

One-Carrier Free Space Charge Motion under Applied Voltage: The General Solution*

P. C. CAMARGO

Departamento de Ciências Físicas e Matemáticas, Universidade Federal de São Carlos, São Carlos SP

and

G. F. LEAL FERREIRA

Departamento de Física e Ciência dos Materiais, Instituto de Física e Química de São Carlos", Universidade de São Paulo, São Carlos SP

Recebido em 13 de Maio de 1976

Extending the method of solution recently presented in this journal, the system of partial differential equations describing the one-carrier free space-charge motion under a given applied voltage is transformed into a system of two ordinary differential equations. The method is applied to find the external current observed with shorted electrodes, after space charge limited current injection.

Extendendo-se o método de solução recentemente apresentado nesta Revista, o sistema de equações diferenciais parciais, que descreve o movimento de carga espacial monopolar, sob voltagem constante, é transformado em um sistema de duas equações diferenciais ordinárias. O método é aplicado ao cálculo da corrente externa fornecida em curto circuito, após injeção de carga espacial.

1. INTRODUCTION

By one-carrier free space charge motion (FSCM), we mean the time development of an excess charge distribution, in which every carrier moves with a velocity proportional to the electric field acting upon it. As

* Work supported by FAPESP and CNPq.

** Postal Address: Caixas Postais 359-378, 13569 - São Carlos SP.

the electrodes (we are assuming planar geometry) may also bear electric charges, the complete specification of the electric field needs a reference to them, as open if unconnected, or as under an applied voltage if they are connected through an e.m.f. source. They are known, respectively, as charge and current modes.

In this article will be given a solution of the FSCM, in the current mode, assuming that the charge distribution, which completely fills the dielectric, is known, at a given time, as well as the applied voltage as a function of time. To achieve this aim, we extended the method of solution recently developed¹ for the case in which the charge distribution touches only one of the electrodes. It turns out that the system of partial differential equations describing the FSCM, namely the Poisson and continuity equations, together with the constraint that the knowledge of the voltage imposes on their solutions, is transformed into a system of two ordinary differential equations (in Ref. 1 we had only one) from whose solution the quantities of interest may be derived.

The method is applied to find the external current delivered by a dielectric which was shorted after being in the stationary space-charge limited current regime. This case has received some attention in the literature (Refs.2,3,4,5), since it is closely connected with experiment. In the sequel, we will often quote Ref. 1 (CALF), on which most of this work is based.

2. THEORY

We use, throughout this paper, dimensionless variables as defined in CALF, p.351. Thus, we write the Poisson and continuity equations as

$$\frac{\partial}{\partial x} E(x, t) = \rho(x, t),$$

$$\frac{\partial}{\partial x} i(x, t) + \frac{\partial}{\partial t} \rho(x, t) = 0$$

$$i(x, t) = \rho(x, t)E(x, t),$$

where, E is the electric field strength, ρ , the charge density, i , the conduction current, x , the depth as measured from the higher potential electrode, and t , the time.

We are given

$$\rho(x,0) = \rho(x) , 0 < x < 1,$$

and

$$\int_0^1 E(x,t) dx = V(t), \quad (1)$$

$V(t)$ being the applied voltage.

Using the method of the characteristics, the following equations are obtained

$$\frac{dx}{dt} = E(x(t), t) , \quad \frac{d}{dt} E(x(t), t) = j(t), \quad \frac{d}{dt} \rho(x(t), t) = -\rho^2(x(t), t),$$

which may be integrated to give the equation of the flow lines

$$x = x_0 + E(x_0)t + \int_0^t dt' \int_0^{t'} j(t'') dt'', \quad (2)$$

and the charge density along them,

$$\rho(x(t), t) = \frac{\rho(x_0)}{1 + \rho(x_0)t} , \quad (3)$$

$E(x_0) = E(x, 0)$ being a known function of the position which may be found from $\rho(x_0)$ and $V(0)$, and j the external current.

3. THE FUNCTION $y(t)$ AND $z(t)$

We assume that both electrodes are receiving carriers; this is surely the case, for all times, if $V(t) = 0$, and for a limited range of time, if

the voltage is not so high as to drift all the carriers in a given direction (in this case the problem would be treated as in Ref. 1). We define, therefore, functions $y=y(t)$ and $z=z(t)$ as giving the initial coordinates, y and z , of the carriers that, at time t , were respectively at $x=0$ and $x=1$. Clearly, we have $y(0)=0$ and $z(0)=1$.

Hence, we may obtain the equations (CALF, p.353)

$$E(0,t) = - [1 + \rho(y)t] \frac{dy}{dt}, \quad (4a)$$

$$E(1,t) = - [1 + \rho(z)t] \frac{dz}{dt}. \quad (4b)$$

With the variables y and z , we may write, from Eq.(2),

$$0 = y + E(y)t + \int_0^t dt' \int_0^{t'} j(t'') dt'', \quad (5a)$$

$$1 = z + E(z)t + \int_0^t dt' \int_0^{t'} j(t'') dt''. \quad (5b)$$

With the help of these relations, Eq.(2) may be rewritten either as

$$x(t) = x_0 - y + t(E(x_0) - E(y)) \quad (6a)$$

or

$$x(t) = 1 + x_0 - z + t(E(x_0) - E(z)). \quad (6b)$$

In Eqs.(5) and (6), $E(y)$ and $E(z)$, like $E(x_0)$, are the electric field, at $t=0$, expressed as a function of the variables y, z and x_0 .

Charge conservation allows us to write

$$E(1,t) - E(0,t) = E(z) - E(y). \quad (7)$$

On the other hand, from Eq.(1), we derive

$$E(1, t) = \int_0^1 x \rho(x, t) dx + V(t) . \quad (8)$$

We, now, change the integration variable, in Eq.(8), from x to x_0 as given by Eq. (6a). Keeping the time fixed, as the integration requires, we differentiate Eq. (6a), obtaining

$$dx = dx_0 (1 + t \frac{d}{dx_0} E(x_0)) = dx_0 (1 + t \rho(x_0)) . \quad (9)$$

Using Eqs.(6a), (9) and (3), in Eq.(8), we obtain

$$E(1, t) = \int_y^z [x_0 - y + t(E(x_0) - E(y))] \rho(x_0) dx_0 + V(t) ,$$

which may be integrated, giving

$$E(1, t) = W(y) - W(z) + E(z) [z - y - t(E(y) + E(z))] + \frac{t}{2} [E^2(y) - E^2(z)] + V(t), \quad (10)$$

with $W(r)$ defined as

$$W(r) = \int_0^r E(x) dx . \quad (11)$$

Subtracting Eq. (5a) from (5b), and using the result in Eq. (10), we obtain

$$E(1, t) = W(y) - W(z) + E(z) + \frac{t}{2} [E^2(y) - E^2(z)] + V(t) . \quad (12a)$$

Using Eq.(7), we may write, for $E(0, t)$,

$$E(0, t) = W(y) - W(z) + E(y) + \frac{t}{2} [E^2(y) - E^2(z)] + V(t) . \quad (12b)$$

Substitution of Eqs. (12a) and (12b), respectively into Eqs. (4a) and (4b), gives rise to a system of two ordinary differential equations in y, z and t :

$$\frac{dy}{dt} = \frac{-1}{1+\rho(y)t} \{W(y)-W(z)+E(y) + \frac{t}{2}[E^2(y)-E^2(z)]+V(t)\} ,$$

$$\frac{dz}{dt} = \frac{-1}{1+\rho(z)t} \{W(y)-W(z)+E(z) + \frac{t}{2}[E^2(y)-E^2(z)]+V(t)\} . \quad (13)$$

It is desirable to add a few words of comment about this system. First, we note that, for $t=0$, $W(0)=0$ (see Eq. (11)) and $W(z)=V(0)$, so $dy/dt > 0$, if $E(y) < 0$, and $dz/dt < 0$, if $E(z) > 0$, as required by the definitions of $y(t)$ and $z(t)$. Suppose now that $V(t)=0$; therefore, as already said, the proposed solution will be valid for all times $t \geq 0$; y will be an increasing function of time, and z a decreasing one. We therefore, expect that, for large times, y and z tend to the same limit, a . This behavior of $y(t)$ and $z(t)$ is, however, very delicate because, for $y-z$, Eq. (13) gives $dy/dt - dz/dt$, what would violate the condition that $y(t)$ must be an increasing, and $z(t)$ a decreasing, function of time.

We have always found that, increasing accuracy of the numerical integration of Eqs. (13), actually increases the time for which $y(t)$ and $z(t)$ behave as expected.

The common limit value of $y(t)$ and $z(t)$, for $t \rightarrow \infty$, is closely related to the total charge $Q(t)$ circulating in the external circuit. To see this, we differentiate Eq. (2) with respect to time:

$$E(x(t), t) = E(x_0) + \int_0^t j(t') dt' = E(x_0) + Q(t). \quad (14)$$

The electric field, acting at large times ($t \rightarrow \infty$), upon those carriers which never reach the electrodes is zero, that is, $E(x(\infty), \infty) = 0$. Clearly, $x_0 = a$, so that

$$E(a) = - \int_0^{\infty} j(t') dt' = -Q(\infty) \quad (15)$$

This equation provides a test for the correctness of our calculation, since a comes out of the integration of Eq. (13), and $j(t)$, the external current, may be found according to the procedure given in the next Section.

4. THE EXTERNAL CURRENT AND THE CHARGE DENSITY

The external current, $j(t)$, is given by

$$j(t) = \rho E + \frac{\partial E}{\partial t}.$$

Integration of this equation in x , from 0 to 1, using Poisson's equation, gives

$$j(t) = \frac{1}{2} [E^2(1,t) - E^2(0,t)] + \dot{V}(t).$$

Using Eqs. (12a) and (12b), we obtain

$$j(t) = (E(z) - E(y)) [W(y) - W(z) + V(t) + \frac{1}{2}(E(z) + E(y)) + \frac{t}{2}(E^2(z) - E^2(y))] + \dot{V}(t). \quad (16)$$

The charge density, at time t , may be found, for any x_0 , using Eq. (3); its position, x , is given by Eq. (6a) (or Eq. (6b)).

Therefore, once $y(t)$ and $z(t)$ are known, the external current and charge density can be directly calculated.

5. APPLICATIONS

In most cases, we do not know the initial charge distribution. If, however, the trap free dielectric is in the stationary space charge limited current regime, the charge density is indeed known, and it will be used to illustrate our method.

We suppose ohmic contact at the injecting electrode during the charge. Using the same dimensionless variables, as in Ref.5, the stationary space

charge density is $\rho(x_0) = 3/4 x_0^{-1/2}$. At $t=0$, the electrodes are shorted, and we want to know the current delivered by the system (besides the capacity current peak, at $t=0$), as well as the charge density as a function of time.

To start with, Fig.1 exhibits y and z as functions of time. These were obtained, by the first order Runge-Kutta method, on a HP-9810-A desk calculator. It is seen that, even for $t=20$, z and y are not too close to their asymptotic value, a . For instance, for $t=26$, we have $y=0.4672$ and $z=0.5017$. It seems safe to put $a=0.4844 \pm 0.0005$.

Figure 2 shows ρ as a function of x and t , for $0 \leq t \leq 1.4$. We see that, at $t=1.4$, ρ is almost uniform. Fig.3 displays the external current $j(t)$, and the charge $Q(t)$ (see Eq. (14)), as a function of t . Observe that j has a very fast initial decay ($0 \leq t < 1$), followed by a rather slow one. The time $t = 1$, mediating these two behaviors, may give a gross indication of the value of the mobility.

Following a hint taken from experiments in KCN crystals, we have found that the function $0.375 \exp(-4.182\sqrt{t})$ very closely represents the external current, in the range $0 < t < 2$.

The asymptotic value of $Q(t)$, that is, $Q(\infty)$, was found to be -0.04426 . Coming back to Eq. (15), we have $E(x_0) = -1 + 3/2 x_0^{1/2}$ and $a=0.4844 \pm 0.0005$, giving $E(a) = 0.04398 \pm 0.00054$. Since a was found in a rather crude way, we think that $Q(\infty)$, as obtained by integration, provides a better value of the external charge than that given by $-E(a)$.

Some years ago, Lindmayer^{7,8} deduced an expression relating the external current with the motion of the zero field plane, namely,

$$j(t) = - \rho(r(t), t) \frac{dr}{dt}, \quad (17)$$

where $r(t)$ gives the position of the zero field plane (that is, $E(r(t), t)=0$). We will discuss some results, arising from Eq. (17), within the FSCM scheme. Integrating Eq. (17) in the time variable, we have

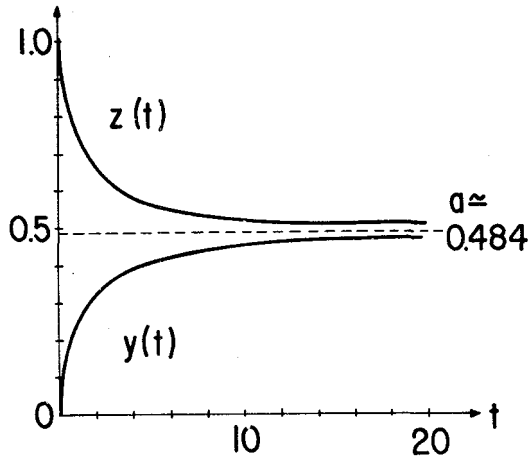


Fig.1 - y and z as functions of time for SCLC discharge. Note the weak convergence to the common limit a .

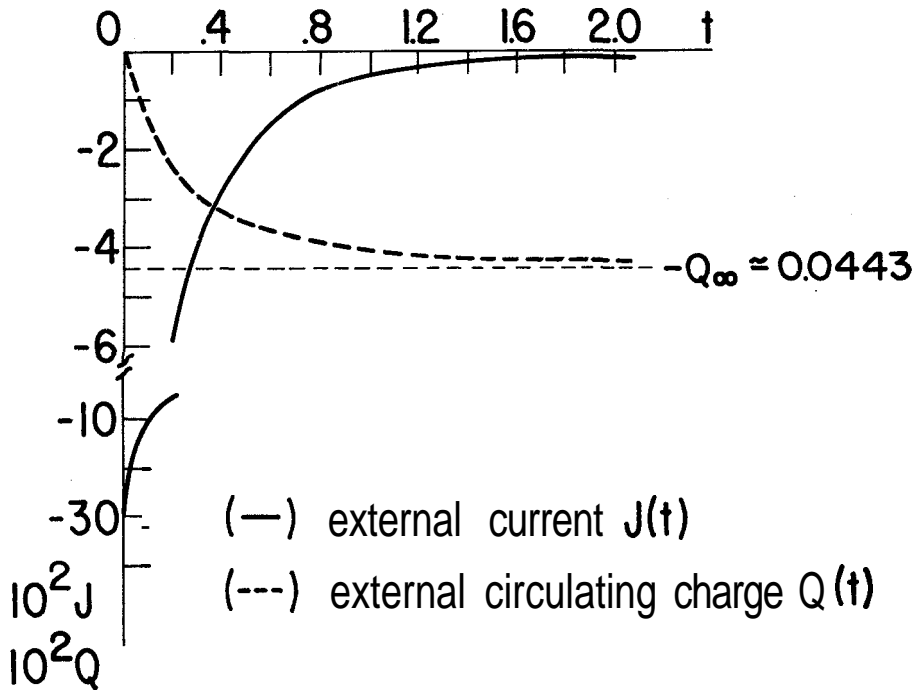


Fig.3 - The external current (full) and charged (dashed) as a function of time. The approximate value of $Q(\infty)$ is also given.

$$-Q(t) = - \int_0^t j(t') dt' = \int_{r_0}^r \rho(r(t), t) dr, \quad (18)$$

where r , is the initial position of the zero field plane. Now, at $r(t)$, the charges are not moving, and so we may say that $-j(t)dt$ is the charge swept out by the moving zero field plane, in a locally stationary charge conservation, we may further say that $-Q(t)$ is equal to the charge lying between the initial value of r , that is r_0 , and the initial position, s_0 , of those carriers that, at time t , are in $r(t)$. For $t \rightarrow \infty$, we have $s_0 \rightarrow a$, and we correspondingly write

$$-Q(\infty) = - \int_0^\infty j(t') dt' = \int_{r_0}^a \rho(s_0) ds_0. \quad (19)$$

For a monotonically decreasing initial charge distribution, Lindmayer puts

$$-Q(\infty) < \rho(r_0) \left(\frac{1}{2} - r_0 \right). \quad (20)$$

Actually, this relation may be derived from Eq.(19), noting that, for a monotonically decreasing $\rho(x_0)$, j is negative, and by Eq.(17), dr/dt is positive. This means that $a > r_0$ and $\rho(r_0) > \rho(a)$. This allows us to write from Eq.(19)

$$-Q(\infty) = \int_{r_0}^a \rho(s_0) ds_0 < \max \rho(s_0) \int_0^a ds_0 = \rho(r_0)(a - r_0). \quad (21)$$

It is easy, now, to show for FSCM that, along a flow line,

$$\frac{\partial}{\partial x} \rho(x(t), t) = \frac{\partial \rho(x_0) / \partial x_0}{(1 + \rho(x_0)t)^3}$$

This relation shows that $\partial \rho / \partial x$ cannot change sign during the charge motion, and hence a monotonically decreasing ρ remains monotonically decreasing as the time goes on. For such charge distributions, $E(1/2, t)$ is always greater than zero, and we conclude that $a < 1/2$, because the char-

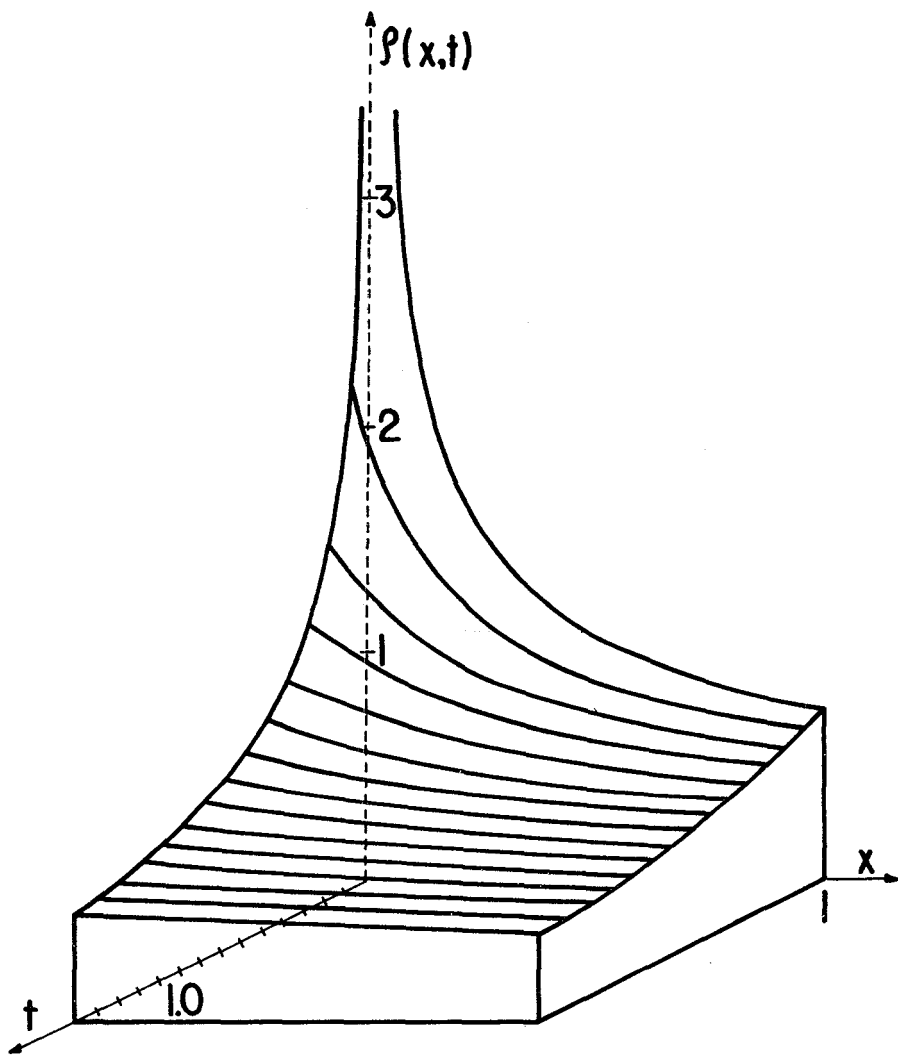


Fig.2 - Tridimensional plot of the charge density as a function of x and t . At $t=1.4$, the charge density is almost uniform.

ges initially at $x \geq 1/2$ actually reach the electrode at $x=1$.

Therefore, Lindmayer's inequality, Eq. (20), has been derived.

Our results satisfy the condition $\alpha < 1/2$, and also the inequality Eq. (21) which is stronger than Eq. (20). From Eq. (21), we have

$$\alpha > \frac{-Q(\infty)}{\rho(x_0)} + x_0$$

We get $\alpha > 0.4838$, which is to be compared with the extrapolated value, namely, $\alpha = 0.4844 \pm 0.0005$.

6. CONCLUSION

We deem that our method greatly simplifies the solution of the FSCM partial differential equations as compared with the direct integration performed by J. van Turnhout¹⁰, in a simpler case (charge touching only one of the electrodes). We also think that approximate solutions of the problem will be welcome inasmuch as the external current does not depend on the fine detail of the charge distribution. In this respect, our solution may be helpful.

We are indebted to L.N. de Oliveira for calling our attention to the meaning of the Lindmayer theorem as expressed in Section 4

REFERENCES

1. L. E. Carrano de Almeida and G. F. Leal Ferreira, Rev. Brasil. Fís., 5, 349 (1975).
2. A. Rose, *Concepts in Photoconductivity and Allied Problems*, Interscience Publ., New York, 1963.
3. D. J. Gibbons, J. Phys. D, Appl. Phys., 7, 433 (1974).
4. B. Gross, J. Appl. Phys. D, Appl. Phys., 7, L 103 (1974).

5. A. Many, G. Rakavy, Phys. Rev. 126, 1980 (1962).
6. M. F. de Souza, private communication.
7. J. Lindmayer, J. Appl. Phys. 36, 196 (1965).
8. B. Gross, M. M. Perlman, J. Appl. Phys. 43, 853 (1972).
9. L. N. de Oliveira and G. F. Leal Ferreira, " Exact Solutions with Non-Uniform Charge Distributions". To be published in J. of Electrostatics.
10. J. van Turnhout, *Thermally Stimulated Discharge of Polimer Electrets*, Elsevier Publ. Co. 1974, Chapter V.