A model for electron avalanches in SF6 with emphases on space charge effects

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A Model for Electron Avalanches in SF₆ with emphases on Space Charge Effects

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Summary

In the High-Voltage and EMC Group (EHC) of The Eindhoven University of Technology (EUT) research is being performed on electrical discharges in insulating gases. As a part of that research this master's study is concentrated on an SF₆ streamer model, which describes electron avalanches in SF₆, and their growth to breakdown.

Fundamental processes occurring in avalanches, such as ionization, strongly depend on the local electrical field, and thereby on the charge density. This space charge effect makes the set of coupled, partial differential equations, which describe the avalanche, strongly non-linear. In this work the set of equations is solved numerically. The resulting simulations make it possible to interpret experimentally observed current waveforms.

The simulation is performed with a program consisting of three parts. The first part is the transport routine which solves the differential equations by means of an algorithm termed Flux-Corrected Transport (FCT). This algorithm handles steep gradients with minimal numerical diffusion while maintaining numerical stability. Although the grid used by the simulation program is two-dimensional (axial and radial) only axial transport is taken into account. The second part of the program is the space charge field calculation routine. Here, power series expansions incorporating Legendre polynomials are used to accurately determine the field resulting from space charge at all locations in the gap. In the third part, the current induced by the motion of charge carriers is determined. These three subsections have been thoroughly tested with analytical and other numerical schemes resulting in a good agreement.

The processes incorporated in the model are electron and ion drift, electron diffusion, ionization, attachment and ion-ion recombination. In the simulated waveforms the space charge effect results in a broadening of the electron swarm, in a decrease in the time in which a current maximum is reached, and in an increase of the current amplitude. Also, it has been observed that a simulation with a fine spatial grid in the radial direction is more accurate in comparison to a one dimensional simulation, only when the swarm diameter is less than half the width of the gap. A few experimental waveforms have been compared with simulation results, confirming the effects of space charge.

Future work in this study should invoke:
- An extension of the program to include radial flow, and ion conversion processes.
- A more extensive comparison of experimental and simulated waveforms.
- A better understanding of the fundamental processes of avalanches in SF₆ so that a more complete description of the pre-breakdown and breakdown process can be obtained.
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1 Introduction

In the High-Voltage and EMC Group (EHC) of The Eindhoven University of Technology (EUT) research is being performed on electrical discharges in insulating gases. A part of this research is concentrated on electron avalanches in such insulating gases. In electron avalanches processes occur which may lead to eventual breakdown of the gas. Although these processes have been investigated for several decades, new insights into the mechanisms behind gas discharges have been obtained by the high time resolution of the experimental setup used in our laboratory.

The research dealt with in this master's thesis concerns electron avalanches in SF$_6$. The project was focused on the development and realization of a model that helps to explain the effects of space charge in electron avalanches in a uniform electrode system. The model developed takes into account the fundamental processes occurring in SF$_6$, solves the associated set of partial differential equations, and determines the space charge field at all locations in the gap. As of present, this appears to be the first work of this kind regarding a complete multi-dimensional study of the development of pre-breakdown conditions in SF$_6$. Although the work primarily involved computer simulations, some experiments were performed and have been presented to support the model.
2 Analysis of electron avalanches

2.1 Current induced by moving charges

The experimental setup that is used in this study consists of two parallel plates, a laser and a current measuring device (figure 1). A DC voltage is applied between the two plates creating a homogeneous electrical field whereby electrons present in the gap are accelerated eventually forming an avalanche. A pulsed nitrogen laser (FWHM 0.6 ns) focused at the center of the cathode is used to release the initial electrons. The motion of these free charges in the gap induces a time varying charge on the cathode surface inducing a current in the electrical circuit.

![Figure 1: the experimental setup.](image)

The complete setup is designed in such a way that the time resolution is small in comparison to the electron transit time (the time it takes an electron to traverse the gap). The transit time of an electron avalanche is of the order of tens of nanoseconds while the time-resolution is approximately 1.4 ns [Verhaart, 1982]. Because of the high time resolution or time response of the setup, it is possible to clearly determine the
beginning, development and exit of the electron avalanche. In order to do measurements at various pressures and various gases, the complete setup is placed in a vessel that can be evacuated.

Avalanches in SF$_6$ are studied in a homogeneous electrical field by measuring the current that is induced by the motion of charged particles. Supposing the diffusion negligible this current can be determined by using the energy equation.(1)

\[ U I(t)\, dt = q(t) \, E\, dx \]  

where:
- U = applied potential (V)
- I(t) = current in the external leads (A)
- q(t) = net charge of species (or particles) (C)
- E = electric field (V/cm) experienced by the charge

The current induced by one type of charged particle is:

\[ I(t) = \frac{en(t)vE}{U} \]  

where:
- v = electron or ion drift velocity in the field direction of the particle (cm/s)
- n(t) = number of particles (ions, electrons)
- e = coulomb charge (1.6X10$^{-19}$ C)

The total current induced by all the moving charged species can be calculated by summing the contribution of each charged species. The current induced by diffusion can be added separately to the drift current. The total current due to the motion of the charged species including diffusion, can be given by the integral:

\[ i(t) = \sum_{\text{species}} \frac{eA \, E}{U} \int_0^d \rho_i(x,t) \, v_i(x,t) + D_i(x,t) \frac{\partial \rho_i(x,t)}{\partial x} \, dx \]  

where:
- \( \rho_i(t,x) \) = density distribution of the charged particles (cm$^{-3}$)
  - (i = electrons, positive or negative ions)
- D = the diffusion coefficient (cm$^2$/s)
- A = the surface area of the charge distribution (cm$^2$)
- d = the gapwidth (cm)

By measuring the current, the development of an avalanche can be traced after its initiation. A more expanded theory about the induced current, which takes the Ramo-Shockly effect into account, is given in chapter four. Also in chapter four, the experimental setup will be presented and discussed in more detail.
One disadvantage in studying the temporal variations of the discharge current is that it doesn’t provide direct information about the distribution of the charge-carriers in the gap (figure 2). Some information regarding the spatial distribution of electrons can be obtained by studying the temporal behavior of electrons leaving the gap. When the charge is very locally concentrated, a sharp discontinuity occurs in the measured current waveform once the electrons have exited the gap (≈ 75 nsec., figure 2). On the other hand, if the electrons are spatially distributed (as in the case of large diffusion) a more gradual discontinuity is observed. The difficulty of extracting information from the measured current is the main reason why modelling and simulation is of vital importance in this study and will be discussed in more detail in chapter 3.
2.2 Processes occurring in an electron avalanche

What occurs in the gap after the first electrons are released? Immediately after release the electrons are accelerated by the applied field and collide with the background gas molecules. The width of the region whereby the electrons are accelerated is a function of the pressure (in vacuum this region is the width of the gap). At the pressures of interest this acceleration width is small compared with the gapwidth. After several collisions with the background gas a constant drift velocity, \( v \), in the direction of the field is reached. This drift velocity is superimposed on the random thermal electron velocity distribution. The thermal velocity shows a Maxwell-Boltzmann distribution.

Collisions of the electrons with the gas molecules can be either elastic or inelastic. In the elastic collision there is only an exchange of kinetic energy and momentum. The internal energy states of the particles involved remain the same. This is contrary to inelastic collisions where a part of the kinetic energy is used to increase the potential energy of the particle. The processes that occur in a gas in which an electrical field is applied resulting in net electron motion, will be described below [Wen, 1989].

When a gas molecule is excited by an inelastic collision, it is lifted to a higher energy state.

\[
e + AB \rightarrow AB^* + e
\]

excitation (4)

The excitation is energetically unstable and after a period of time the gas molecule will fall back to a state of lower energy by emission of a photon

\[
AB^* \rightarrow AB + hv
\]

emission (5)

or by transferring some of the excess energy to another gas molecule via a collision (quenching).

\[
AB_1^* + AB_2 \rightarrow AB_1^{*'} + AB_2^{*''}
\]

where \( *' \) energetic state + \( *'' \) energetic state = \( * \) energetic state (eV). The latter is the dominating process at higher pressures. When a molecule is excited to an energy level higher then the ionization potential, this results in the release of an electron. This process is called ionization. The excitation isn’t always necessarily due to a single inelastic collision, multiple inelastic collisions can occur before the ionization level is reached. Ionization can be described by the following reactions, where AB represents a gas molecule.
\[
e + AB \rightarrow AB^+ + 2e \quad \text{single ionization (7)}
\]
\[
e + AB \rightarrow A^+ + B + 2e \quad \text{dissociative ionization (8)}
\]

Here the molecule AB may already be excited by previous collisions. The ionization coefficient, \( \alpha \), is defined as the mean number of ionizing collisions for one electron per unit length travelling in the direction of the field (cm\(^{-1}\)).

**Attachment**, the capture of an electron by a neutral gas molecule may occur in three different ways as described by the following reactions:

\[
e + AB \rightarrow A^- + B \quad \text{dissociative attachment (9)}
\]
\[
e + AB \rightarrow AB^- \quad \text{non-dissociative attachment (10)}
\]
\[
e + AB_1 + AB_2 \rightarrow AB_1^- + AB_2^+ \quad \text{three-body attachment (11)}
\]

The last reaction can be seen as the result of two separate processes.

\[
e + AB_1 \rightarrow AB_1^- + AB_2 \rightarrow AB_1^- + AB_2^+ \quad (12)
\]

Two forms of the negative ion occur: stable and unstable. The difference between the unstable and a stable version is expressed in their respective lifetimes. The lifetime of a stable ion is significantly longer. This is a result of the structure of the molecule (or atom) which has attached the electron. The energy of an unstable negative ion is higher than that of its ground state configuration, while the energy of a stable negative ion is lower. The lifetime of a negative ion depends on the type of gas, pressure and field. It can vary between sub-picoseconds to several seconds. In addition, the unstable negative ion can convert to a negative ion of stable form. The attachment coefficient, \( \eta \), can be viewed as the sum of the attachment resulting in a stable negative ion, \( \eta_{st} \), and the attachment resulting in an unstable negative ion, \( \eta_{un} \). The attachment coefficient is given as the number of attachments per unit length travelled by an electron in the direction of the field (cm\(^{-1}\)).

An unstable negative ion can become stable via the following processes.

\[
AB_1^- + AB_2 \rightarrow AB_1^- + AB_2^+ \rightarrow AB_1 + AB_2^- \quad \text{conversion (13)}
\]

This stabilization process is called **conversion**. The conversion coefficient, \( k_c \), is defined as the number of conversions that occur per second per unstable negative ion (s\(^{-1}\)).
Electrons can be released by negative ions in various ways, this process is termed detachment. As mentioned above, unstable negative ions are more sensitive to this process than stable negative ions. The first detachment process mentioned is termed autodetachment whereby the unstable negative ion spontaneously loses its extra electron. Since no collision with another molecule (atom) is needed for autodetachment, detachment of this type cannot occur for stable negative ions.

\[ AB^{-\ast} \rightarrow AB + e \]  

autodetachment (14)

Collisions with neutral gas molecules can also force a negative ion to release its extra electron. This process can occur in various ways:

\[ AB_1^{-\ast} + AB_2 \rightarrow AB_1 + AB_2 + e \]  
direct detachment (15)

\[ A^{-\ast} + B \rightarrow AB + e \]  
associative detachment (16)

\[ AB_1^{-\ast} + AB_2 \rightarrow A + B + AB_2 + e \]  
dissociative detachment (17)

Detachment requiring collisions (15, 16, 17) is considered to be the most dominant mechanism under normal gas-discharge conditions [Schmidt and Van Brunt, 1982]. The detachment coefficient, \( k_d \), is defined as the number of detachments occurring per second per negative ion (s\(^{-1}\)).

**Photodetachment**, the release of the additional electron from the negative ion via photon absorption.

\[ AB^{-\ast} + \nu \rightarrow AB + e \]  
photodetachment (18)

In a gas discharge the photons are produced via excited molecules falling back to a lower state or via recombination. The former process is considered to be the most dominant.

Photons can also release electrons from neutral particles. The photo-ionization of the atoms comprising the cathode surface is the mechanism responsible for the initial release of the electron swarm in our setup (photoelectron-emission).
\[ h\nu + A \rightarrow A^+ + e \]

\[ h\nu + A \rightarrow A^+ + e \]

One of the conditions for photoelectron-emission is that the photons should contain more energy than the work-function of the cathode material. It's believed to be the mechanism causing a complete breakdown when the electrical field is below the critical field value for in nitrogen [Kennedy, 1993].

Another loss process is ion-ion-recombination. This process results in the formation of a neutral species via the collision of a positive and a negative ion. The recombination can be termed direct or indirect.

\[ AB^- + AB^+ \rightarrow AB^+ + AB^- \]

\[ AB^- + AB^+ \rightarrow (AB^- AB^+) \]

\[ (AB^- AB^+) \rightarrow AB_1 + AB_2 + AB_3 \]

The final loss process to be mentioned, is the neutralization of the various charged species at the electrodes. In response to the electrical field the electrons and negative ions drift toward the anode and the positive ions drift toward the cathode. Electrons and negative ions recombine at the anode with the positive net charge residing at the anode surface due to the applied field and to the repulsion of any negative charge by the proximity of the electrons and negative ions. Similarly, a positive ion will be annihilated at the cathode through recombination with the net negative charge resulting both from the applied potential and the attraction of electrons by the positive ions. A summary of the loss and gain processes is given in table 1.
Table 1: The loss and gain processes in the gap

<table>
<thead>
<tr>
<th>charge carriers</th>
<th>gain</th>
<th>loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>electrons</td>
<td>ionization ((\alpha))</td>
<td>attachment ((\eta)) neutralized at the anode*</td>
</tr>
<tr>
<td></td>
<td>photo-ionization*</td>
<td></td>
</tr>
<tr>
<td></td>
<td>detachment ((k_6))</td>
<td></td>
</tr>
<tr>
<td>positive ions</td>
<td>ionization ((\alpha))</td>
<td>neutralized at the cathode*</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ion-ion recombination ((k_r))</td>
</tr>
<tr>
<td>stable negative ions</td>
<td>attachment ((\eta))</td>
<td>neutralized at the anode*</td>
</tr>
<tr>
<td></td>
<td>conversion ((k_c))</td>
<td>ion-ion recombination ((k_r))</td>
</tr>
<tr>
<td>unstable negative ions</td>
<td>attachment ((\eta))</td>
<td>detachment ((k_6))</td>
</tr>
<tr>
<td></td>
<td></td>
<td>conversion ((k_c))</td>
</tr>
</tbody>
</table>

* these processes occur only at the metal surfaces

Most of the above mentioned processes are in a way dependent on the field strength or density or both. For example a two body collision process with a charged particle involved is linearly dependent on \(E/N\). The mean energy of an electron involved can be determined by looking at the electrical field as a force which accelerates an electron over a mean free path \(\lambda\)

\[
U_e = qE\lambda
\]  

(23)

where \(U_e\) is the mean energy of an electron, and \(q\) is the charge of an electron.

The mean free path is dependent on the reciprocal of the density \(N\) of the background gas molecules. Hence the energy is:

\[
U_e \propto \frac{E}{N}
\]  

(24)

In an avalanche having a low charge density the field will be constant and only depend on the voltage applied to the electrodes and the electrode separation (i.e. Laplacian field). Hence, the coefficients can be considered constant. At high charge densities however, the homogeneous field becomes distorted by a resulting space charge field which is superimposed on the Laplacian field. This distortion of the Laplacian field is termed: space charge effect. As mentioned above, because the coefficients depend on the electric field, they can no longer be considered constant during the spatio-temporal
evolution of an avalanche. Since the line integral of the total field must equal the Laplacian potential, it is quite possible that the front region of the avalanche experiences a velocity much higher than that in the back region and indeed this does occur. This causes the electron avalanche to grow in length. Similarly, because attachment decreases with increasing E/N while ionization increases, both ionization and attachment may occur in the same avalanche even when the (Laplacian field)/N value states that either one or the other occurs.
2.3 Theoretical description of an electron avalanche

The following coupled set of partial differential equations [Wen, 1989] describe the spatio-temporal growth of charges in the gap. One should keep in mind that the coefficients depend on the local field and pressure as described in section 2.2.

\[
\frac{\partial \rho_s}{\partial t} + \nabla (\rho_s v_s) = (\alpha - \eta_{nu} - \eta_{nm}) \rho_s |v_s| + k_0 \rho_{nu} - (\alpha - \eta_{nm}) D (\vec{v} \cdot \nabla \rho_s) + \nabla \cdot \nabla \rho_s \tag{25}
\]

\[
\frac{\partial \rho_p}{\partial t} - \nabla (\rho_p v_p) = \alpha \rho_s |v_s| - k_v \rho_p (\rho_{nu} + \rho_{nm}) - \alpha D (\vec{v} \cdot \nabla \rho_p) \tag{26}
\]

\[
\frac{\partial \rho_{nu}}{\partial t} + \nabla (\rho_{nu} v_{nu}) = \eta_{nu} \rho_s |v_s| - k_v \rho_p \rho_{nu} - (k_v + k_d) \rho_{nu} - \eta_{nu} D (\vec{v} \cdot \nabla \rho_p) \tag{27}
\]

\[
\frac{\partial \rho_{nm}}{\partial t} + \nabla (\rho_{nm} v_{nm}) = \eta_{nm} \rho_s |v_s| - k_v \rho_p \rho_{nm} + k_c \rho_{nm} - \eta_{nm} D (\vec{v} \cdot \nabla \rho_p) \tag{28}
\]

\[
\nabla \cdot \vec{E}_{sp} = e (-\rho_s + \rho_p - \rho_{nu} - \rho_{nm}) / \varepsilon_0 \tag{29}
\]

Where $\rho_s$ is the electron density (cm$^{-3}$); $\rho_p$ is the positive ion density (cm$^{-3}$); $\rho_{nu}$ is the unstable negative ion density (cm$^{-3}$); $\rho_{nm}$ is the stable negative ion density (cm$^{-3}$); $D$ is the diffusion coefficient of electrons in cm$^2$/s; $v_{s,p,nu,nm}$ are respective drift velocities; $E_{sp}$ is the space charge field (V/cm).

Detachment from stable negative ions, and ion diffusion are not included in this study. The metal surfaces are viewed as a transparent grid whereby the differential equations are solved in the area beyond so that the boundary conditions are properly handled. The current however, is only calculated for the region between the grids.

This set of equations may have no analytical solution because of the dependency of the coefficients on the density and the derivatives in time and space. Under the assumption that space charge effects can be ignored, by setting recombination to zero and stating that the initial electrons released are a delta function, the above set of equations can be solved analytically [Wen, 1989]. In this study, a numerical technique is used to solve this set of coupled, non-linear, partial differential equations.
In the numerical technique used in this study no difference is made between stable and unstable negative ions because of the limited amount of data on stable and unstable negative ions. This has the consequence that conversion has not been taken into account. Equation 27 and 28 can be rewritten to:

\[
\frac{\partial \rho_n}{\partial t} + \nabla (\rho_n \mathbf{v}_e) = \eta \rho_e |\mathbf{v}_e| - k \rho_e \rho_n - k \rho_n - \eta D \mathbf{v} \nabla \rho_n
\]  

where \( \rho_n \) is the negative ion density (cm\(^{-3}\)).
2.4 Processes in $\text{SF}_6$

In the following section $E$ is the local electrical field (V/m), $N$ is the background gas density (m$^{-3}$) and $T$ is the temperature (K).

In $\text{SF}_6$ ionization is a simple two body process in which an electron and a positive ion are formed.

$$e + \text{SF}_6 \rightarrow \text{SF}_6^+ + 2e$$  \hspace{1cm} (31)

The ionization coefficient, $\sigma$, is dependent on the pressure and field as shown in the following relation [Morrow, 1986]:

$$\frac{\sigma}{N} = \begin{cases} 
3.44 \times 10^{-24} \left( \frac{E}{N} \right)^{2.085} \text{m}^2, & \frac{E}{N} < 4.6 \times 10^{-19} \text{V} \cdot \text{m}^2 \\
11.269 \left( \frac{E}{N} \right)^{1.159} \text{m}^2, & \frac{E}{N} > 4.6 \times 10^{-19} \text{V} \cdot \text{m}^2 
\end{cases}$$  \hspace{1cm} (32)

The dominating attachment process in $\text{SF}_6$ is the formation of an unstable negative ion.

$$e + \text{SF}_6 \rightarrow \text{SF}_6^{--}$$  \hspace{1cm} (33)

The data on attachment show the following dependence on $(E/N)$ [Morrow, 1986]:

$$\frac{n}{N} = \begin{cases} 
2.0483 \times 10^{-20} - 0.25379 \left( \frac{E}{N} \right) + 1.4705 \times 10^{-18} \left( \frac{E}{N} \right)^2 - 3.0078 \times 10^{26} \left( \frac{E}{N} \right)^3 \text{m}^2, & 5.0 \times 10^{-20} < \frac{E}{N} < 2.0 \times 10^{-19} \text{V} \cdot \text{m}^2 \\
7.0 \times 10^{-21} \exp \left( -2.25 \times 10^{18} \left( \frac{E}{N} \right) \right) \text{m}^2, & \frac{E}{N} > 2.0 \times 10^{-19} \text{V} \cdot \text{m}^2 
\end{cases}$$  \hspace{1cm} (34)

The autodetachment process of these unstable negative ions has a large time constant (> 1 µs), so its role during an avalanche is not significant. More often the unstable ion collides with a neutral molecule, resulting in the following reactions: [Yicheng Wang et al., 1989; Teich].

$$\text{SF}_6^{--} + X \rightarrow \text{SF}_6 + e + X$$ collisional detachment (35)
The negative $\text{SF}_6$ ion can also collide:

$$\text{SF}_6^- + X \rightarrow \text{SF}_6 + F^- + X$$  \hspace{1cm} (36)

$$\text{SF}_6^- + X \rightarrow \text{SF}_6 + F + X$$  \hspace{1cm} (37)

As can be seen, the first equation of both sets are detachment processes while the others are conversion reactions. The above mentioned processes are the most important. More processes occur and are described in literature [Olthoff, 1989; O’Neill, 1973]. The process of photo-detachment in $\text{SF}_6$ is considered to be of minimal importance [Van Brunt, 1983].

A relationship between the detachment frequency with field and pressure has been extracted from measurements [Hilmert, 1991]. This relation is:

$$K_d = N \cdot 10^{(3.375 \times 10^4 \frac{E}{N} - 28.4)} s^{-1}$$  \hspace{1cm} (40)

Recombination in $\text{SF}_6$ is a two step process. The ions of $\text{SF}_6$ in this reaction are $A^+$ and $B^-$ while M represents a neutral molecule. The process can be represented by [Cornell, 1987]:

$$\text{SF}_6^+ + \text{SF}_6^- + \text{SF}_6 \rightarrow (\text{SF}_6^+\text{SF}_6^-)^+ + \text{SF}_6 \rightarrow 3\text{SF}_6$$  \hspace{1cm} (41)

The recombination coefficient is more or less independent on the E/N ratio [Cornell, 1986]:

$$K_r = 5.6 \times 10^{-6} \text{ cm}^3 \text{s}^{-1}$$  \hspace{1cm} (42)

Photo-ionization of a $\text{SF}_6$ molecule is described by the following reaction [Mitsuke, 1990]:

$$\text{SF}_6 + h\nu \rightarrow \text{SF}_6^+ + (6-k)F^- + e^- \quad (k \leq 5)$$  \hspace{1cm} (43)

Whether this is happening in an avalanche or not is not yet clear. It is also a question whether photons produced by the avalanche in $\text{SF}_6$ can release electrons from the metal surface. The result of photoelectron-emission from the cathode is observed as a second peak located at about two electron transit times in a discharge current.
waveform. In a previous study [Wen, 1989], a second peak was not observed, thus suggesting photoelectron-emission is of minimal importance in SF₆ discharges.

The electron velocity $v_e$, positive ion velocity $v_p$, and negative ion velocity $v_n$, are given by [Morrow, 1986]:

$$v_e = 1.027 \times 10^{10} \left( \frac{E}{N} \right)^{0.7424} \text{ m/s}$$

$$10^{-20} < \frac{E}{N} < 2 \times 10^{-18} \text{ Vm}^2$$

(44) 

$$v_p = \frac{P_0}{P} \frac{T}{T_0} E \cdot 6.0 \times 10^{-5} \text{ m/s},$$

$$\frac{E}{N} < 1.2 \times 10^{-19} \text{ Vm}^2$$

$$= \frac{P_0}{P} \frac{T}{T_0} E \cdot 1.216 \times 10^{-5} \ln \left( \frac{E}{N} \right) + 5.89 \times 10^{-4} \text{ m/s},$$

$$1.2 \times 10^{-19} < \frac{E}{N} < 3.5 \times 10^{-19} \text{ Vm}^2$$

$$= \frac{P_0}{P} \frac{T}{T_0} E \cdot -1.897 \times 10^{-5} \ln \left( \frac{E}{N} \right) - 7.346 \times 10^{-4} \text{ m/s},$$

$$\frac{E}{N} > 3.35 \times 10^{-19} \text{ Vm}^2$$

(45) 

$$v_n = \frac{P_0}{P} \frac{T}{T_0} E \cdot 1.89 \times 10^{32} \left( \frac{E}{N} \right)^2 + 5.3 \times 10^{-5} \text{ m/s},$$

$$\frac{E}{N} < 5.0 \times 10^{-19} \text{ Vm}^2$$

(46) 

Where $P_0 = 1013.25$ mBar and $T_0 = 273.16$ K.

The electron diffusion coefficient can be described by [Morrow, 1986]:

$$D = \frac{v_e}{E} \cdot 8.6488 \times 10^9 \left( \frac{E}{N} \right)^{1/2} \text{ m}^2/\text{s}$$

$$\frac{E}{N} < 6.5 \times 10^{-19} \text{ Vm}^2$$

Summarizing the above processes in SF₆ the following coefficients are considered important:

- Ionization, $\alpha$, is a two body process.
- Attachment, $\eta$, is a two body process forming an unstable negative ion with a long lifetime.
- Detachment, $k_e$.
- Recombination, $k_r$, is a two step process in which three particles are involved.
- All species drift velocities as well electron diffusion.
3 Simulation

As mentioned previously, the discharge current does not give direct information concerning the density and distribution of the charged (and uncharged) species present in the gap. Therefore, simulations are needed to comprehend the observed waveforms in the measurements.

The method used to simulate a discharge in \( \text{SF}_6 \) (or any gas type) will be described shortly. The problem of simulating an avalanche can be split into three distinct parts repeated for each time step:

1. calculation of the electrical field created by the charged particles;
2. solution of the continuity equations describing the spatio-temporal motion and growth of the particles;
3. implementation of the additional processes like boundary conditions, feedback mechanisms and calculation of the current.

The first step to be taken in writing the simulation program is how should the charges be represented and what kind of grid system should be used. The situation to be described is three dimensional but since swarms of charge carriers are presumed to have rotational symmetry about the direction of motion, a 2D grid is used. The charge-carriers are distributed over discrete rings about the axis of symmetry. (figure 3). Each ring is presumed to be uniformly filled with electrons and/or positive and negative ions.

![Set of rings](image)

**Figure 3:** The distribution of rings in the gap.
The simulation starts with electrons occupying the first set of rings immediately adjacent to the cathode. As long as the simulation time is less than the laser pulse time (0.6 ns) electrons are added to these rings. For each point on the grid the field due to the space charge is calculated (see section 3.2) and added to the Laplacian field. This resulting field is used to calculate the aforementioned coefficients that describe the spatio-temporal behaviour of the discharge. These coefficients are then used in the transport algorithm (section 3.1), which solves the continuity equation for each point at that certain moment in time. This results in an overall movement and subsequent growth or decay of the particle densities. The simulated discharge current is calculated with equation (3). Once all the data is calculated for that timestep, the time is incremented and the complete procedure begins again with the calculation of the field at each grid point.

Although the field calculation, and hence the coefficients, are defined in the \( r,z \) space only transport in the \( z \)-direction was studied. The main routines in the simulation program are explained in the following sections.
3.1 **Transport routine**

The partial differential equations previously described in section 2.3, in one dimension and without diffusion take the form:

\[
\frac{\partial p}{\partial t} + \frac{\partial}{\partial x}(p v) = S
\]

(48)

where S represents the source terms. Setting S = 0 equation (48) represents a waveform moving in the x-direction.

A problem in simulating the transport of such a wave is that the wave is discretized. As can be seen in the next figure (figure 4) the sampling of two identical waves may result in different numerical waves. This is termed the Gibbs error and can only be avoided by refining the discretization.

![Figure 4: Sampling of two identical pulses showing the Gibbs error.](image)

Another problem that occurs is that the shape of the pulse becomes altered due to other numerical errors that occur when the pulse is propagated. The steep gradients that comprise the pulse create a type of error termed dispersion. Several methods to solve equation (48) have been developed [Book, 1975][Boris, 1973]. The quality of these methods can be tested by simulating the propagation of a rectangular pulse through several timesteps after which a comparison with the original is made (table 2)[Book, 1975].
Table 2: Methods of pulse propagation and their resolution.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Mean absolute error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Donor cell</td>
<td>.260</td>
</tr>
<tr>
<td>Leapfrog (zero diffusion)</td>
<td>.245</td>
</tr>
<tr>
<td>Law-Wendorff (zero diffusion)</td>
<td>.175</td>
</tr>
<tr>
<td>Flux-corrected diffusion</td>
<td>.082</td>
</tr>
<tr>
<td>Flux-corrected donor cell</td>
<td>.064</td>
</tr>
<tr>
<td>Flux-corrected leapfrog</td>
<td>.074</td>
</tr>
<tr>
<td>SHASTA FCT (explicit)</td>
<td>.057</td>
</tr>
<tr>
<td>SHASTA FCT (implicit)</td>
<td>.049</td>
</tr>
<tr>
<td>SHASTA FCT (phoenical)</td>
<td>.052</td>
</tr>
</tbody>
</table>

The transport method used in the simulation program is selected on the following criteria:
- The densities should remain positive (stable)
- The total charge should be conserved
- It should propagate a pulse as accurately as possible.
- It should be easy to implement source terms

Flux corrected transport (FCT) easily satisfies these above requirements. Here we use a particular version termed phoenical SHASTA LPE flux-corrected transport [Boris, 1976]. The principle of flux-correction is explained in section 3.1.1 and the flux-correction used in the simulation is described in section 3.1.2. This version of FCT handles steep density gradients with minimal residual diffusion.

3.1.1 Flux-corrected transport

Rewriting equation (48) with $S=0$ the differential equation to be solved is:

$$\frac{\partial p}{\partial t} = -\frac{\partial pv}{\partial x} \quad (49)$$

The left hand side can be approximated by a simple upwind difference:
\[
\frac{\partial \rho}{\partial t} = \frac{\rho^{\text{new}} - \rho^{\text{old}}}{\Delta t}
\]  
(50)

The timestep \( \Delta t \) is chosen in a manner that the fastest particle always travels less than \( \Delta x \), where \( \Delta x \) is the spatial width between grid locations \( j \) and \( j+1 \).

\[
\Delta t < \frac{\Delta x}{v_{\text{max}}}
\]  
(51)

where \( v_{\text{max}} \) is the velocity of the fastest particle.

Because refining the spatial step \( \Delta x \) will increase the calculation time significantly, a term similar to the right hand side of equation (50) can not be used for the spatial gradient term in equation (49). To find a numerical solution to the right hand side of the equation, it is expanded into a Taylor series:

\[
f_{j+1} = f_j + \frac{df_j}{dx} \Delta x + \frac{1}{2} \frac{d^2f_j}{dx^2} \Delta x^2 + \frac{1}{3!} \frac{d^3f_j}{dx^3} \Delta x^3 + H.O.T.
\]  
(52)

\[
f_{j-1} = f_j - \frac{df_j}{dx} \Delta x + \frac{1}{2} \frac{d^2f_j}{dx^2} \Delta x^2 - \frac{1}{3!} \frac{d^3f_j}{dx^3} \Delta x^3 + H.O.T.
\]  
(53)

where H.O.T. stands for the Higher Order Terms, \( f = \rho v \), and the subscript \( j \) is the discrete position in the gap.

When equation (53) is subtracted from (52), an expression for the gradient can be found:

\[
\frac{df_j}{dx} = \frac{(f_{j+1} + f_j) - (f_{j-1} + f_j)}{2 \Delta x} - \frac{1}{3!} \frac{d^3f_j}{dx^3} \Delta x^2 + H.O.T.
\]  
(54)

This expression is only useful when the third and higher order terms are ignored. This however makes the solution unstable [Morrow, 1981][Oran, 1987]. To avoid this problem a second order term is added to replace the third and higher order terms. The second order term is derived by adding equations (52) and (53) ignoring the third and higher order terms. The expression for the gradient in equation (48) becomes:

\[
\frac{df_j}{dx} = \frac{(f_{j+1} + f_j) - (f_{j-1} + f_j)}{2 \Delta x} + K \frac{(f_{j+1} - 2f_j + f_{j-1})}{\Delta x^2}
\]  
(55)

where \( K \) is a factor in units of distance.

The complete description of equation 50 is:
\[ \frac{\rho_{\text{new}} - \rho_{\text{old}}}{\Delta t} = -\frac{1}{2\Delta x}
\left[ v_{j+\frac{1}{2}}(\rho_{j-1} + \rho_j) - v_{j-\frac{1}{2}}(\rho_{j-1} + \rho_j) \right] 
+ \frac{1}{\Delta x^2}
\left[ K v_{j-\frac{1}{2}}(\rho_{j-1} - \rho_j) + K v_{j+\frac{1}{2}}(\rho_{j-1} - \rho_j) \right] \] 

This can be rewritten into:

\[ \rho_{j_{\text{new}}} = \rho_{j_{\text{old}}} - \frac{1}{2}
\left[ \epsilon_{j+\frac{1}{2}}(\rho_{j_{\text{old}}} + \rho_{j+1}) - \epsilon_{j-\frac{1}{2}}(\rho_{j_{\text{old}}} + \rho_{j-1}) \right] 
+ \chi_{j+\frac{1}{2}}(\rho_{j_{\text{old}}} - \rho_{j+1}) - \chi_{j-\frac{1}{2}}(\rho_{j_{\text{old}}} - \rho_{j-1}) \] 

where

\[ \epsilon_{j+\frac{1}{2}} = \frac{v_{j+1/2}\Delta t}{\Delta x} \] 

and

\[ \chi_{j+\frac{1}{2}} = \frac{v_{j+1/2}\Delta t}{\Delta x^2} \] 

The factor \( K v_{i+\frac{1}{2}} \) can be regarded as a diffusion coefficient (units cm²/s). The added diffusion is necessary to maintain stability, but has as a consequence, diffusion like distortion of discontinuities.

The FCT routine first adds diffusion as outlined above and later on in the same timestep subtracts a part of this diffusion (antidiffusion). In this method first provisional values, \( \tilde{\rho}_{\text{new}} \), are calculated which are then used in the antidiffusion stage. Thus, the first step is:

\[ \tilde{\rho}_{j_{\text{new}}} = \rho_{j_{\text{old}}} - \frac{1}{2}\left[ \epsilon_{j+\frac{1}{2}}(\rho_{j_{\text{old}}} + \rho_{j+1}) - \epsilon_{j-\frac{1}{2}}(\rho_{j_{\text{old}}} + \rho_{j-1}) \right] 
+ \chi_{j+\frac{1}{2}}(\rho_{j_{\text{old}}} - \rho_{j+1}) - \chi_{j-\frac{1}{2}}(\rho_{j_{\text{old}}} - \rho_{j-1}) \] 

next, the correction is done in the antidiffusion stage

\[ \rho_{j_{\text{new}}} = \tilde{\rho}_{j_{\text{new}}} - f_{j+\frac{1}{2}}^{\text{ad}} + f_{j-\frac{1}{2}}^{\text{ad}} \] 

where

\[ f_{j+\frac{1}{2}}^{\text{ad}} = \mu_{j+\frac{1}{2}}(\tilde{\rho}_{j+1} + \tilde{\rho}_{j_{\text{new}}}) \] 

where \( \mu_{i+\frac{1}{2}} \) is a positive antidiffusion coefficient. Antidiffusion reduces the strong diffusion, but also reintroduces the possibility of instability. Therefore, if the amount of antidiffusion is too large instabilities occur and positivity is no longer maintained, but if it is too small numerical diffusion occurs resulting in a distorted waveform. To avoid such problems the antidiffusion is modified by a process that is called flux-correction.
The antidiffusion flux is corrected in such a manner that it will not generate new maxima or minima in the solution, but still reduces the numerical diffusion. The new antidiffusion stage will be then
\[ \rho_j^{\text{new}} = \rho_j^{\text{new}} - f_{j+\frac{1}{2}}^c + f_{j-\frac{1}{2}}^c \]  
(63)

where the corrected flux, \( f_{j+\frac{1}{2}}^c \), satisfies
\[ f_{j+\frac{1}{2}}^c = S \cdot \max \left[ 0, \min \{ S(\rho_{j+2}^{\text{new}} - \rho_{j-1}^{\text{new}}), \left| f_{j+\frac{1}{2}}^{\text{old}} \right|, S(\rho_{j-2}^{\text{new}} - \rho_{j-1}^{\text{new}}) \} \right] \]  
(64)

where
\[ S = \text{sign}(\rho_{j+1}^{\text{new}} - \rho_j^{\text{new}}). \]  
(65)

This procedure in limiting the flux ensures that the corrected flux cannot push \( \rho_i \) below \( \rho_{i+1} \), which would produce a new minimum, or push \( \rho_{i+1} \) above \( \rho_{i+2} \), which would produce a new maximum. In the next section this technique is used.

### 3.1.2 Phoenical SHASTA LPE flux-correction routine

In the presentation of the principal of flux-corrected transport in the previous section the source terms were not incorporated. The source terms are incorporated via a two step method and the diffusive and antidiffusive coefficients are chosen in such a way that the shift in phase is as low as possible (Low Phase Error (LPE)) [Boris, 1976]. The term ‘phoenical SHASTA’ refers to the way the antidiffusion flux is calculated. The complete procedure is described below.

In the first step the densities are transported over half the actual timestep after which new source terms are calculated. These are used in the second step where the densities are transported over the complete timestep [Boris, 1993]. The timestep is given by the following equation:
\[ \Delta t = \frac{K^i \Delta x}{v_{\text{max}}} \]  
(66)

where \( K^i \) is about 0.01, to ensure stability. The first step (t = ½Δt) is:

Advance the density and add the source term (which is dependent on the density):
\[ \rho_j^{\text{TI}} = \rho_j^{\text{old}} - \frac{1}{2} \epsilon_{j+\frac{1}{2}}^{\text{old}} (\rho_{j+1}^{\text{old}} + \rho_j^{\text{old}}) + \frac{1}{2} \epsilon_{j-\frac{1}{2}}^{\text{old}} (\rho_j^{\text{old}} + \rho_{j-1}^{\text{old}}) + \text{source}(\rho_j^{\text{old}}) \]  
(67)

Calculate the raw antidiffusion fluxes:
Apply diffusion:
\[ \rho_{j}^{TDI} = \rho_{j}^{TI} + \kappa_{j-\frac{1}{2}}(\rho_{j+1}^{old} - \rho_{j}^{old}) - \kappa_{j+\frac{1}{2}}(\rho_{j}^{old} - \rho_{j-1}^{old}) \]  

(69)

Limit the corrective fluxes:
\[ f_{j-\frac{1}{2}}^{cl} = S \cdot \max \left[ 0, \min (S(\rho_{j+1}^{TDI} - \rho_{j}^{TDI}), |f_{j-\frac{1}{2}}^{old}|, S(\rho_{j}^{TDI} - \rho_{j-1}^{TDI})) \right] \]  

(70)

\[ S = \text{sign}(f_{j-\frac{1}{2}}^{old}) \]  

(71)

Apply the antidiffusion:
\[ \rho_{j}^{new} = \rho_{j}^{TDI} - f_{j-\frac{1}{2}}^{cl} + f_{j-\frac{1}{2}}^{old} \]  

(72)

This half timestep calculation is done for electrons and all ions prior to implementation of step two.

The second step (t = \( \Delta t \)) is the same except for the calculation of the source term and the timestep:

\[ \rho_{j}^{T2} = \rho_{j}^{old} - \frac{1}{2}e_{j-\frac{1}{2}}(\rho_{j+1}^{old} + \rho_{j}^{old}) + \frac{1}{2}e_{j+\frac{1}{2}}(\rho_{j}^{old} + \rho_{j-1}^{old}) + \text{source}(\rho_{j}^{T}) \]  

(73)

\[ f_{j-\frac{1}{2}}^{old} = \mu_{j-\frac{1}{2}}(\rho_{j+1}^{T2} - \rho_{j}^{T2}) \]  

(74)

\[ \rho_{j}^{TD2} = \rho_{j}^{T2} + \kappa_{j-\frac{1}{2}}(\rho_{j+1}^{old} - \rho_{j}^{old}) - \kappa_{j+\frac{1}{2}}(\rho_{j}^{old} - \rho_{j-1}^{old}) \]  

(75)

\[ f_{j-\frac{1}{2}}^{cl2} = S \cdot \max \left[ 0, \min (S(\rho_{j+1}^{TD2} - \rho_{j}^{TD2}), |f_{j-\frac{1}{2}}^{old2}|, S(\rho_{j}^{TD2} - \rho_{j-1}^{TD2})) \right] \]  

(76)

\[ S = \text{sign}(f_{j-\frac{1}{2}}^{old2}) \]  

(77)

\[ \rho_{j}^{new} = \rho_{j}^{TD2} - f_{j-\frac{1}{2}}^{cl2} + f_{j-\frac{1}{2}}^{old2} \]  

(78)

The diffusion and antidiffusion coefficients are equal
\[
\begin{align*}
\chi_{\text{j}^{-1}} & = \nu_{\text{j}^{-1}} = \frac{1}{2}\left(1 + \frac{\Delta t}{6\Delta x^2}\right) \\
\epsilon_{\text{j}^{-1}} & = \frac{1}{2}\left(v_{\text{j}} + v_{\text{j}^{-1}}\right) \frac{\Delta t}{\Delta x}
\end{align*}
\] (79) (80)

As it can be seen this method is quite straightforward. Errors of less then 1\% have been obtained with regards to the incorporation of the source terms when compared to simple analytical solutions. In addition, incorporation to a multi-dimensional simulation is quite straightforward (not included in this study) using the FCT algorithms.

The source terms are calculated twice, the first time for equation (67) using the old densities, and the second time for equation (70) using the densities calculated after the first step (½\Delta t). The field is not recalculated for the second calculation of the source terms. These source terms are:

\[
S_{e,j} = (a_j - \eta_j)v_{e,j} \rho_{e,j} \Delta t + k_{e,j} \rho_{e,j} \Delta t
\] (81)

\[
S_{p,j} = a_j v_{e,j} \rho_{e,j} \Delta t - k_{i,j} \rho_{p,j} \rho_{n,j} \Delta t
\] (82)

\[
S_{n,j} = \eta_j v_{e,j} \rho_{e,j} \Delta t + k_{i,j} \rho_{p,j} \rho_{n,j} \Delta t
\] (83)

where \(S_{e,j}\) represents the source term of the electron transport; and \(S_{p,j}\) and \(S_{n,j}\) represent the source terms for the positive and negative ion transport respectively.

Electron diffusion is implemented by a term added onto the diffusion term of the transport routine, the diffusion term now becomes:

\[
\chi_{\text{j}^{-1}} = \frac{1}{2}\left(1 + \frac{\Delta t}{6\Delta x^2}\right) + \frac{D}{\Delta x^2} \Delta t
\] (84)

where \(D\) is the ‘real’ diffusion coefficient resulting from collisions with the background gas density.
3.2 Field calculation

The electrical field in the gap consists of two components, the Laplacian field induced by the voltage applied to the electrodes and the space-charge field created by the charged species in the gap. The Laplacian field, which is homogeneous, can be determined easily from the equation:

$$E_{lep} = \frac{V_{lep}}{d}$$ (85)

where $V_{lep}$ is the applied voltage and $d$ is the distance between the electrodes.

The space-charge field in the gap is determined using a routine that calculates the field at all locations in the gap due to each uniformly distributed ring of charge. The complete field is then the summation of all these individual fields. For the calculation of the field from one ring a mirror charge scheme is used to represent the electrodes which are assumed perfectly conducting (figure 5).

![Figure 5: Ring of charges with several image charges.](image)

In practice, two or three pairs of mirror images are sufficient to determine the field accurately (see section 3.4.2).
3.2.1 The field due to one ring of charge

The method used to calculate the space charge field will be discussed for one ring of charge. The overall field is the superposition of the contributions of all rings including the images. This calculation is done by initially determining the potential at the axis of symmetry and expanding the equation for the potential to the off-axis points with the use of Legendre polynomials. The electrical field is determined by taking the gradient of the potential. The calculation of the potential distribution (i.e. a scalar field) is done for a plane ring with a surface charge density \( \sigma \), an inner radius \( a \), and an outer radius \( a + \Delta a \). (figure 6).

![Diagram of a ring](image)

**Figure 6: Description of a ring**

The charge on a ring located between \( a \) and \( a + \Delta a \) of radius \( R \) is given by:

\[
dQ = \left[ (R + dR)^2 \pi - R^2 \pi \right] \sigma \\
= \left[ 2RdR + dR^2 \right] \pi \sigma = 2\pi \sigma R dR
\]

(86)

The potential of a point on the axis at a distance \( x \) from the ring is
Following the procedure used to determine the potential at all locations on and off the axis of symmetry from a distribution of charge having axial symmetry, equation (88) needs to be in the form [Arfken, 1985]:

\[
\phi(x) = \frac{\sigma}{2\varepsilon_0} \left( \frac{a^2}{r^2 + (a^2)^2 - (a^2)^2} \right)
\]

Equation (88) is in the spherical coordinate system.

Applying equation (89) to the problem suggests that equation (88) should be expanded into a power series of the binomial type. Equations (90),(91),(92) are the result of such an expansion. Notice that three discrete regions now exist.
x < a:

\[
\phi(x) = \frac{\sigma}{2\varepsilon_0} \left[ (a + \Delta a) \sum_{n=0}^{\infty} \left( \frac{x}{a + \Delta a} \right)^{2n} - a \sum_{n=0}^{\infty} \left( \frac{x}{a} \right)^{2n} \right]
\] (90)

a < x < a + \Delta a:

\[
\phi(x) = \frac{\sigma}{2\varepsilon_0} \left[ (a + \Delta a) \sum_{n=0}^{\infty} \left( \frac{x}{a + \Delta a} \right)^{2n} - \left| x \right| \sum_{n=0}^{\infty} \left( \frac{x}{x} \right)^{2n} \right]
\] (91)

x > a + \Delta a:

\[
\phi(x) = \frac{\sigma}{2\varepsilon_0} \left[ \left| x \right| \sum_{n=0}^{\infty} \left( \frac{a + \Delta a}{x} \right)^{2n} - \left| x \right| \sum_{n=0}^{\infty} \left( \frac{a}{x} \right)^{2n} \right]
\] (92)

Here \( \binom{1}{n} \) is the binomial coefficient of power 1/2.

Applying equation (89) to equation (90...92) and after rearranging terms, the required equations for the potential for locations on and off the axis of symmetry are:

r < a:

\[
\phi(r, \theta) = \frac{\sigma}{2\varepsilon_0} \left[ (a + \Delta a) \sum_{n=0}^{\infty} \left( \frac{r}{a + \Delta a} \right)^{2n} P_{2n}(\cos \theta) - a \sum_{n=0}^{\infty} \left( \frac{r}{a} \right)^{2n} P_{2n}(\cos \theta) \right]
\] (94)

a < r < a + \Delta a

\[
\phi(r, \theta) = \frac{\sigma}{2\varepsilon_0} \left[ (a + \Delta a) \sum_{n=0}^{\infty} \left( \frac{r}{a + \Delta a} \right)^{2n} P_n(\cos \theta) - r P_1(\cos \theta) - a \sum_{n=0}^{\infty} \left( \frac{r}{a} \right)^{2n-1} P_{2n-2}(\cos \theta) \right]
\] (95)

r > a + \Delta a

\[
\phi(r, \theta) = \frac{\sigma}{2\varepsilon_0} \left[ (a + \Delta a) \sum_{n=1}^{\infty} \left( \frac{r + \Delta a}{r} \right)^{2n-1} P_{2n-2}(\cos \theta) - a \sum_{n=1}^{\infty} \left( \frac{r}{r} \right)^{2n-1} P_{2n-2}(\cos \theta) \right]
\] (96)

It is to be noted that no convergence will occur when \( r = a \) or \( r = a + \Delta a \). The field in the \( r \) and \( \theta \) directions can be calculated by taking the gradient of the potential.
r < a:

$$\varepsilon_r'(r, \theta) = \frac{\partial \phi(r, \theta)}{\partial r} = \frac{a}{2\varepsilon_0} \sum_{n=0}^{\infty} \left( \frac{1}{2n} \right) 2n \frac{P_{2n}(\cos \theta)}{(r^{2n-1})} - \frac{r^{2n-1}}{(a+\Delta a)^{2n-1}}$$

(97)

$$\varepsilon_\theta'(r, \theta) = \frac{1}{r} \frac{\partial \phi(r, \theta)}{\partial \theta} = \frac{a}{2\varepsilon_0} \sum_{n=0}^{\infty} \left( \frac{1}{2n} \right) \frac{\partial P_{2n}(\cos \theta)}{\partial \theta} \left[ \left( \frac{r}{a+\Delta a} \right)^{2n-1} - \left( \frac{r}{a} \right)^{2n-1} \right]$$

(98)

a < r < a + \Delta a:

$$\varepsilon_r(r, \theta) = \frac{a}{2\varepsilon_0} \sum_{n=0}^{\infty} \left( \frac{1}{2n} \right) 2n \left( \frac{r}{a+\Delta a} \right)^{2n-1} P_n(\cos \theta) - P_1(\cos \theta)$$

+ \sum_{n=1}^{\infty} \left( \frac{1}{2n-1} \right) \left( \frac{a}{r} \right)^{2n} P_{2n-2}(\cos \theta) \right]$$

(99)

$$\varepsilon_\theta(r, \theta) = \frac{a}{2\varepsilon_0} \sum_{n=0}^{\infty} \left( \frac{1}{2n} \right) \frac{\partial P_{2n}(\cos \theta)}{\partial \theta} - \frac{\partial P_1(\cos \theta)}{\partial \theta} - \sum_{n=1}^{\infty} \left( \frac{1}{2n-1} \right) \left( \frac{a}{r} \right)^{2n} \frac{\partial P_{2n-2}(\cos \theta)}{\partial \theta} \right)$$

(100)

r > a + \Delta a:

$$\varepsilon_r(r, \theta) = -\frac{a}{2\varepsilon_0} \sum_{n=1}^{\infty} \left( \frac{1}{2n-1} \right) P_{2n-2}(\cos \theta) \left[ \left( \frac{a+\Delta a}{r} \right)^{2n-1} - \left( \frac{a}{r} \right)^{2n-1} \right]$$

(101)

$$\varepsilon_\theta(r, \theta) = \frac{a}{2\varepsilon_0} \sum_{n=1}^{\infty} \left( \frac{1}{2n-1} \right) \frac{\partial P_{2n-2}(\cos \theta)}{\partial \theta} \left[ \left( \frac{a+\Delta a}{r} \right)^{2n-1} - \left( \frac{a}{r} \right)^{2n-1} \right]$$

(102)

Transforming from spherical into cylindrical coordinates the electrical field in the z direction becomes:

$$\varepsilon'_z = \cos \theta \varepsilon'_r - \sin \theta \varepsilon'_\theta$$

(103)

Repeating the above procedure the net $\varepsilon'_z$ resulting from all the charges located in the gap can now be determined.
3.3 Determination of current

3.3.1 Current calculation

The current is given by the integral:

\[ i(t) = \sum_{\text{species}} \sum_{\text{rings}} \left( \frac{eA_{\text{ring}}F_{\text{RS}}}{U_{\text{RS}}} \int_{0}^{d} \rho_{i}(x,t)v_{i}(x,t) + D_{i}(x,t) \frac{\partial \rho_{i}(x,t)}{\partial x} \, dx \right) \]

where \( A_{\text{ring}} \) is the surface area of the ring involved, the subscript \( i \) expresses the type of species and \( F_{\text{RS}} \) and \( U_{\text{RS}} \) are respectively the Ramo-shockley field and potential (see section 4.1.1).

The integral is solved with the Simpson's rule. The gradient in the diffusion term is solved by backward differencing. The Simpson's rule can be defined as:

\[ \int_{x=0}^{d} \arg(x) \, dx = \frac{1}{3} \Delta x (\arg(0) + 4 \cdot \arg(\Delta x) + 2 \cdot \arg(2\Delta x) + 4 \cdot \arg(3\Delta x) + \ldots + \arg(d)) \]

where

\[ \arg(x) = \left[ \rho(x)v(x) + D\frac{\rho(x) - \rho(x-\Delta x)}{\Delta x} \right] \]

The contribution of the diffusion term to the total current is small but is included for completeness.
3.4 **Accuracy tests for program verification**

3.4.1 **Flux-corrected transport tests**

The transport routine can be tested by three features.
1. Are the particles transported with the correct velocity?
2. Are the coefficients handled correctly?
3. Does the routine conserve charge?
4. Is the residual numerical diffusion minimal?

The velocity can be checked by placing a rectangular pulse of electrons in the middle of the gap, set the space-charge field calculation off, and set all coefficients to zero. The electrons should now move with a constant velocity towards the anode. The velocity of the pulse should be constant and identical to the drift velocity for an electron. (figure 7). In addition condition 4 is checked by observing that the rectangular pulse keeps its original shape.

![Figure 7: Pulse before and after transport over 20 nsec.](image)

Accurate incorporation of the source terms can easily be checked by including only ionization in the above mentioned test for velocity. After the pulse has travelled a
time \( t \), the total amount of electrons is counted and should be equivalent to the result of:

\[ N(t) = N_0 \exp(a v t) \]  

(107)

where \( N_0 \) is the initial amount of electrons and \( N(t) \) is the amount of electrons after time \( t \). The initial number of electrons in the test was 2050, after \( t = 20 \) ns the amount of electrons grew to 15153. The velocity \( v \) is \( 2.0 \times 10^7 \) and the ionization coefficient set to \( \sigma = 5 \), using equation (107) this gives 15148 electrons. The deviation was thus 0.04%. Attachment was tested in a similar way (replace \( \sigma \) by \( \eta \)). Due to the increased complexity the other coefficients were not tested except for conservation of charge.

The conservation of charge test requires that the net charge located in the gap remains constant. The test is done by running the transport routine for about 20 nanosecond with again a block of electrons in the gap afterwhich the net charge is determined. Charge conservation requires that the net charge should be equal to the net charge of the initial electrons. In this test the charge of the initial electrons is \(-3.28 \times 10^{-16} \) C, and after 20 nanoseconds the net charge was still \(-3.28 \times 10^{-16} \) C.

### 3.4.2 Field calculation tests

The field calculation is tested in two ways. The result of a line-integral of the space charge field over the x-axis (from cathode to anode) should be zero. In addition, the resulting field from one ring located in the gap is compared with results of a field simulation program (ELECTRO) with the same configuration.

When the simulation program is running, it plots the results of the line integral of the first three rings on the screen, it also plots the space-charge fields graphically. In all the simulations the result of the line integrations were small compared to the applied potential.

The comparison with ELECTRO is done with the configuration shown in figure 8:
Figure 8: configuration of rings used in ELECTRO field calculation.

The plots of the fields show that the deviation is small (Figure 9).

Figure 9: Comparison of the field calculation of the simulation program (solid) and the simulation of the field by ELECTRO (dashed).
4 Experiment

4.1 Experimental setup

The experimental setup used in the measurements is shown below (figure 10). The cathode is subdivided into an outer ring and an inner disk to provide a well-defined coupling capacitor close to the gap for optimum time resolution.

![Figure 10: Experimental setup.](image)

The equivalent electrical circuit is shown in figure 11. $C_p1$ is the capacitance between the outer ring of the cathode and the anode, $C_g$ is the capacitance between the inner disk and the anode, $C_p2$ is the capacitance between the two sections of the cathode. The current due to motion of charged particles in the gap is represented as a current source [Verhaart, 1982; Wen, 1989].
The dimensions of the cathode construction are chosen in a way that the ratio $C_g/C_{p1} \approx 0$ (i.e. $C_{p1} >> C_g$). The current now becomes:
The remaining capacitances in the equation should be as low as possible in order to obtain a high frequency response. The capacitance $C_g$ is already small, $C_{p2}$ is, however, one of the impeding factors of the time-resolution. This capacitor can be reduced by making the inner disk of the cathode smaller, but then the measured current no longer resembles the motion of the charged particles due to the Ramo-Shockley effect (section 4.1.1).

4.1.1 Ramo-Shockley effect

The subdivided cathode increases the time-resolution of the measuring circuit considerably, but the inner disk is bound to a minimum size if the gap width is kept fixed. When the disk radius becomes too small, the moving charges in the gap also induce current in the outer ring, which is not detected. There is a relation between the width $d$ of the gap and the radius of the inner disk regarding the measured current. In an earlier study the optimum for the disk radius was determined as [Verhaart, 1982]:

$$\frac{R}{d} \approx 2 \tag{110}$$

Here $R$ is the radius of the inner disk and $d$ is the gap width. In the experimental setup the gap distance is 10 mm and the the radius of the inner disk is 20 mm. The dependency of the measured current on the radius of the inner disk is expressed by not using the Laplacian field but the Ramo-Shockley field $\mathbf{E}_{\text{RS}}$ in equation (2) [Ramo, 1939; Shockley, 1938; Verhaart, 1982]:

$$R(t) = \frac{en(t)}{U_{\text{RS}}} (\mathbf{v} \cdot \mathbf{E}_{\text{RS}}) \tag{111}$$

Here, $\mathbf{E}_{\text{RS}}$ is the field created by the inner disk when a 'hypothetical voltage' $U_{\text{RS}}$ is applied to it and the other electrodes are grounded (figure 13). Due to the dot product of the velocity and the Ramo-Shockley field only the velocity component in the direction of the $\mathbf{E}_{\text{RS}}$ results in the measuring disk "seeing" the moving charge. Remember, the direction of the velocity vector is determined by the ‘real’ electric field ($\mathbf{E}_{\text{ap}} + \mathbf{E}_{\text{space charge}}$).
Figure 13: The Ramo-Shockley field of the inner cathode.
4.2 Results

4.2.1 Experimental results

In this study the emphasis was on the development of the model rather than on experiments. Still a few measurements have been made. Two of these current measurements will be presented in this study. The measurements were done with a gapwidth of 1 cm and surface area radiated by the laser of 0.16 cm$^2$. The first current versus time plot is shown in figure 14.

![Current waveform](image)

Figure 14: A current waveform measured by 14.97 kV and 163 mBar.

The oscillations in the tail of the avalanche is probably the result of resonance in the experimental setup. It can be seen that the avalanche develops within 50 nanoseconds ($T_e$) and the peak is flattened at the top. This latter effect could be the result of broadening of the electron cloud in axial direction. The front electrons are located in a higher field than the rear electrons, and are thus moving faster. This causes the cloud to be broadened, or even split into two more or less distinct clouds [Kennedy, 1992]. A large aftercurrent (current occurring later than $T_e$) due to the drift of the ions is quite apparent. By plotting the measured current on a logarithmic scale (figure 15) space charge effects can be seen.
Figure 15: A semi-logarithmic plot of current waveform of figure 14.

One of the observed effects due to space charge is that the effective ionization coefficient \((a - \eta)\), observed as the slope of the curve in figure 15, is not constant but increasing. With no space charge, the effective ionization coefficient should not change because the coefficients \(a\) and \(\eta\) are constant.

In figure 16 the measuring time is longer (1 \(\mu\)sec.). This was done in the hope that the initiation of a breakdown could be seen. The breakdown however, did not occur in one \(\mu\)sec. but later. The breakdown is believed to have caused the large number of observed spikes in the waveform and believed to be an artifact of the digitizer and no way associated with the gaseous processes leading to breakdown.
Figure 16: A current waveform measured by 14,90 kV and 143 mBar.

It can be seen that shortly after $T_e$ there is a slight increase in the aftercurrent upto 0.42 $\mu$sec. after which a slow decrease is observed. The increase may be explained by the detachment of electrons (see figure 17). At some point in time the net detachment of electrons decreases due to the process of conversion, and thus may explain the decrease in current after 0.42 $\mu$sec. Current waveforms incorporating various combinations of detachment and conversion can be found in the thesis of Wen [Wen, 1989].
4.2.2. Simulation results

In figure 17 two simulations with and without space charge effects of an electron avalanche are shown. The shape of the pulse can be compared to that of the measured pulse of figure 14. Contrary to experimental observations and simulations made in nitrogen [Kennedy, 1992] space charge effects resulted in an increase in the current. This may be due to the formation of negative space charge resulting from net electron attachment ($\sigma-\eta$ negative) in the back of the electron pulse. The increased growth is due to the enhanced ionization occurring in the front region of the electron pulse.

![Graph showing current waveforms](image)

**Figure 17:** Current waveforms by 18.05 kV and 200 mBar simulated with four rings with a total diameter of 6.3 mm. The upper curve is with space charge effects included. The lower curve without.

In both simulations the aftercurrent increases due to electron detachment. It remains growing because the possible stabilizing process, conversion, is not taken into account in the simulation model. The Te value decreases when space charge effects are included, again supporting the idea that the field is increased in the front region of the swarm. In the plot of the electron densities (figure 18) it can be seen that there is no separation of the cloud. The electron swarm however, is slightly broadened. The fact that no apparent separation of the cloud is observed also suggests that the positive ion space charge is greatly neutralized by the large presence of negative ions.
In the plots of the density distribution it can be noticed that there is almost no difference in densities between the rings, implying an uniform charge distribution. On the other hand, the slight increase of growth in the outer ring implies that the field is not radially uniform.
5 Conclusions

A program was made that is capable of performing simulations of electron avalanches in SF$_6$ including space charge effects. The individual parts of the program have successfully passed several tests and initial simulations have been made.

Direct comparison with measured waveforms is difficult. This is partly due to the fact that too few simulations have been run for an accurate systematic comparison. The emphasis in this study is on the development of the model. Continuation of this work will lead to a better understanding of the experimental results. Some conclusions may still be drawn with respect to the simulations and experiments:

- Simulating with one ring (i.e. a disk) is accurate when the total diameter of the set of rings is larger than half the gapwidth.
- Spatial broadening of the electron swarm is observed, indicative of the occurrence of space charge effects.
- Regarding current waveforms, space charge effects result in an increase in the $i_{\text{max}}$ value and a decrease in the time whereby $i_{\text{max}}$ occurs.

It is believed that one or both of the following mechanisms is responsible for breakdown.

- The breakdown may be due to detached electrons responding to the positive ion space charge left by the initial avalanche.
- Impact of positive ions on the cathode surface may release new electrons. If the number of new electrons exceeds the initial number then a breakdown eventually occurs. In addition, these new electrons may also respond to any remaining positive ion space charge.

Suggestions for future study on this subject are:

- Implementation of the process of conversion so that stabilization of the detachment process is simulated.
- Implementation of radial flow.
- Further study regarding the secondary electron emission mechanism including, cathode photoelectron emission, electron emission by positive ion impact, and gas phase photo-ionization.
- Extensive comparison with experimental waveforms for different gasses and conditions.
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