1. Introduction

Titan’s atmosphere is an important end point for studies of atmospheric escape and evolution (e.g., Chamberlain and Hunten, 1986; Griffith and Zahnle, 1995; Johnson, 2004). Prior to Cassini’s arrival at Saturn, Titan’s atmospheric mass loss was thought to be dominated by loss of hydrogen (~2 × 10^23 amu/s; Lebonnois et al., 2003; Wilson and Atreya 2004) with much smaller mass loss rates for the heavier molecules (~2–5 × 10^22 amu/s; Shematovich et al., 2003; Michael et al., 2005). Recent analyses of the structure of Titan’s thermosphere from data attained by the ion neutral mass spectrometer (INMS) on Cassini have lead to substantially larger loss rate estimates (0.3–5 × 10^23 amu/s) (De La Haye et al., 2007; Yelle et al., 2008; Strobel, 2008; Johnson, 2009). If the largest loss rates suggested are correct, then a significant fraction of the present atmospheric mass would have been lost in 4 Gyr.

The loss of hydrogen has been clearly confirmed by the INMS data of density vs. altitude by allowing a net upward flow at the exobase. Large mass flow rates were extracted and interpreted due to thermally driven escape to space at a rate that is orders of magnitude larger than the Jeans escape rate. This process is referred to as slow hydrodynamic escape. Direct simulation Monte Carlo (DSMC) models are used here to describe the transition region of Titan’s atmosphere where the gas changes from being dominated by collisions to being dominated by ballistic transport. When normalized at an altitude below the exobase to the densities and temperatures calculated in the recent continuum descriptions of the Cassini ion neutral mass spectrometer data, these simulations show no evidence for slow hydrodynamic escape. In addition, above the nominal exobase there is no evidence for the proposed enhancement in the tail of the molecular speed distribution that would be required at these temperatures to give the suggested escape rates. Even simulations at Titan for artificially small Jeans parameters do not give thermal escape rates that deviate enormously from the Jeans estimate. Therefore, we conclude that the suggested upward flow rates extracted from the INMS data, if confirmed, must be due to mass loss by non-thermal processes and/or global transport.

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Thermally driven atmospheric escape: Monte Carlo simulations for Titan’s atmosphere

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1. Introduction

Titan’s atmosphere is an important end point for studies of atmospheric escape and evolution (e.g., Chamberlain and Hunten, 1986; Griffith and Zahnle, 1995; Johnson, 2004). Prior to Cassini’s arrival at Saturn, Titan’s atmospheric mass loss was thought to be dominated by loss of hydrogen (~2 × 10^23 amu/s; Lebonnois et al., 2003; Wilson and Atreya 2004) with much smaller mass loss rates for the heavier molecules (~2–5 × 10^22 amu/s; Shematovich et al., 2003; Michael et al., 2005). Recent analyses of the structure of Titan’s thermosphere from data attained by the ion neutral mass spectrometer (INMS) on Cassini have lead to substantially larger loss rate estimates (0.3–5 × 10^23 amu/s) (De La Haye et al., 2007; Yelle et al., 2008; Strobel, 2008; Johnson, 2009). If the largest loss rates suggested are correct, then a significant fraction of the present atmospheric mass would have been lost in 4 Gyr.

The loss of hydrogen has been clearly confirmed by the INMS data of density vs. altitude of H_2 (Waite et al., 2005; Yelle et al., 2006) and by the ENA imaging of Titan’s corona (Garnier et al., 2007). The rate extracted is roughly consistent with pre-Cassini estimates, although it was suggested that the Jeans estimate for loss of H_2 needs modification (Cui et al., 2008).

Three different one dimensional (1-D) models were used to estimate the heavy molecule loss rate based on INMS data for density vs. altitude (for summaries see Johnson, 2009; Johnson et al., 2009). In a fluid dynamic model, the heating rate and the mass density profile vs. altitude were used to extract a net average upward flux below the exobase (Strobel, 2008). In a diffusion model, the diffusion of methane through nitrogen was described below the exobase allowing for upward flow (Yelle et al., 2008). In a third model the coronal structure above the exobase was simulated using the observed density vs. altitude dependence was due to a non-thermal process occurring near the exobase of a roughly isothermal thermosphere (De La Haye et al., 2007). The latter model calculated the hot recoils produced by exothermic chemistry and atmospheric sputtering (e.g., Johnson 1990, 1994) and concluded that the incident plasma drove escape (e.g., Michael et al., 2005). In the two continuum models it was assumed that the upward flow extracted from the averaged INMS data below the exobase is driven by heat conduction from below. They further assumed that conduction continues to act above the nominal exobase producing enhanced thermally driven escape, a process referred to as slow hydrodynamic escape (e.g., Strobel, 2008; Johnson et al., 2008).

Slow hydrodynamic escape was defined as an organized outflow of gas in which the atmospheric flow rate directly...
overcomes the gravitational well due to heating from below. Such a process is thought to occur at Pluto (McNutt, 1989; Krasnopolsky, 1999), where the Jeans parameter, $\lambda_J$, the ratio of the gravitational energy of a molecule to the thermal energy, is $\sim 10$ at $r_{exo} \sim 3.5 \text{~P_{Triton}}$ (Strobel, 2007). This process has recently been suggested to occur at Titan where the Jeans parameter is relatively large, $\sim 45$ at $r_{exo} \sim 1.6r_{P_{Triton}}$ (Strobel, 2008).

Here we examine that suggestion using a direct simulation Monte Carlo (DSMC) description of the 1-D atmosphere near the exobase. Marconi et al. (1996) used a DSMC simulation to test a fluid model in the transition region for an Io-like atmosphere and found significant differences for a model in which escape was forced to occur. The DSMC simulation is a suitable test to the fluid models applied in Titan’s atmosphere because it makes no assumptions about how atmospheric flow is driven by conduction or convection. With DSMC we can apply an observed density and inferred temperature to a lower boundary, and calculate how conduction and convection would alter the atmosphere. In order to test the escape rate from the slow hydrodynamic model, we can connect a DSMC simulation to the continuum model using the properties of the atmosphere below the exobase in Strobel (2008) for a single component atmosphere and in Yelle et al. (2008) for a two component atmosphere. We carry out DSMC simulations of Titan’s transition region assuming no additional escape process is occurring other than thermally driven escape. Based on these simulations, we find that mass loss driven by thermal conduction is not significantly enhanced over the Jeans rate at the relevant temperatures or even at temperatures made artificially larger. Therefore, if upward flow is occurring at the exobase, as suggested by models of the INMS data, it must be associated with transport to other regions of the atmosphere or to non-thermal escape mechanisms (e.g., Johnson, 2008; Johnson et al., 2009).

3. DSMC model

To describe the transition region in the atmosphere from below the exobase to above, solutions to the Boltzmann equation or Monte Carlo simulations are required. Here we use a DSMC model (Bird, 1994). The atmosphere is described using a set of representative molecules and its evolution is calculated by following the motion of these particles subject to gravity and collisions. A 1-D simulation is carried out, consistent with the 1-D continuum models being tested. In the main flow direction, radially outward from Titan, the space is divided into cells with sizes less than the local mean free path for collisions between atmospheric neutrals. For the results presented below the typical diffusion cross did not change the conclusions.

\[ \lambda_J = \frac{\phi^*_J}{\phi_J} \]

Thermally driven escape from the exobase, $r_{exo}$, occurs in two different limits which are categorized by the Jeans parameter, $\lambda_J$, the ratio of the gravitational energy to thermal energy of molecules: $\lambda_J = \frac{(GMm(H_{exo})/kT_{exo})}{(1/2)}\frac{\sigma_d}{(Mm)}$, where $G$ is the gravitational constant, $M$ the object’s mass, $m$ the molecular mass, and $T_{exo}$ is the temperature at the exobase or critical level. This can also be written as $\lambda_J = r_{exo}/H_{exo}$, the exobase radius over the scale height. When $\lambda_J$ is large, the molecules have to overcome a significant gravitational barrier. In this limit Jeans escape occurs due to the fraction of the molecules at the exobase which have velocities that are above the escape speed and directed outward. In this case the escape flux is

\[ \phi_J = \left[(n_{exo}(\phi_J)/4)\frac{(1 + \lambda_J)^{1/2}}{}\right] \]

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We describe Titan’s atmospheric corona over radial distances 3875–7000 km, with the upper boundary dependent on the Jeans parameter involved. Fixed densities and temperatures taken from the continuum models were applied at the lower boundary which is below the exobase. The upper boundary was placed many scale heights above the exobase to include any effects of collisions which may have occurred above the nominal exobase. Upward moving molecules with speeds greater than the
escape speed were assumed to escape while the others were specularly reflected back into the simulation region. The reflected, non-escaping molecules represent ballistic particles that are returning allowing a shorter time to achieve steady state. Variations in the upper boundary did not affect the results presented below. Typically, on the order of one million particles were used to represent the atmosphere in order to have at least a few hundred particles in the very top cells. The weights for the representative molecules were determined in order to meet that condition. Using this number of representative molecules, we were able to obtain results with relatively small statistical scattering. Even with this number of particles we cannot accurately simulate the escape that might occur well above the exobase if our lower boundary is the same as in the continuum models (∼3450 km). Therefore, we use the continuum results at an altitude closer to the exobase and simulate the transition region. In Strobel (2008), a model which included no EUV or UV heating was used to determine the lower limit to the escape rate from Titan using the approximate hydrodynamic model. For this case a thermally driven escape flux of $3.3 \times 10^{18} \text{amu/cm}^2/\text{s}$ normalized to the physical surface was obtained by the approximate fluid model. Since this flux was assumed to apply globally, for the surface area of $0.84 \times 10^{18} \text{cm}^2$ the net atmospheric loss rate was estimated to be $-2.8 \times 10^{28} \text{amu/s}$ Strobel (2008).

Fixing the temperature and density at our lower boundary, ∼3875 km, to that calculated for the same altitude from the hydrodynamic model, the DSMC results in (Fig. 1a) were obtained. It is seen that, unlike in the temperature profile in Strobel (2008) the atmosphere is essentially isothermal throughout the transition region, where the nominal exobase in our simulations is ∼4000 km. In addition, since no test particles escaped during the simulation, consistent with our estimate of the Jeans escape rate and the simulation time, we can obtain an upper limit on the escape flux. If one representative particle would have escaped from our model during the simulation the escape rate would be more than six orders of magnitude less than the rate estimated in Strobel (2008).

The sense of these results did not change by changing the lower boundary or increasing the upper boundary. We also compared our simulations in which radial cells were used to simulations in which rectangular cells were used. In both cases the gravitational field is assumed to vary with radial distance. The results are very close for our altitude range and cell sizes; i.e., $dr = dz = 20 \text{km}$.

In addition, we carried out simulations in which the collisions were described by a forward-directed cross section (Johnson, 1990, 1994). This meant that escape could occur from deeper in the thermosphere (i.e., a slight lowering of the effective exobase level as discussed earlier). This also did not change the results in Fig. 1a within the uncertainties. Simulations of the transition region were carried out for the other cases that included EUV and UV heating in Strobel (2008) by normalizing to the temperatures and densities at 4000 km, and using the appropriate heating rates. In all cases the escape was negligible.

For the case in which no heating was assumed to occur above 3450 km, Strobel (2008) obtained a net upward thermal flux due to heat conduction. At the lower boundary, this flux was $-4.7 \times 10^9 \text{eV/cm}^2/\text{s}$. At the lower boundary in our radial simulations, 3875 km, this would be $-4 \times 10^8 \text{eV/cm}^2/\text{s}$. This flux is, of course, smaller than the total upward thermal flux of $\sim 1.3 \times 10^9 \text{eV/cm}^2/\text{s}$, which in the absence of escape is balanced by a downward thermal flux. Because heat conduction was suggested to drive the large escape rate obtained in Strobel (2008), we tested the effect of an additional heat flux of the size suggested. Therefore, at our lower boundary we increased the upward heat flux by $4 \times 10^8 \text{eV/cm}^2/\text{s}$ and allowed the system to evolve. The new temperatures and densities are also indicated in (Fig. 1a) by the dashed lines. On achieving steady state this lead to an undetectable increase in escape, but the temperature increased slightly (Fig. 1a) until the increased upward heat flux was balanced by an increase in the downward heat flux. These simulations indicate that thermal conduction, included here by explicitly including all collisions up to a few scale heights above the nominal exobase, is not efficient at driving molecules over their gravitational barrier for the relevant $\lambda_2$ values.

To simulate the presence of an additional escape process, we artificially removed molecules at the upper level, consistent with a non-thermal loss mechanism, such as plasma-induced sputtering.
(e.g., Johnson, 2009; Johnson et al., 2009). A removal rate was used equivalent to an escape flux of $4.5 \times 10^{25}$ amu/s. The effect on the density profile is relatively small over this range of altitudes but, not surprisingly, as seen in (Fig. 1b) the temperature decreases with altitude slowly, consistent with adiabatic cooling induced by atmospheric loss. A decreasing temperature profile is suggested by the HASI experiment on Cassini (Fulchignoni et al., 2005). However, above the exobase the form for thermal conduction changes when the mean free path for collisions is long (e.g., Marconi et al., 1996), so that the temperature profile for the same escape flux differs from that in Strobel (2008).

4. DSMC results for smaller $\lambda_j$

In the description of escape from Pluto, $\lambda_j$ for the principal N$_2$ component ranged from $\sim$5–16 depending on the case examined (Krasnopolsky, 1999; Strobel, 2007). The approximate hydrodynamic escape model led to an estimate that was four orders of magnitude larger than the Jeans rate at $\lambda_j$$\sim$16 for the principal N$_2$ component, and became smaller than the Jeans rate for the cases in which $\lambda_j$$<$$\sim$5. Therefore, we examine the escape rate from Titan for a lower $\lambda_j$ as might occur, for example, due to additional heat sources which would yield higher temperatures. We increased $T$ at the lower boundary in the simulations using a fixed starting altitude ($r = 4000$ km), which was a number of scale heights below the exobase, with a density $(n = 3.25 \times 10^7$ cm$^{-3}$) consistent with that used in the above simulations. In this way we ensured that at a sufficiently high $T$ thermal escape would occur. Changing $T$ in this manner also increases the scale height and the nominal exobase level. As the scale height and exobase level increased, we also increased the upper boundary, keeping the collision probabilities in each radial box approximately the same.

Thermal escape is seen to occur in the simulations when the $T$ is increased significantly. However, unlike the hydrodynamic model applied to Pluto and Titan, with a temperature at the lower boundary as high as 500 or 600 K ($\lambda_j$$\sim$14 and $\sim$11 at the exobase), the escape rate is only $\sim$1.5 that of Jeans escape rate calculated using the exobase temperature and exobase density. Results for the 600 K case are shown in (Fig. 2). The decreasing temperature vs. radial distance from Titan in (Fig. 2a) are consistent with the fact that in these simulations escape is occurring, as was the case in (Fig. 1b) when molecules were simply removed for the exobase region. In (Fig. 2b) the rate of escape vs. radial distance from Titan is shown as is the flux of particles at each altitude with sufficient energy to escape. Results are shown for two different upper boundaries, indicating that the upper boundary conditions chosen do not influence the escape rate. For these cases, $\lambda_j$$<$$\lambda$ at the exobase (indicated in both panels) giving a Jeans rate of $4.6 \times 10^{25}$ N$_2$/s. The actual (simulated) escape rate is $2.0 \times 10^{25}$ N$_2$/s. This again emphasizes that the very large hydrodynamic escape rates obtained by the approximate fluid model are incorrect at Titan, and, possibly, incorrect at Pluto. This aspect will be described more thoroughly in a separate paper.

5. Speed distributions

It has been suggested, that thermally induced escape is enhanced when an accurate description of the transition region is used. That is, thermal conduction was suggested to produce an enhancement in the tail of the particle energy distribution above the exobase (Cui et al., 2008; Yelle et al., 2008). Such an enhancement was shown using a DSMC model attached to a fluid model when escape was forced to occur in an Io-like atmosphere (Marconi et al., 1996). In Fig. 3 we show results from our simulations of thermal escape. It is seen that for the no heating case in Strobel (2008) the speed distributions are well fit by Maxwellians. Even for energies well above the peak, there is no evidence for an enhancement in population of the tail of the distribution in these simulations. This is the case for all the coronal temperatures in all of the models in Strobel (2008) and Yelle et al. (2008). When the temperature of the lower boundary was raised so that thermal escape became significant as in the examples in Fig. 2, both depletions, due to escape, and enhancements due to collisions eventually occur, which will also be discussed in a separate paper.

6. DSMC result: N$_2$+CH$_4$

Although Strobel (2008) solved the approximate fluid equations for the net mass flux, the principal escaping component was...
assumed to be CH$_4$. Yelle et al. (2008) on the other hand solved the coupled diffusion equations for CH$_4$ and N$_2$ and came to roughly the same conclusion. That is, they found an upward flow of $\sim 4 \times 10^{28}$ amu/s for CH$_4$ which they assumed escaped to space. This was also roughly consistent with the model in Müller-Wodarg et al. (2008). Therefore, we carried out another set of DSMC simulations for an atmosphere having both methane and nitrogen. At the lower boundary, in this case $r = 3800$ km, we again fixed the temperature and the density of each species to the values taken from Bondi (1964). Molecular diffusion, included here explicitly by the molecular collisions, dominates over eddy diffusion above $\sim 3400$ km (Yelle et al., 2008). As seen in Fig. 3, the model can reproduce the INMS averaged density measurements, but results in a different temperature structure. Again, only an upper bound on the escape rate for CH$_4$ is obtained from these simulations and this is many orders of magnitude smaller than the suggested rate. Although including some eddy mixing above our lower boundary might affect these results slightly, the conclusion that thermal conduction can drive large escape rates at these values of $\lambda_J$ does not borne out. As in our earlier discussion, there is no evidence for a significant enhancement in the tail of the speed distribution and the Jeans model appears to adequately describe escape unless the Jeans parameter is much smaller as in Fig. 2. Including in our simulations the other important molecule in Titan’s upper atmosphere, H$_2$, did lead to a significant H$_2$ escape rate as predicted, which we will also described in a separate paper. Here we point out that the upward flowing H$_2$ did not significantly modify the CH$_4$ escape rate, but does, not surprisingly, have an affect on the temperature profile, as the escaping H$_2$ are energized by the background gas leading to adiabatic cooling (Fig. 4).

7. Discussion and summary

Recent Cassini measurements of density vs. altitude (Waite et al., 2005; Fulchignoni et al., 2005) have lead to continuum models of Titan’s upper atmosphere below the exobase. These models suggest that there is a net upward mass flux of the principal atmospheric components at the exobase (Strobel, 2008; Yelle et al., 2008; Müller-Wodarg et al., 2008). In these papers the authors concluded that, at the temperature and densities expected at Titan’s exobase, an escape flux many orders of magnitude larger than the Jeans flux could be driven by thermal conduction. This process was also suggested to be the case at Pluto (Krassnopolsky, 1999; Strobel, 2007). The approximate fluid model used is often referred to as the slow hydrodynamic escape model (e.g., Johnson et al., 2008). Here we used DSMC simulations of the exobase region to show that, for expected temperatures and densities, the large escape rates predicted by the slow hydrodynamic model are not occurring either in the one component atmosphere or the two component atmosphere. In addition, as seen from the comparison in Figs. 1a and 4, the density profiles below the exobase are not good constraints on the escape rate.

The results here also appear to contradict those found for Pluto earlier using the slow hydrodynamic model. That is, for a Jeans parameter $\sim 11$ at Titan (the 600 K case) with exobase at $\sim 1.8 r_T$, we found the actual escape rate was about 1.5 times the Jeans rate. Whereas at Pluto, when $\lambda_J \sim 10$ at an exobase $\sim 3.5 r_P$, the hydrodynamic model predicts escape rates orders of magnitude larger than the Jeans rate (Strobel, 2007). Therefore, either the model is incorrect or the size of the Jeans parameter alone is not sufficient to describe when significant deviations from Jeans escape occur. Simulations for Pluto are in progress.

DSMC simulations include thermal conduction explicitly by directly calculating the molecule–molecule collisions. These collisions were described using both isotropic and forward-directed models of the angular scattering. Here we showed that in the transition region, thermal conduction did not cause a significant enhancement in the tail of the speed distribution even when the exobase temperature was significantly larger than that expected. The difference with the result in Strobel (2008, 2009) is because the thermal conduction model used does not apply above the exobase and also the hydrodynamic equations were scaled by the escape flux so that solutions with negligible escape cannot be obtained but solutions with large fluxes are favored.
However, we also showed that if an escape process other than thermal escape is operative above Titan’s exobase (e.g., De La Haye et al., 2007; Johnson, 2009), then, not surprisingly, the temperature vs. altitude dependence is more consistent with that proposed. Therefore, if the net upward flux below the exobase is confirmed, that flow must be due to non-thermal loss mechanisms acting in the exobase region and/or to net flow to other regions of the atmosphere.

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