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A computer code to calculate the fast induced signals by electron swarms in gases

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Abstract. To aid the data analysis of pulsed Townsend experiments, a special code has been developed to calculate the induced pulse by solving the electron continuity equation including growth, drift and diffusion. A realistic profile of the initial laser beam is taken into account as well as the boundary conditions at the cathode and the anode. The approach is either semi-analytic, based on the expression derived by P.H. Purdie and J. Fletcher, or fully numerical, using a finite-difference scheme introduced by J. de Urquijo et al. A new improved scheme is also proposed and compared with the other two methods under typical experimental conditions. A brief discussion on the stability of the numerical procedures is given. The new finite-difference scheme allows a detailed investigation of the importance of back diffusion to the cathode, a subject seldom tackled in the past.

Keywords: electron transport parameters, pulsed Townsend technique, cathode back-diffusion

PACS: 51.50.+v, 52.25.Fi, 52.80.Dy, 02.70.Bf

INTRODUCTION

The study of electron transport parameters (i.e. drift velocity, diffusion coefficients and first Townsend coefficient) in gases is very important in several areas of applied nuclear science. For example, they are a relevant input to the design of particle detectors employing micro-structures (MSGC's, micromegas, GEM's) and RPC's (resistive plate chambers). Moreover, if the data are accurate and complete enough, they can be used to derive a set of electron impact cross-sections with their energy dependence, that are a key ingredient in micro-dosimetry calculations. Despite the fundamental need of such data and the long age of the field, the gases of possible interest are so many and the effort of obtaining good quality data is so time demanding, that an important contribution can still be made. As an example, electrons drift velocities at moderate field strengths (up to 50 Td) in pure Isobutane (a tissue-equivalent gas) have been measured only recently by the IPEN-LIP collaboration using a dedicated setup [1]. The transport parameters have been derived from the recorded electric signal induced by a swarm started with a fast discharge laser shining on the cathode. This is a kind of pulsed Townsend technique, first successfully employed by J.A. Hornbeck [2]. Over the years, several groups adopted again the method and made improvements [3–5].

To complement the experimental effort undergoing within the mentioned IPEN-LIP

collaboration, a computer code has been developed to calculate the expected signal. Its utility is twofold: during the commissioning phase of the setup it can be employed to compare the calculations and the measurements performed with a very well known gas (like Nitrogen) to identify possible problems, while in the operational phase it allows to fit the data and extract the values of the transport parameters.

This is not a new topic and the program originated as a simple reimplementation of the approximate analytical formula of P.H. Purdie and J. Fletcher [3] and of the finite-difference scheme introduced by J. de Urquijo [7] et al. The presence in the former of an initial spike, absent in the latter, motivated a critical reexamination of the finite-difference scheme, which has been improved. A detailed study of the effect of back diffusion to the cathode has been performed with the new, unconditionally stable, algorithm.

THE FORMULATION OF THE PROBLEM

To measure electron transport parameters in a well-defined condition, a uniform electric field must be employed imposing a parallel plate configuration to the experimental cell. This results in a one dimensional problem. In the pulsed Townsend technique, the same pair of parallel plate electrodes is used to polarise the gas and to record the induced signal. Then, according to Ramo's theorem, the induced fast current by an electron swarm is

$$i(t) = \frac{e}{d} W_v \int_0^d n(z,t) dz , \quad (1)$$

where e is the elementary charge, $n(z,t)$ is the 1d-electron spatial density and d is the distance between the planar parallel electrodes. A constant average drift velocity W_v is assumed. If the swarm is in hydrodynamic equilibrium (i.e. the energy acquired on average from the electric field is balanced by the energy lost to collisions with gas molecules) then $n(z,t)$ must obey the electron continuity equation

$$\frac{\partial n(z,t)}{\partial t} = R_i n(z,t) - W_r \frac{\partial n(z,t)}{\partial z} + D_L \frac{\partial^2 n(z,t)}{\partial z^2} , \quad (2)$$

where R_i , W_r and D_L are the PT ionisation rate, drift velocity and longitudinal diffusion coefficient, respectively.

The electrodes are modelled as perfectly absorbing ideal electron sinks, resulting in boundary conditions of the Dirichlet type

$$\begin{cases} n(0,t) = n_0 \delta(t) \\ n(d,t) = 0 \end{cases} , \quad (3)$$

where the Dirac- δ represents the external initial ionisation produced e.g. by shining a laser on the cathode. The initial condition is that there shall be no previous ionisation in the gap

$$n(z,0) = 0 . \quad (4)$$

THE HUXLEY ANALYTIC SOLUTION

A standard approach to solve eq. (2) would be to first derive its Green function in free space and then incorporate the boundary conditions by the classical method of images. Because of the particular configuration of eq. (3), in the present case an infinite number of images is actually required, resulting in a series. L.H.G. Huxley [6] first succeeded in finding an approximate solution $n(z, t)$ of the electron continuity equation of good quality by devising a careful truncation procedure. In this expression, the boundary condition at the anode is exactly verified, while the boundary condition at the cathode is only approximately satisfied. Because the electrons are moving toward the anode, the former condition is the most important one to obtain the induced signal, while the latter is relevant only to describe the perturbation arising from back-diffusion to the cathode.

P.H. Purdie and J. Fletcher [3] were able to integrate analytically Huxley's result arriving at a closed expression for the induced current

$$\begin{aligned}
 i(T) = & \frac{en_0}{2d} W_v \exp(R_i t_0 T) \\
 & \cdot \left\{ \left(\frac{\beta}{\pi T} \right)^{1/2} \exp\left(-\frac{T}{\beta}\right) \left[1 + \exp\left(-\frac{4}{\beta T}\right) - 2 \exp\left(\frac{2}{\beta} - \frac{1}{\beta T}\right) \right] \right. \\
 & + \operatorname{erf}\left(\frac{1-T}{(\beta T)^{1/2}}\right) + \operatorname{erf}\left(\frac{T}{(\beta T)^{1/2}}\right) \\
 & \left. + \exp\left(\frac{4}{\beta}\right) \left[\operatorname{erf}\left(\frac{2+T}{(\beta T)^{1/2}}\right) - \operatorname{erf}\left(\frac{1+T}{(\beta T)^{1/2}}\right) \right] \right\}, \quad (5)
 \end{aligned}$$

where $T = t/t_0$ with $t_0 = d/W_r$, $\beta = 4D_L/(W_r d)$.

THE FINITE-DIFFERENCE SCHEME OF J. DE URQUIJO ET AL.

A common method to find a numerical solution of eq. (2) is to discretise n as $u_j^n = n(z_j, t_n)$ at the points of a rectangular mesh ($z_j = j\Delta x, t_n = n\Delta t$) with constant space and time sizes Δx and Δt , respectively. The partial derivatives can then be approximated by finite-differences and the solution of eq. (2) is transformed into the solution of a, possibly large, system of coupled linear algebraic equations in the unknowns u_j^n . It has to be emphasised that such procedure is not unique and several finite-difference schemes can be devised, all corresponding to eq. (2). The standard definitions of the finite-difference calculus $\delta_0 u_i = u_{i+1} - u_{i-1}$, $\delta_- u_i = u_i - u_{i-1}$, $\delta_+ u_i = u_{i+1} - u_i$ and $\delta^2 u_i = u_{i+1} - 2u_i + u_{i-1}$ will be employed in what follows.

A particularly simple scheme for eq. (2) has been introduced, as mentioned, by J. de Urquijo et al. [7]

$$u_j^{n+1} - u_j^n = -r\delta_- u_j^n + s\delta^2 u_{j-1}^n + t u_j^n \quad (6)$$

where $r = W_r/v_0$, $s = D_L/(v_0 \Delta x)$, $t = R_i \Delta t$ and $v_0 = \Delta x/\Delta t$. Its main advantage is the fully explicit nature in u_j^{n+1} : the knowledge of all u_j^n at time n can be immediately

propagated one step forward in time calculating all the u_j^{n+1} at time $n + 1$ and by successive iterations the complete evolution at all later times can be obtained. Such procedure is quite efficient in terms of both memory usage and number of arithmetic operations. In the same work, it has been adopted to investigate several features of the induced signals including the effect of positive and negative ions (present at longer timescales), which remain beyond reach here. In particular, the distortion due to the time profile of the initial ionisation (e.g. laser pulse) has been studied in detail.

Nevertheless, scheme (6) has a fundamental limitation: its stability. The sizes of the meshes Δt and Δx can not be decreased at will, at some point a situation is reached where the rounding errors amplify catastrophically at each step forcing u_j^n to diverge. From the general theory, it is very well known that, in the present case, a necessary and sufficient condition [8] for stability can be found with the von Neumann analysis, which replaces u_j^n by $\xi^n e^{ikj\Delta x}$ in eq. (6) and solves for the time amplifying factor ξ of the space mode e^{ikx} . The stability condition requires $|\xi|$ to be less or equal to 1 for all values of k . For scheme (6), the most critical mode is the $k = \pi$ imposing

$$|\xi_\pi| = \left| 1 - 2 \left(\frac{W_r}{v_0} - \frac{2D_L}{v_0 \Delta x} \right) \right| \leq 1 . \quad (7)$$

To actually avoid that numerical diffusion spoils the accuracy of the solution, the condition $W_r/v_0 = 1$ has also to be imposed [8], implying that there exists a minimum mesh size below which the scheme becomes unstable $\Delta x \geq 2D_L/W_r$.

THE CRANK-NICOLSON SCHEME

To overcome the limited stability of scheme (6), the present code can also utilise an extension of the classical Crank-Nicolson scheme to eq. (2)

$$u_j^{n+1} - u_j^n = -r \frac{1}{4} (\delta_0 u_j^{n+1} + \delta_0 u_j^n) + s \frac{1}{2} (\delta^2 u_j^{n+1} + \delta^2 u_j^n) + t \frac{1}{2} (u_j^{n+1} + u_j^n) . \quad (8)$$

It is second-order accurate in both space and time and the von Neumann stability analysis shows that it is unconditionally stable (i.e. it is stable independently from the values of r , s and t). To avoid any adverse impact of numerical diffusion, the condition $r = W_r/v_0 = 1$ shall also be satisfied. The main disadvantage, as compared to scheme (6), is that now a tridiagonal matrix has to be inverted at each time step.

A typical result obtained with the present code is reproduced in Fig. 1. On the left panel all three options are compared: the approximate analytic formula eq. (5), the numerical solution with scheme (6) and with scheme (8). The signal shows the characteristic asymmetry between the rising and falling parts due to diffusion. The stability of scheme (6) limits the minimum mesh sizes and the beginning of the signal can not be investigated in detail, but the analytic solution already exhibits signs of a sharp spike absent in the numerical ones. With the new scheme (8) the mesh sizes can be greatly refined fully revealing such a feature, as illustrated in the right panel of Fig. 1. The initial drop is due to the electrons which are first extracted and then diffuse back to the cathode and are reabsorbed. J.A. Hornbeck reports, in his pioneering work [2],

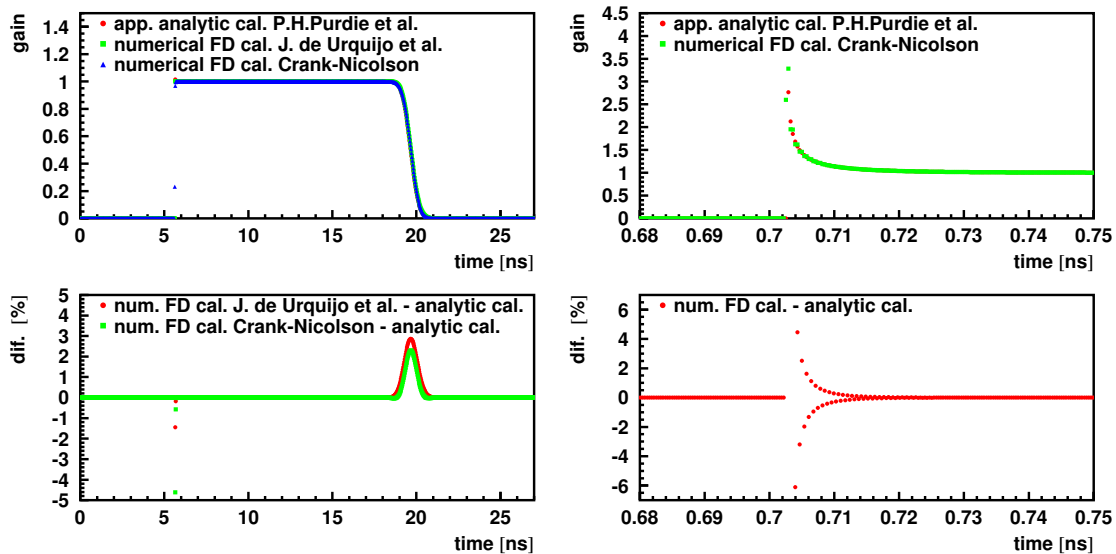


Figure 1. Example of a calculation for the induced signal in Nitrogen at atmospheric pressure and room temperature ($T = 300$ K). The gap is 1 mm and the electric field is $E/N = 61$ Td ($E = 15$ kV/cm). The left panel refers to mesh sizes limited by the stability of the scheme (6). The right panel refers to the initial part only, obtained with a much finer mesh allowed by the unconditional stability of scheme (8).

the experimental observation of this effect in Neon and Argon at very low electric field strengths $E/N < 1$ Td. The agreement between eq. (5) and the numerical solution with scheme (8) is excellent, confirming the high quality of the truncation procedure devised by L.H.G. Huxley. A tendency of scheme (8) to oscillate, which is expected [8], is also visible in the right panel of Fig. 1. It is presently being investigated in detail.

The fraction f_s of initially injected electrons surviving back-diffusion and finally being collected at the anode is given in Fig. 2 as a function of the initial position of their release z_i . As expected, once the electrons are produced well inside the gap f_s saturates to 1. Two values of the electric field $E/N = 61$ ($E = 15$ kV/cm) and $E/N = 143$ Td ($E = 35$ kV/cm) have been considered in Fig. 2 corresponding to a case where $R_i = 0$ and $R_i \neq 0$, respectively. To distinguish the effect of the term with R_i in eq. (2) from the effect of the dependence of the transport parameters on E/N , a case with the values of W_r and D_L corresponding to $E/N = 143$ Td, but with $R_i = 0$, is also plotted in Fig. 2. Clearly, the concentration gradient present when $R_i \neq 0$, plays a minor role in back diffusion under ordinary conditions. Two different choices of mesh sizes are also compared to demonstrate that no residual inaccuracy is present.

CONCLUSIONS

A computer code has been developed to calculate the fast signals induced by electron swarms in gases under the effect of a uniform electric field. The initial options, employing the approximated analytic expression of P.H. Purdie and J. Fletcher and the finite-difference scheme introduced by J. de Urquijo et al., have been supplemented by

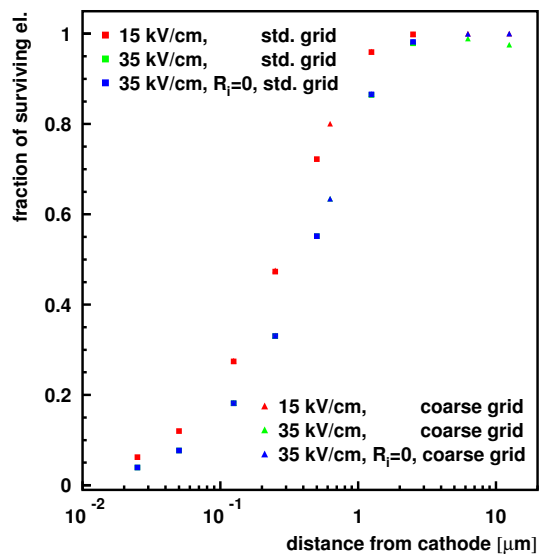


Figure 2. Fraction of surviving electrons f_s , after back diffusion has become negligible, as a function of the initial cloud position inside the gap z_i . A 1 mm gap filled with Nitrogen at atmospheric pressure and room temperature ($T = 300$ K), as in Fig. 1, has been chosen.

a new finite-difference scheme, first introduced here, generalising the Crank-Nicolson one to the present case. Although more demanding in terms of the number of arithmetic operations involved, its unconditional stability allowed a detailed investigation of back diffusion to the cathode.

Finally, the agreement between the approximate analytic and the exact numerical solutions is so good, that it has been decided to use directly the former to fit the measured signals. More results concerning this part of the code will be presented in the future.

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