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COMPUTATIONAL MODELING OF HIGH PRESSURE GAS BREAKDOWN AND STREAMER FORMATION IN EXTERNAL ELECTRIC FIELDS *

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Abstract

The development of new computational models of gas breakdown for use in particle-in-cell (PIC) codes is described. These modeling efforts include fundamental processes associated with the breakdown of high pressure gases and represent key components in the comprehensive study of the physics of high-pressure gas switches. Two computational algorithms are discussed; a Monte Carlo type collision (MCC) model whereby PIC macro-particles undergo random elastic and inelastic interactions, and a semi-fluid scattering model.

A newly implemented attachment algorithm, important for electronegative gases such as SF_6, has been developed. Cross-section compilations for H_2 and SF_6 for use in the MCC algorithm are summarized along with the modeling assumptions used to make this model computationally tractable. The results of detailed swarm calculations using these cross-sections are presented along with comparisons to experimental data.

An implicit semi-fluid collision PIC model is used to carry out the streamer simulations. These simulations track the formation and evolution of a streamer from a small seed electron population in different applied electric fields. The results of H_2 and SF_6 streamer simulations are discussed, including comparisons between the semi-fluid and MCC model for streamer formation and evolution in H_2.

I. INTRODUCTION

Computational modeling of the fundamental processes associated with the breakdown of high pressure gases is an important aspect in the design of a number of pulsed power switching components [1-4]. New models of high pressure gas breakdown are presently under development for use in particle-in-cell (PIC) codes. These modeling efforts are key steps in comprehensive and fundamental studies of the physics of high-pressure gas switches. The computational algorithms described here are of two types; a Monte Carlo collision (MCC) model whereby PIC macro-particles undergo random elastic and inelastic interactions, and a semi-fluid scattering model.

In Sec. II, a description of a newly implemented attachment algorithm, important for electronegative gases such as SF_6, is given along with a detailed description of the modeling assumptions that are made to make this model computationally tractable. A brief summary of the cross-section compilations for H_2 and SF_6 for use in the MCC algorithm are given in Sec. III. This section also includes a discussion of the results of detailed swarm calculations using these cross-sections and comparisons with experimental data. In Sec. IV, the existing implicit collision model in the PIC code LSP [5] is used to carry out 2D (r,z) streamer simulations. These simulations track the formation and evolution of a streamer from a small seed electron population in different applied electric fields. Conclusions are given in Sec. V.

II. ATTACHMENT ALGORITHM

We have developed a MCC model which has been used to simulate breakdown in weakly-ionized gases [1]. This model, including electron elastic, inelastic, and ionization processes with neutrals, was benchmarked for noble gases, such as He and Ar, in which no significant electron sink is present [3]. For an electronegative gas such as SF_6, electron attachment processes play a key role in inhibiting breakdown at low field values. To facilitate SF_6 modeling, an attachment algorithm has been developed and added to the MCC model. The algorithm has also been adapted to work with the more approximate scattering model in Lsp.

At this time, the Monte Carlo attachment algorithm has been ported into Lsp with some notable simplifications: only a single attachment channel for each neutral species ($e+X \rightarrow X^-$) is enabled. This simplifies the input, and keeps the number of ion species down. For example, for SF_6 the three significant attachment cross sections (for production of the negative ions SF_6^-, SF_5^-, and F^-) are summed to get a total attachment cross-

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section, and all ion macro-particles are created as SF_6^-. Unless detailed ion dynamics become important this simplification should be adequate for a weakly ionized gas. The algorithm may be easily extended to a more general form allowing for multiple attachment processes if necessary. Next, the neutral species temperature is not considered in the Lsp implementation. This assumption is justified in the limit that the electron temperature is much greater than the neutral temperature. Finally, recombination (a second order effect in a weakly ionized gas) and electron detachment of negative ions (believed to occur on very long time scales) are not included. Also note that ion neutral collisions can also be modeled by the MCC model in Lsp, but are not included in the calculations presented here.

One constraint associated with the MCC model is the need to resolve to the electron-neutral collision frequency. The approximate scattering algorithm allows LSP to be run at time steps which exceed the inverse of the collision frequency, although with a loss of detailed kinetic information regarding the electron distribution. This algorithm assumes like particles scatter off locally-constructed drifting Maxwellian distributions. Collisions between dissimilar particles such as between electrons and neutrals (and ions) are handled with a lumped frictional force and Ohmic heating term. In contrast, the MCC algorithm typically requires relatively small (sub-picosecond) time steps for parameter ranges of interest. The relative accuracy of the two scattering methods has been accessed and reported in [1]. One important goal is to find and validate an algorithm that may sacrifice some detailed kinetic information, but which provides approximately the right transport coefficients when used with a larger time step.

III. CROSS SECTIONS FOR H_2 AND SF_6

Ultimately the use of the MCC model requires accurate cross section data for gases of interest. While some measured data is available for these gases, cross-sections cannot be directly measured for all important processes. As an example, for SF_6, the excitation cross-section is not well known, although the threshold is roughly 10 eV [6]. The transport properties, such as drift velocity, temperature, and effective ionization rates of electron swarms in a gas can be readily measured. One common technique for determining a self-consistent set of cross-sections for a gas is to numerically solve for the transport coefficients while iteratively adjusting the unknown cross-sections (a lumped excitation cross-section in the case of SF_6) until good agreement is found with measured data. This is not a trivial procedure as the cross-sections are, in general, functions of electron energy. So both the functional shape and magnitude of the cross-sections can be adjusted to match the transport coefficients over some range of applied electric field values. Typically, the numerical values of the transport coefficients are calculated by a Boltzmann code. For this work, the EEDF code [7] was used which iteratively solves for the steady-state electron energy distribution function $f(E)$ where E is the electron energy. The transport coefficients are then calculated by appropriate integrals of the distribution function. Note that the electron number density can increase or decrease exponentially, but the shape of the distribution function and values of the transport coefficients are time independent. The standard method of solution is to expand the distribution function in spherical harmonics and then to truncate the expansion to two terms: an isotropic leading term, and a small anisotropic correction term which is due to the applied field. Clearly this perturbative treatment is only valid when the electron drift velocity is small compared to the thermal velocity. A more careful analysis[8] of the higher order terms in the expansion shows that the two term expansion is, in addition, only valid for electron energies for which the elastic cross-section is much larger than the cross-section for inelastic processes. If these conditions are not satisfied, higher order terms in the expansion are required [9]. An alternate method is to directly simulate a swarm of particles using a PIC code. We used LSP to push electron macro-particles in a background neutral gas with a uniform applied electric field. The simulations were performed in a single cell. The particles were confined to the cell by suppressing the position push. Since the particles are not allowed to move spatially, spatial transport coefficients like the diffusion coefficient can not be determined. Note also that only the applied electric field is present, the particle charges and currents were not allowed to feed back onto the fields. The electron neutral scattering was modeled by the MCC algorithm described in the previous section. The LSP-MCC swarm simulations must push electron macro-particles in the time-domain for a given set of initial conditions until steady-state conditions are achieved. Since the MCC algorithm does not make any assumptions a priori about the distribution function, it should generate the correct kinetic behavior to all orders for an adequately small time step and sufficiently large particle number. As reported in [1], the results of the two methods were found to be the same as long as the two term expansion is valid for H_2 and SF_6 comparisons. Some subtle differences were apparent in the analysis of SF_6 [1], however, and some additional study is warranted.

IV. SIMULATION OF STREAMER PROPAGATION IN H_2

An implicit collisional electromagnetic-PIC method [10] was used to study the evolution and propagation of a streamer in an atmosphere of hydrogen. In 2D cylindrical (r,z) simulations, streamer evolution initiated from wispy electron swarms is followed to high density without the

need to resolve the plasma electron oscillation frequency or the Debye length while maintaining reasonable energy conservation. These constraints severely hamper the densities that can be simulated with explicit PIC algorithms. In these calculations, a coax feeds a forward-going voltage wave giving electric fields of roughly 6-100 kV/cm across an 8-mm anode-cathode gap. A 3×10^8 cm^{-3} plasma was initialized 1-mm from the cathode on axis. We found that in all but the lowest electric field values, a streamer evolved and propagated with increasing speed towards the anode. The streamer front velocities increased from 10 to 160 cm/μs. Typically, as shown in Fig. 1 for the 30 kV/cm field, a weak streamer initially formed a small distance from the seed. As the streamer drifted and the density increased, eventually the tail of the electrons became anchored in space by the increasing space charge. At this point the density of the plasma electrons and ions became comparable and the plasma begins to shield out the electric field. Shown in Fig. 2, the field is enhanced at the streamer edges to roughly twice the initial field. The electron temperature at the edges is roughly 4-eV enable a weak avalanche that sustains the streamer.

The sensitivity of the electron avalanche to time step is illustrated in Fig. 3. Here the time step was varied from 0.67--2.67 ps with electron-neutral collision times, τ_{en}~0.28 ps. Thus, the time step is actually as high as $10\tau_{en}$. We see that except for early time initiation, the exponential growth of the electrons in the three simulations is quite close. (We note that this agreement required some algorithm modifications which are described in [1].) The calculated avalanche rates were found to be within 10% for a factor of 4 variation in time step with steps as high as 10 collision times.

V. SUMMARY

A MCC model has been implemented and tested in swarm calculations for H_2 and SF_6. The algorithm includes an attachment processes that is important for electronegative gases such as SF_6.

A series of hydrogen breakdown simulations have been carried out with the Lsp simulation code. Swarm simulations calculate electron avalanche rate, drift velocity and electron temperatures in reasonable agreement with experiments. Sensitivity of the results to simulation time step was investigated. Results were shown to be insensitive to time step after handling of ionization and the Ohmic heating term were modified. Two dimensional simulations of streamer propagation were carried out showing front velocities 3-5 times that of the 1D mean electron drift velocity. These results were consistent with a factor of 2-3 enhancement of the ambient electric field due to 2D geometry of the streamer. Electric fields are increasingly shorted within the streamer, and enhanced at edges as the streamer density increases. Electron temperatures are typically 4-5 eV at edge, sufficient for a weak avalanche in > 6 kV/cm fields. Although not discussed here, an advanced particle management algorithm has been developed to speed simulations that will allow for larger scale simulations [11].

Streamer calculations have been carried out using the MCC model in 2D. Initial results show good agreement with streamer simulations using a semi-fluid scattering model in both H_2 and SF_6. A complete report on these streamer calculations in both H_2 and SF_6 will be presented in a future publication.

VI. REFERENCES

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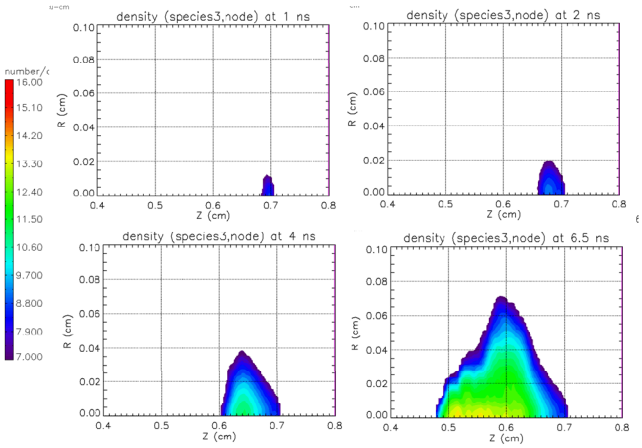

Figure 1. The plasma ion density (Log_{10} contour levels) is plotted 1, 2, 4 and 6.5 ns into the 30 kV/cm-atm 2D LSP simulation. A small $3x10^8$ cm^{-3} plasma seed is initialized at t=0.

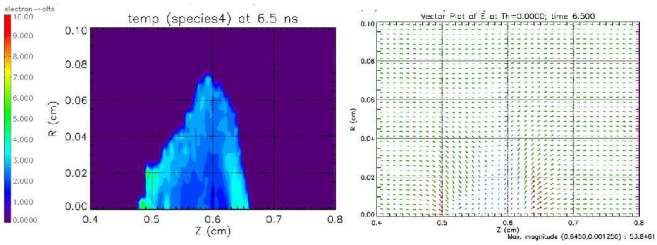

Figure 2. For the 30 kV/cm-atm 2D simulation, the electron temperature (left) and electric field vectors (right) are plotted after 6.5 ns.

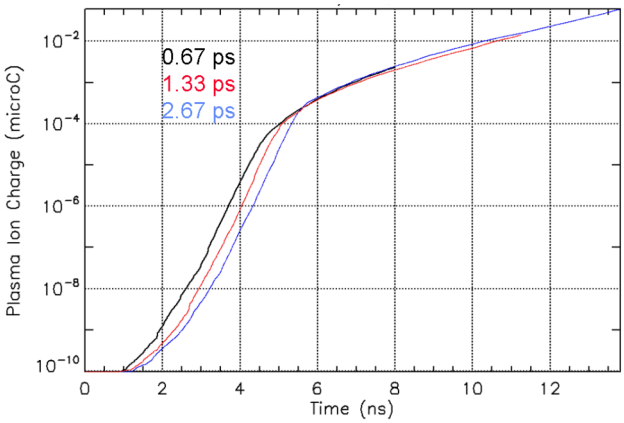

Figure 3. The total ion charge in three streamer simulations with time steps of 0.67, 1.33 and 2.67 ps are shown as a function of time.