

# The one-particle approximation in the reflecting discharge simulation

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**Abstract.** The method of some reflecting discharge (Penning discharge) characteristics computation, based on the one-particle approximation is proposed. This discharge is widely used in ion sources aimed at surface modification. However, only the steady state of this discharge is sufficiently described, whereas pulsed modes are preferable in many cases. In fact, the proposed method is similar to the approach used in the early times of first glow discharge investigations and crossed fields ion sources. It may be applied for the early discharge stages (the Townsend regime) description. It is somehow simpler than the diffusion-drift approximation used as a rule for the stationary state description, because plasma does not exist yet. On the other hand, one need not use most of usual diffusion-drift simplifications e.g. 1 or 2D models, uniform magnetic field etc. So the process of discharge formation may be described exactly for different kinds of Penning cells geometries and fields configurations. The discharge ignition condition for the Penning cell, analogous to the Townsend law is evaluated. It allows one to appreciate the discharge formation time as a function of cell geometric parameters, field configurations, anode voltage and Townsend’s coefficients  $\alpha$  and  $\gamma$ . This time, or exactly the trajectory length during this time, plays the role of the Townsend parameter  $d$  – the distance between electrodes. The calculated values of such times show good agreement with experimental data.

## 1. Introduction

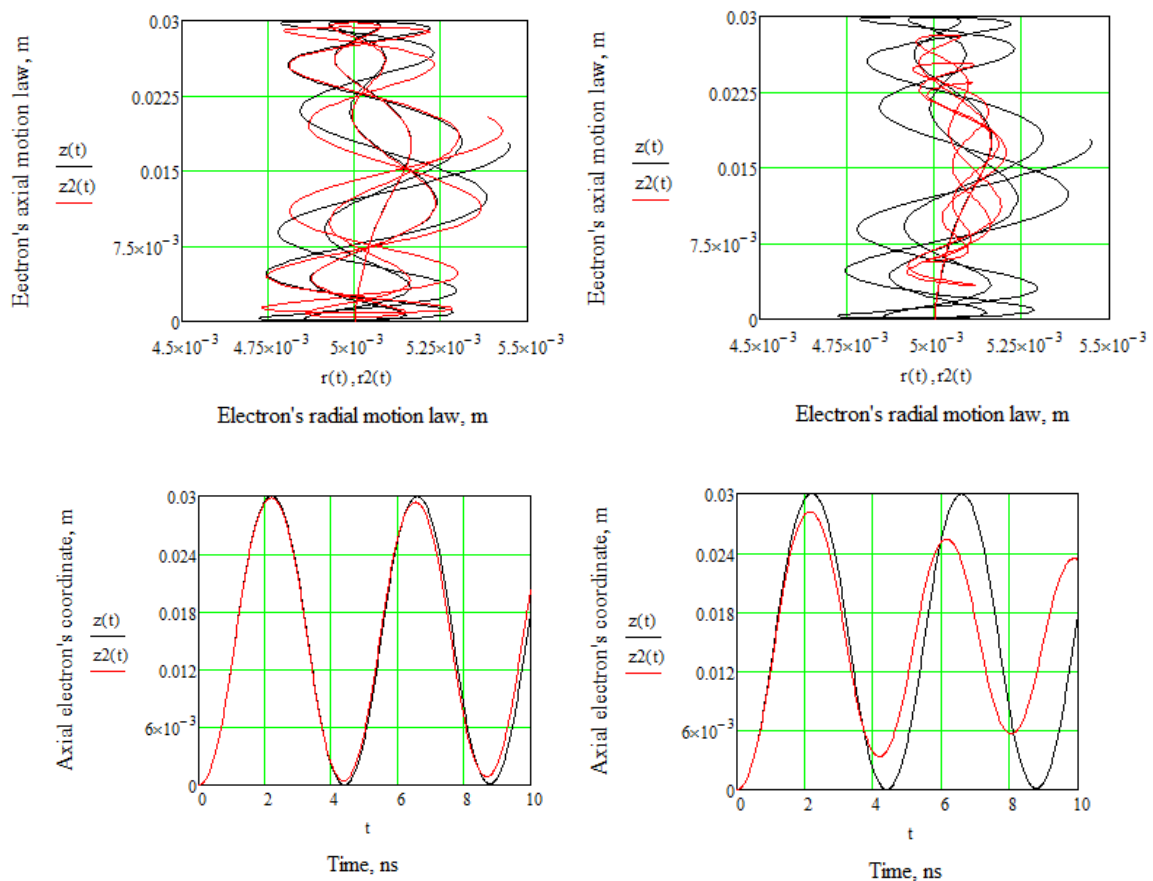
The diffusion-drift approximation used as a rule in Penning discharge simulation [1-3] allows one to evaluate key dependencies of the discharge characteristics upon the process parameters in a steady state. However, the initiation or discharge formation regime is quite interesting for some applications. Its adequate description is important from the fundamental point of view too. On the other hand, such description is somehow simpler than the one for the steady state as plasma does not exist yet and fields are not disturbed by free charges and currents. Charge trajectories may be easily calculated exactly even including “friction” due to charge-neutral collisions. Moreover, in the Townsend mode, when plasma does exist, charges do not disturb fields significantly. That is why the so called “one-particle approximation” may be used allowing one to calculate the exact trajectory. It makes possible to give the proper formulation of the discharge ignition condition analogous to Townsend’s law because in a Penning cell one need to employ the trajectory length instead of the inter-electrode distance and consequently to determine the time needed to strike the discharge.



## 2. The calculation of non-uniform fields and electron trajectories in a Penning cell

The calculation of the electrostatic field  $\mathbf{E}$  distribution implies the Laplace equation solution with the constant scalar potential  $\varphi(\vec{r})$  boundary conditions on metallic surfaces and calculated on the basis of the “image method (mirror-image method)” on dielectric ones. The solution for the simple Penning cell geometry in series expansion form is given in [4, pp 490-491]. The magnetic fields  $\mathbf{B}$  as well as vector potential are also calculated by the instrumentality of series expansion with known (measured)  $\mathbf{B}$  axial component [5]. The three terms approximation of the vector potential is quite approved. It is not evident *apriori* which field is better (from the discharge ignition time viewpoint) – uniform or nonuniform creating magnetic traps, “plugs” etc.

The electron trajectories calculation in the residual atmosphere is performed according to nonrelativistic equation of motion:  $m\dot{\vec{v}} = e\vec{E} + e[\vec{v}, \vec{B}] - m\nu_m \vec{v}$  (by inserting the transport cross-section  $\nu_m$  – [6], system SI, cylinder coordinates, electron starting from cathodes). The deceleration due to the ionization is not separated in this equation from other processes but the ionization frequency is much smaller as a rule than the transport one [6]. But the transport frequency itself in the case of the Penning cell is much smaller than the electron oscillation frequency. For example, the hydrogen transport frequency is  $\nu_m = 4.8 \cdot 10^9 \text{ s}^{-1}$  [6], that is around 5 MHz at 10 mTorr which is significantly smaller (three orders of magnitude) than the oscillation one and even more the cyclotron frequency.

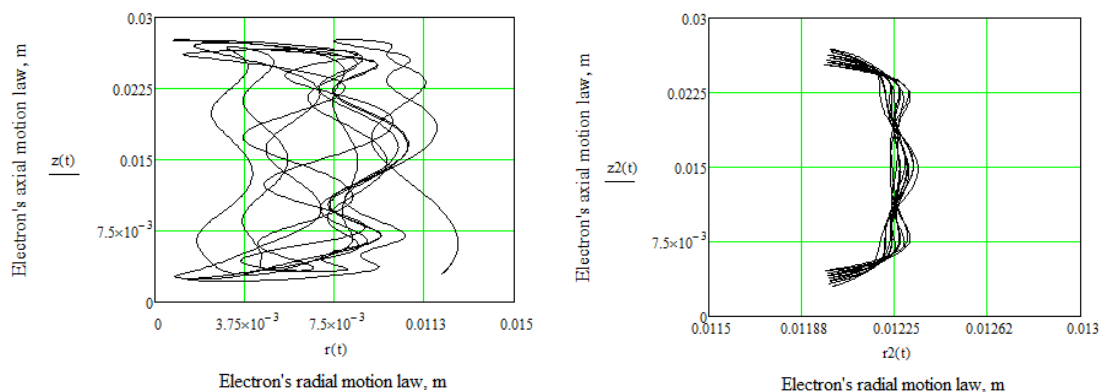


**Figure 1.** The electron trajectories and motion laws along the Z axe in the Penning cell taking into account the friction (red lines) and without friction (p=2 mTorr – left, 20 mTorr – right).

Figure 1 shows the projections of the electron trajectories  $z(r)$  and  $z2(r2)$  on the  $\{r,0,z\}$  plane as well as their motion laws  $z(t)$ ,  $z2(t)$  calculated according to the solution mentioned above [4, pp 490-

491]. The geometrical parameters of the cell are as follows: radius – 1 cm, length – 3 cm, anode height – 5 mm. The anode potential – 2 kV. The initial conditions are as follows: an electron starts from the cathode point 5 mm aside from its axis with zero initial velocity in the uniform and constant magnetic field 50 mT. The motion laws are given taking account the friction (index 2) and without it with the transport frequency  $10^7$  Hz (left plots) which approximately corresponds to 2 mTorr pressure. It is seen that the oscillation period is of 4 ns order whereas the cyclotron period for such an induction is only 0.715 ns. So during the oscillation period an electron makes approximately 6 turns around its trajectory. On the right plots, the trajectories and motion laws are given for the case when the transport frequency is equal to  $10^8$  Hz, corresponding to 20 mTorr pressure – an order of magnitude greater. The difference is well seen but as in the former case, it influences only the oscillation damping decrement but practically does not change its period. Consequently, one may not take into account the friction due to different collisions in the electron trajectories calculation in the before-discharge stage.

The magnetic field nonuniformity introduces naturally big changes in the trajectory forms. The examples of the electron trajectory at hydrogen pressure 1.5 mTorr calculated in uniform and nonuniform fields are shown in figure 2. The electron trajectories starting from the point ( $r=12$  mm,  $z=3$  mm) calculated during 40 ns are shown: in the 29 mT uniform (equal to the averaged across the cell nonuniform field) – at the right, and nonuniform magnetic field – at the left. It is well seen that in the nonuniform field the electron moves practically across the whole cell volume, its trajectory is much longer than in the case of the uniform field. In the uniform magnetic field electron oscillates practically along the straight line declining from it towards anode only by few mm tenths.



**Figure 2.** The trajectories of electrons starting from the same cathode point in the uniform (at the right) and nonuniform magnetic fields,  $U_{an}=800$  V.

### 3. The Penning discharge ignition condition

The discharge ignition condition (the Townsend rule) [5]:  $\gamma(\exp(\alpha d) - 1) = 1 \Rightarrow \alpha d = \ln(1/\gamma + 1)$  in which Townsend's coefficients are implied –  $\alpha$  (ionization) and  $\gamma$  (or generally  $\Gamma$ ), characterizing the secondary ion-electron emission as well as other near electrodes electron generation processes and the inter-electrode distance –  $d$ , cannot be used in the genuine form and must be modified. The Penning cell differs significantly from the two parallel flat infinite electrodes investigated by Townsend. That is why the inter-electrode distance –  $d$  in the Townsend's law must be substituted by the trajectory length  $L(t)$  along which an electron generated on the cathode (or anticathode) moves oscillating between cathodes until it recombines or falls on the anode. However, the whole current is not determined by these “falls”, as in the parallel flat electrodes system.

While determining the ignition time one has to calculate the trajectory length during the given time interval. Besides, as the 1<sup>st</sup> Townsend's coefficient strongly depends upon the electron energy which is the function of the cell point (or the time if trajectories are time parameterized) the integral must be in the exponent instead of the simple product  $\alpha l$ . The 2<sup>nd</sup> Townsend's coefficient –  $\gamma$  – depends upon the

electron energy too, but because of the weak (logarithmic) dependence of the Townsend's law may be taken constant. Finally, one has to take into account the fact that the trajectory type and length may largely depend on the start point (distance from the cathode axis) and the whole current is the integral upon the cathodes surfaces.

All these circumstances urge one to modify the ignition condition this way:

- It is not the current density that must become infinite in the arbitrary point of the infinite cathode, but the whole electron current from the cathode and anti-cathode, in some points the density may be zero;

- The ions generated in the cell's part (half for symmetric) adjacent to the cathode may fall only on the cathode, not anti-cathode because of their small initial energy and large anode potential, the same for the cell's part adjacent to anti-cathode;

- In the last case one has to account the fact that part of them quit the cell through the exit orifice, which will not generate secondary electrons from anti-cathode.

Assuming the knowledge of the  $\alpha$  dependence upon the energy let us repeat the Townsend law evaluation taking into account the proposed obvious amendments. However, the Townsend's 1<sup>st</sup> coefficient explicit form  $\alpha = A \cdot p \cdot \exp(-Bp/E)$  does not suit. One has to approximate experimental dependencies by some appropriate functions. For example, the  $H_2$   $\alpha$  dependency [6] upon the electron energy may be approximated by the sum of the parabola and exponent.

The electron motion law knowledge allows one to write the explicit form of such an approximation and the whole ionization probability as time functions:

$$\alpha_{apr}(t) = \alpha_{apr}(T_{kin}(t)) = \alpha_{apr}((\dot{r}(t))^2 + (\dot{z}(t))^2 + (r\dot{\psi}(t))^2), P_{ion}(\tau) = \int_0^\tau \alpha(t) \cdot p \cdot dl(t)$$

The electrons trajectories and consequently the ionization coefficients are the start point functions or the distance from the axis –  $r_0$  (for cathode) and  $\rho_0$  (for anti-cathode). Accounting for the point dependence of  $\alpha$  and different contributions of ions born in different cell parts in the secondary electrons generation on the cathode and anode let us introduce the short denominations for different integrals that will appear in the next evaluation:

$$In_{k,1}(r_0, \tau) = \begin{cases} \int_0^\tau \alpha(r_0, t) dl(r_0, t), & z \leq Lc/2 \\ 0, & z > Lc/2 \end{cases} \quad In_{k,2}(r_0, \tau) = \begin{cases} \int_0^\tau \alpha(r_0, t) dl(t), & Lc/2 < z \leq Lc \\ 0, & z < Lc/2 \end{cases}$$

$$In_{ak,1}(\rho_0, \tau) = \begin{cases} \int_0^\tau \alpha(\rho_0, t) dl(\rho_0, t), & Lc/2 < \zeta < Lc \\ 0, & \zeta < Lc/2 \end{cases} \quad In_{ak,2}(\rho_0, \tau) = \begin{cases} \int_0^\tau \alpha(\rho_0, t) dl(\rho_0, t), & \zeta < Lc/2 \\ 0, & Lc/2 < \zeta < Lc \end{cases}$$

Let us account now the possible difference in generalized 2<sup>nd</sup> Townsend coefficients for the cathode and anti-cathode introducing coefficients  $\Gamma_\kappa$  and  $\kappa\Gamma_{ak}$ . The  $\kappa$  coefficient describes the part of ions born in the anticathode cell half-part (they will be extracted in the acceleration gap). In the first approximation this coefficient may be taken as the cathodes surface area ratio. Repeating Townsend let us introduce the following functions to reduce the notations:

$$f_1(r_0, \tau) = \exp(In_{k,1}(r_0, \tau)) - 1, \quad f_2(r_0, \tau) = \exp(In_{k,2}(r_0, \tau)) - 1,$$

$$f_3(\rho_0, \tau) = \exp(In_{ak,1}(\rho_0, \tau)) - 1, \quad f_4(\rho_0, \tau) = \exp(In_{ak,2}(\rho_0, \tau)) - 1.$$

Then introducing initial currents from the cathode and anti-cathode –  $I_{k0}$ ,  $I_{ak0}$ , let us write the current expressions taking into account the electrons contributions on the cathode and anticathode ( $R_{ap}$  is the exit aperture radius):

$$2\pi j_k \int_0^{R_k} r0(1 - \Gamma_k f1(r0, \tau)) dr0 = I_{k0} + \Gamma_{ak} 2\pi j_{ak} \int_{R_{ap}}^{R_{ak}} \rho0 f4(\rho0, \tau) d\rho0$$

$$2\pi j_{ak} \int_{R_{ap}}^{R_{ak}} \rho0(1 - \kappa \Gamma_{ak} f3(\rho0, \tau)) d\rho0 = I_{ak0} + \kappa \Gamma_{ak} 2\pi j_k \int_0^{R_k} r0 f2(r0, \tau) dr0.$$

Solving this system of equations relatively to the current density on the cathode  $j_k$ , for instance, we will get the ignition condition as the coefficient at this density vanishing:

$$\int_0^{R_k} (1 - \Gamma_k f1(r0, \tau)) r0 dr0 \int_{R_{ap}}^{R_{ak}} (1 - \kappa \Gamma_{ak} f3(\rho0, \tau)) \rho0 d\rho0 = \kappa \Gamma_k \Gamma_{ak} \int_0^{R_k} f2(r0, \tau) r0 dr0 \int_{R_{ap}}^{R_{ak}} f4(\rho0, \tau) \rho0 d\rho0$$

This is the Penning cell ignition condition during  $\tau$  according to all assumptions made above. It is not so easily interpreted as the classical Townsend law and even hardly calculated if more simplifying assumptions due to the electrons and ions trajectories properties are not made. Fortunately, the calculations show that the ionization probability as a point function is almost constant (in contrast to trajectory length). It permits one to significantly simplify the ignition condition by retrieval of the averaged current density from the integral. Introducing the electrodes areas –  $S_k$  and  $S_{ak}$  and assuming  $\kappa = S_{ak}/S_k$  (for the 1<sup>st</sup> approximation) we will obtain this condition in such a form:

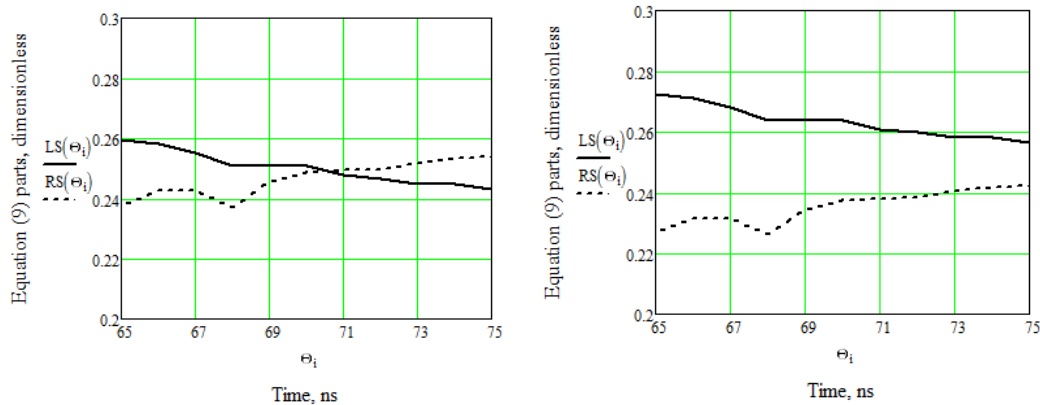
$$(1 - \Gamma_k f1(\tau))(1 - \frac{S_{ak}}{S_k} \Gamma_{ak} f3(\tau)) = \kappa \cdot \Gamma_k \Gamma_{ak} f2(\tau) f4(\tau) \quad (1)$$

As it can be easily seen besides the absence of the integration the condition does not contain the start point dependencies of the  $f_i$  but only the discharge ignition time  $\tau$  (because of the dependencies absence one can take the only one trajectory, e.g. with the start point in the middle of the distance from the axis). If the anti-cathode area tends to zero (for example if it is made from the high transparency mesh) the ignition condition becomes practically Townsend's:

$$(1 - \Gamma_k f1(\tau)) = 0 \Rightarrow \int_0^{\tau} \alpha(l) dl \Big|_{z \leq 0, 5L_c} = \ln(1 + \Gamma_k^{-1})$$

with a simple modification consisting in the interchange of the inter-electrodes gap  $d$  by the ignition time  $\tau$  and the integral is calculated in the cathode part of the cell. To solve graphically the equation (1) is to find out the crossover of its left side – LS(t) and right side – RS(t) (dimensionless) time dependencies – figure 3 (argument  $\Theta_i$  varies discretely – 0.5 ns per step – to truncate the calculation time,  $p=15$  mTorr). For example, the ignition condition is achieved during 200 ns in the symmetric cell (2 cm long, 2 cm diameter, 1 cm anode height) in hydrogen residual atmosphere (1.5 mTorr), magnetic induction 50 mT and anode potential 1 kV if cathodes areas are practically equal and  $\Gamma$  coefficients are equal to 0.514. If only the cathode secondary emission is accounted its value must be raised to a factor 3, that is approximately 1.5 to conserve the ignition time. So this time strongly depends upon the “integer” coefficients  $\Gamma$ . For the stainless steel electrodes and hydrogen pressure

around 1 mTorr the calculated ignition time is around 400 ns which agrees well with the experimental data.



**Figure 3.** Two examples of calculated plots with slightly different parameters ( $\Gamma_k=1.1$  – at the left,  $\Gamma_k=1.05$  – at the right).

Varying different cell parameters, residual pressure and anode potential one can see the ignition time dependencies upon these parameters. One need not every time find out the crossover of the (1) left and right hand sides plots – it takes too much time. To determine the trends, it is sufficient to investigate the dependence of the e.g. the right part upon these parameters during a rather short integration time. It is possible because the left side is always greater in the beginning. That is why the right side rise during given time at some parameter variation means the ignition time reduction and vice versa. One can also use the “two point linear approximation” of the equation (1) left and right sides, thus radically shortening the calculation, but it leads to greater ignition times. For instance, this approximation gives 88 ns ignition time instead of 70 ns in the figure 3 (left) example.

We need to note that with the one-particle approximation usage the calculation of the ignition and extinction potentials in the Townsend mode may also be done with the introduction of explicit dependence of the ionization coefficient on the electric field strength similar to the Townsend’s way with all modifications made above.

#### 4. Conclusion

The use of the one-particle approximation at the early Penning discharge stages simulation allows one to avoid numerous simplifications used in diffusion-drift models. Particularly the influence of nonuniform fields in asymmetric cells on the discharge formation rate and ignition/extinction potentials may be investigated numerically. The characteristic times and potentials may be calculated using the ignition condition introduced above analogous to the Townsend law for flat infinite electrodes system. This approach allows one to optimize different Penning ion sources parameters according to specific surface modification tasks.

#### References

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