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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 N_2 from Titan due to the interaction of Saturn's magnetospheric N^+ ions and molecular pick-up ions with its N_2 atmosphere. Based on estimates of the ion flux into Titan's corona, atmospheric sputtering is an important source of both atomic and molecular nitrogen for the neutral torus and plasma in Saturn's outer magnetosphere, a region now being studied by the Cassini spacecraft.
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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, and produces, for instance, the Io torus and Na cloud (McGrath et al., 2004). Using Voyager 1 observational data Hartle et al. (1982) found evidence for mass loading of the Saturn's magnetospheric plasma by material from Titan's upper atmosphere. Later Neubauer et al. (1984) showed that the incident plasma interacts with the atmosphere of Titan. 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., 2004; Smith et al., 2004).

Calculations of the atmospheric loss induced by the corotating magnetospheric ions, with assumed energies of 2.9 keV, 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 (energies less than 750 eV) and the re-impact of heavy, newly created atmospheric pick-up ions (energies less than 1.25 keV), Shematovich et al. (2003) used a 1-D model to show that atmospheric sputtering could be as important as or dominate the photo-dissociation-induced loss. This is critical as molecular nitrogen ejection only occurs efficiently by

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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 N_2^+ 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 collision-less 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 is 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 to about 1000 km above the surface of Titan. The domain is divided in such a way that the cells are of altitude 10 km and there are 30 and 60 cells in the latitudinal and longitudinal direction respectively. Recoils generated below 1000 km will be thermalized quickly and will have a small effect on the coronal population and escape. The upper boundary is optimized for the best results and minimum simulation time. Since the dominant species at Titan's exobase is N_2, a pure N_2 atmosphere is considered with a density profile described by Keller et al. (1998). 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 N_2 particles are followed until they escape from Titan's atmosphere, until they collisionally lose energy and 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 $2R_T$ from the surface of Titan they are assumed to have escaped if they have sufficient energy. Increasing this altitude significantly has only a few percent effect on the yield and the distributions presented. This procedure is carried out for each time step in each cell. A similar simulation procedure was used to study the solar wind interaction with Mars and more details are given in Leblanc and Johnson (2001, 2002).

In these calculations we use estimates of the incident fluxes of ambient flowing N^+ and molecular pickup ions from Brecht et al. (2000). These are globally averaged fluxes based on the statistics of individual ion trajectories that intersect the exobase. The energy and angular distributions are given in Shematovich et al. (2003). These spectra were used to describe the distribution of angles for the incident ions with respect to the local vertical and the incident flux and energy distribution.

The slowed and deflected co-rotating N^+ have energies that are much smaller than the co-rotation energy (2.9 keV) (Hartle et al., 1982; Sittler et al., 2005), 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. Keller et al. (1992, 1998) and Fox and Yelle (1997) suggested that the dominant ion close to the exobase is $HCNH^+$ or $C_2H_5^+$. Brecht et al. (2000) used $C_2H_5^+$ (mass 29) in their model. Because the heavy atoms in the molecular pick-up ions contribute much more to the sputtering than does the attached hydrogen, the effect of such ions can be described using energetic incident nitrogen molecules. Since at very high altitudes (∼1500 km) smaller carbon molecules, such CH_4^+, may be more important pick-up ions than the mass 28–29 ions above (Sittler et al., 2005), their effect would be roughly approximated by the incident N^+ considered here.

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 are fit to those in Johnson et al. (2002) and at low energies to those of Tully and Johnson (2002) as corrected (Tully and Johnson, 2003). In Shematovich et al. (2003) we used integrated momentum transfer and dissociation cross sections and mean energy transfers to estimate the recoil energies, rather than true differential cross sections. Here the recoils are directly obtained from the differential cross sections obtained from molecular dynamics calculations discussed above.

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. Hartle et al. (1982) provided observational evidence for pickup ions of mass 29 having velocity components towards Titan, where the direction of electric field points towards Titan. In particular the pickup ions are locally created in the surrounding exosphere. 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 in agreement with the suggestion of Hartle et al. (1982). The energy deposited by the co-rotating 2.9 keV N^+ ions if they could reach the exobase would be, roughly, 2.1×10^9 eV cm^{-2} s^{-1} while the energy deposited by the deflected N^+ ions (50–750 eV) and the pickup ions (50–1250 eV) is, roughly, 4.8×10^9 eV cm^{-2} s^{-1}. The solar UV photons carry an energy flux ($\sim 2 \times 10^{10}$ eV cm^{-2} 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 that energy is deposited at greater depths on the average. Using our 3-D Monte Carlo model the low energy N^+ ions and N_2^+ ions are allowed to collide with the atmosphere of Titan and the atmospheric loss is studied. Figure 1 presents the energy distributions for escaping nitrogen atoms and molecules produced by the incident N^+ and N_2^+ ions. These distributions are globally averaged at the upper boundary independent of the location from where they escape. The distribution is dominated by low energy atoms and molecules but with a high-energy tail typical of atmospheric sputtering (Johnson et al., 2000). More than 70% of the escaping particles are of energy less than 2 eV. However, due to the slow decay at the higher energies the mean energy of escaping nitrogen is much higher than the energies of the majority of the escaping particles and a significant fraction of the ejecta escape from Saturn's system.

The inset picture of Fig. 1 shows the coronal density of 'hot' (>0.1 eV) N driven by the incident N^+ ions in the equatorial x–y plane. Here the incident flux is in the $-x$ direction. If the average flow was along the co-rotation direct, this would be onto the trailing hemisphere with the z-axis Titan's axis of rotation and y the radius vector from Saturn to Titan. Based on the gyro-motion, the mean flow is actually onto a quadrant on the Saturn facing side (Brecht et al., 2000). Since the atmosphere is spherically symmetric the incident axis can be rotated to the appropriate flow direction, which will be measured by Cassini. 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

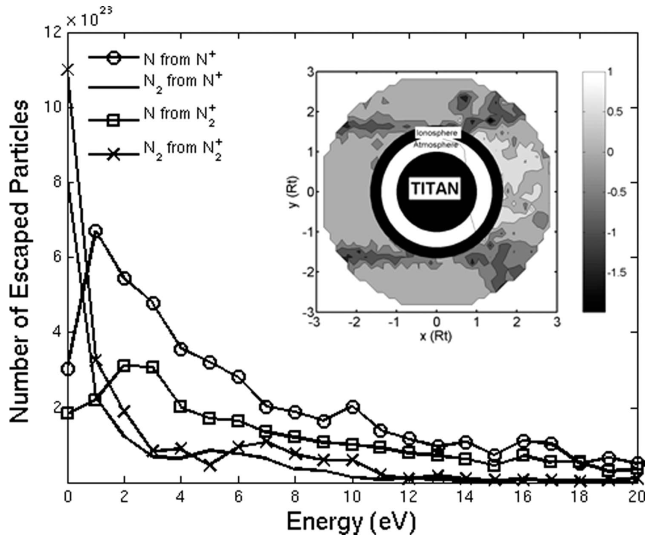

Fig. 1. Energy Distribution of the escaping nitrogen atoms and molecules ejected by incident N^+ and N_2^+ ions. The picture in inset shows the enhancement of density ($\log_{10}$ of cm^{-3}) of hot N (>0.1 eV) in the corona produced by incident N^+ ions. A similar distribution is produced by the incident molecular ions.

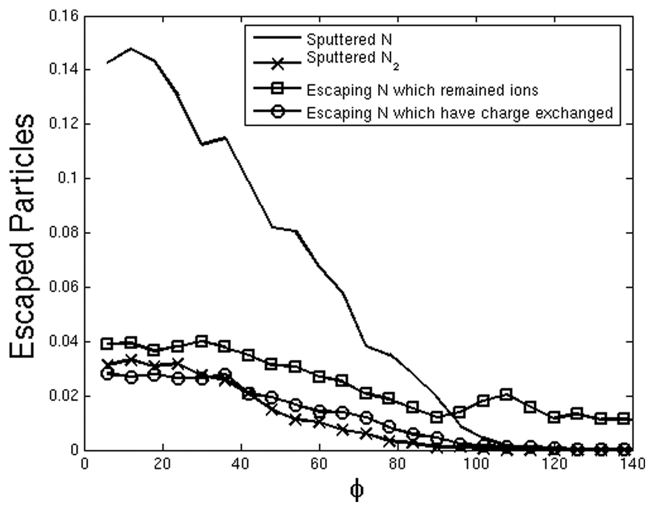

Fig. 2. Spatial distribution of the escaping particles averaged over the azimuthal angle about the direction of incidence. $\phi = 0$ represent backscattered particles. Solid line represents ejected N and line with crosses represents ejected N_2. Line with squares represent the incident N^+ which escape 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.

the atmosphere and transfer energy to the atmospheric molecules.

Figure 2 gives the direction in which nitrogen atoms and molecules are ejected by incident N^+ ions. Integrating over the azimuthal angle around the direction of incidence, $\phi = 0°$ describes back-scattered particles and $\phi = 180°$ 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 pen-

Table 1
Escape flux of N and N_2 by incident N^+ and N_2^+ ions

Incident ions	Escape flux ($\times 10^{25}$ s^{-1})					
	3-D Model			1-D Model (Shematovich et al., 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
N_2^+	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 N_2. Brackets include those incident N^+ which are neutralized and escape as N in the case of 3-D model. Exobase area is $\sim 2.1 \times 10^{18}$ cm^2 and the surface area is $\sim 0.85 \times 10^{18}$ cm^2. Incident flux is 1.1×10^7 N^+ cm^{-2} s^{-1} and 1.4×10^7 $C_2H_5^+$ cm^{-2} s^{-1} (treated as N_2^+ in the model) (Shematovich et al., 2003).

etrate 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.

The local and integrated escape flux of N and N_2 and the altitude profile for the production of suprathermal 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 yields for the incident N^+ but somewhat different relative amounts of dissociated and non-dissociated species for the incident molecular ion. Table 1 presents the escape flux of N and N_2 by N^+ and N_2^+ incident ions along with the results of 1-D model. Collision of the incident N^+ and N_2^+ 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 N_2^+ 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 N_2^+ ions. The increase in N escape by the incident N_2^+ ions can be attributed primarily to the difference in our treatment of the dissociation of N_2 molecules. However, the 3-D model also better estimates the contribution from forward scattering and knock-out from the edges.

Ledvina and Cravens (1998), Kabin et al. (1999), Kopp and Ip (2001), and Chiu et al. (2001) recently calculated the mass loading near Titan using 3-dimensional magnetohydrodynamic models. Their estimates range from 10^{24} to 3.8×10^{25} s^{-1}. Our net atmospheric loss rate, including the photo-induced loss, is $\sim 4.6 \times 10^{25}$ N s^{-1} as either N or N_2. Based on the energies in Fig. 1, ~60% are on trajectories that will escape from the gravitational attraction of Saturn. Therefore, the net nitrogen lost that is likely to be ionized in the magnetosphere is 1.8×10^{25} N s^{-1}, which is within the range suggested above. This does not include pick-up in the corona and the ejected nitrogen atoms and molecules described here are ionized over a large spatial region as shown in Smith et al. (2004).

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, 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 are described in Smith et al. (2004) and the inward and outward diffusion of the resulting ions, as well as the interactions with the inner icy satellites have been reported in Sittler et al. (2004).

4. Summary

We calculated the ejection of N and N_2 due to the bombardment of Titan's atmosphere by slowed and deflected magnetospheric N^+ and by the molecular pick-up ions ($C_2H_5^+$, $HCNH^+$ or N_2^+). 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 at present atmospheric sputtering rates (Johnson, 2004). 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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