CORONA STREAMER MODELING WITH AN ADVANCED SEMI-TWO DIMENSIONAL MODEL

MAY-JUNE-JULY 1992
BY : B.H.T. SMEETS
EG/92/609

student of Eindhoven University of Technology

AT : I.V.T.A.N. MOSCOW
SUPERVISION : Yu.M. Solozobov

The faculty of electrotechnics of the Eindhoven University of Technology is not responsible for the contents of this report.

TECHNISCHE UNIVERSITEIT EINDHOVEN
ABSTRACT

In the Moscow institute for high temperatures, IVTAN, a program has been developed with which a positive corona streamer can be simulated. The program is based on solving the one dimensional continuity equations of charged particles, using a flux corrected transport method, coupled with a semi two dimensional Poisson solver called disk method. It takes into account kinetic processes and photo ionization as sources of charged particles.

In this report the first results of simulations with this program are shown. At first these results showed the program didn’t simulate all physical mechanisms satisfactory. Because of this the program was improved and new simulations were done giving different results. Finally the results show that the program simulates the streamer phenomenon satisfactory. Unfortunately this report includes only the results of one simulation with this final version.

The simulations can be done on any 386 of higher based computer. Computational time depends on streamer radius and length of the streamer. For instance the first 10 ns of a 200μm streamer will take about one hour on the above computer, but 30 ns of a 50μm streamer will probably take days.

In future the program will include a more complete kinetic model. Diffusion, two dimensional modeling and non local effects might also be taken into account.
CONTENTS

Abstract 2

1 Introduction 4
2 Physical basics 6
3 Numerical basics 10
4 Program structure 12
5 Simulation conditions 14
6 Results of simulations 15
   6.1 Initial stage 15
   6.2 Quasi stationary propagation 19
7 Calculations on kinetic reactions 22
8 Discussion 25
9 Conclusions and recommendations 26

References 27

Figures 28
CHAPTER 1 INTRODUCTION

Positive corona streamers have many applications, e.g. in ozonizers, in laser printers and in flue gas cleaning stations. For optimal use of corona in each of these applications, this highly complex phenomenon has to be understood in detail. For this reason streamers have been modeled by many scientists in many different ways.

In IVTAN, Moscow’s institute for high temperatures, an effort is made to compete in this research. A model has been developed which, with the help of a computer, solves the one dimensional continuity equations for charged particles using a Flux Corrected Transport (FCT) method and the semi two dimensional Poisson equation. With this it is possible to model the corona streamer through every stage of its existence using a simple 386 based desk computer.

As the program is being developed it is tested thoroughly. In this report these tests are described and the results are interpreted with respect to physical meaning and numerical techniques.

In chapter two of this report the basics of the models physical mechanisms are explained. The continuity and Poisson equations are discussed as well as boundary conditions and source terms of charged particles including photo ionization.

Chapter three deals with the numerical aspects of the program. It gives a brief explanation of how the differential equations are solved and what the advantages are of the method used.

Chapter four contains a block scheme of the computer program. The function of every block is explained.

To do an investigation with a simulation program like this, a plan has to be made. In this plan a typical situation has to be chosen and some parameters have to be varied keeping all other parameters constant and equal to the typical situation. Chapter five describes this plan.

In chapter six the results of the simulations of both initial stage and quasi stationary stage simulation are shown and a physical explanation is given for shapes and trends of curves.

In chapter seven a brief description of the 'KINEL' program (for zero dimensional simulation of kinetic reactions in gases) is
given as well as the results of a few simple simulations. In chapter eight the results of the simulations with the streamer modeling program are being compared with measurements. Chapter number nine, the last chapter of this report, holds conclusions and recommendations for future scientific work.
CHAPTER 2 PHYSICAL BASICS

The simulation of positive corona streamers consist of solving the continuity equations for charged particles coupled with Poisson equation. The particles are presumed to be located in a narrow cylinder with radius \( r \). All parameters are assumed to be depending only on the axial coordinate. If no particles are getting lost or being produced the one dimensional continuity equation will look as follows (not taking into account diffusion):

\[
\frac{\partial N_j}{\partial t} + \frac{\partial N_j v_j}{\partial x} = 0 \tag{2-1}
\]

In which \( x \) is the distance from the anode, \( t \) is time, \( N_j \) is the density of the particle and \( v_j \) its velocity as a result of the electrical field.

If attachment, ionization, detachment and recombination are taken into account, the one dimensional continuity equations for all charged particles present look as follows:

\[
\begin{align*}
\frac{\partial N_e}{\partial t} + \frac{\partial N_e v_e}{\partial x} &= S_e \\
\frac{\partial N_{p,1}}{\partial t} + \frac{\partial N_{p,1} v_{p,1}}{\partial x} &= S_{p,1} \\
\cdots & \cdots \cdots \\
\frac{\partial N_{p,k}}{\partial t} + \frac{\partial N_{p,k} v_{p,k}}{\partial x} &= S_{p,k} \\
\frac{\partial N_{n,1}}{\partial t} + \frac{\partial N_{n,1} v_{n,1}}{\partial x} &= S_{n,1} \\
\cdots & \cdots \cdots \\
\frac{\partial N_{n,1}}{\partial t} + \frac{\partial N_{n,1} v_{n,1}}{\partial x} &= S_{n,1}
\end{align*}
\]

The coefficients \( e \) and \( p, j \) \( j \in \{1..k\} \) and \( n, j \) \( j \in \{1..l\} \) refer to electrons, \( k \) different positive ion species and \( l \) different negative ion species. \( S_x \) is the source term of the charged particle species \( x \) which is equal to:
\[
S_e = (\alpha - \eta)v_e N_e - N_e \sum_{y=1}^{k} \beta_y N_p, y + \sum_{y=1}^{1} \xi_y N_n, y + s_{ph}^e
\]

\[
S_{p,j} = \alpha v_e N_e - \beta_j N_e P_{p,j} - N_{p,j} \sum_{y=1}^{1} \xi_{j,y} N_n, y + s_{ph}^e
\]

\[
S_{n,j} = \eta v_e N_e - \zeta_j N_n, j - N_{n,j} \sum_{y=1}^{1} \xi_{j,y} N_p, y
\]

In which \( \alpha \) and \( \eta \) are the ionization and attachment coefficients, \( \beta_x \) is the coefficient of recombination between electrons and positive ion species \( x \), \( \zeta_x \) is the detachment coefficient of the detachment process of the negative ion species \( x \), \( \xi_{x,y} \) is the reaction coefficient of the reaction between a positive ion of species \( x \) and a negative ion of the species \( y \), and \( s_{ph}^e \) is the electron production rate as a result of photo ionization.

If divided by \( p \) (gas pressure), \( \alpha \), \( \beta \), \( \zeta \) and \( v_x \) are dependent of \( E/p \). All other coefficients are independent of pressure and reduced field.

The boundary conditions are given by:

\[
N_e(d) = 0
\]

\[
N_{p,j}(0) = 0 \quad j \in \{1..k\}
\]

\[
N_{n,j}(d) = 0 \quad j \in \{1..l\}
\]

These are the densities at the electrodes which the particles are moving away from. The production of the particles at the surface of the electrodes is non-existing (for \( N_{p,j} \) and \( N_{n,j} \)) or negligible during the time of simulation (for \( N_e \)).

In positive corona streamers the most important process of generation of secondary electrons is the process of photo ionization in the volume. As previously shown by Zheleznyak et al. (lit. 1,2) for oxygen-nitrogen mixtures, molecular bands of nitrogen in vacuum ultraviolet are a source of ionizing photons while electrons emerge as a result of direct photo ionization of oxygen molecules. It was found that photo ionization is governed by radiation in the wavelength range of \( \lambda=980-1025\AA \). The short
wavelength limit is associated with the onset of intensive absorption of ionizing radiation by nitrogen and the long wavelength limit corresponds to the potential of oxygen ionization ($\approx 12.1$ eV). The rate of photo ionization $S_{e}^{ph}(r_1) \, (\text{cm}^{-3}\text{s}^{-1})$ is determined by the expression (lit. 1) (3 dimensional):

$$S_{e}^{ph}(r_1) = \int_{V} A \alpha v_{e} N_{e}(r_2) f(|r_1-r_2|) d^3 r_2$$

(2-5)

$$A = \zeta \frac{\omega p_{T}}{\alpha (p + p_{T})} ; \quad f(x) = \frac{\exp(-k_{\text{min}}x) - \exp(-k_{\text{max}}x)}{x \ln(k_{\text{max}}/k_{\text{min}})}$$

Where $r_1$ is the point where the production rate of electrons is to be calculated, $r_2$ is the integration parameter (the point from which radiation may occur), $V$ is the set of values $r_2$ will go through during integration (in our case a cylinder with radius $r_{str}$), $\omega$ is the amount of ionizing photons generated by one electron along a 1 cm path in the absence of processes of extinction by heavy particles, $\zeta \leq 1$, the efficiency of photo ionization which is equal to the number of electrons produced per absorbed quanta, $p$ is the gas pressure, $p_{T}$ is a parameter resulting from the inclusion of the extinction by heavy particles for air $p_{T}=30$ Torr (lit. 3), $k_{\text{min}}$ and $k_{\text{max}}$ are the minimum and maximum coefficients of absorption in the gas in the range $\lambda=980-1025\text{Å}$.

Then, there is the phenomenon of current being induced in the external circuit. The formula describing this induction law is given by the Sato integral (lit. 4):

$$I = e \pi r^{2} \int_{0}^{d} \left( N_{e} v_{e} + \sum_{y=1}^{k} N_{p,y} v_{p,y} + \sum_{y=1}^{l} N_{n,y} v_{n,y} \right) E_{1} dx / V$$

(2-6)

In which $e$ is the electron charge, $V$ is the voltage difference between the electrodes and $E_{1}$ is the Laplacian field (field as a result of the electrodes without any charge distorting it).

As discussed in (lit. 5) it is important to solve Poisson equation in three dimensions to allow for the finite radial extent of the charge distribution. Thus the axial electric field $E(x)$ is
evaluated using the method of disks (lit. 6) which represents the
discharge as a cylinder with a uniform radial distribution and
variable axial distribution of charge. In such a model the axial
component of the electric field at point \( x \) is given by:

\[
E(x) = \frac{1}{2\varepsilon_0} \left[ \int_{-x}^{0} \rho(x+x') \left( -1 - \frac{x'}{r^2} - \frac{1}{2} \right) dx' + \right. \\
\left. + \int_{0}^{d-x} \rho(x+x') \left( 1 - \frac{x'}{r^2} + \frac{1}{2} \right) dx' \right] \quad (2-7)
\]

Where \( \rho(x) \) is the net charge density at \( x \), \( r \) is the cylinder
radius and the gap extends from \( x=0 \) to \( d \). In applying this
equation, the electrode boundary conditions are implemented by
including "images" of the charge \( \rho(x) \) reflected appropriately at
the surface of the perfectly conducting electrodes (lit. 7).
The program is based on the assumption that the energy
distribution of electrons in a spot is a function of the electric
field, pressure and temperature in this point. The possibility of
electrons being injected from a nearby area of high field is
excluded. Because of this reaction's coefficients and drift
velocities are functions of local parameters. This assumption is
not correct in areas of extremely high electric field.
CHAPTER 3 NUMERICAL BASICS

To simulate the positive corona streamer a method has been used that solves the continuity equations in one dimension (Flux Corrected Transport method) and Poisson equation with the disk method (semi two dimensional). Some properties of the method used are:
- The parameters only vary in the \( x (=\text{axial}) \) direction.
- The parameters are calculated only in the mesh points on discrete moments.
- For the field calculation the charge is presumed to be spread homogeneous over a disk with radius equal to the discharge radius. Solving equation (2-1) (the source terms \( S_x \) are being integrated separately) for a time step \( \Delta t \) leads to:

\[
\Delta N_j = \int_{t_1}^{t_1 + \Delta t} \frac{\partial N_j}{\partial t} \, dt = - \int_{t_1}^{t_1 + \Delta t} \frac{\partial N_j \cdot v_j}{\partial x} \, dt \approx - \Delta t \frac{\partial N_j \cdot v_j}{\partial x} \quad (3-1)
\]

This equation can be solved in many different ways. The methods have different ways of calculating the derivative of \( N_j \cdot v_j \) with respect to the distance \( x \). Linear methods all have certain disadvantages like, large numerical diffusion, oscillations and artificial negative values. The non linear Flux Corrected Transport (FCT) methods are more precise and do not show these disadvantages taking small computational time (lit. 8).

The mesh of points used is inhomogeneous because there are some regions in the gap where a fine mesh is necessary and a fine mesh everywhere leads to big computational time loss. Because of this, where possible, an expanding mesh is used. The mesh regions are (from fine to course):
- The streamer head region. A very fine mesh is used because of its high gradients in field and density.
- The streamer channel. A moderate mesh is used because of the use of the disk method.
- The region between streamer head and cathode. An expanding mesh is used because of no need for a fine mesh.

The mesh will not be rebuilt every step because it would consume
to much time to calculate the influence matrix for the disk method. Instead a small area in front of the streamer head also has a fine mesh. Only if the streamer head gets to close to the end of the fine mesh the mesh will be rebuilt.

The time step $\Delta t$, after which the parameters of the streamer will be calculated again, is calculated every step, and depends on the Courant condition:

$$
\Delta t = \text{cour} \times \min\left(\frac{\Delta x}{v_j}\right) \quad (3-2)
$$

Where $\Delta x$ is the distance between two mesh points and $v_j$ is the velocity of any charged particle in this mesh point as a result of the electric field and cour is the Courant number which is the proportionality coefficient. The value of the Courant number has got a theoretical maximum which is 0.5 for our (explicit) method. Mostly a smaller value (cour=0.3) is chosen to get a solution which is more stable and more precise.

The process of numerical diffusion was mentioned before. With help of an example this phenomenon will be explained. In figure 3-1 the approximation of a triangular function by uniform sampling is shown (top curve). If this triangle would drift to the right the solution after a time step $\Delta t$ (satisfying $\Delta t \cdot v_d = 0.5 \cdot \Delta x$ with $v_d$ the drift velocity and $\Delta x$ the distance between mesh points) would be (using linear interpolation) given by the second curve from the top. The third curve is the solution after $2 \cdot \Delta t$ and so on. As can be seen the triangle loses its shape as if diffusion would occur. This process is called numerical diffusion.

Although numerical diffusion is very small in FCT methods it can have influence on the calculation.
CHAPTER 4 PROGRAM STRUCTURE

Figure 4.1 contains a block diagram of the program structure. There are two main loops. The one at the right occurs if the routine calculation is done for one time step $\Delta t$ without a new mesh being generated.

The other loop (at the left) contains some additional blocks which all have the function of generating a new mesh and calculating its properties. In this chapter the function of the parts of the program as shown in the left margin of figure 4.1 will be discussed.

**Initial part:**
The physical and internal parameters are given their initial values. A very important parameter is the initial electron density. It should be chosen carefully because it might affect the streamer forming and propagation (or no streamer may be formed). Then, the first mesh is chosen and the photo ionization and influence disk method (for calculation of the electric field) matrix are calculated.

The final part of this block is the calculation of the Laplacian (= undistorted) field.

**Calculation of the parameters after $\Delta t$:**
At first the velocities of the charged particles in all mesh points are calculated. After that time step $\Delta t$ can be calculated using the Courant condition. Then equation 2-1 is solved using the Flux Corrected Transport method, by which the convective part of the continuity equation is found. Then the kinetic constant rates are calculated in every mesh point and using these the source terms (including the photo ionization term) are obtained.

Adding convective, source and photo ionization terms to the old value of $N_j(n)$ gives the values of the densities after $\Delta t$. By these the net charge is known and the electric field as it is nowwill be calculated using the disk method.

**Block of choices:**
If time has reached a certain limit the output will be presented.
The current induced in the external circuit is calculated using the Laplacian field (saved earlier). The limit of output time will be shifted.

If time has passed a specified limit the program will be terminated.

If the streamer head has moved close to the edge of the fine mesh a new mesh will be built (the left loop will be chosen). If not, this would only consume time (the right loop is chosen). This decision is made at the end of the block of choices

New mesh generation block II:
If the streamer has reached the end of the fine mesh zone, a new mesh will be built. First the x-coordinates of the mesh points will be calculated, then the densities have to be interpolated. After that the process starts all over again at the New mesh generation block I, which is described in the initial part description (except that in stead of the Laplacian field the distorted field will be calculated).

The program calculates the streamer propagation by executing the steps described above. If all physical parameters have been set for the type of gas that the streamer is propagating in, an initial electron and ion density can be set. Then, if the voltage dependence of time is known the simulation can start. The time to end the calculation and the time step between two successive output times can be set.
CHAPTER 5 SIMULATION CONDITIONS

The most important parameters which have to be chosen and the values assumed for our simulations are:

<table>
<thead>
<tr>
<th>configuration</th>
<th>wire-plate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>wire radius= 0.03 cm</td>
</tr>
<tr>
<td></td>
<td>electrode separation= 3.5 cm</td>
</tr>
<tr>
<td>pressure</td>
<td>1 atm</td>
</tr>
<tr>
<td>temperature</td>
<td>273 K</td>
</tr>
<tr>
<td>gas</td>
<td>air</td>
</tr>
<tr>
<td>applied voltage, V</td>
<td>Heaveyside function</td>
</tr>
<tr>
<td></td>
<td>11, 13, 15 kV (initial stage study)</td>
</tr>
<tr>
<td></td>
<td>Heaveyside function</td>
</tr>
<tr>
<td></td>
<td>17.5, 20, 22.5 kV (st. prop. study)</td>
</tr>
<tr>
<td>streamer radius, R_{str}</td>
<td>200, 100, 50 \mu m</td>
</tr>
<tr>
<td>initial electron</td>
<td>10^5 \text{cm}^{-3} if 0&lt;x&lt;5*R_{str}</td>
</tr>
<tr>
<td>distribution</td>
<td>0 \text{cm}^{-3} if 5*R_{str}&lt;x</td>
</tr>
</tbody>
</table>

For the initial stage study the typical values were V=15kV and R_{str}=200\mu m, from this setting the V and R_{str} were varied. For the quasi stationary stage study this typical values are V=20kV and R_{str}=200\mu m.
CHAPTER 6 RESULTS OF SIMULATIONS

6.1 The initial stage.

It is important to study the initial stage of the streamer for two reasons:
1) It is an important part of the existence of the streamer (the fundamental part) and future propagation depends on it.
2) To improve analytical modeling of the initial stage, the results of which can be used in semi qualitative models of streamers which describe only quasi stationary stage. The initial values are given by analytical approximations.

This stage is essentially different from the quasi stationary stage in which the streamer propagates through the gas. The initial stage is started if two demands are satisfied:
- At first there must be a region where the electrical field is higher than the critical value. This region must be big enough to get a steady multiplication of electrons in an avalanche and to have an electron production rate (secondary electrons) by photo ionization that is high enough to maintain and even increase the avalanche in time (and by this satisfying Townsend criterion).
- Initial electrons must be provided in this region to get the electron avalanche started. These electrons can originate from a constant emitting cathode (constant density throughout the gap), flash lamp radiation (half Gaussian peak), electron beam (Gaussian peak) or background radiation.

The first demand is satisfied by creating a high voltage pulse on the wire. The second by defining an initial electron distribution. For the study of the initial stage of the streamer an initial electron distribution is defined that is constant in the range between the wire and 5 streamer radii from the wire. This initial electron distribution is equal to $10^5 \text{ cm}^{-3}$, this corresponds to one electron in a cubic space with a sided of 215 $\mu$m. With the radius of the streamer in the simulations between 50$\mu$m and 200$\mu$m this value of the initial electron distribution is quite low (1/5 respectively 12 electrons present in the channel).

The mechanism of streamer forming is that in the electron avalanche the number of electrons and positive ions grows very
fast (exponential in the beginning), the electrons moving to the anode and the positive ions remaining almost in the spot where they are originated. Because of this a positive net charge will occur after some time. This net charge will change the initial, also called Laplacian, field. If the net charge is big enough (>10^{10}\text{cm}^{-3}) , the electric field may get a maximum somewhere close to but free from the anode. In this maximum the electron multiplication in the avalanche will be the highest and the positive net charge will increase the fastest. Because of this the maximum of electric field and with it the phenomenon of the largest electron multiplication will move away from the anode. This is a continuous process and is called streamer propagation. Behind the maximum of electric field the Laplacian field is reduced by the positive net charge. This region is called the channel of the streamer.

If the streamer propagation and the streamer channel are present the initial stage is ended and the acceleration stage of the quasi stationary streamer propagation will start.

To study the initial stage of the streamer a number of simulations have been done. These simulations were done:
- With a Heaveyside function applied to the wire.
- With initial electron distribution as described above.
- From t=0 to the time (t_{end}) where the maximum of electric field is at the distance from the anode equal to 1.5 times the streamer radius (typical distance of field distortion by net charge in one disc).

The following simulations have been done:

<table>
<thead>
<tr>
<th>V (kV)</th>
<th>r_{str} (\mu m)</th>
<th>t_{end} (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11</td>
<td>200</td>
</tr>
<tr>
<td>2</td>
<td>13</td>
<td>200</td>
</tr>
<tr>
<td>3</td>
<td>15</td>
<td>200</td>
</tr>
<tr>
<td>4</td>
<td>15</td>
<td>100</td>
</tr>
<tr>
<td>5</td>
<td>15</td>
<td>50</td>
</tr>
</tbody>
</table>

* = no streamer present

The first simulation is done at a voltage that is not high enough for streamer initiation in 30ns. The net charge that is produced is not big enough to cause any relevant distortion of the electric field. This is caused by the low multiplication rate in the
electron avalanche and insufficient photo ionization. The images of the electron, positive ion and negative ion densities are shown in figure 6.1-1. Also a graph of the Sato current is present in this figure. From this last picture we can see that the avalanche is no longer exponentially rising which means that no streamer is expected to appear. All electrons will drift to the anode wire.

In figures 6.1-2 to 6.1-5 the results of simulations 2 to 5 are shown. For every simulation a graph is made for the electron, positive ion and negative ion density and the electric field for three moments of the discharge. The first is for t=0, the second is the moment of the first maximum in the electric field not at x=0 and the third moment is the moment for which t=t_{end}. Also for every simulation a graph is present with Sato current versus time and streamer velocity versus distance of the propagation. The streamer velocity is defined as the velocity of the maximum of the electric field. Because the initial maximum appears at a certain distance from the anode and the top of the electric field is rather smooth (changing of shape will be interpreted as high velocity), the velocity has an irregular shape at the beginning. In this region there is no real streamer structure present so the first irregular part (including the sharp maximum) of the velocity graph is not of any physical importance.

Because the mechanism for streamer initiation is the same for simulations 2-5 and the x and t axis are changed for different simulations, the pictures of fields, densities, current and velocity have the same shape. Characteristic values of these parameters however are depending on the simulation. Current and velocity for instance are decreasing dramatically with decreasing streamer radius.

Also N_{net} = N_p - N_e - N_n has been calculated and is shown for simulation 3 in figure 6.1-6. The maximum value of N_{net} for t=t_{end} was found to be proportional to 1/r_{str}'.

The high value of t_{end} (6.3ns) of simulation 5 is caused by two factors:

1 Because the initial electron distribution was created over a length proportional to r_{str}. Setting the initial distribution to the same as for simulations 1-3 resulted in t_{end} = 3.0ns.
2 Because inception voltage is higher for smaller r_{str}.
Then in figure 6.1-7 two particle fluxes of electrons from simulation 2 and 3 are shown, the convective flux \( N_e v_e \) and the diffusive flux (which was not included in solving the continuity equations) \( D \frac{\delta N_e}{\delta x} \). For this last calculation the diffusion coefficient is assumed constant and equal to \( 5.1 \times 10^3 \) (lit. 9). In this figure also are the graphs for the ratio of the convective and diffusive particle flux. From this graph can be seen that the diffusive particle flux is not really important to get a close to true solution.

In figure 6.1-8 the fields and electron densities for \( t = t_{\text{end}} \) of simulations 3, 4 and 5 are shown in graphs with on the x axis distance divided by \( r_{\text{str}} \). It can be seen that for simulation 3 and 4 the result at \( t = t_{\text{end}} \) can without doubt be called a streamer. For simulation 5 this is not so clear. The maximum of the electric field is quite round and a channel is not really present. Also the slope of electron density is not steep enough. After this stage the electric field maximum and its velocity will increase, this is called the acceleration stage of the quasi stationary streamer propagation.
6.2 Quasi stationary propagation

For these simulations a new and better variant of the program has been used. The method for calculation of the impact and photo ionization term as well as the mesh generation algorithm were changed in order to get a more stable and precise calculation. At first calculations were done for some cases:

<table>
<thead>
<tr>
<th>V (kV)</th>
<th>r_{str} (μm)</th>
<th>t_{end} (ns)</th>
<th>order of ionization calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>a 17.5</td>
<td>200</td>
<td>30</td>
<td>low</td>
</tr>
<tr>
<td>b 20.0</td>
<td>200</td>
<td>20</td>
<td>low</td>
</tr>
<tr>
<td>b* 20.0</td>
<td>200</td>
<td>20</td>
<td>high</td>
</tr>
<tr>
<td>c 22.5</td>
<td>200</td>
<td>20</td>
<td>low</td>
</tr>
<tr>
<td>d 20.0</td>
<td>100</td>
<td>10</td>
<td>low</td>
</tr>
</tbody>
</table>

These calculations have been done with Courant number equal to 0.3. The results of simulations a, b, c and d are shown in figures 6.2-1 to 6.2-4. The mechanism for streamer propagation is explained in the previous section so now we will directly start discussing the results.

A big difference is noticed with the results from the former chapter. The inception voltage (lowest voltage at which a streamer is formed) became higher after the changes made. The reason for this is the changes made in the calculation of the impact ionization source term for which streamer models are very sensitive and thus results in a rise of the inception voltage from 12 to 16 kV for streamers with a radius equal to 200μm.

In the plots for electric field in figures 6.2-1 to 6.2-4 it can be seen that the sharp maximum of the field moves from the anode towards the cathode. The maximum increases with increasing wire voltage and decreasing streamer radius. Electron concentrations show a steep slope at the point of the field maximum where ionization is the highest. In the area between streamer head and cathode there is a low non zero electron concentration which is due to photo ionization. The plots for positive ions show a similar view.

The negative ion concentration is lower because they arise from attachment which is not a very fast process. Distance and velocity
plots show the movement of the electric field maximum and the current plot shows the current induced in the external circuit. After these calculations the ionization source term was changed because in the region of high field the ionization time is close to the time step made. This makes it necessary to use a high order method for calculation of this term. The result of this improvement was a dramatic change of all parameters. For distance and Sato current verses time and velocity verses distance the plot before and after the change are shown in figure 6.2-5.

Then the check was made to prove the time step the program uses is justified. For this the same calculation was done with different Courant number. The simulation included a 200μm streamer radius, a 20kV (Heaveyside function) applied voltage and an initial electron distribution that is constant in the region of the fine mesh and zero elsewhere. Position and value of the electric field maximum were noted after 2ns of simulation. In figure 6.2-6 the result of this test is shown. As can be seen the two parameters looked at change dramatically with varying Courant number. Two conclusions are possible:

-The Courant number has to be very small (for precise solution of the convection equation) because the parameters seem to have a limit for small values.

-There is a process that depends on the Courant number strongly and either for small or high values results in big errors.

Tests have shown that the second conclusion is the right one. The process involved is the process of numerical diffusion. If the Courant number is smaller more calculations have to be made for a simulation of 2ns and numerical diffusion will increase. The mechanism that influences the calculation is that if numerical diffusion is big in front of the streamer the electron concentration will be higher than would be expected if only photo ionization would supply electrons in that region. Because of this more seed electrons are present for the moving avalanche and all parameters of the streamer are influenced.

Because of a lack of time only the results of one simulation with the new version of the program, in which the problem of numerical diffusion is solved, are included in this report. The changes made to diminish the influence of numerical diffusion
are:
- More mesh points in the region where numerical diffusion may be of influence.
- Taking a different initial electron distribution (so the end of the constant distribution is not in the end of the fine mesh). The distribution chosen is a constant distribution of $10^8 \text{cm}^{-3}$.
- Keeping the Courant number close to the value 0.5. Whereas in linear methods numerical diffusion is proportional to $(1-COUR)$ in the FCT methods it is proportional to $(COUR+1/COUR)$. Minimal numerical diffusion is to be expected near $COUR=0.5$.

The results of this simulation are shown in figure 6.2-7. The simulation was executed for a value of $r_{str}=200 \mu\text{m}$, a 20 kV applied voltage (Heaveyside function) and the above initial electron distribution. The results shown in figure 6.2-7 are very much alike previous results. Also some new graphics are shown. Apart from $i(t)$, $x(t)$ and $v(x)$ there are graphics containing the average density of three kinds of radicals ($O$, $N$ and $N_2^*$ radicals) in the active streamer volume (cylinder with radius $r_{str}$ and length $x(t)$). Also a graph containing G factor versus time is included. The G factor is defined as the amount of radicals produced per 100 eV energy input.
CHAPTER 7 THE CALCULATION ON KINETIC REACTIONS

Another program created in IVTAN moscow is 'KINEL'. This program calculates concentrations of molecules, ions, radicals and exited molecules in a gas versus time. A set of kinetic reactions (only gas reactions, no aerosol) can be defined which contain the information about creation and termination of particles. An analytical description of this system leads to a large number of non linear differential equations which cannot be solved analytically so a numerical approach is chosen.

The initial concentration of particles obtained from measurements (pollutants) and calculation, with the hydro dynamic streamer simulation model (radicals and ions), are input for the program. Then it calculates for one point in space the reactions as they proceed in time.

For the flue gas from a coal flame through which a streamer has just passed the initial concentrations are shown in table 7.1.

<table>
<thead>
<tr>
<th>particle</th>
<th>Concentration (1/cm⁻³)</th>
<th>particle</th>
<th>Concentration (1/cm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂</td>
<td>1.43E19 (74%)</td>
<td>e⁻</td>
<td>2.09E14</td>
</tr>
<tr>
<td>O₂</td>
<td>9.71E17 (5%)</td>
<td>N₂⁺</td>
<td>2.14E14</td>
</tr>
<tr>
<td>CO₂</td>
<td>2.91E18 (15%)</td>
<td>O₂⁺</td>
<td>2.40E11</td>
</tr>
<tr>
<td>H₂O</td>
<td>1.16E18 (6%)</td>
<td>N₂⁺</td>
<td>6.76E14</td>
</tr>
<tr>
<td>NO</td>
<td>7.77E15 (0.04%)</td>
<td>O²⁻</td>
<td>3.80E12</td>
</tr>
<tr>
<td>SO₂</td>
<td>1.94E16 (0.1%)</td>
<td>O³⁻</td>
<td>1 E9</td>
</tr>
<tr>
<td>OH</td>
<td>1.16E16 (0.06%)</td>
<td>O₄⁺</td>
<td>5.13E11</td>
</tr>
<tr>
<td>O</td>
<td>2.14E15</td>
<td>O₂⁻</td>
<td>5.01E15</td>
</tr>
</tbody>
</table>

The densities of some important particles, taking into account all important reactions, look as shown in figure 7.1 (simulation nr. 1, see later on in this chapter). Some calculations have been done to look at the influence of some particles on the flue gas cleaning, see table 7.2.
### TABLE 7.2 Results of the simulations

<table>
<thead>
<tr>
<th>nr</th>
<th>O₂ ini.</th>
<th>O ini.</th>
<th>OH ini.</th>
<th>REACTIONS</th>
<th>SO₂ cl.</th>
<th>NO cl.</th>
<th>NO₂, end ( \frac{\text{NO₂, end}}{\text{NO, ini}} ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9.70E17</td>
<td>2.14E15</td>
<td>1.16E16</td>
<td>ALL</td>
<td>5.5</td>
<td>34.8</td>
<td>15.5</td>
</tr>
<tr>
<td>2</td>
<td>9.70E17</td>
<td>2.14E15</td>
<td>1.16E16</td>
<td>[715L]</td>
<td>5.5</td>
<td>34.8</td>
<td>14.6</td>
</tr>
<tr>
<td>3</td>
<td>9.70E17</td>
<td>2.14E15</td>
<td>1.16E16</td>
<td>[715L]</td>
<td>5.4</td>
<td>32.1</td>
<td>11.9</td>
</tr>
<tr>
<td>4</td>
<td>1.94E18</td>
<td>2.14E15</td>
<td>1.16E16</td>
<td>ALL</td>
<td>5.5</td>
<td>37.3</td>
<td>17.9</td>
</tr>
<tr>
<td>5</td>
<td>9.70E17</td>
<td>2.14E15</td>
<td>2.32E16</td>
<td>ALL</td>
<td>7.0</td>
<td>40.9</td>
<td>16.7</td>
</tr>
<tr>
<td>6</td>
<td>9.70E17</td>
<td>2.14E15</td>
<td>0</td>
<td>ALL</td>
<td>1.1</td>
<td>19.5</td>
<td>15.8</td>
</tr>
<tr>
<td>7</td>
<td>9.70E17</td>
<td>2.14E15</td>
<td>1.16E16</td>
<td>ALL</td>
<td>2.5</td>
<td>44.4</td>
<td>31.8</td>
</tr>
</tbody>
</table>

The first calculation was the calculation in which the initial densities of table 7.1 were used and all relevant reactions (about 500) were taken into account. In table 7.2 we can see in the first column the number of the simulation then three columns with initial concentrations of particle densities that were varied in different calculations, then a column in which the number of reactions taken into account are shown, the next two columns show the cleaning percentage of SO₂ and NO, and the last column shows the NO₂ (initial concentration=0) produced as a percentage of the initial concentration of NO. The ideal cleaning results would be 100% removal of SO₂ and NO and 0% production of NO₂.

Simulation nr. 2 and 3 are done to look at the influence of O₃ on the cleaning of the flue gas. Most of the O₃ is produced in reaction 715L:

\[
O₂ + O + M \rightarrow O₃ + M
\]

(reaction 715L)

In which M can be any particle. Excluding this reaction (sim. nr. 2) reduces the density of O₃ in the gas to about 1% of its value in sim. nr. 1. This however has no direct effect on the cleaning of the gas. Excluding all other O₃ producing reactions from the system (sim. nr. 3) results in an almost unchanged O₃ density. However, it has some influence on the gas cleaning. From this we can conclude that O₃ doesn’t directly react with SO₂ and NO but that NO is oxidized to NO₂ (a little) in reactions (but not 715L) where O₃ is produced.
In simulations 4 to 7 the influence of initial concentrations of $O_2$, OH and O particles is investigated. It can be seen that OH radicals have the biggest influence on removing $SO_2$ and NO (without forming $NO_2$). Increasing the $O_2$ density only results in NO to $NO_2$ oxidation. Increasing the O density does the same and has a bad influence on $SO_2$ removing.

The conclusion of this short investigation is that OH radicals are the most important particles in flue gas cleaning. Optimizing the corona streamer on its OH production rate is desirable.
CHAPTER 8 DISCUSSION

In this section a comparison will be made between the calculations and measurements done at Eindhoven University of Technology. Unfortunately there was only little measurement data available at the time of writing this report. This data is:

For a streamer which propagates in the same configuration as the simulations are done for with an applied voltage of 25 kV (zero rise time), the velocity as a function of the distance is known (figure 8.1) and the total charge induced in the external circuit is 10nC. Also it is known that the radius of discharge is smaller than 50µm.

Because of a lack of time the simulation for a streamer with radius of 50µm is not executed. A comparison with the v(x) graph of the last (most reliable) calculation of chapter 6.2 shows that the order of magnitude is correct. However because of the difference in applied voltage and discharge radius any other conclusion is impossible. In comparing the induced charge also the time of integrating the Sato current is a crucial point. Because the current is only known for 10 ns and it is necessary to integrate at least 10 times longer comparison is impossible.

For a decent comparison the simulation with above setting should have to be done for 20 ns (velocity comparison) or >100 ns (induced charge comparison). However this last calculation might take several days on a 50MHz 486 based computer.
CHAPTER 9 CONCLUSIONS AND RECOMMENDATIONS

The most important conclusion is that the program is working properly. The results show that the physical mechanisms of streamer initiation and propagation are simulated satisfactory well. The only disadvantage concerning the mechanism is that the phenomenon of numerical diffusion might have some influence on the propagation of the streamer. Besides, this numerical diffusion is smaller then the physical diffusion would be if it were included. The practical use of the program is restricted to computers based on a 386 processor or higher. On this type of machine a simulation for a streamer with radius of 200\(\mu\)m for 10 ns would take about one hour (estimation). The computational time rises fast (first or second order) with decreasing streamer radius. Also if the streamer grows longer (more mesh point) the computational time would increase.

This program can be of use in any research program in which detailed information about positive corona streamers is desired.

A decent comparison with measurements will show the influence of assumptions made like absence of diffusion, constant radius of discharge and absence of non local processes.

In future the program can be improved. The following physical mechanisms can be taken into account:
- All important kinetic processes for for example flue gas cleaning.
- Cathode electron emission by photo effect and ion impact.
- Diffusion
- 2 dimensional effects (varying radius of discharge)
- non local effects (electron beam model)
REFERENCES


FIGURE 3-1 Example of numerical diffusion.
FIGURE 4.1 Block scheme of the program structure.
FIGURE 6.1-1 Initial stage simulation V=11kV r=200μm.
FIGURE 6.1-2 Initial stage simulation $V=13$kV $r=200\mu$m.
FIGURE 6.1-3 Initial stage simulation V=15kV r=200μm.
FIGURE 6.1-4 Initial stage simulation V=15kV r=100μm.
FIGURE 6.1-5 Initial stage simulation $V=15kV \ r=50\mu m$. 
FIGURE 6.1-6 Net charge particle density at $t=t_{\text{red}}$ for $V=15\text{kV}$ $r=200\mu\text{m}$. 
FIGURE 6.1-7 Convective and diffusive particle fluxes and their ratio for $V=13kV \ r=200\mu m$ (a-c) and $V=15kV \ r=200\mu m$ (d-f).
FIGURE 6.1-8 Electric field and electron density in graphs with normalised x axis V=15kV t=t_{\text{end}}.
FIGURE 6.2-1 Streamer propagation simulation $V=17.5$ kV $r=200\mu$m.
FIGURE 6.2-1 g

FIGURE 6.2-2 Streamer propagation simulation V=20kV r=200µm.
FIGURE 6.2-3 Streamer propagation simulation $V=22.5\text{kV} \ r=200\mu\text{m}$.
FIGURE 6.2-4 Streamer propagation simulation V=20kV r=100µm.
FIGURE 6.2-5 Comparison of results before and after changes.

FIGURE 6.2-6 Result of the Courant number check.
FIGURE 6.2-7 Simulation with the final version of the program $V=20\text{kV}$ $r=200\mu\text{m}$. 
FIGURE 6.2-7 Simulation with the final version of the program $V=20kV$ $r=200\mu m$. 
FIGURE 7.1 A typical 'KINEL' plot (result of simulation 1).
FIGURE 8-1 the velocity of the streamer head.