Multiple ion species fluid modeling of sprite halos and the role of electron detachment of O\textsuperscript{−} in their dynamics

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[1] A two-dimensional fluid model with multiple charged species is developed for simulating the ionospheric responses to the lightning quasi-static electric (QE) field. In addition to electrons, the model takes into account four symbolic ion species and O\textsuperscript{−} ions that are considered separately to investigate the role of the fast electron detachment process from O\textsuperscript{−} in the ionospheric response. The modeling results of a sprite halo driven by positive cloud-to-ground lightning indicate that the halo can descend to lower altitude with much higher electron density behind its front when the O\textsuperscript{−} detachment process is included. Electron density ahead of the halo front is not significantly reduced from the ambient value, so there is no attachment “hole” forming in that region that is commonly observed in previous modeling studies. The fast O\textsuperscript{−} detachment process affects the dynamics of the halo by allowing the growth of electron density in the upper atmosphere under sub-breakdown condition, i.e., the electric field is smaller than the conventional breakdown threshold field. The implications of the results reported here to sprite streamer initiation include (1) low ambient electron density at sprite initiation altitude may be the only means to avoid avalanche overlapping before the avalanche-to-streamer transition; and (2) the large downward extent of the halo may offer an explanation for the initiation of sprites at the altitude as low as 65–70 km, which was observed in previous studies.


1. Introduction

[2] The direct coupling between the lower and upper atmosphere through thunderstorm/lightning activities is manifested by transient luminous events (TLEs) in the mesosphere and lower ionosphere. Compared to other classes of TLEs, sprite halos exhibit a relatively homogeneous glow structure that is centered around 78–80 km altitude with horizontal extension of tens of kilometers and vertical thickness of several kilometers [e.g., Barrington-Leigh et al., 2001; Wescott et al., 2001; Pasko, 2010]. On average they occur once every minute on Earth, according to the global survey of the TLE occurrence by the ISUAL instruments on the FORMOSAT-2 satellite [Chen et al., 2008]. It has been generally accepted that sprite halos are driven by the quasi-electrostatic (QE) field of cloud-to-ground lightning (CG) [Pasko et al., 1997; Barrington-Leigh et al., 2001]. They normally appear within 1–2 ms after their parent CG and last for several milliseconds [Barrington-Leigh et al., 2001; Wescott et al., 2001; Cummer et al., 2006]. They occur either as a single event or are accompanied by elves and/or sprites. In comparison to sprites that are predominantly caused by strong positive CG (+CG) [e.g., Boccippio et al., 1995; Barrington-Leigh et al., 1999; Williams et al., 2006; Taylor et al., 2008], the occurrence of halos does not show a strong dependence on the polarity of CG. Negative CG that quickly transfers a large amount of charge from thunderclouds to the ground can produce halos as effectively as positive CG [Bering et al., 2004; Frey et al., 2007].

[3] Recent high-speed images show that when halos are accompanied by sprites, some sprite streamers appear to be initiated from the structures formed in the halos [e.g., Cummer et al., 2006; McHarg et al., 2007; Stenbaek-Nielsen and McHarg, 2008], those observations have motivated modeling efforts in investigating the role of halos in the initiation of sprite streamers. Formation of sprite streamers from halos was simulated by Luque and Ebert [2009] using a plasma fluid model with adaptive computational grid, and it was concluded that the descending halo front continues to sharpen and eventually collapses into a sprite streamer. However, Qin et al. [2011] noted that there could be spatial and temporal separation between the luminosities of observed halos and sprite streamers, which suggests that the initiation of sprite streamers is not necessarily a continuous development of halos. They reported simulation results of halos obtained using a fluid model and the modeling results of the avalanche-to-streamer transition with a particle level description. They found that the initiation of sprite streamers can be roughly determined by the condition that the conventional breakdown threshold field $E_b$ is reached at an...
altitude with a sufficiently small electron density which is on the order of \(10^3 \text{ m}^{-3}\). Such a low electron density at the sprite initiation altitude may result from both low ambient electron density and depletion of electrons below the halo front due to electron attachment process [Qin et al., 2011].

[5] In the above mentioned modeling studies, typical processes taken into account for electron density time variation include electron impact ionization, dissociative attachment, photoionization, recombination, etc. However, recent studies on sprite streamer chemistry suggested that electron detachment from \(O^-\) is an important source for electrons in sprite streamer channel where electric field is typically below \(E_k\) [Gordillo-Vázquez, 2008; Liu and Sentman, 2010]. This process can lead to net production of electrons even when electric field is smaller than \(E_k\) if \(O^-\) ions are abundant. As the lightning QE field can last for tens of milliseconds around typical sprite initiation altitude, this process may turn out to be important for the dynamics of halos and/or the initiation of sprites.

[5] The purpose of this paper is to report a modeling study to understand the dynamics of sprite halos driven by CG lightning and particularly, to investigate how the electron detachment from \(O^-\) affects the response of the lower ionosphere to the lightning electrostatic inputs. A two-dimensional fluid model with multiple ion species was developed for the study. The ion chemistry model implemented is a modification and expansion of the one developed by Lehtinen and Inan [2007] that was used to analyze the dynamics of ionization perturbations produced in the region from thundercloud top to the lower ionosphere such as those produced by gigantic jets. In their model, charged particles are classified as electrons, simple positive and negative ions, and cluster positive and negative ions. Here we include \(O^-\) as an additional species in order to consider the electron detachment process. We report simulation results of sprite halos caused by a +CG stroke resulting in 600 C km charge moment change with and without the \(O^-\) detachment process. It is found that when the detachment process is included the halo can descend through a longer distance and the electron density can increase even in the region where the lightning field is smaller than \(E_k\). The halo brings down the lower ionosphere right above the parent lightning by about 15 km through raising the electron density behind the halo front to a value comparable to the ambient value at 85 km altitude. It is also found that no significant electron density reduction is present below the halo front, so the attachment "hole" commonly observed in previous modeling studies is absent.

2. Model Formulation

2.1. Model Equations

[6] To model the ionospheric response to the quasi-electrostatic field produced by cloud-to-ground lightning, the continuity equations of charged particles are solved together with Poisson’s equation. The model equations are

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot \vec{J}_i = S_i - L_i, \tag{1}
\]

\[
\nabla^2 \phi = -\frac{\rho}{\varepsilon_0}, \tag{2}
\]

where \(n_i\) is the density of the \(i\)th charged species, \(\vec{J}_i\) the flux density, \(S_i\) and \(L_i\) the source and sink for the \(i\)th species; \(\phi\) is the electric potential and electric field \(\vec{E} = -\nabla \phi\), \(\rho\) the charge density, and \(\varepsilon_0\) the permittivity of free space. The flux density \(\vec{J}_i\) is defined as \((n_i \vec{v}_i - D_i \nabla n_i)\), where \(\vec{v}_i = \mu_i \vec{E}\) is the drift velocity, \(\mu_i\) the mobility of the \(i\)th charged species, and \(D_i\) the diffusion coefficient of that species. The terms \(S_i\) and \(L_i\) account for the change of the density due to ionization, attachment, recombination and detachment, which are discussed in more detail in the next section. The photoionization process is ignored here, because it only plays a minor role in halo dynamics as shown by Qin et al. [2011, Figure 8], who compared the halo modeling results with and without this process. Although this process is known to be important for streamer propagation, its relatively minor role in the dynamics of halos likely results from the following factors: (1) the maximum field in the halo is much smaller than the streamer head field. The production of UV photons responsible for photoionization is less efficient at a lower electric field. (2) The spatial scales involved in the halo are much larger than the photon absorption length, which is about 100–200 m at halo altitude. The introduction of \(O^-\) further makes the photoionization less important, because it can also generate free electrons ahead of the halo front.

2.2. Model Species and Reactions

[7] As demonstrated by recent studies on sprite chemistry [e.g., Sentman et al., 2008; Sentman and Stenbaek-Nielsen, 2009; Gordillo-Vázquez, 2008; Liu and Sentman, 2010], many charged species can be produced by electric discharges in the mesosphere/lower ionosphere. In general, simple ions are produced by electron impact reactions during the active stage of the discharge process and then converted to complex ions such as hydrated positive ions and cluster negative ions following a chain of reactions. Tens of ion species and hundreds of reactions have been considered in the aforementioned studies of sprite chemistry, where a zero dimensional model was typically used.

[8] However, it is computationally unrealistic to take into account such a large number of charged species and reactions for a two-dimensional model, and it is necessary to simplify the ion chemistry in order to be able to simulate the principle physics and chemistry of sprite halos in a tolerable computation time. Lehtinen and Inan [2007] recently improved the ion chemistry model developed earlier by Glukhov et al. [1992], to study the dissipation of ionization perturbations produced by gigantic jets. According to their work, the charged species created by electric discharges in the upper atmosphere can be grouped into electrons (e), light negative ions (M−), cluster negative ions M−\(_c\), light positive ions M\(^+\), and cluster positive ions M\(_c^+\). On the other hand, recent work by Gordillo-Vázquez [2008] and Liu and Sentman [2010] showed that electron detachment of \(O^-\) could be an important source for electrons when \(O^-\) ions accumulate to certain level in sprite streamer discharges, which requires a separate treatment of \(O^-\) ions from the rest of light negative ions. In the present study, we therefore include the five charged species considered by Lehtinen and Inan [2007] and \(O^-\) ions in our ion chemistry model. It should be noted that although such a simplified chemistry model works well within the first several hundred milliseconds after the beginning of the
discharges, when the ion chemistry is dominated by a few number of of ion species and electron impact reactions. It may lead to invalid results at longer timescale as various forms of ions can be produced and characterizing the ion chemistry at this stage by just using such a small set of ion species unavoidably introduces inaccuracy in the obtained results.

The model species and reactions are summarized in Tables 1 and 2, respectively. To make the simplified ion chemistry model as accurate as possible, the symbolic ions should represent the dominant ions that are found in the discharges as well as in the lower ionosphere. According to negative ion chemistry in the D-region ionosphere [Brasseur and Solomon, 2005, p. 575], stable CO$_3^-$, HCO$_3^-$ and Cl$^-$ are the dominant negative ions. For plasma chemistry initiated by sprites, O$^-$, O$_2^-$, O$_3^-$ and O$_4^-$ are the major ions within ~1 s of the discharges, and ions like CO$_3^-$, Cl$^-$ and NO$_3^-$ take over afterwards [Sentman et al., 2008; Sentman and Stenbaek-Nielsen, 2009; Liu and Sentman, 2010]. O$_3$ and O$_4$ are the gateway species for the formation of CO$_5^-$ and NO$_5^-$. CO$_3^-$ and NO$_3^-$ ions are very stable and virtually impossible to lose electrons, while O$_2^-$ and O$^-$ ions can lose electrons when colliding with N$_2$ and O$_3$ molecules as well as N and O atoms. It is therefore reasonable to classify the negative ions as the light negative ions M$^-$ and more stable M$_x^-$. Conversion between the light negative ions and more complex ions is taken place through intermediate O$_3$ and O$_4$ species. Reactions producing O$_3$ and O$_4$ from O$^-$ and O$^-$ are considered to be the formation reaction for M$_x^-$, while those from O$_3$ and O$_4$ to O$^-$ and O$^-$ to be the conversion from M$_x^-$ to M$^-$.

The dominant positive ions in the D-region ionosphere are O$_2^+$, NO$^+$, proton hydrates and NO$^+$ ion clusters [Brasseur and Solomon, 2005, p. 559]. During sprite discharges, O$_2^+$ and O$_4^+$ are the most abundant positive ions initially, and positive ion hydrates dominates at the later stage [Sentman et al., 2008; Sentman and Stenbaek-Nielsen, 2009; Liu and Sentman, 2010]. It is necessary to differentiate O$_2^+$ from the rest of the major positive ions because they recombine with electrons at different rates. Hence, M$^+$ is introduced in the model to represent O$_2^+$ and M$_x^+$ for the rest.

### Table 1. Model Species

<table>
<thead>
<tr>
<th>Charged Species</th>
<th>Neutral Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>e, O$^-$, M$^-$, M$_x^-$, M$^+$, M$_x$</td>
<td>Q, M, M$_x$, M$_x$</td>
</tr>
</tbody>
</table>

### Table 2. Reaction Set

<table>
<thead>
<tr>
<th>Reaction Number</th>
<th>Reaction</th>
<th>Rate Constant</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>(R1)</td>
<td>Q + M → e + M$^+$ + Q</td>
<td>1e-25</td>
<td>see text</td>
</tr>
<tr>
<td>(R2)</td>
<td>e + M → e + e + M$^+$</td>
<td>f(E/N)</td>
<td>Hagelaar and Pitchford [2005]</td>
</tr>
<tr>
<td>(R3)</td>
<td>e + O$_2$(M) → O$^-$ + O(Mac)</td>
<td>f(E/N)</td>
<td>Hagelaar and Pitchford [2005]</td>
</tr>
<tr>
<td>(R4)</td>
<td>e + M + M → M$^+$ + M</td>
<td>f(E/N)</td>
<td>Hagelaar and Pitchford [2005]</td>
</tr>
<tr>
<td>(R5)</td>
<td>e + M$^-$ → Mac + Mac</td>
<td>3e-13</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R6)</td>
<td>e + M$_x^-$ → M + M</td>
<td>1e-12</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R7)</td>
<td>M$^+$ + M$^+$ → M + M</td>
<td>5e-13</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R8)</td>
<td>M$^+$ + M$_x^-$ → M + M$_x$</td>
<td>5e-13</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R9)</td>
<td>O$^+$ + M → O(Mac) + M</td>
<td>5e-13</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R10)</td>
<td>O$^+$ + M$_x^-$ → O(Mac) + M$_x$</td>
<td>5e-13</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R11)</td>
<td>M$_x^+$ + M$_x^+$ → M$_x$ + M$_x$</td>
<td>5e-13</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R12)</td>
<td>M$_x^+$ + M$_x^-$ → M$_x$ + M$_x$</td>
<td>5e-13</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R13)</td>
<td>M$^+$ + M$^+$ + M → M + M + M</td>
<td>5e-37</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R14)</td>
<td>M$^+$ + M$_x^+$ + M → M$_x$ + M + M</td>
<td>5e-37</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R15)</td>
<td>O$^+$ + M$^+$ + M → O(M$_x$)$_2$ + M + M</td>
<td>5e-37</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R16)</td>
<td>O$^+$ + M$_x^+$ + M → O(M$_x$)$_2$ + M$_x$ + M</td>
<td>5e-37</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R17)</td>
<td>M$_x^+$ + M$^+$ + M → M$_x$ + M + M</td>
<td>5e-37</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R18)</td>
<td>M$_x^+$ + M$_x^+$ + M → M$_x$ + M$_x$ + M</td>
<td>5e-37</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R19)</td>
<td>M$^+$ + M + M → M$_x^+$ + M</td>
<td>2e-42</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R20)</td>
<td>M$_x^+$ + M → M$^+$ + M + M</td>
<td>2e-22</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R21)</td>
<td>M$_x^+$ + M$_x^-$ → M$^+$ + M</td>
<td>1e-16</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R22)</td>
<td>M$^+$ + M + M → M$_x^+$ + M</td>
<td>1e-43</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R23)</td>
<td>O$^+$ + M + M → O$^-$ + O(M$_x$)</td>
<td>3e-43</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R24)</td>
<td>M$_x^+$ + M$_x^-$ → M$^+$ + M</td>
<td>2e-16</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R25)</td>
<td>M$^+$ + M → e + M + M</td>
<td>2e-29</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R26)</td>
<td>M$^+$ + M$_x^-$ → e + M + M$_x^-$</td>
<td>2.5e-16</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R27)</td>
<td>O$^+$ + M → e + M$_x$</td>
<td>f(E/N)</td>
<td>Raymont and Moruzzi [1978]</td>
</tr>
<tr>
<td>(R28)</td>
<td>O$^+$ + M → e + M$_x$</td>
<td>1e-21</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
<tr>
<td>(R29)</td>
<td>O$^+$ + M$_x^-$ → e + M$_x$</td>
<td>4e-16</td>
<td>see text and Sentman et al. [2008]</td>
</tr>
</tbody>
</table>

*The species of O$_2$ and O appear in the reaction table to make the stoichiometry correct when O$^-$ ions are included separately. The term in the parentheses is the actual species implemented in the model.

*Units are m$^3$/s for two body reaction or m$^3$/s for three body reaction. The ambient temperature is assumed to be 200 K.*
Figure 1. Comparison of the rate constants for the O$^-$ detachment, electron impact ionization, and two body attachment. The rate constants are referenced to neutral air density.

of the major ions. The recombinations between ions generally have very similar rate coefficients that differ by a factor of three at most [Sentman et al., 2008], and therefore lumping various forms of positive ions into $M_e$ seems to be appropriate.

Besides the charged particles mentioned above, the species included in the model are $M$ (nitrogen and oxygen molecules), $M_{ac}$ (active neutrals such as oxygen atom, nitrogen atom, excited states), $M_c$ (cluster molecules), and $Q$ for cosmic ray background ionization. In the simulation, the densities of neutral species are kept constant at the background level that is discussed in the next section. The ionization provided by cosmic ray background is taken into account by reaction (R1), in a similar manner as the rest of the reactions, which simplifies the code implementation. The rate constant of this reaction can be chosen rather arbitrarily because the cosmic ray background ionization contributes to the kinetics through the product of this constant and the value of $Q$. The number given in Table 2, $1 \times 10^{-25}$ m$^{-3}$, results in a value of $Q$ comparable to the background density of the charged particles when $Q$ is determined self-consistently from the model ion chemistry and ambient electron density profile, which is discussed in the next section.

The rate constants for electron impact reactions (R2)–(R4) depend on electric field and can be obtained with the solution to the Boltzmann equation [Hagelaar and Pitchford, 2005; Moss et al., 2006]. The rate constants for the rest of the reactions except (R27) are determined by considering the dominant one among all the possible reactions from the chemistry model of Sentman et al. [2008] represented by a symbolic reaction. For example, the reaction $e + O_2 \rightarrow O + O_2^+$ is the fastest one among all possible recombinations between $e$ and $O_2$. It has a rate constant of $1.13 \times 10^{-11} (T/300)^{-0.7}$ m$^3$/s $= 3 \times 10^{-13}$ m$^3$/s, if the air temperature $T$ is 200 K. This gives the reaction constant for (R5), while the constant for (R6) is taken from the recombination between $e$ and $O_2^+$.

[15] For the reactions involving O$^-$ except the detachment reaction (R27), their reaction constants are set to resemble the behavior of light negative ions $M_e^-$. The O$^-$ ion has an electron affinity about 1.46 eV, and the O$^-$ detachment process from colliding with $N_2$: $O^- + N_2 \rightarrow e + N_2O$, proceeds very fast at moderate electric field condition [Rayment and Moruzzi, 1978]. Comparison between the rate constants $k_r$, referenced to neutral air density, of the detachment (R27), the electron impact ionization (R2), and two-body dissociative attachment (R3) is shown in Figure 1. The O$^-$ detachment rate constant increases with increasing electric field and reaches $\sim 1 \times 10^{-18}$ m$^3$/s at the breakdown threshold field $E_k = 120$ Td. It is larger than the two-body attachment reaction constant in the reduced field range of 10–50 Townsend but becomes smaller for stronger field. It should be noted that (R27) proceeds with a rate of $k_e[O^-][M]$ but (R2) and (R3) with $k_e[M]$, where the notation of a species surrounded by square brackets represents the density of that species. Only when the densities of O$^-$ and $e$ are comparable to each other, the reaction constant $k_r$ alone determines which reaction goes faster or slower.

[14] Overall, the model should provide an accurate description of the sprite halo chemistry within several hundreds of milliseconds after the parent lightning stroke, because electron impact reactions and electron detachment from O$^-$ dominate the chemistry that can be quite accurately described by the symbolic reactions (R2)–(R4) and (R27). For the chemistry at the later stage, the simple ion conversion scheme between $M^-$ and $M_c$ may not work well for representing the much more complex negative ion chemistry studied by Sentman et al. [2008].

2.3. Background Density Profiles

[15] Employing self-consistent background density profiles in the model provides possibility for modeling the mesospheric and ionospheric response to lightning inputs on long timescale. In our model, the densities of M and $M_{ac}$ are taken from the MSIS profile (http://omniweb.gsfc.nasa.gov/vitmo/msis_vitmo.html), and as the species $M_c$ does not participate as reactant in any reaction, its density is unimportant.

[16] The background profiles are determined with the goal that under quiet condition at night (i.e., no electron impact ionization (R2) and two-body associative attachment (R3)) and without any O$^-$ ions (i.e., no reactions (R9), (10), (15), (16), (23), (27)–(29)) the steady state solution of electron density from equation (1), with electron and ion transport ignored, matches a realistic profile. The electron density profile from the work by Wait and Spies [1964], which was suggested to represent the realistic ambient electron density profile when some observed sprites occurred [Pasko and Stenbaek-Nielsen, 2002], is used as the target profile to match. The procedure of calculating the background density profiles is briefly described below. Given the electron density, the unknowns are the densities of $M^-$, $M_e^-$, $M_c^-$, and $M_{ac}$, and the value of $Q$. Due to charge neutrality, the system of equations represented by equation (1) is not independent, and one of them should be replaced by this condition. The steady state solution can then be found by setting the left hand side of equation (1) to zero and solving the resulting nonlinear equation system with a numerical solver such as the KINSOL module of the SUNDIALS software package.
developed by Lawrence Livermore National Laboratory (https://computation.llnl.gov/casc/sundials/main.html).

[17] The obtained background profiles are shown in Figure 2a. Figure 2b shows the corresponding conductivity profiles by taking the mobilities of electrons, positive ions, and negative ions at ground pressure as 1.4856 (the value at small electric field measured by Davies [1983]), 2.3 × 10^{-4}, and 2.75 × 10^{-4} m^2/V/s [Morrow and Lowke, 1997], respectively, and scaling those values with neutral density for a particular altitude. It can be seen that the electronic conductivity \( \sigma_e \) dominates above 70 km altitude while the ion conductivity dominates below. The ion conductivity profile \( \sigma_{ion} \) was reported by Holzworth et al. [1985] based on balloon and rocket measurements above active thunderstorms. Interestingly, the conductivity profile from the calculation with this simple set of ion chemistry differs only slightly from the measured values in the region where the ion conductivity dominates. The deviation from the measured value above 70 km is unimportant because electronic conductivity is much larger there.

[18] To further validate the model, we compare the steady state densities of the symbolic ions calculated above to the background densities of major ions obtained by Sentman et al. [2008]. The densities of \( M^- \), \( M_x^- \), \( M^+ \), and \( M_x^+ \) at 70 km altitude are found to be 1.7 \times 10^5, 3.0 \times 10^5, 1.8 \times 10^7, and 2.8 \times 10^8 m^{-3}, respectively, given an ambient electron density of 2.2 \times 10^5 m^{-3} from the profile discussed above. According to Sentman et al. [2008, Table 2], for a given electron density of 1.0 \times 10^6 m^{-3} at this altitude, the steady state density of O_2^- is 1.5 \times 10^6 m^{-3} and the density of dominant negative ions CO_2^- or NO_3^- is about a factor of 10^3 larger. The density of dominant positive ions N_2O_7^+ or hydrated protons is about 10^3 times larger than the electron density. According to Liu and Sentman [2010], two fast ion conversion processes were not considered by Sentman et al. [2008]: N_2O_7^+ + N_2 \rightarrow O_2^- + N_2 + N_2 and N_2O_7^- + O_2 \rightarrow O_2^- + N_2 with rate coefficients of 7.19 \times 10^{-17} and 1 \times 10^{-15} m^3/s [Kossyi et al., 1992], respectively. The two reactions quickly convert N_2O_7^+ to O_2^- or O_2^- ions. As the density of N_2 is about 4 times larger than the O_2 density, the formation of O_2^- proceeds at a rate of 3–4 times slower than O_2^- Therefore, the density O_2^- should be roughly an order of magnitude smaller than the total density of complex positive ions including O_2^- and other cluster ions in the work of Sentman et al. [2008, Table 2], which is consistent with the density ratio between \( M^- \) and \( M_x^- \). In summary, although the absolute densities of symbolic ions at 70 km altitude are about an order of magnitude smaller than those of their representing species calculated by a more complete chemical kinetics model [Sentman et al., 2008], the difference is largely caused by the different prescribed electron densities at that altitude and the relative density ratio between \( M^- \) and \( M_x^- \) as well as between \( M^+ \) and \( M_x^+ \) agrees reasonably well with the ratio of the species they represent from the work of Sentman et al. [2008]. Therefore, it is expected that the ion chemistry model used here does allow a relatively accurate description of the ion chemistry induced by sprites/sprite halos.

2.4. Lightning Model

[19] Previous studies on sprites/sprite halos have established that the most important factors to determine the ionospheric responses to the lightning quasi-static electric field are the polarity of CG, the charge moment change, the duration of charge removal, and the ambient conductivity profile [e.g., Pasko et al., 1997; Cummer and Inan, 1997; Asano et al., 2008; Qin et al., 2011]. Pasko et al. [1997]
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Figure 3. Simulation geometry.

showed that charge removal from thunderclouds to the ground can be effectively modeled by depositing the same amount of charge of opposite polarity at the same location in thunderclouds when the QE effects in the upper atmosphere are concerned. It should be noted that such an equivalent model may result in different electric fields in the lower mesosphere at long timescale [Pasko et al., 1997], but at that time the electric field is very small and the resulting chemical effects could be negligible. The charge depositing model is therefore used in our study to simulate CG. [20] The following expression is used to describe the deposited charge \( Q(t) \) as a function of time \( t \) [Pasko et al., 1997]:

\[
Q(t) = Q_0 \frac{\tanh(t/\tau_f)}{\tanh(1)}, \quad 0 \leq t < \tau_f,
\]

\[
Q(t) = Q_0, \quad t \geq \tau_f,
\]

where \( \tau_f \) and \( Q_0 \) are the duration of the lightning and the total amount of charge deposited, respectively. The simulation starts at \( t = 0 \), which is the onset of the lightning discharge, and \( \tau_f \) is set to 1 ms in this study. The deposited charge \( Q(t) \) is distributed in space following a Gaussian distribution, which is centered at 10 km altitude and has a characteristic spatial scale 3 km. 

2.5. Numerical Implementation

[21] Starting with the background density profile, the solution to the densities of the charged species is advanced over time using the CVODE solver of the SUNDIALS software package. The finite volume method is used to discretize the simulation region for the continuity equation (1), and the flux density \( \vec{J}_i \) is calculated using a modified Scharfetter-Gummel algorithm [Kalikovsky, 1995]. Poisson’s equation (2) is discretized with finite difference method and the resulting linear equation system is solved using the successive over-relaxation method [e.g., Hockney and Eastwood, 1988, p. 179]. The same set of methods except a different time integrator was previously used to solve sprite streamer model equations [Liu et al., 2009a, 2009b].

[22] Cylindrical symmetry is assumed in the model and the simulation region is shown in Figure 3. The electric field solution is sought from the ground to 90 km altitude while the densities from 40 km to 90 km altitude. The reason to use different solution regions is to avoid numerical complications due to thundercloud source charge when solving continuity equation as well as to reduce computation time. Numerical tests with different lower boundaries of the simulation domain for the continuity equation show that 40 km altitude is a good choice.

[23] Electric potential is set to zero on all boundaries. The boundary conditions for the continuity equation are

\[
\frac{\partial n_i}{\partial r} = 0, \quad r = 60 \text{ km},
\]

\[
\frac{\partial n_i}{\partial z} = 0, \quad z = 40, 90 \text{ km}.
\]

Each simulation consists of three phases: (1) 0–1 ms. In this phase, transport of ions is ignored to avoid numerical problems that may arise due to zero initial density of O^-.

(2) 1–400 ms. All terms in equations (1) and (2) are taken into account. And (3) > 400 ms. In this phase, the focus is to follow the dissipation of the disturbances created by sprite halos. Transport of both electrons and ions is ignored in equation (1) so there is no need to solve Poisson’s equation. In this paper, we only report the results from the first two phases.

3. Results

[24] We report simulation results of a sprite halo caused by a +CG discharge removing 60 C charge from 10 km altitude in 1 ms. The corresponding charge moment change 600 C km is around the upper limit of the charge moment change threshold for production of short delayed sprites [Cummer and Lyons, 2005; Hu et al., 2007]. Figure 4 shows the cross-sectional view of the distributions of the normalized electric field, the electron density and the O^- density at four different moments of time: 1, 1.9, 6.3 and 20 ms. It shows that a convex curvature of the lower ionosphere forms and develops above the parent lightning, which generally agrees with previous modeling studies on sprite halos [e.g., Barrington-Leigh et al., 2001; Qin et al., 2011]. The lightning field points predominantly downward so electrons drift upward (noting that ion motion is negligible for the timescale under consideration). The electrons therefore move in the same direction as the gradient of the ambient electron density shown in Figure 2, and the descending sprite halo on such a short timescale can only be explained by the development of ionization wave. The O^- ions exist only in the region the halo occupies or has passed through as there is no initial background density for this species. After production, they persist for a while.

[25] The altitude profiles of the same three quantities on the symmetry axis at more time instants are shown in Figure 5. The profiles of the normalized electric field show that the region of strong electric field descends as time progresses.

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progresses and the peak normalized field decreases after 1 ms. It can also be seen that the strong electric field only lasts for ~1 ms above 80 km altitude but an extended time period of 10s ms around 69 km altitude. In addition, the electric field only exceeds $E_k$ in a small altitude range around 80 km. The lowest altitude where $E$ exceeds $E_k$ is 76–77 km that is reached at $t = 1.9$ ms. Without the electron detachment from $O^-$ ions, it would be expected that the strong field region would move down very slowly from 77 km to 69 km altitude because the ambient electron density decreases rapidly in this region and it could be further reduced by the two body dissociative attachment due to $E < E_k$ in this region so that the Maxwellian relaxation timescale would be very long. However, as shown by the field profiles, the peak field can still move relatively rapidly downward for a considerable distance even under the condition of $E < E_k$.

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**Figure 4.** Simulation results of a halo caused by a +CG lightning flash transferring 60 C charge from 10 km altitude to the ground in 1 ms. Cross-sectional view of the distributions of (a) normalized electric field, (b) electron density, and (c) $O^-$ density at $t = 1, 1.9, 6.3$ and 20 ms.

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**Figure 5.** Simulation results of a halo caused by a +CG stroke transferring 60 C charge from 10 km altitude to the ground in 1 ms: altitude profiles of (a) normalized electric field, (b) electron density, and (c) $O^-$ along symmetry axis for various moments of time.
although the speed decreases as it moves down. The front reaches about 69 km altitude at ∼50 ms and stays there until numerical instability occurs at ∼70 ms due to steepening electron density profile around that altitude that is further discussed below.

Figure 5b shows that the electron density in the altitude range of 70–85 km is highly elevated. It reaches a value close to the ambient electron density at about 85 km altitude. The sprite halo essentially brings down the lower ionosphere right above the parent lightning by about 15 km altitude. The increase in the electron density below 77 km altitude is quite interesting, where \( E \) never exceeds \( E_k \). This increase of the electron density in the sub-breakdown condition \( E < E_k \) is caused by the electron detachment from \( O^- \). Figures 4c and 5c show that \( O^- \) ions are produced abundantly on the timescale of the halo dynamics and their density in the altitude range of 70–85 km is comparable to electron density. The growth of electron density in \( E < E_k \) when there are abundant \( O^- \) ions in space can be understood as follows. Electrons are still produced below the breakdown threshold field due to electron impact ionization and they are constantly converted to \( O^- \) by the attachment process at the same time. Therefore, the total density of e and \( O^- \) increases as long as the ionization is effective (recombination takes place on a much longer timescale). When \( O^- \) ions accumulate to certain level, the detachment process becomes faster than the attachment process and then electron density increases together with the \( O^- \) density if significant ionization is continuously produced by the electron impact ionization. This is discussed in more detail in the next section.

After about \( t = 50 \) ms, the halo stops descending but the electron density front becomes steeper and steeper, which eventually leads to numerical instability. In the end, a sharp electron density profile around 70 km is formed by the halo, but this is mostly caused by the increased electron density above and not by the loss of electrons below due to the attachment.

As a comparison, Figures 6 and 7 show simulation results for the same setup except that the \( O^- \) detachment process is not included. It can be clearly seen that an attachment “hole” is formed below the sprite halo as the density of electrons is greatly reduced by the dissociative

![Figure 6](image-url)  
Figure 6. Simulation results without the inclusion of the \( O^- \) detachment process for the same lightning stroke as for Figure 4: (top) electron density distribution and (bottom) normalized electric field distribution.

![Figure 7](image-url)  
Figure 7. Comparison of halo simulation results with (solid line) and without (dashed line) the inclusion of \( O^- \) ions: (a) electric field profile and (b) electron density profile.
attachment. The electron density profiles at 6.3 ms differ significantly for the two simulation cases. The large electron density gradient forming at 73–74 km for the case without the O\(^-\) detachment is mainly caused by the depletion of electrons in the E < E\(_k\) region.

4. Discussion

4.1. Electron Density Growth at Sub-breakdown Condition E < E\(_k\)

[30] To further understand the effects of the detachment process in the ionization in the upper atmosphere, a simple zero dimensional ionization model is formulated below. Considering the density changes of electrons and O\(^-\) ions under the influence of constant electric field, the governing equations after ignoring slow processes such as recombination are

\[
\frac{dn_e}{dt} = (\nu_i - \nu_a)n_e + \nu_d n_{O^-}, \tag{5}
\]

\[
\frac{dn_{O^-}}{dt} = \nu_d n_e - \nu_a n_{O^-}, \tag{6}
\]

where \(n_e\) and \(n_{O^-}\) are the densities of \(e\) and \(O^-\), respectively; \(\nu_i\), \(\nu_a\), and \(\nu_d\) are the corresponding reaction frequencies of the ionization, attachment, and detachment. For constant electric field, \(\nu_i\), \(\nu_a\), and \(\nu_d\) are fixed, and the two linear ordinary differential equations can be solved analytically. Assuming that the initial densities of electrons and O\(^-\) ions are \(n_{e0}\) and zero m\(^{-3}\) respectively, the solution is

\[
\begin{bmatrix} n_e \\ n_{O^-} \end{bmatrix} = \frac{n_{e0}}{\bar{\nu}} \left( \begin{bmatrix} \nu_d + \nu_a \\ \nu_i \end{bmatrix} \exp(\nu_i t) - \begin{bmatrix} \nu_d + \nu_a \\ \nu_i \end{bmatrix} \exp(\nu_a t) \right), \tag{7}
\]

where \(\bar{\nu} = \sqrt{(\nu_i - \nu_d - \nu_a)^2 + 4\nu_i \nu_d} \) and \(\nu_\pm = 0.5[(\nu_i - \nu_d - \nu_a) \pm \bar{\nu}]\). Figure 8 shows the variation of the densities at various normalized electric field \(E/E_k\) at 80 km altitude given an initial electron density of 10\(^6\) m\(^{-3}\). The figure shows that the electron density decreases initially and then either stays constant for lower field cases: 0.17 and 0.33 \(E_k\) or increases for other cases in the time window of 0–100 ms. The initial decrease is caused by the second term on the right hand of equation (7) while the increase by the first term. It should be emphasized that even when \(E = 0.67E_k\) a considerable increase in the electron density can be reached in a time period of 100 ms. In addition, changing \(n_{e0}\) only results in vertical shifting of the curves in the figure while the shapes of the curves are preserved according to the solution (7).

[31] It is illustrative to see the dependence of the growth rates \(\nu_\pm\) on the reduced electric field, which is shown in a neutral density independent form in Figure 9, where electron impact ionization and two body attachment frequencies are also shown for comparison. Note that \(|\nu_\pm|\) is plotted here and the corresponding exponential term in solution (7) only contributes initially for the ionization change. In the altitude range of 75–90 km, \(N_0/N\) varies from \(5 \times 10^4\) to \(5 \times 10^5\) and the reduced field must be greater than 70–80 Td, i.e., \(E/E_k > 0.6\) to 0.7, to have a noticeable increase in electron density in several to tens milliseconds.

With this possible electron density growth at sub-breakdown condition, a question arises naturally: Is it possible that an electron avalanche develops and transforms into a streamer even under the condition of \(E < E_k\)? Consider a region where a uniform sub-breakdown field exists. Both the densities of electrons and O\(^-\) ions are growing exponentially (shown in Figure 8) with the rate \(\nu_\pm\). Suppose that an electron avalanche at an intermediate stage somehow appears at

![Figure 8](https://example.com/f8.png)

Figure 8. Density change of (a) electrons and (b) O\(^-\) ions at constant electric field from the simple ionization model. The number labeling each curve is the value of \(E/E_k\).
some location. As the avalanche moves in the opposite direction of the electric field, its electrons are quickly converted to $O^-$ ions due to $\nu_a \gg \nu_i$. So the avalanche becomes weaker and weaker until it is dissipated, while leaving a trail of enhanced $O^-$ density. The original compact avalanche head spreads out along its trail and is therefore unable to make to the avalanche-to-streamer transition.

### 4.2. Effects on Sprite Streamer Initiation

[32] How sprite streamers are initiated in the upper atmosphere is not well understood. Recent triangulation analysis on multistation sprite videos has concluded that the initiation altitude of sprite streamers varies between 65 and 90 km [e.g., Stenbaek-Nielsen et al., 2010; Gamerota et al., 2011], which overlaps with the altitude extent of sprite halos. According to high-speed video observations, sprite streamers appear to be initiated either at the bottom of halos or out of the dark background [e.g., Stenbaek-Nielsen et al., 2000; Cummer et al., 2006; McHarg et al., 2007; Stenbaek-Nielsen et al., 2010]. The role played by sprite halos in the initiation of sprite streamers has been investigated by several recent modeling studies [e.g., Luque and Ebert, 2009; Qin et al., 2011]. In particular, Qin et al. [2011] considered the response of the lower ionosphere to the lightning QE field as a system of electron avalanches. On the basis of their modeling results on the halos and the electron avalanche-to-streamer transition, they have suggested that an ambient electron density about $10^3$ m$^{-3}$ is required to avoid overlapping of electron avalanches before they transform into individual streamers. This density value is derived by considering the transverse size of electron avalanches at the avalanche-to-streamer transition moment and possible density fluctuation on particle level at sprite initiation altitudes. According to Figures 4, 5, and 8, due to the detachment process of $O^-$, electron density is not significantly reduced from its ambient value in the region below the halo front. Therefore, the ambient electron density profile at sprite streamer initiation altitude should be close to $10^3$ m$^{-3}$ if this value is required for formation of individual streamers.

[33] On the other hand, a combined analysis of sprite images, remote measurement of lightning current moment, and finite difference time domain simulations of lightning electromagnetic fields indicated that the simulated lightning electric field at the time of sprite initiation could be well below the breakdown threshold field $E_b$ [Hu et al., 2007; Li et al., 2008; Gamerota et al., 2011]. A hypothesis to explain such results is that sprite streamers can be initiated from ionospheric inhomogeneities in the lower ionosphere. Recent streamer simulations confirm that it is indeed possible for sprite streamer initiation in a lightning field below $E_b$ if an ionization patch with enhanced density exists at the sprite initiation altitude [Kosar et al., 2011]. The simulations also reproduce many aspects of observed sprite streamers at their initiation such as preferential formation of positive streamers over negative streamers and luminous structure above the initiation point [McHarg et al., 2007; Stenbaek-Nielsen et al., 2007; Stenbaek-Nielsen and McHarg, 2008]. However, more work is needed to be done to investigate what are the requirements for the inhomogeneity such as its dimension and density.

[34] If there is no existing ionospheric inhomogeneity, it is generally difficult to explain the initiation of sprites at 70–80 km altitudes due to lightning with charge moment change as small as 120 C km $^{-1}$ [Hu et al., 2002; Pasko, 2010]. Qin et al. [2011] found that a sharp variation of the ambient electron density profile at the sprite initiation altitude reduces the charge moment change threshold for sprite initiation. Or equivalently, a sharp variation in electron density profile allows a lower initiation altitude of sprites given a charge moment change. Following this principle, a simple model can be formulated to estimate the lowest possible sprite initiation altitude for a given charge moment change. Consider the configuration shown in Figure 10a. A point charge is placed between the ground and the ionosphere that are assumed to be perfectly conducting, and the region between the ground and the ionosphere is free space. This configuration models the extreme case of the sharp increase in the electron density profile at the lower ionospheric boundary. Under such configuration, sprites should always be initiated at the lower boundary of the ionosphere if the parent lightning is strong enough, because the lightning electrostatic field $E$ always reaches $E_b$ first at this boundary and this field will last long enough for streamer formation due to zero conductivity below the ionosphere. The zero conductivity also prevents the overlapping between adjacent electron avalanches, so an electron appearing in that high field region is very likely to develop into a streamer to initiate sprites.

[35] The solid lines in Figure 10b show the electrostatic field $E$ at the lower edge of the ionosphere right above a point charge of 10, 30, 50, 90 and 150 C at 10 km altitude, as a function of the ionosphere height $H$, i.e., for every point on the solid line the electric field is calculated by setting the lower ionosphere boundary at that altitude. If the lower boundary of the ionosphere is fixed at 90 km altitude, the electric field as a function of altitude due to the same point charges is illustrated by the dashed line in the figure. As shown by the figure, lowering the ionosphere height $H$ results in larger electric field. Triangulated initiation altitudes of five sprite events (including both short- and long-delayed sprites) together with charge moment changes at the
initiation moment are reported in [Stenbaek-Nielsen et al., 2010; Gamerota et al., 2011]. The initiation altitudes are 80, 76, 75, 74 and 66 km, and the corresponding charge moment charges are 350, 500, 700, 1000 and 1200 C km. Here, for the event consisting of multiple sprite elements separated in time, only the first element is selected for consideration. With those charge moment changes, the condition $E = E_k$ is reached at 79, 76, 73, 69, and 67 km altitude from the simple model. For all five events, the triangulated initiation altitudes are higher or very close to the calculated altitudes, which suggests it is possible to explain the observed initiation altitudes without invoking ionospheric inhomogeneities but this requires that the lower ionosphere descends to the observed initiation altitude of sprites. It should be noted that the simple model assumes a uniform plane boundary for the lower ionosphere and therefore does not take into account the field enhancement due to the possible curvature of this boundary such as that resulted from sprite halos. 

[36] Without the O$^-$ detachment process, the halo front stops descending after reaching 75 km altitude according to Figure 7. The region with increased electron density behind the front is very limited and the initiation of sprite streamers at altitude around 70 km [Stenbaek-Nielsen et al., 2010; Gamerota et al., 2011] is difficult to be explained with this result. However, when the O$^-$ detachment process is included, the halo front can descend to $~$70 km and the elevated density behind the front is much higher than the other case, which approaches the Figure 10a configuration. The field at 45.7 ms in Figure 5 is about 0.5$E_k$. If additional 500 C km charge moment change is introduced by either the continuing current of the parent CG or another CG, the field will be raised by $>0.5E_k$, estimated from Figure 10, and then $E_k$ will be reached around 70 km to initiate sprite streamers. The total charge moment change is 1100 C km, which is a reasonable value compared to the numbers reported by Gamerota et al. [2011].

5. Summary and Conclusions

[37] The results reported in this paper can be summarized as follows.

1. A two-dimensional fluid model with multiple ion species is developed to simulate the ionospheric responses to the lightning quasi-electrostatic field. The model takes into account four symbolic ion species and O$^-$ ions that are considered separately to investigate the role of the fast electron detachment process from O$^-$ in these responses. In this model, the background ion density profiles are self-consistently obtained with the model ion chemistry and a realistic ambient electron density profile.

2. The modeling results for a sprite halo caused by a +CG stroke with 600 C km charge moment change show that the front of the halo can descend to $~$70 km altitude and the electron density behind the halo is elevated to a value close to 85 km altitude. The halo brings down the lower ionosphere boundary by about 15 km altitude that is much larger than that by a halo without the O$^-$ detachment process. The large descending extent of the sprite halo enabled by the detachment process may be critical for initiation of sprites at 70 km altitude.

3. Electron density below halo front is not significantly reduced from the ambient value, i.e., there is no pronounced attachment hole forming below the halo front. To have a small electron density about $10^3$ m$^{-3}$ at sprite initiation altitude for formation of individual streamers [Qin et al., 2011], the ambient electron density at this altitude must be close to this value.

4. Electron density can increase even in the sub-breakdown condition $E < E_k$ at sprite/sprite halo altitudes.
This is because the total density of electrons and O\(^{-}\) ions increases as long as the electron impact ionization takes effect. The electron density decreases initially if the density of O\(^{-}\) is low, but both densities eventually increase with the same rate if the electric field is maintained at a moderate level. However, this does not imply that an electron avalanche is able to proceed and transform into a streamer in \(E < E_K\).

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