NONSTATISTICAL MODELS OF DISCHARGE DEVELOPMENT

For many years there has been great interest in trying to predict theoretically the growth of a gaseous discharge from its initiation to the stage where currents of many amperes may be flowing and the gas has undergone a rapid transition from the insulating to the conducting state.

The basic problem is that a self-consistent description of processes associated with the discharge development must take into consideration the collective interaction between the charged particles via the space-charge fields, i.e., the fields produced by the space charge generated in the gap must be taken into account. In general, the space charge is characterized by large density gradients and dynamics range. In such conditions the gas properties such as the ionization coefficient and electron drift velocity are not more in equilibrium with the electric field. In a consequence of this detailed information on discharge development in these conditions can be obtained only from a non-equilibrium electron distribution function. The distribution function can be found using a Monte Carlo technique or by the solution of the Bolzmann equation.

When the Monte Carlo technique is used for solving the dynamic behaviour of the electrons the simulation is divided into small time sections. An initial group of electrons, with specified energy distribution, is started from the cathode in random directions toward the anode. Each electron and the secondaries generated by ionization collisions with the gas molecules are tracked until the end of the time section, when a new sections begins, with the electrons present at the end of the section as primary electrons, etc. In a very short time, however, the number of electrons in the assembly grows to unmanageable proportions for further simulations. To avoid this limitation, a procedure must be used that transforms the existing large electron assembly into another consisting of less test particles.

In the Boltzmann equation

$$\frac{\partial f_j}{\partial t} + v.\frac{\partial f_j}{\partial x} + \frac{q_j}{m_j}.(E + v \times B).\frac{\partial f_j}{\partial v} = \sum_k C_k . f_k \qquad (1)$$

a distribution function f_j (x,v,t) is defined for each species in the discharge, such that $f_j$dxdv represents the number of particles of species j contained in the volume in the velocity-space defined by x ± dx, v ± dv at time t. In the equation (1) q_j and m_j are the particle charge and mass, E and B are the local electric and magnetic fields respectively and the operator C_k describes all collisional processes (elastic and inelastic) experienced by the particles of species k resulting in changes to f_i . The greatest problem in the application of the Bolzmann equation is the lack of data regarding cross sections. Also, the solution of BE for many kinds of particles needs inordinately long computing time. This is why a large number of models have concentrated on noble gases for which a great deal of information on important processes is known.

Due to the metioned obstacles in the applications of the above mentioned kinetic models ((*see also "particle in cell" method* https://boltzplatz.eu/intro-particle-in-cell/) simplified models have been introduced, which usually attempt to describe discharge development in terms of the continuity equations that must be satisfied to ensure charge conservation of each particle species active in the discharge. Such discharge models are based on the continuity and momentum transfer equations coupled with Poisson`s equation. The transport coefficients (drift velocity, diffusion coefficient, and ionization coefficient) which are involved in these

equations depend, in fact, on the local velocity distribution function which is unknown. However, one generally assumes that the local distribution function depends only on the local electric field. Consequently, the transport coefficients are considered to be represented by the conventional Townsend parameters and determined by the local value of the ratio electric field/gas number density (E/N), i.e, it is supposed that any swarm of charged particles comes almost instantaneously into a dynamic equilibrium. This assumption in usually termed as "local field approximation" or "equilibrium approximation".

This classical equilibrium approach has provided a basic insight into discharge behaviour, however the local field approximation becomes questionable when the space variations of the electric field over an electron mean free path are large.

A typical example is the cathode fall region of a glow discharge, where because of the strong field gradient the electrons are not longer in equilibrium with the electric field. If the electrons leaving the cathode are emitted with low energy, then no ionisation can occur until their energy has increased sufficiently, by acceleration in the electric field to exceed the ionization energy of the parent gas molecules. Thus α_{eff} at the cathode is zero, whereas "equilibrium α" gives too large values because this is the point where the field tends to a maximum as the discharge current grows, which is illustrated in Figure 2 for the cathode region of a normal glow discharge in Ar at 1 Torr (Tran Ngoc An, E. Marode, P.C. Johnson: **J.** Phys. D: Appl. Phys., Vol. 10, 1977:

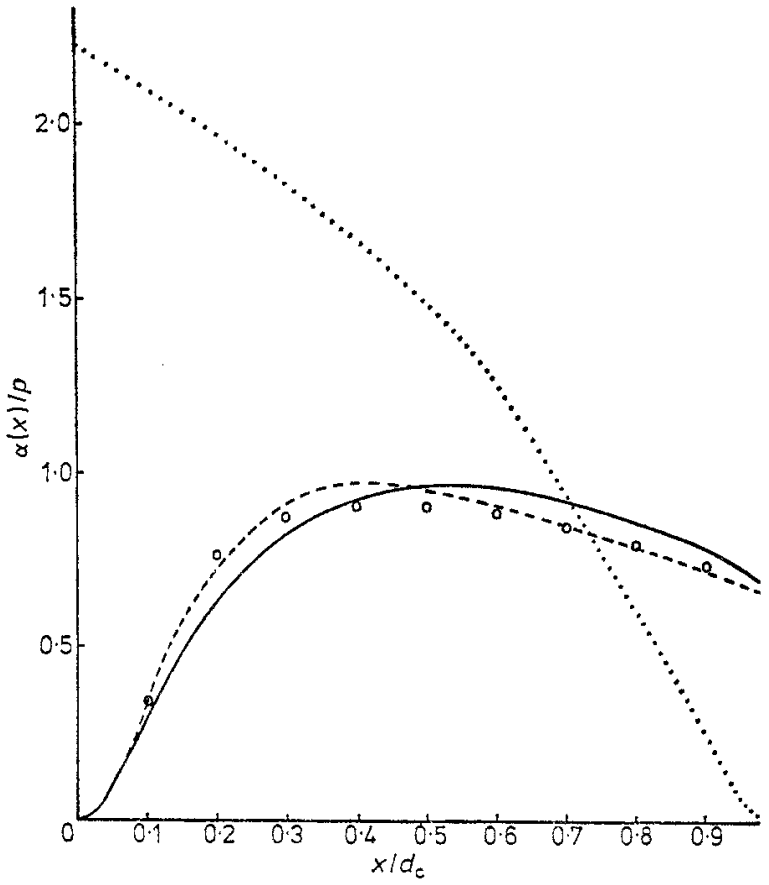

Figure 2. α coefficient from the Monte Carlo results (○) compared with values computed from equation (17) (. . .), from the solution to the differential equation (18) (———), and from the approximation (19) (– – –).

(17) $$\frac{\alpha(x)}{p} = 6{\cdot}5 \exp\left[-16{\cdot}4\left(\frac{p}{E(x)}\right)^{1/2}\right]$$

high or varies rapidly in space (for example in a streamer head and in nonuniform-field geometries), it is no longer permissible to assume instantaneous equilibrium of the charged particles with the field and it is necessary to introduce modified models which take into account non-equilibrium effects. As already indicated, these models have used Monte-Carlo methods or solutions of the Boltzmann equation to simulate the discharge growth, but recently possible extension to the macroscopic simulation techniques have also been put forward.This is based on the use of so-called "electron beams models".

In the equilibrium hydrodynamic model, for the case where the operative gas ionising processes are primary ionisation by electron impact and electron attachment, (neglecting, for example, detachment, recombination, and photoionisation), the evolution of gas discharge can be determined from the following set of equations:

$$\frac{\partial N_e}{\partial t} + \nabla . N_e v_e = \alpha . N_e . v_e - \eta . N_e v_e + S_p \qquad (2)$$

$$\frac{\partial N_p}{\partial t} = \alpha . N_e v_e + S_p \qquad (3)$$

$$\frac{\partial N_n}{\partial t} = \eta . N_e v_e \qquad (4)$$

where (2),(3),and (4) are the continuity equations for electrons, positive and negative ions, respectively, and N_e : electron density, N_p : positive ion density, N_n : negative ion density, v_e : electron fluid velocity, and η: electron attachment coefficient. The electron fluid velocity is determined from the expression:

$$N_e . v_e = -D . \nabla N_e - \mu_e . N_e . \left(E_s + E_o\right) \qquad (5)$$

where D is the diffusion tensor for electron with components D_L and D_T (the longitudial and transverse diffusion coefficient), μ_e is the electron mobility, and E_s and E_o are the space-charge and applied field, respectively. The space-charge field is determined from Poisson`s equation:

$$\nabla . E_s = \frac{q}{\varepsilon} . \left(N_p - N_e - N_n\right) \qquad (6)$$

where q is the elementary charge and ε is the dielectric constant.

To solve the above equations it is necessary to specify the boundary conditions at the electrodes, and we must thus consider the possible secondary ionisation processes that can occur at the cathode. In general the current density of electrons leaving the cathode ($J_e = N_e . v_e$) is:

$$J_e(x=0,t) = J_o(x=0,t) + \sum J_r(x=0,t) \qquad (7)$$

where J_r is the current density produced by the r-th secondary process and J_o is an externally generated source of cathode electrons (e.g. due to ultraviolet illumination).

If electrons are emitted from the cathode by the incidence of positive ions a term

$$\gamma_i . J_{i+}(x=0,t) \qquad (8)$$

appears on the right hand side of eqn.7 where γ_i is the probability of electron emission per incident ion.

Note: A slow ion, approaching a metal surface with thermal velocity, distorts the potential barrier by reason of its electric field and gives electrons in the upper Fermi levels an opportunity to tunnel through the barrier. In order that electron emission shall be observed, two electrons must leave the metal, one of which neutralizes the ion. The total energy reguired to extract the electron is $2q\phi$ (where ϕ is the work function), and the energy available is the potential energy of the ion eV_i .The process is thus only possible when $V_i > 2\phi$. If the ions are fast, i.e., having kinetic energy as well as potential energy, their effectiveness in releasing electrons is only slightly increased on clean metal surfaces indicating that under common conditions the chief mechanism is due to the distortion of the surface potential barrier.

Similarly, if electrons are produced by the incidence of non-resonance photons then , in the one-dimensional approximation describing parallel-plane geometry of electrodes,a term

$$\gamma_p . \int_o^d \alpha . n_e . v_e . dx \qquad (9)$$

(where d is the gap separation) must be added to (6), where γ_p is defined to be the probability of electron emission by photoemission per ionising collision in the gas. The expression (8) presumes immediate decay of excited gas molecules. If photons have a delay time τ (due, for example, to the finite lifetime of the excited states) then the term

$$\frac{\eta_p}{\tau} . \int_o^t \exp\left[-\frac{(t-t')}{\tau} \right] . \int_o^d \alpha . n_e . v_e . dx . dt' \qquad (10)$$

would appear (assuming the delay times to have an exponential distribution). Note that a decrease in γ_p with increasing gas pressure is characteristic of a photon secondary effect, which is reduced by increased collisional quenching of photon-emitting excited states and absorption of photons in the gas. The decrease may also be due to increased electron attachment near the cathode surface.

In expressions (9) and (10) it is implicitly assumed that the electrodes are of infinite size so that γ_p is independent of the position in the gap that excited atoms are created. Thus, to take into account a more complex gap geometry and the photon absorption, it would be more logical to write (9) and (10) in terms of the excitation coefficient α_{ex} corresponding to α when they become:

$$\frac{\Gamma_p}{\tau} \int_o^d \alpha_{ex} . n_e . v_e . dx \qquad (11)$$

and $$\frac{\Gamma_p}{2.\tau} . \int_o^t \exp\left[-\frac{t-t'}{\tau} \right] . \int_o^d \alpha_{ex} . n_e . v_e . dx . dt' \qquad (12)$$

where Γ_p the photoelectric efficiency of the cathode, is now the number of secondary electrons produced per incident photon. The factor 1/2 is appears because, for infinite parallel electrodes, each photon emitted by an exited atom will have a probability 1/2 of reaching the cathode.

Experimentally it is found that if J_o (t) is constant (see equation (7)) and the gap voltage is less than the discharge onset voltage V_s , then the current flowing between the electrodes remains constant in time and the steady-state current densities can be found by setting the left-

hand sides of eqns. 2 to 4 equal to zero. In one-dimensional approximation the resulting expression for the current density at the anode is

$$J = J_o \cdot \frac{\left[\exp\{(\alpha - \eta).d\} - \frac{\eta}{\alpha} \right]}{\frac{\alpha - \eta}{\alpha} - \gamma_T \cdot \left[\exp\{(\alpha - \eta).d\} - 1 \right]} \qquad (13)$$

Eqn. 13 is the well-known Townsend steady-state equation and $\gamma_T = \gamma_i + \gamma_p$ is the generalized Townsend secondary ionisation coefficient. This relation is the basis of most of the steady-state experiments which have been used to determine the coefficients α, η and γ_T.

For temporally growing discharges, however, no exact formal solution of the continuity equations (except the work of Davidson (Brit.J.Appl.Phys.4, 1953), where space-charge field was not taken into account) and it is necessary to use modern computational techniques to obtain numerical solutions.