given by (30):

\[
\bar{\psi}_{sh} = \frac{T_e \left( \frac{L}{\epsilon_{sh}} \right)^2}{2} \left( \frac{3}{8} \sin 2\phi - \frac{\phi}{4} \cos 2\phi - \frac{\phi}{2} \right)^2, \quad \text{for } \phi = \pi
\]

\[
= \frac{T_e L^2 (9 + 2\pi)^2}{2592 \epsilon_{sh}^2}
\]

(42)
Performing the surface integration:

\[
\int_S e n_i v_i \psi_{sh} dS
\]  

(43)

over the surface of the discharge space, and assuming as before a simplified geometry of circular electrodes of equal area \(A\), and a symmetric discharge, we find that this term contributes

\[
\frac{1}{V_a} \int_S e \Gamma \psi_{sh} dS = -K \left( \frac{2e}{m_i} \right)^{1/2} \frac{\psi_{sh}^{3/2}}{s_m} \frac{D_{sh}}{\psi_{sh}} \epsilon_{sh} V_a
\]  

(44)

where \(D_{sh}\) is given by (38).

In going from (29) to (30), we have made the assumption that \(\epsilon_{sh}\) is independent of \(\phi\). Since \(\epsilon_{sh}\) is, in fact frequency dependent:

\[
\epsilon_{sh}(\omega) = \epsilon_{sh} \infty + \frac{\epsilon_{sh s} - \epsilon_{sh \infty}}{1 - i\omega \tau}
\]

(45)

where \(\tau\) is the sheath relaxation time, it cannot be trivially factored out of the integral. One must use the relation: \(\omega t = \phi\) before performing the integration over \(\phi\).

**Discussion**

We have shown that the time-dependent version of Sato’s equation is not independent of the space charge electric field. We consider the specific example of the Godyak-Lieberman model for a capacitative RF discharge, and show that the sheath field gives a non-negligible contribution to the gap capacitance of the discharge tube. Space charge effects in a discharge tube can be analysed using energy balance methods, by modelling the system as a two-layer Maxwell-Wagner capacitor. For frequencies below RF frequencies also, the argument above shows that the electric field and potential of the space charge can give a non-zero contribution to the external current in the circuit, when the potential drop across the space charge is appreciable. The diffusion terms could also give a non-trivial contribution in these cases to the terms coming from space charge effects: \(\int_S D \nabla n_l \psi_{sh} dS\), \((l = i, e)\), \(D\) being the ambipolar diffusion constant. For a symmetric discharge and circular electrodes of equal area \(A\), this surface term would contribute a factor: \(\frac{2}{16} \frac{D_{sh \infty}}{e_{sh}} \left(1 + \frac{4 \rho_s}{e_{sh}}\right)^{-2} D_{sh}\) from the ion flux, \(D_{sh}\) being given by (38).

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