

Ejection of Nitrogen from Titan's Atmosphere by Magnetospheric Ions and Pick-up Ions

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Abstract

A 3-D Monte Carlo model is used to describe the ejection of N and N₂ from Titan due to the interaction of Saturn's magnetospheric N⁺ ions and pick-up C₂H₅⁺ ions with its N₂ atmosphere. Based on estimates of the ion flux into Titan's corona, this atmospheric sputtering process is an important source of both atomic and molecular nitrogen for the neutral torus and plasma in Saturn's outer magnetosphere, a region soon to be studied by the Cassini spacecraft.

Keywords: Titan, Satellites of Saturn, Magnetospheres, Collisional physics

1 Introduction

The flow of plasma onto the atmosphere of a planet or planetary satellite produces a series of energy transfer events that can lead to atmospheric loss, a process often called atmospheric sputtering (e.g., Johnson 1990; 1994). When an energetic ion intersects Titan's exobase and collides with an atmospheric atom or molecule, a direct transfer of momentum occurs which initiates a cascade of collisions between atmospheric particles. During this process atoms or molecules at the exobase can be knocked upward into ballistic trajectories populating the corona or can have sufficient momentum in the right direction in order to escape the gravitational field. Atmospheric sputtering can be produced by impacting solar wind ions, pick-up ions or magnetospheric plasma ions. Magnetospheric ion sputtering of Io leads to the formation of its plasma torus and Na cloud (McGrath *et al.* 2004). The interaction of magnetospheric ions and pick-up ions with the atmosphere of Titan, studied here, results in the escape of nitrogen atoms and molecules (Shematovich *et al.*, 2003). These neutrals form a toroidal cloud of nitrogen that is a distributed source of heavy ions for Saturn's magnetosphere (Barbosa, 1987, Lammer and Bauer, 1993, Sittler *et al.*, 2003, Smith *et al.* 2004).

Calculations of the atmospheric loss induced by the co-rotating magnetospheric ions showed that the atmospheric sputtering rate was much smaller than the photo-dissociation-induced escape rate (Shematovich *et al.* 2001). However, taking in account the slowing of the heavy, co-rotating plasma ions close to Titan and the re-impact of heavy, newly created atmospheric pick-up ions, Shematovich *et al.* (2003) used a 1-D model to show that atmospheric sputtering could be as important as the photo-dissociation-induced loss or could dominate. This is critical as molecular nitrogen ejection only occurs efficiently by atmospheric sputtering. Therefore, the character of the nitrogen plasma trapped in Saturn's magnetosphere will differ

depending on the relative importance of these atmospheric loss processes. A 3-D Monte Carlo model is developed here to describe the sputtering of Titan's atmosphere by the deflected magnetospheric N^+ and C_2H_5^+ pick-up ions. The flux of escaping particles is typically formed over a wide transition region in which the character of the gas flow changes from a thermospheric collision dominated regime to an exospheric collisionless regime. In this paper we calculate the production of suprathermal atoms and molecules, their escape and their supply to the nitrogen torus. The implications of these results for Saturn's neutral clouds and magnetospheric plasma are discussed.

2 Monte Carlo Model

A three dimensional Monte Carlo model is developed to simulate the penetration of ions into Titan's atmosphere. The cascade of collisions initiated by the incoming ions and the recoil atoms and molecules are described. In this simulation only suprathermal nitrogen with a kinetic energy above 0.1 eV are followed in order to limit the computing time. These particles move under Titan's gravity and collide with N_2 in the atmosphere. The incident and recoil particles are followed from 1700 km to about 1000 km. Recoils generated below 1000 km will be thermalized quickly and will have a small effect on the coronal population and escape. Since the dominant species at Titan's exobase is N_2 , a pure N_2 atmosphere is considered. Both recoil N_2 molecules and recoil N atoms from a dissociation event are tracked.

The particle tracking is described using the algorithm of Bird (1994). If collisions of magnetospheric ions with ambient N_2 molecules are accompanied by the formation of suprathermal recoils, N or N_2 , with kinetic energies higher than the cut-off energy, then these particles are created in the cell. This means that the numerical model evolves with a variable number of modeling particles representing the suprathermal populations of atomic and molecular

nitrogen. In the same time step, the transport of each modeling particle in the transition region is calculated. The N and N₂ modeling particles are followed until they escape from Titan's atmosphere, until they collisionally lose energy so their kinetic energy falls below the cut-off energy, or until they penetrate deep into the atmosphere. When recoil particles cross the upper boundary they become ballistic and are subject only to the gravitational attraction of Titan. These ballistic particles are followed until they again cross the upper boundary of the domain and are reintegrated with the population of the colliding fast particles. Above a distance of 2 R_T from the surface of Titan they are assumed to have escaped. This procedure is carried out for each time step in each cell. A similar model was used to study the solar wind interaction with Mars (Leblanc and Johnson 2001; 2002).

In these calculations we use estimates of the incident fluxes of ambient flowing N⁺ and C₂H₅⁺ pickup ions from Brecht *et al.* (2000). These are globally averaged fluxes based on the statistics of individual ion trajectories that intersect the exobase. We assumed the distribution of the angles of ion incidence with respect to the local vertical, and the incident flux and energy distribution, were represented by the average distribution from the simulation. The incident ion fluxes adopted (Table I) are obtained using a single set of conditions. Although Titan experiences a range of conditions in Saturn's magnetosphere and in the solar wind, Voyager encounter ambient conditions were used. In addition, simplified conditions were assumed for the incident magnetospheric ion temperature and for the description of the upper atmospheric source of pick-up ions. The impacting ions are not uniformly distributed over the ram face of Titan because of the large ion gyroradii. This implies that there are regions where the flux can be larger or smaller by an order of magnitude than the average incident ions flux used here. Though the magnetospheric flow past Titan is expected to be sub-magnetosonic (Ness *et al.*, 1982), later

models suggested that the flow might be super-magnetosonic when Titan is on the dusk side of the magnetosphere (Nagi *et al.*, 2001). Brecht *et al.* (2000) assumed that the flow is super-magnetosonic. The consequences of these assumptions will be addressed in a future work.

The slowed and deflected co-rotating N^+ have energies that are much smaller than the co-rotation energy (2.9 keV), allowing them to interact more efficiently near the exobase. The heavier pick-up ions also have large cross sections for momentum transfer to the atmospheric molecules and, therefore, are also more efficient at ejecting species near the exobase. Because the heavy atoms in the molecular pick-up ions contribute much more to the sputtering than does the attached hydrogen, they are treated as energetic incident nitrogen molecules. Since many of the energetic atmospheric recoils are N atoms, both $N + N_2$ and $N_2 + N_2$ cross sections are required over a large range of energies. We constructed tables of such cross sections using appropriate interaction potentials and the results of molecular dynamics calculations and then interpolated. The calculated cross sections at high energies agree with those in Johnson *et al.* (2002) and at low energies with those of Tully and Johnson (2002) as corrected (Tully and Johnson 2003). In Shematovich *et al.* (2003) we had used integrated momentum transfer and dissociation cross sections and mean energy transfers to calculate the recoil energies, here they are directly obtained from the molecular dynamics calculations.

3 Results and Discussion

It was initially thought that the co-rotating N^+ ions (~ 2.9 keV) would be the most efficient sputtering agents at Titan. However, the slowed and deflected N^+ and the newly created pick-up ions interact more efficiently with atmospheric molecules and the area from which ions have access to the atmosphere is larger. In particular the pickup ions are locally created in the

surrounding exosphere, and so those picked up in the hemisphere opposite to the $E=-v \times B$ corotation electric field direction are directed toward the exobase in that hemisphere. Moreover they do not travel far before they impact the exobase, and they deposit much of their obtained picked up energy near the exobase. The energy deposited by the co-rotating 2.9 keV N^+ ions if they could reach the exobase would be, roughly, $2.1 \times 10^9 \text{ eV cm}^{-2} \text{ s}^{-1}$ while the energy deposited by the deflected N^+ ions (50 – 750 eV) and the pickup ions (50-1250 eV) is, roughly, $4.8 \times 10^9 \text{ eV cm}^{-2} \text{ s}^{-1}$. The solar UV photons carry an energy flux ($\sim 2 \times 10^{10} \text{ eV cm}^{-2} \text{ s}^{-1}$) that is larger than that carried by the ions considered here and larger than the energetic magnetospheric ions (Luna *et al.* 2003), but it is deposited at greater depths on the average.

Using our 3-D Monte Carlo model the low energy N^+ ions and $C_2H_5^+$ ions are allowed to collide with the atmosphere of Titan and the atmospheric loss is studied. Figure 1 presents the energy distribution of the escaping N_2 molecules produced by the incident N^+ ions. The distribution is dominated by low energy N_2 but with a high-energy tail typical of atmospheric sputtering (Johnson 2000). About 70% of the escaping nitrogen molecules have energies less than 2 eV with about 35% of the escaping N_2 having energy less than 0.5 eV. Due to the slow decay at the higher energies the mean energy of escaping N_2 ($\sim 2.7 \text{ eV}$) is much higher than the energies of the majority of the escaping particles.

The local and integrated escape flux of N and N_2 and the altitude profile for the production of supra-thermal N_2 and N in the thermosphere of Titan were determined earlier using a 1-D model (Shematovich *et al.* 2003). Although the method of determining the outcome of individual collisions differs here, we obtained comparable results for the incident N^+ but somewhat different results for the incident molecular ion. Using the 3-D model, Fig. 2 shows the coronal density of ‘hot’ ($>0.1 \text{ eV}$) N driven by the incident N^+ ions in the equatorial xy plane.

Here the incident flux is in the $-x$ direction, onto the trailing hemisphere. Titan's axis of rotation is along the z -axis and y represent the radius vector from Saturn to Titan. Based on the gyro-motion, the mean flow is actually onto a hemisphere in the xy quadrant on the Saturn facing side. Since the atmosphere is spherically symmetric the incident axis can be rotated to the appropriate flow direction. It is seen that a fraction of the particles leave the corona where the flow direction is nearly tangential to the exobase. Some of these are energetic forward scattered nitrogen not included in the 1-D model. Others are the incident ions that make weak collisions before leaving with very high energy. Ions with an angle of incidence close to the normal to the exobase penetrate into the atmosphere and transfer energy to the atmospheric molecules. As seen in Fig. 2, the resulting recoils can be scattered backwards in multiple collisions, which is the usual sputter contribution. A distribution of energetic N_2 similar to that in Fig. 2 is produced with its component of forward scattered particles.

Figure 3 gives the direction in which N atoms are ejected by incident N^+ ions. Integrating over the azimuthal angle around the direction of incidence, $\phi = 0^\circ$ describes back-scattered particles and $\phi = 180^\circ$ the forward scattered. It is seen that a major portion of the sputtered particles are back-scattered. The probability of neutralization of the incident ions by charge exchange was also studied. Those ions that enter closest to the normal and penetrate into the atmosphere have a higher probability of neutralization than the grazing incident ions. The neutralized component is represented by the solid curve with squares and those that exit as ions are represented by the solid curve with circles.

Table 1 presents the escape flux of N and N_2 by N^+ and $C_2H_5^+$ incident ions along with the results of 1-D model. Collision of the incident N^+ and $C_2H_5^+$ with atmospheric N_2 leads to the formation, through momentum transfer and dissociation collisions, of both N and N_2 with

relatively high kinetic energies. Momentum transfer collision of $C_2H_5^+$ pick-up ions with the ambient N_2 molecules are more efficient than collisions of N^+ ions because they are heavier and more energetic on the average. It is seen that the loss rate is similar for our 1-D and 3-D simulations except for the N loss driven by $C_2H_5^+$ ions. The 3-D model better estimates the contribution by forward scattering and knock-out from the edges. The increase in N escape by the incident $C_2H_5^+$ ions can be attributed to the difference in treating the dissociation of N_2 molecules.

Earlier we showed that if the fluxes estimated from Brecht *et al.* (2000) are correct, sputter-loss is at least equivalent to and may be more important than photo-induced loss at Titan (Shematovich *et al.* 2003). The calculations here give a sputtering rate that is 40-50% larger and a more accurate ratio on N to N_2 . Therefore, motivation exists to construct a 3-D model with detailed dissociation cross sections is required to obtain a good estimate of the spatial and velocity distribution of the sputtered N and N_2 . These ejecta generate Titan's nitrogen torus. Calculations of morphology of the torus, inward and outward diffusion of the resulting ions, and interactions with the inner icy satellites are in progress.

4 Summary

Here we calculate the ejection of N and N_2 due to the bombardment of Titan's atmosphere by slowed and deflected magnetospheric N^+ and by the pick-up $C_2H_5^+$. The atmospheric recoils are set in motion by momentum transfer collisions and by collisional dissociation. Earlier we showed that the plasma-induced sputtering of Titan is an important contribution to the atmospheric loss rate. Using the 3-D model and a simplified description of the flow, it is observed the total escape flux of N, as either atomic or molecular nitrogen, is about 40-50% larger than in our earlier 1-D model due to knock-out from the edges of the atmosphere,

forward scattering, and difference in treating dissociation of N_2 . The ejected neutrals are characterized by low energies but with a very energetic tail. We described the spatial distribution of suprathermal corona nitrogen relative to the incident direction and we give the escape flux. Combining this with earlier estimates of the photo-dissociation contribution and accounting for increased EUV flux in the early solar system only a few percent of Titan's atmosphere would have been removed in ~ 4 Gyr, consistent with Titan retaining much of the present nitrogen content. The ejected species are also the source of the N and N_2 neutral tori in Saturn's outer magnetosphere (Sittler *et al.* 2004; Smith *et al.* 2004) so that a significant fraction of the fresh nitrogen in Titan's plasma torus will be molecular if atmospheric sputtering is important. Therefore, Cassini measurements of the production of ions at Titan's orbit can determine to what extent atmospheric erosion by the magnetospheric ions and pick-up ions is important. Here we described atmospheric loss, but this model can also describe the spatial distribution of plasma heating near the exobase (e.g., Johnson 1994) once an accurate spatial distribution of the incident ions is available from Cassini measurements. Together the CAPS ion spectrometer and the ion neutral mass spectrometer (INMS) on the Cassini orbiter will provide observations of the incident ions energy and angle distribution, and the exobase composition, allowing detailed comparison with our calculation in the next year.

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Table 1. Escape flux of N and N₂ by incident N⁺ and C₂H₅⁺ ions

Incident Ions	Escape flux ($\times 10^{25} \text{ s}^{-1}$)					
	3-D Model			1-D Model (Shematovich <i>et al.</i> 2003)		
	N atoms	N ₂ molecules	Total N	N atoms	N ₂ molecules	Total N
N ⁺	0.88(0.19)	0.17	1.2(1.4)	0.79	0.23	1.2
C ₂ H ₅ ⁺	1.6	0.46	2.5	0.14	0.59	1.3

Total N is estimated as the sum of the ejected N and twice the ejected N₂. Brackets include those incident N⁺ which are neutralized and escape as N. Exobase area is $\sim 2.1 \times 10^{18} \text{ cm}^2$ and the surface area is $\sim 0.85 \times 10^{18} \text{ cm}^2$. Incident flux is $1.1 \times 10^7 \text{ N}^+ \text{ cm}^{-2} \text{ s}^{-1}$ and $1.4 \times 10^7 \text{ C}_2\text{H}_5^+ \text{ cm}^{-2} \text{ s}^{-1}$ (Shematovich *et al.* 2003).

Figure Captions

Figure 1. Energy Distribution of the escaping N_2 ejected by incident N^+ ions. Mean energy of the escaping N_2 is 2.7 eV.

Figure 2. Enhancement of density (\log_{10} of cm^{-3}) of hot N (>0.1 eV) in the corona produced by incident N^+ ions. A similar distribution is produced by the incident molecular ions.

Figure 3. Spatial distribution of the escaping particles averaged over the azimuthal angle about the direction of incidence. $\phi=0$ represent backscattered particles. Solid line represents ejected N and line with crosses represents ejected N_2 . Line with squares represent the incident N^+ which escape as ions and the solid line with circles represent the neutralized N^+ ions which escape as N atoms. The affect on the ion motion of the fields below the exobase will be included in subsequent work.

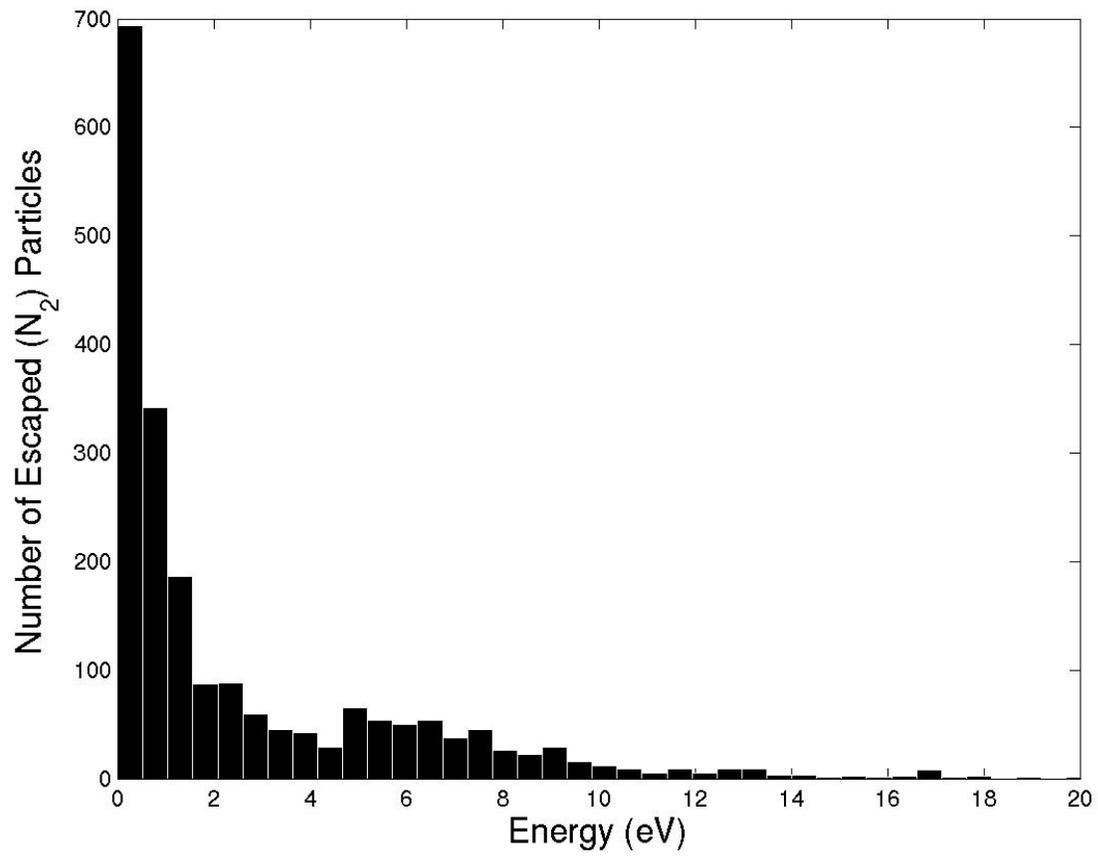


Figure 1. Energy Distribution of the escaping N₂ ejected by incident N⁺ ions. Mean energy of the escaping N₂ is 2.7 eV.

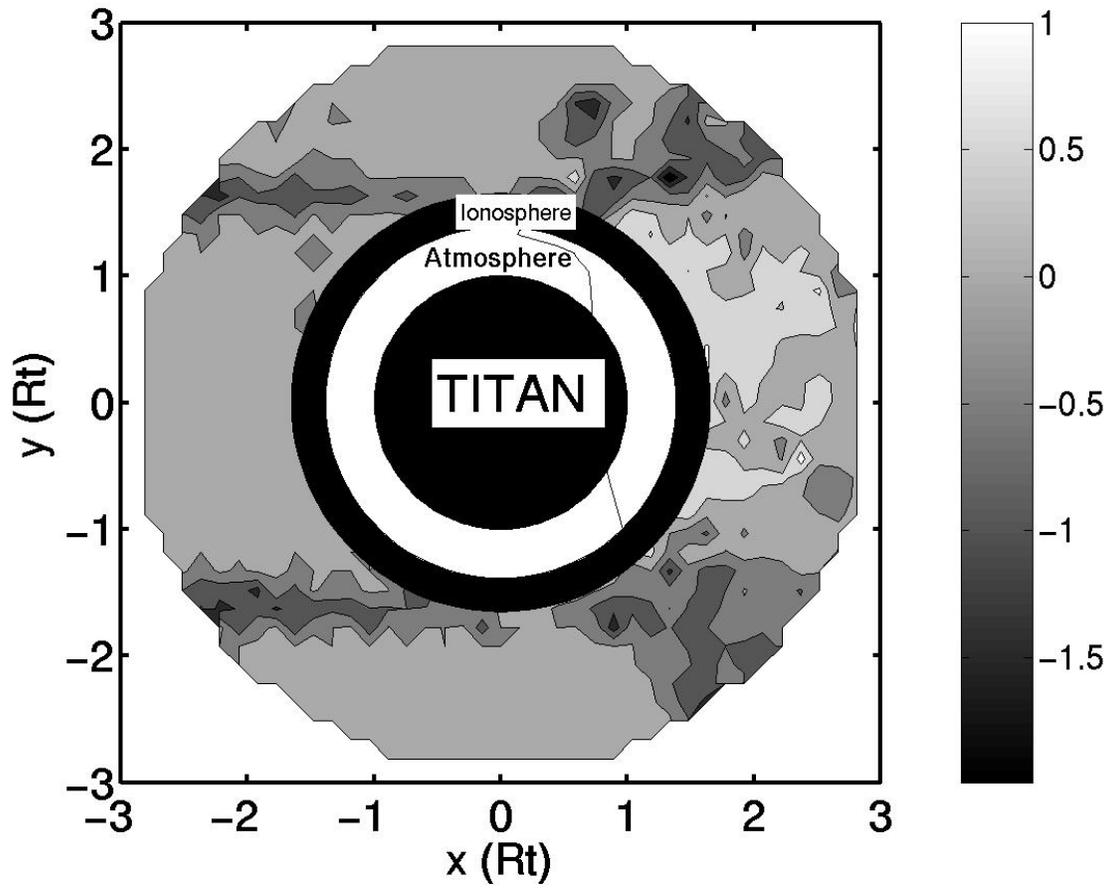


Figure 2. Enhancement of density (\log_{10} of cm^{-3}) of hot N (>0.1 eV) in the corona produced by incident N^+ ions. A similar distribution is produced by the incident molecular ions.

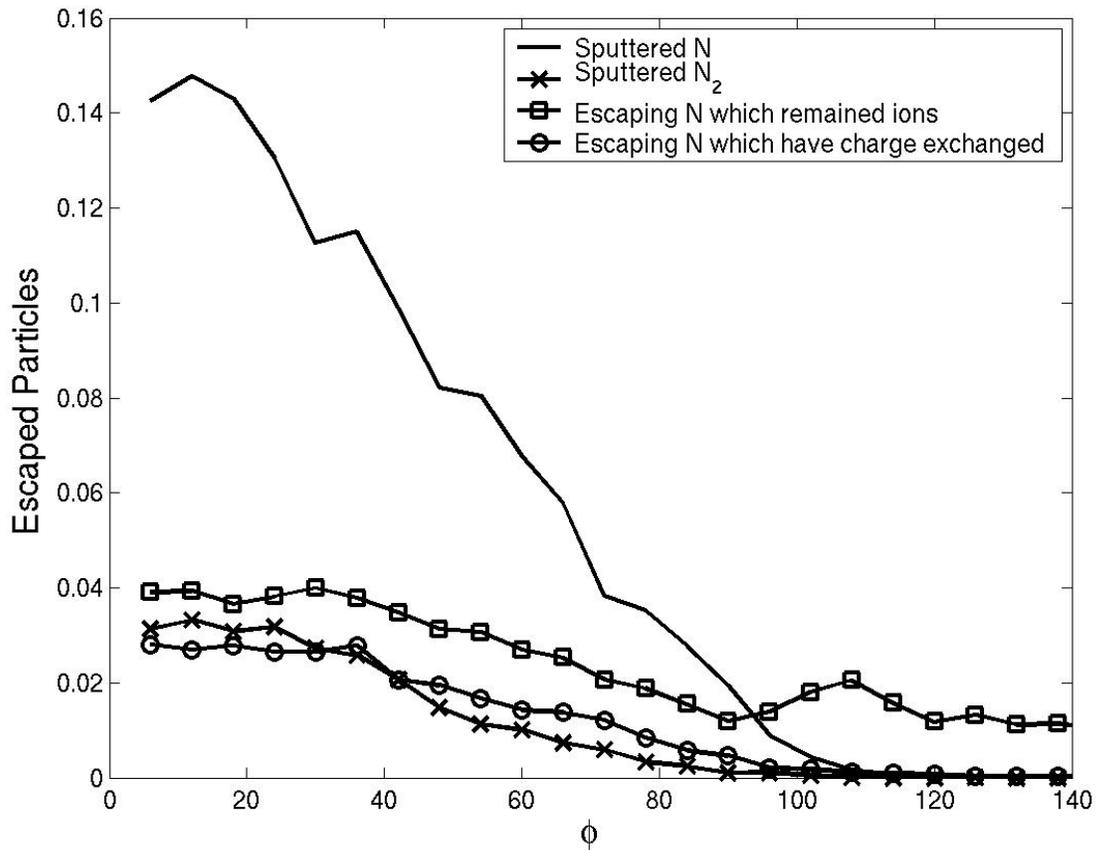


Figure 3. Spatial distribution of the escaping particles averaged over the azimuthal angle about the direction of incidence. $\phi=0$ represent backscattered particles. Solid line represents ejected N and line with crosses represents ejected N_2 . Line with squares represent the incident N^+ which escape as ions and the solid line with circles represent the neutralized N^+ ions which escape as N atoms. The affect on the ion motion of the fields below the exobase will be included in subsequent work.