Breakdown simulations from arc initiation to stable arcs: Challenges for accurate PIC-DSMC simulation

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Simulation of breakdown is important for understanding and designing a variety of applications such as trigger spark gap switches, gaseous micro-optoelectronics systems, and mitigating/shunting undesirable discharge events These simulations must be numerically accurate from early time arc initiation to late time stable arc behaviour. The present work examines numerical accuracy constraints for particle-in-cell (PIC) kinetic simulations [1] that model particle-particle collisions using the direct simulation Monte Carlo (DMSC) method [2]. Accurate simulation of even a simple electron avalanche across a fixed voltage drop and a reduced field of 1000 Td has been found to require a timestep ~1/100 of the mean time between collisions. Additionally, even though the electric field and neutral density are constant across the gap, the collision mesh must still be resolved at less than ~1/25 the mean free path for converged electron multiplication across the gap. These constraints are much smaller than the typical PIC-DSMC requirements for timestep size (plasma frequency, mean collision time, CFL) and element size (Debye length and mean free path) [1, 2]. However, both of these constraints seem related to the fact that charged particles are accelerated each timestep by an external force across an element and therefore gradients in the electron energy distribution function (EEDF) can exist at scales smaller than the collision time/length. For numerical accuracy, the EEDF must also be resolved in order to capture gradients in the electron-neutral cross sections versus energy. We have found if a simulation does not accurately resolve these scales then even with an external circuit model providing stabilizing feedback, the simulation can go unstable at late times.

1. Introduction

There is considerable interest in simulation capability for breakdown between electrodes. In the present work we outline several challenges for numerically accurate simulation of arc breakdown. Depending on the neutral gas pressure and device length scales, the plasma may be in non-equilibrium throughout the gap during breakdown. However, even in large gaps at high pressure the plasma can be in non-equilibrium in the cathode fall region where the majority of ionization occurs. Therefore PIC kinetic simulations [1] that model collisions using the direct simulation Monte Carlo (DMSC) method [2] are often used.

In PIC-DSMC simulations particles are pushed, collided, and the field updated on a finite timestep. Obviously the timestep size will affect numerical accuracy and stability. For PIC simulations of collisionless plasma this is well understood [1]; similarly it is well understood for DSMC simulations of collisional neutral flows. However, breakdown involves a collisional partially ionized gas, and we show below that traditional timestep constraints are not always sufficient with charged particles.

In order to solve for the field and perform collisions, PIC-DSMC sorts particles into spatial mesh elements. Again, accuracy and stability constraints on the mesh size relative to the Debye length and mean free path are relatively well understood [1, 2]. In this case DSMC is explicit in stating that gradients (in density, the EEDF, etc.) across an element affect the simulation accuracy and that these changes in gas properties across an element need to be minimized. Traditionally in collisional DSMC simulations it is assumed that the gradients scale with the mean free path; however, we find that external forces on the particles can create (and sustain) gradients at scales less than the mean free path. We find that this can be recast as an element voltage drop constraint for breakdown simulations that is likely dependent on the gas species and reduced field.

2. Results

In order to demonstrate the timestep and mesh size constraints we simulate electron avalanche in a fixed field (the field is not coupled to the simulated space charge). In the simulations a small number (10^5) of electrons are seeded at the cathode (0 V) and then the simulation proceeds until all electrons have left the domain via the anode boundary (held at 200 V). During transit, the electrons have three possible interactions with the simulated neutral gas particles: elastic, excitation, or ionization interactions. Simplified artificial cross sections are

used for the simulations and are shown in Figure 1. The present avalanche simulations assume isotropic scattering for all collisions. Ionization creates a secondary electron with energy, E_S:

$$E_s = E_{iz} tan\left(Rand_{\#} atan\left(\frac{E_r - E_{iz}}{2E_{iz}}\right)\right)$$

where E_{iz} is the ionization energy, $Rand_{\#}$ is a uniform random number, and E_r is the relative energy.

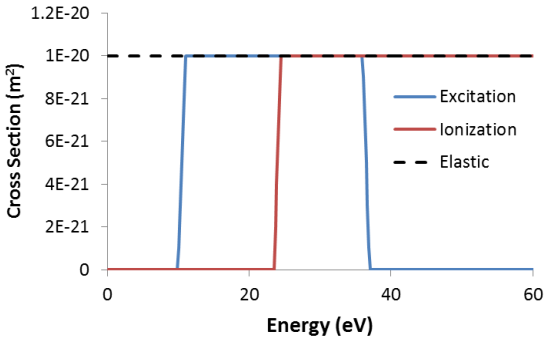

Figure 1: Cross sections used in simple electron avalanche simulations.

2.1. Timestep size

Figure 2 shows the electron multiplication (number of electrons crossing the anode divided by the number seeded at the cathode) versus timestep size for three different gap sizes and pressures such that the reduced field (1000 Td) is the same for each case. The product of density and gap length is constant, so from Paschen curve arguments [3] one expects that the electron multiplication factor for the three cases can be collapsed onto a single curve if the timestep is scaled by the mean time between collisions (which scales with the background density). If instead one were to plot the electron multiplication versus the physical time or the CFL condition, then the curves would not collapse.

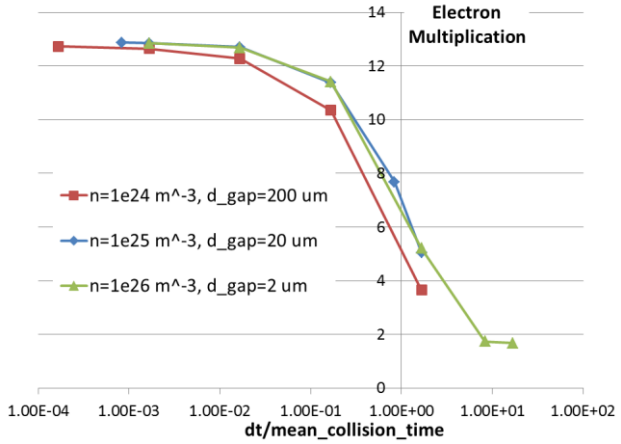

Figure 2: Electron multiplication across gap versus timestep size.

These simulations do not couple the space charge to the field solve and therefore the plasma frequency is not a meaningful timestep constraint. On the other hand, neutral particle DSMC timestep convergence would be expected for timestep sizes on the order of the mean collision time. However in these simulations with charged particles (and a reduced field of 1000 Td) it can be seen that a timestep of 10^{-2} times the mean collision time is required for reasonable accuracy.

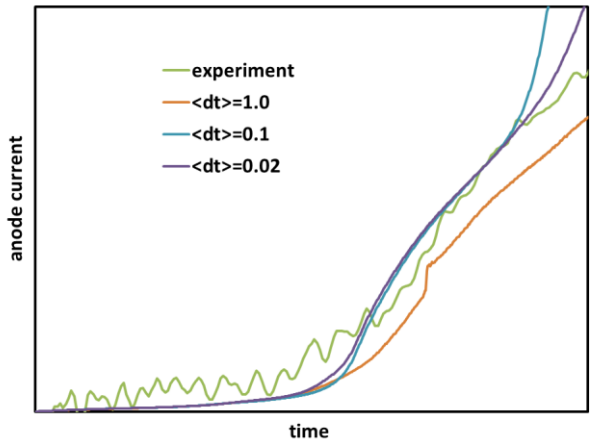

Figure 3: Anode current vs. time for 1D simulation of vacuum breakdown at several different timestep sizes (normalized).

A more applied example with realistic cross sections and particle creation at the electrodes is shown in Figure 3, which plots the anode current versus time for a simulation of the initiation of a vacuum arc breakdown. Traditionally, one would expect a normalized timestep of 1.0 (that resolves both plasma frequency and mean collision time) to be sufficiently small for accurate simulation. However, it is clear that the anode current requires normalized timesteps much smaller than 1.0 to show convergence. In fact, the late-time behaviour still shows the simulation might not be converged even at a normalized timestep of 0.02.

2.2. Mesh Size

For accurate simulations, DSMC requires that the mesh size be less than any gradient length scales. For gas flows with only neutral particle collisions, gradients are not sustained over length scales much smaller than the mean free path. However, external forces on the particles (e.g., electrical or gravitational fields) can result in gradients with smaller length scales. In the case of electron multiplication across a fixed field, the EEDF controls the ionization rate and the change in the EEDF across the gap must be well resolved by

collision elements in order to get the correct ionization rate.

Finally, Figure 4 shows the electron multiplication across a 20 μm gap with a background gas density of 10^{25} m^{-3} and an anode voltage of 200 V (reduced field of 1000 Td). It is interesting to note that there is no spatial mesh convergence unless the timestep is sufficiently small. In this instance, convergence in spatial mesh is achieved when the timestep drops to 1 fs. If one uses a converged timestep, then it is seen that the mesh must be ~1/25 of the mean free path.

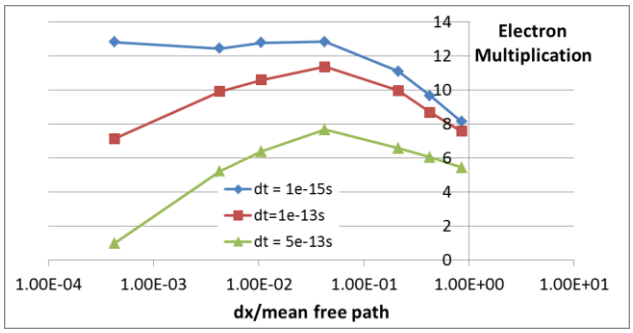

Figure 4: Electron multiplication vs. element size.

3. Conclusions

We have found additional constraints on numerical parameters necessary for accurate simulation of arc initiation through stable arc behaviour. Charged particles accelerated by an external force per timestep and across an element can develop gradients in the EEDF at scales smaller than the collision time/length. Therefore the mean time between collisions and the mean free path can provide misleading estimates of accuracy limits for the timestep and mesh size respectively.

4. References

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4. Acknowledgments

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