ionization because the dissociation energy is also required.[5] Electronic excitation, rotational and vibrational excitations of water molecules are important energy loss mechanisms at the electron energy less than 10 eV.[6] Dissociative attachment of the electrons to water molecules to form negative ions, H^-, O^- and OH^- is another loss mechanism.[7] The cross sections for these processes are well-known and are employed in our simulation code.

The initial injection energy of the beam electrons is 10–20 keV and the initial beam radius is 1 mm. The cross section of ionization collisions at 10 keV beam energy is about 10^{-17} cm^2 so that the mean free path is about 3×10^{-3} cm at one atmospheric pressure. The cross section becomes larger by more than a factor of 10 at lower beam energy reaching the maximum value of 2×10^{-16} cm^2 at around 100 eV and decreases for smaller energies. The threshold energy for ionization of the water molecule is 12.61 eV. For energies below the ionization energy of water molecules, dissociative electron attachment which produces negative ions including OH^-, H^- and O^- can occur. The cross sections for these processes are 10^{-18}–6.4×10^{-18} cm^2 for the beam energy of 4.3–12 eV. It is well-known that the negative H^- and O^- ions immediately react with water molecules to produce OH^- ions. Energy losses caused by the electronic excitation, as well as rotational and vibrational excitations of water molecules are also included in the present simulations. The elastic collisions in which no kinetic energy is consumed for atomic and chemical processes can cause transfer of electron kinetic energy to the water molecules. The cross section for the elastic collision is 10^{-15} cm^2 for low energy electrons, less than 10 eV and decreases thereafter monotonically with increasing energy. While the fractional energy loss to the water molecules from the electrons is only the electron to molecule mass ratio, elastic collisions can cause energy drain at low energy where few other loss mechanisms exist.

A three dimensional particle simulation model in slab geometry was developed adding various collisional processes to a conventional collisionless simulation model.[8] An electron beam at 20 keV energy and 4 μA current is injected into one-half atmospheric pressure water vapor through a 1 mm diameter hole at the center of a conducting plate located at $z=0$. At the other end of the system, a positively biased conducting wall at 1 keV potential is located at $z=1.6$ cm. A $64\times64\times64$ spatial grid was used for all the simulations reported in this paper.

Injected beam electrons lose their energy via ionization and non-ionizing collisions as they propagate into water vapor. Each beam electron produces about 100 ions in our simulations. Note the high energy collisions produce predominantly forward scattered electrons so that electrons tend to propagate forward into water vapor. When the electron energy reaches below the ionization energy, some of the beam and secondary electrons are attached to form OH^- negative ions. At earlier times less than a few nanoseconds after injection, the electrostatic repulsion is weak due to low net charge density so that a quasi-steady state is reached in which the beam electrons are converted into secondary electrons, positive ions and negative OH^- ions whose density

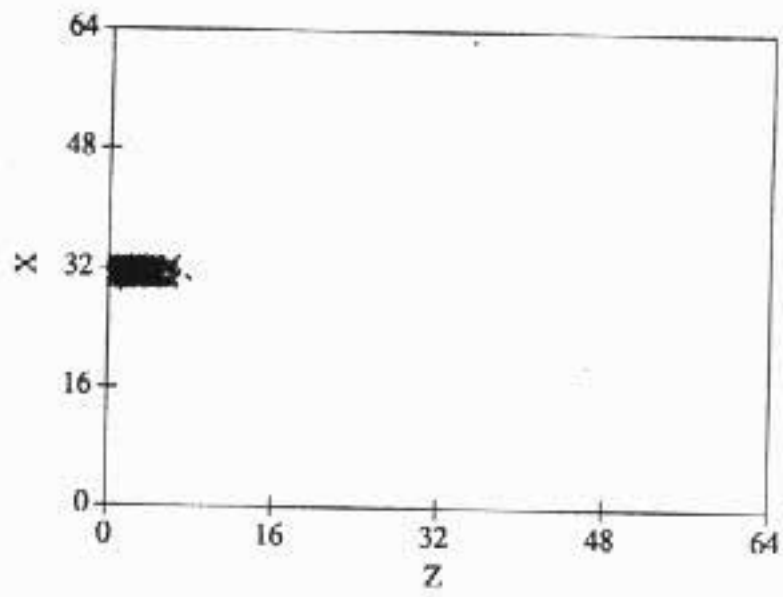

FIG. 7. Result of a simulation at t=5 ns after injection. Shown is a scatter plot of 1024 H_2O^+ ions penetrating about 1 mm into water vapor. The profile of the ions does not change until the electric potential pulls the electrons and ions toward the biased wall.

profiles do not change in time. The tip of the propagation is about 1 mm away from the injector.

Shown in Fig. 7 is a result of a simulation at $t=5\times10^{-9}$ sec where the scatter plot of 1024 H_2O ions projected onto the (x,z) plane is shown. By the time beam electrons propagate 1 mm into water vapor, electrons lose most of their energy via ionizing and non-ionizing collisions and at the same time electrostatic repulsion is weak so that the injected beam and secondary particles stay more or less the same shape.

In order to speed up the calculations in real time, notice that most of the beam electrons are converted into low energy (less than 10 eV) electrons within the 1 mm propagation distance. Since the conversion process remains the same so long as the background water vapor is not modified, one can model the initial conversion process without directly following beam particles. This allows us to use a much larger time step of integration since beam electrons need not be directly followed in time. Another numerical technique developed in this model is to lump electrons and ions into macroparticles as more and more new born particles are created in the course of the simulations. Particles located nearby in phase space move together for a short time. These particles can be lumped together thereby reducing the number of simulation particles. This technique is particularly useful in a collisional gas where rapid collisions cause large diffusion in phase space. Another technique we have tested is to assume that the electrons are trapped by the water molecules and move together in the presence of an electric field. The rationale behind this idea is that since the collisions are so frequent that the electrons are trapped by the water molecules and they tend to move together. This would increase the effective mass of an electron thereby a much larger time step can be employed. These techniques must be carefully tested before they are employed in the production runs. We show only some of preliminary results using these techniques.

Shown in Fig. 8 is OH^- ions at t=0.27 μs showing that they propagate away from the injector and at the same time spread out radially. The simulation was continued without