Diffusion and thermal escape of H$_2$ from Titan's atmosphere: Monte Carlo simulations

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**Abstract**

The Direct Simulation Monte Carlo (DSMC) technique is used here to describe the transition region in Titan's atmosphere where the gas flow goes from being collisional to collisionless. We expand on our previous study (Tucker, O.J., Johnson, R.E. [2009]. Planet. Space Sci. 57, 1889–1894) by including H$_2$ in addition to CH$_4$ and N$_2$. We again find that thermal escape of CH$_4$ is Jeans-like, contrary to what has been suggested by some fluid/continuum models. However, we also show that the temperature of molecular hydrogen separates from the background gas well below the exobase, and its escape cools the background gas. This results in a non-isothermal CH$_4$ density profile without requiring an upward CH$_4$ flux and, therefore, fits using the diffusion equation can overestimate the escape flux. These simulations also reproduce the Cassini H$_2$ density versus altitude data averaged over flybys for which Titan is orbiting in Saturn’s plasma sheet, but with a somewhat different escape rate than suggested by the diffusion equation. However, for flybys for which Titan is not in Saturn’s plasma sheet our simulations result in H$_2$ densities that diffusively separate from the N$_2$ densities at lower altitudes than typically indicated by the Cassini data. By tracking ballistic transport in the H$_2$ corona we show that a global, as well as temporal description of the exobase region is required.

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1. Introduction

One of the principal goals of the Cassini mission to Saturn is to characterize the mechanisms driving escape of the major molecular species, N$_2$ (~98%), CH$_4$ (~1.6%) and H$_2$ (~0.1%), from Titan’s atmosphere. Prior to the availability of Cassini data, thermal escape was assumed to occur at the theoretical Jeans rates in which case only H$_2$ had a significant escape rate. Escape of N$_2$ and CH$_4$ was assumed to be driven primarily by non-thermal processes (e.g., Michael et al., 2005; Michael and Johnson, 2005; Shematovich et al., 2003). Surprisingly, recent diffusion models were used to fit Cassini density data of the upper atmosphere that inferred CH$_4$ escape rates orders of magnitude larger than the corresponding Jeans rates (e.g., Yelle et al., 2006, 2008). A series of papers (e.g., Strobel, 2008, 2009, 2010) investigated the possibility of a significant CH$_4$ escape rate powered by thermal conduction in a process referred to as slow hydrodynamic escape (SHE). However, recent Monte Carlo models, which include thermal conduction and diffusion implicitly, suggest that thermal escape of methane is evaporation and therefore Jeans-like (e.g., Tucker and Johnson, 2009; Volkov et al., 2011a,b). Here, we expand our molecular kinetic study (Tucker and Johnson, 2009) to consider how diffusion and thermal escape of H$_2$ shape the density structure of Titan's upper atmosphere. We compare our results to the Cassini Ion Neutral Mass Spectrometer (INMS) density data and recent continuum model results in which it is assumed the mean free path for collisions is much shorter than the length scales associated with any gradients. Since such models break down in the vicinity of the exobase either higher moment (Boqueho and Blelly, 2005; Cui et al., 2009) or molecular kinetic simulations, such as those described here, are required to obtain accurate density and temperature profiles near the exobase.

2. Exosphere and Jeans escape

Titan’s thermosphere is heated primarily by molecules and molecular fragments energized via solar UV/EUV absorption and by interactions with precipitating ions and electrons from Saturn’s magnetosphere. In this region, molecular collisions are relatively frequent, and the energized molecules are thermalized via collisions heating the atmosphere. Therefore, the energy distribution of molecules in the thermosphere is close to a Maxwellian. In the uppermost region of Titan’s atmosphere, referred to as the exosphere, molecular collisions are infrequent and molecules directed
outward with energy greater than the planetary binding energy, \( \Phi_b(r) = GM_p m_r / r \), have a high escape probability. Here \( G \) is the gravitational constant, \( M_p \) is the planet's mass, \( m_r \) is the molecular mass and \( r \) is the radial distance from the planetary center. Although the species energized by the incident radiation and plasma interactions can directly escape, referred to here as non-thermal escape (e.g., Johnson, 2009; De La Haye et al., 2007a,b), the aim of this study is to characterize the escape of molecules heated by conduction from below, referred to here as thermal escape.

In diffusive equilibrium, the density profile of each molecular species, \( s \), in an isothermal atmosphere will decrease exponentially with increasing altitude according to its scale height:

\[
n_s(r) = n_s(r_0) \exp\left(-\frac{r - r_0}{H_s(r)}\right)
\]

where \( H_s(r) = rK_s \) is the atmospheric scale height and \( n_s(r) \) is the density with \( K_s \) the Boltzmann constant and \( T \) the temperature. The local Knudsen number, \( K_s(r) = \lambda_{\text{mfp}} / H_s(r) \), which is the ratio of the local mean free path for a collision, \( \lambda_{\text{mfp}} \), to the atmospheric scale height, characterizes how rarefied the atmosphere is at a particular altitude. The exosphere region is defined at altitudes where \( K_s \gg 1 \) and the lower boundary to this region \( r_s \) is referred to as the exobase, \( K_s \sim 1 \); (e.g., Chamberlain, 1963; Johnson et al., 2008; Johnson, 2010). Therefore, thermal escape is commonly estimated at the exobase using the so-called Jeans parameter \( r_{\text{ex}} = r_s / H_s(r_s) \) (Jeans, 1916).

Assuming the velocity distribution at the exobase is Maxwellian the theoretical Jeans formula for the global escape rate is given as:

\[
\dot{N}_{\text{ex}} = \frac{4\pi r^2 n_s(r_s) \langle v \rangle_s}{n_s} \left(1 + \frac{\lambda_{s,\text{ex}}}{r_s}\right) \exp\left(-\frac{\lambda_{s,\text{ex}}}{r_s}\right)
\]

where subscript 's' refers to quantities evaluated at the exobase and \( \langle v \rangle_s = (8KT_s / \pi m_s)^{1/2} \) is the mean thermal speed. For large values of the Jeans parameter the atmosphere is strongly bound by gravity, and for small values the escape rates approach values similar to that for free expansion.

In the comparisons below, the exobase altitude is estimated using the \( \lambda_{\text{mfp}} \) and \( H_s \) of the principal collision species, \( N_2 \). Likewise, the theoretical Jeans rate for the minor species, \( CH_4 \) and \( N_2 \), is evaluated using their corresponding densities at the exobase but with the background \( N_2 \) temperature. The collective INMS density profiles indicate characteristic \( N_2 \) temperatures ranging from \( \sim 100 \) K to \( 200 \) K in Titan’s upper atmosphere, \( r > 3500 \) km, and the corresponding exobase altitudes vary from \( r_s \sim 3900-4300 \) km (e.g., Cui et al., 2011, Table 1; Westlake et al., 2011, Fig. 4). At \( T_s = 188 \) K the Jeans parameters evaluated at the exobase are \( \lambda_{N_2,\text{ex}} \approx 38 \), \( \lambda_{CH_4,\text{ex}} \approx 22 \) and \( \lambda_{N_2,\text{ex}} \approx 3 \), and the corresponding Jeans escape rates at \( r_s = 4125 \) km are \( \dot{N}_{\text{ex},N_2} \sim 10^{15} \) \( N_2/\text{s} \), \( \dot{N}_{\text{ex},CH_4} \sim 10^{21} \) \( CH_4/\text{s} \), and \( \dot{N}_{\text{ex},N_2} \sim 10^{28} \) \( H_2/\text{s} \) (e.g., T36 flyby in Table 1 in Cui et al., 2011). These rates for \( CH_4 \) and \( N_2 \) are much smaller than both pre-Cassini, \( \sim 10^{25} \) molecules/\( \text{s} \), and post-Cassini, \( \sim 10^{26}-10^{27} \), estimates for non-thermal escape (e.g., Johnson et al., 2009).

### 3. Summary of continuum model results

The vast amount of Cassini data on molecular densities versus altitude in Titan’s upper atmosphere has allowed atmospheric scientists to quantitatively consider the dominant factors determining its structure and driving escape. Yelle et al. (2006) suggested that the non-isothermal nature of the INMS \( H_2 \) and \( CH_4 \) density profiles was determined by upward diffusion and escape. Subsequently, several diffusion models have been used to fit the \( CH_4 \) and \( H_2 \) INMS densities and thereby infer escape rates (e.g., Cui et al., 2008, 2009, 2011; Yelle et al., 2008).

The diffusive flow rate, \( \varphi_{\text{DL,s}} \), for binary molecular diffusion of trace species through a hydrostatic planetary atmosphere is given by:

\[
\varphi_{\text{DL,s}} = -4\pi r^2 D_n \left[ \frac{1}{H_s} \frac{\partial n_s}{\partial r} + \frac{1}{H_s} \right] + \left(1 + \frac{\lambda_{s,\text{ex}}}{r_s}\right) \frac{dT}{dr}
\]

where \( D_n \) is the binary diffusion coefficient and \( \lambda_{s,\text{ex}} \) is the thermal diffusion factor (Hunten, 1973). Although \( H_2 \) escape produces a modest temperature decrease in \( N_2 \) (<10 K over the region \( r > 3500-4100 \) km), as discussed below, diffusion is driven primarily by the pressure gradient (e.g., at \( T = 200 \) K, \( 1/H_s \sim 10^{-3} \) and \( \lambda_{s,\text{ex}}/r_s \sim 10^{-6} \) km\(^{-1}\) where \( x_s < 1 \)). Neglecting the thermal diffusion term, as is typical (e.g., Cui et al., 2008, 2009; Hunten, 1973; Yelle et al., 2006, 2008), then

\[
\varphi_{\text{DL,s}} = -4\pi r^2 n_s D_n \left[ \frac{1}{H_s} \frac{\partial n_s}{\partial r} + \frac{1}{H_s} \right]
\]

The maximum diffusive flow rate, \( \varphi_{\text{DL,s}} \), for a trace species is obtained when the mixing ratio is constant with altitude. Below Eq. (3b) is rewritten in terms of the mixing ratio, \( f_s = n_s / n_p \) where \( n_p \) is the number density of the dominant species.

\[
\varphi_{\text{DL,s}} = \left[ \varphi_{\text{DL,s}} - 4\pi r^2 n_s D_n \frac{df_s}{dr} \right]
\]

For a constant mixing ratio with increasing altitude above the homopause, the molecular diffusion limited flow rate is:

\[
\varphi_{\text{DL,s}} = 4\pi r^2 b_s T_s^4 f_s \left[ \frac{1}{H_s} \frac{1}{H_p} \right]
\]

where \( b_s \), \( T_s \), \( f_s \) are related to the viscosity exponent, \( H_s \) is the scale height of the dominant species and \( n \) is the total number density of the atmosphere (e.g., Chapman and Cowling, 1970). Because the diffusion coefficient is roughly proportional to temperature, the limiting rate is primarily determined by the mixing ratio in the homosphere (Bertaux and Kokkarts, 1983; Hunten, 1973; Strobel and Cui, 2012).

The collective results of continuum models for molecular hydrogen suggest it escapes thermally, essentially at the diffusion limited rate, e.g., \( \sim 9.2 \pm 1.2 \times 10^{27} \) \( H_2/\text{s} \) (e.g., Bell et al., 2010a,b; Cui et al., 2008, 2009, 2011; Strobel, 2009; Strobel and Cui, 2012; Yelle et al., 2006). However, the corresponding results for methane escape disagree on both the escape rate and whether it is driven primarily by non-thermal or thermal processes (e.g., Bell et al., 2010a,b; Cui et al., 2012; Strobel, 2009, 2010). In these works INMS density data is used to constrain the eddy diffusion coefficient for Titan’s atmosphere that is in turn used along with the molecular diffusion to calculate the methane escape rate. Initially Yelle et al. (2006) used a diffusion model to show the \( CH_4 \) densities could be fit with a large escape rate and a small eddy diffusion...
coefficient or vice versa. Since argon is inert in Titan’s atmosphere and strongly bound by gravity, Yelle et al. (2008) subsequently constrained the eddy diffusion coefficient using the averaged $^{40}$Ar INMS density data to derive a homopause distance of 3425 km, and suggested that escape, on average, occurs at a rate of 2.5–2.7 × $10^{17}$ CH$_4$/s. Later, Bell et al. (2011) constrained the eddy diffusion coefficient using an updated $^{40}$Ar mixing ratio and $^{14}$N/$^{15}$N isotopic ratios. They derived a higher homopause radius of 3575 km, and suggested that escape, at most, occurs at a rate of 8.3 × $10^{17}$ CH$_4$/s. Cui et al. (2012) recently re-analyzed the CH$_4$ density structure in Titan’s upper atmosphere using improved data reduction techniques and obtained similar results to their previous work in Yelle et al. (2008). These homopause radii are smaller than the lower bounds used in our simulations described below.

Two different numerical models which solve the Navier Stokes fluid equations constrained by the INMS density data have been used to interpret the methane diffusion rates considering the effects of solar EUV/UV heating, magnetospheric heating, and chemistry. Strobel (2008, 2009, 2010) postulated that the escape rate is the result of a slow hydrodynamic expansion of Titan’s atmosphere that leads to supersonic escape of CH$_4$ at rates of 1.7 × $10^{17}$ CH$_4$/s dominantly driven by the conduction of heat from solar UV and EUV radiation. This escape rate, possibly fortuitously, is consistent with the diffusion model results in Yelle et al. (2008). As stated above, Bell et al. (2010a,b) using the Titan Global Ionosphere and Thermosphere model (T-GITM) proposed a broad range of CH$_4$ escape rates. A principal difference between the T-GITM and SHE models was whether or not the flow became supersonic. This was the case since the escape rate is a parameter in such models poorly constrained by fitting the vertical density structure to INMS data (Tucker and Johnson, 2009). In that work we also showed that molecular kinetic models are well suited to calculate escape rates. That is, molecular kinetic models calculate escape explicitly, and the atmospheric structure is determined by the local velocity distribution, which evolves due to collisions, gravity and escape. Here we do not consider the effects of eddy diffusion in the upper atmosphere but use a lower boundary that is above the expected homopause, reducing its importance, and consider the effects of molecular diffusion and thermal escape on atmospheric structure using a kinetic model. A description of our model is given below.

4. Description of the kinetic model

To describe the transition of the atmosphere from collisional flow below the exobase to collisionless flow above the exobase, solutions to the Boltzmann equation or Monte Carlo simulations are required. Here we use the direct Monte Carlo simulation technique (DSMC) (e.g., Bird, 1994). The atmosphere is described using a set of representative particles subject to gravity and mutual collisions as described in more detail in Tucker and Johnson (2009) and Volkov et al. (2011a,b). In the radial flow direction outward from Titan, the space is divided into radial cells on the order of or smaller than the local mean free path of gas molecules. At the lower boundary we impose a constant density and temperature assuming a Maxwell–Boltzmann velocity distribution. The atmospheric structure is driven by heat transport from the lower boundary via collisions, and molecular escape from the upper boundary. At the upper boundary, a few scale heights above the exobase, molecules with velocities equal to or larger than the escape velocity are removed and all other molecules are specularly reflected. The reflected molecules represent ballistic molecules that would eventually return to the simulation domain. Occasional collisions still occur above the exobase so the upper boundary is chosen such that further increases in altitude result in a variance in the escape rate of less than 10%. After the atmospheric flow reaches steady state the macroscopic properties are obtained from the local velocity distributions of the molecules within the cells. We follow the general constraints suggested in Bird (1994); the flow properties are independent of the number of representative molecules, the time step is smaller than the mean collision time and the nature of molecular collisions is independent of the motion of molecules between collisions.

The DSMC results discussed below were obtained using the variable hard sphere (VHS) collision model to evaluate velocity dependent molecular collisions and the Larsen–Borgnakke (LB) approximation to include the subsequent transfer of translational and internal energy between molecules, as given by Bird (1994). The VHS collision cross-section is parameterized using a temperature dependent thermal conductivity $\kappa(T) = \kappa_0 T^{\alpha}$, for which the cross-section, $\sigma = \sigma_{\text{ref}} (v_{\text{ref}}/v)^{\alpha - 0.5}$, depends on the relative collision speed, $v_{\text{ref}}$, and the average relative velocity $v_{\text{ref}}$ at a reference temperature $T_{\text{ref}}$ assuming a Maxwell–Boltzmann velocity distribution. Here all reference parameters for the individual molecular species are taken from Appendix A in Bird (1994), and intermolecular parameters are taken as mean values. At temperatures characteristic of Titan’s upper atmosphere, the N$_2$, CH$_4$, and H$_2$ vibrational modes are assumed not to be excited. Therefore, the LB model is parameterized only for the number of rotational degrees of freedom: two for N$_2$ and H$_2$ and three for CH$_4$. In addition, we neglect changes in rotational levels due to IR cooling between collisions. The initial internal energy for each molecule is chosen from a Maxwell–Boltzmann energy distribution for the temperature at the lower boundary.

We used two different implementations of DSMC method referred to as the “3-component DSMC” and “DSMC-H$_2$” simulations to obtain the results discussed below. Due to the small H$_2$ mixing fraction, achieving good statistics in the 3-component DSMC simulations for Titan’s atmosphere is computationally demanding. Using the full 3-component DSMC simulation it is seen that the N$_2$ and CH$_4$ temperatures and densities are affected by H$_2$ escape which will be discussed further below. After considering the results for the steady state atmosphere using the 3 primary components, we modified the code to dynamically track the H$_2$ molecules in a stationary background gas composed of the dominant species CH$_4$ and N$_2$ (e.g., Brinkmann, 1970; Chamberlain and Campbell, 1967; Chamberlain and Smith, 1971). In these DSMC-H$_2$ simulations we start deeper in the atmosphere. When a collision occurs between a H$_2$ molecule and a background gas molecule, an artificial N$_2$ or CH$_4$ molecule is created with a velocity and internal energy sampled from a Maxwell–Boltzmann distribution. For simplicity we neglect bulk motion of the background gas which is very small. After the collision, only the subsequent motion and internal energy change of the H$_2$ particle is tracked. The DSMC-H$_2$ simulations are completed in less time than the 3-component DSMC simulations and provide better statistics.

5. DSMC results

DSMC studies were carried out in order to interpret two sets of averaged INMS data, which showed that plasma heating affects Titan’s upper atmosphere (e.g., Magee et al., 2009; Westlake et al., 2011). Colleagues at the Southwest Research Institute provided these data, referred to as lobe and plasma sheet data. The individual Titan flybys have been classified as plasma sheet or lobe for encounters in which Titan was orbiting in high or low density plasma regions of Saturn’s magnetosphere (e.g., Rymer et al., 2009; Simon et al., 2010). Westlake et al. (2011) averaged the INMS N$_2$ densities versus altitude and obtained effective temperatures of $T \sim 161$ K and 132 K for the plasma sheet and lobe encounters respectively. The averaged density data sets, measured as the
spacecraft penetrated into Titan’s atmosphere, are shown in Fig. 1. It is seen that N₂ and CH₄ exhibit a steeper density gradient for plasma sheet encounters, but the averaged molecular hydrogen density profile does not. We investigate these data using DSMC simulations with Table 1 summarizing the lower boundary conditions for the various simulations discussed below.

5.1. Three component simulations

In the 3-component DSMC simulations, the lower boundary was set at a radial distance just below that at which H₂ appears to diffusively separate from N₂, approximately at r₀ = 3685 km in Fig. 1. The lower boundary densities consistent with the INMS data sets are given in Table 1. The temperatures used at the lower boundary are not measured, but are obtained from hydrostatic fits to the N₂ INMS density profiles, T₀ = 118 K and 161 K for the lobe and plasma sheet conditions respectively, similar to the temperatures mentioned above. The difference in the inferred lobe temperature from that in Westlake et al. (2011) is due to using a different lower boundary when fitting the N₂ data. To more rapidly obtain steady state densities versus altitude the simulation densities were initialized using the isothermal hydrostatic equation and the final results were shown not to depend on the initial state of the atmosphere. We do not include heating from solar radiation within the simulation domain. That is, the dominant heating, whether solar or by the plasma, is assumed to occur below r₀. The upper boundary was set at r = 5000 km which was found to give sufficient accuracy. Increasing the upper boundary by several N₂ scale heights to 6000 km increased the H₂ escape rate by less than 10%.

The 3-component DSMC simulations for Titan’s atmosphere are computationally demanding. Approximately 6 × 10⁵ representative particles were used with a total of 6300 particles in the lower boundary cell of which ~25 represent H₂ particles. At every time step we re-distribute velocities to all the particles in bottom cell, according to a Maxwell–Boltzmann velocity distribution, so that on average the velocity distribution is well sampled. For example, in the lobe simulations, the statistical scatter in the temperature at the lower boundary was T₁₁₂ = 118 ± 0.04, T₁₁₄ = 118 ± 0.07 and T₁₁₂ = 118 ± 0.3. Furthermore, the fluctuation in the H₂ temperature is greatest at the bottom of the simulation domain where its mixing ratio is smallest. Conversely, in the upper most regions (r > 4300 km) the N₂ and CH₄ temperatures fluctuate more than that of H₂.

After 1.4 × 10⁶ time steps of 0.1 s each, which is about a tenth of a Titan orbital period (~1.4 × 10⁶ s), the density versus altitude for N₂ and CH₄ in the 3-component DSMC simulations reach steady state. However, the initial isothermal H₂ density profile is very different than the final result obtained, and the H₂ densities versus altitude take roughly half a Titan day to achieve steady state. The resulting N₂ density profiles are seen to be similar to both the INMS lobe (Fig. 2a) and plasma sheet (Fig. 2b) averaged data. The simulated methane densities at the higher altitudes are somewhat larger than the averaged INMS densities for both data sets, but within the variation of the collective data indicated by the error bars. Therefore, consistent with the simulations in Tucker and Johnson (2009) we find the thermal escape of CH₄ is not many orders of magnitude larger than the Jeans rate. That is, over the duration of our simulations no molecular nitrogen or methane representative particles escaped. If one representative particle would have escaped, the loss rate would have been ~10²⁷ CH₄/s, which is several orders of magnitude smaller than the escape rate inferred using the diffusion equation to fit the data (e.g., Yelle et al., 2008). For characteristic temperatures of Titan’s upper atmosphere, this result is consistent with thermal escape of N₂ and CH₄ occurring on a molecule-by-molecule basis and not as a fluid-like outflow as has been suggested (e.g., Strobel, 2008, 2009). Even for the highest temperatures inferred by the INMS density data, i.e. T ~ 200 K (e.g., Cui et al., 2011; Westlake et al., 2011), the Jeans parameter for methane, JCH₄ ~ 20, is much larger than the value suggested for a hydrodynamic-like loss in our extensive DSMC studies of thermal escape (e.g., Volkov et al., 2011a,b).

We derive a nominal exobase distance (Kn ~ 1) of rₓ ~ 4000 km and 4100 km for the lobe and plasma sheet encounters respectively. The hydrogen escape rates obtained in the simulations are 1.0 × 10²⁸ H₂/s for the lobe and 1.4 × 10²⁸ H₂/s for the plasma sheet. These are both similar to the Jeans rate, ϕJ / ϕH ~ 1.1 × ϕH. The Jeans rates are evaluated using the corresponding H₂ densities (2.9 × 10⁶ cm⁻³, 1.2 × 10⁶ cm⁻³) and background gas temperature, Tₓ ~ (114 K, 154 K), at the exobase (Table 2). Removing energy at a rate of 4.3 × 10⁻⁴ erg cm⁻² s⁻¹, H₂ escape adiabatically cools all three species (Fig. 2c and d). As a result, the N₂ and CH₄ densities are not isothermal as previously implied in Fig. 4 in Tucker and Johnson (2009). The H₂ temperatures are seen to separate from both N₂ and CH₄ at r ≈ 3800 km and ≈3900 km (Kn ~ 0.2) for the lobe and plasma sheet respectively. Therefore, even well below the exobase H₂ is not in thermodynamic equilibrium with the background gas. In addition, the translation and internal temperatures for H₂ deviate from each other as shown in Fig. 2e and f. Because the background gas does not have a significant escape rate, the translation and internal energy modes for N₂ and CH₄ are nearly in thermodynamic equilibrium. The slight departures above the exobase occur as H₂ is the dominant collision partner above the exobase. These results are in qualitative agreement with our previous DSMC simulations of a one-component atmosphere (Volkov et al., 2011a,b), where the breakdown of translational equilibrium was also observed well below the exobase.

For higher thermosphere temperatures, H₂ cooling of the background gases is significant and can, falsely, suggest thermal escape rates for CH₄ that are much larger than the Jeans rate. For example, using the diffusion equation including the eddy diffusion coefficient, as given in Yelle et al. (2008), we could incorrectly attribute the difference between the isothermal CH₄ density profile and our DSMC density profile for the plasma sheet case in Fig. 3 to require an escape rate of ~4 × 10²⁸ CH₄/s. However, to the extent that the DSMC profile is, on average, above the measured profile, additional escape processes are likely contributing. Therefore, the non-thermal processes discussed in Johnson et al. (2009) may contribute at a rate of a few times 10²⁸ CH₄/s. In addition, Hartle et al. (2012) have pointed out that the high speed horizontal flows in
Titan’s thermosphere (e.g., Müller-Wodarg et al., 2008) can enhance the estimates of both the thermal and non-thermal escape rates. Another interesting result of the 3-component DSMC simulations is the disagreement of the H$_2$ density profile with INMS averaged data for the lobe encounters (Fig. 2a). The lobe simulations indicate the H$_2$ densities diffusively separate from the N$_2$ density at altitudes above $\sim$3750 km, whereas the averaged INMS H$_2$ densities appear to not diffusively separate until altitudes above $\sim$3800 km. In both the lobe and plasma simulations, the H$_2$ density profiles began to separate from N$_2$ at altitudes where the $n_{\text{N}_2} \sim 10^{10}$ cm$^{-3}$.

5.2. H$_2$ in a fixed background of N$_2$ and CH$_4$: DSMC-H$_2$

Because the 3-component DSMC simulations are computationally intensive we performed simulations in which we tracked the H$_2$ molecules in a stationary background atmosphere of N$_2$ and CH$_4$, which we refer to as DSMC-H$_2$. Although the N$_2$ and CH$_4$ temperature and density profiles are affected by H$_2$ escape, in the remainder of this paper we focus on H$_2$ diffusion and escape. To that end, now the background densities in the DSMC simulations discussed below are hydrostatic fits or taken directly from the INMS data and are not simulation results.

This method allows us to perform simulations that start more than 200 km deeper in the atmosphere encompassing the INMS data set from 3548 to 4600 km and use $\sim 2 \times 10^3$ representative H$_2$ particles with $\sim 100$ particles in the bottom cell. For these simulations, the fluctuations in temperature in the bottom cell are approximately an order of magnitude smaller than the previous 3-component DSMC simulations. The lower boundary conditions are given in Table 1 at $r_0 = 3548$ km for the averaged lobe and plasma sheet DSMC-H$_2$ simulations. This altitude is more than two N$_2$ scale heights below that used earlier, starting deeper into the region in which H$_2$ has been suggested to be well mixed (e.g., Cui et al., 2009; Yelle et al., 2008). Furthermore, at $r_0 = 3548$ km the mixing ratio of the averaged data sets is $f_{\text{H}_2} = 0.003$, which is a 25% decrease from that at 3685 km indicating that diffusive separation of H$_2$ likely begins below $r = 3685$ km. In these simulations we also assume the dominant heating occurs below $r_0$. 

Fig. 2. Density (a and b) and temperature (c–f) versus radial distance. The left panels shows INMS density data for N$_2$ (squares), CH$_4$ (circles) and H$_2$ (triangles) for the lobe (filled shapes) and plasma sheet (open shapes) against DSMC results for density (solid curves). The middle and right panels show DSMC results for the temperature of N$_2$ (dashed curve), CH$_4$ (dotted curve) and H$_2$ (solid curve). Middle panel: Total temperature $T = (3T_{\text{TRANS}} + N T_{\text{INT}}) / (3 + N)$ where $T_{\text{TRANS}} = (2T_0 + T_{\text{INT}}) / 3$ and $T_{\text{INT}}$ are the temperatures defined by the translational and internal energy modes respectively, and $N$ is the number of internal degrees of freedom. Left panel: (e) Ratio of perpendicular $1 / 2kT_0 + 1 / 2m v_0^2$ and parallel $1 / 2kT_{\|} = 1 / 2m (v_\| - \text{u})^2$ temperatures where $T_0$, $v_0$, $v_{\|}$, and $u$ are the parallel, perpendicular and bulk velocities respectively. (f) Ratio of translational to internal temperatures.

Fig. 3. The DSMC CH$_4$ density profiles (solid curve) are not barometric as a result of adiabatic cooling from H$_2$ escape lowering the scale height. The barometric profile is represented by the (dashed curve). Using the diffusion equation to fit the DSMC (open squares) and averaged INMS plasma sheet densities (dash dot curve) require significant escape rates.
The exobase distances are located Table 2

The deviations in the velocity distributions for the N₂, CH₄, and CH₂ from a Maxwell–Boltzmann obtained by the 3-component DSMC simulation do not affect the bulk of collisions with H₂. Since we do not include cooling of the N₂ and CH₄ due to H₂ escape in the DSMC-H₂ simulations, their temperatures are few degrees higher at the exobase: 4 and 10 K for the plasma sheet and lobe respectively.

The DSMC-H₂ molecular temperature profile is seen to cool with altitude as a result of escape and again departs from the fixed N₂ and CH₄ temperatures at altitudes well below the exobase (Fig. 4b). The simulated escape rates are now 1.3 × 10⁻²⁸ H₂/s and 1.4 × 10⁻²⁸ H₂/s, both ~0.93 × Jeans, for the lobe and plasma sheet using the corresponding exobase parameters: \( n_e = 3.4 \times 10^9 \text{ cm}^{-3} \) and \( T_e (118 \text{ K}, 161 \text{ K}) \).

The plasma sheet DSMC-H₂ and the 3-component DSMC simulations produce very similar results. For example, the escape rates are the same for both simulations, and at \( r = 3700 \text{ km} \) the densities differ by <20%. However, the DSMC-H₂ lobe simulations had an escape rate 20% larger than the 3-component DSMC lobe simulation. This difference can be attributed to the altitude at which H₂ begins to approach diffusive equilibrium. In the lobe simulations, diffusive separation begins at lower altitudes as compared to the plasma sheet. Even though in the 3-component DSMC simulations H₂ is in thermal equilibrium with the other species at 3700 km, the DSMC-H₂ lobe simulations show that H₂ diffusive separation occurs below 3700 km. For example, the density at this altitude is 1.3 times larger than that in the 3-component DSMC simulation resulting in a larger inventory of escaping molecules.

### 5.3. H₂ density profiles and diffusion

Both the 3-component DSMC and the DSMC-H₂ simulations produce H₂ temperatures lower than the background gas and densities that separate from N₂ at lower altitudes than what appears to be shown by the averaged INMS data. To examine this trend we performed a series of DSMC-H₂ simulations for a range of temperatures, \( T_{N₂} = 100–200 \text{ K} \), and a fixed mixing ratio, \( f_{H₂} \sim 0.003 \), at the lower boundary, characteristic of Titan’s upper atmosphere. In these simulations, we considered H₂ in a background isothermal N₂ atmosphere and \( T_{N₂} \) refers to the imposed N₂ temperature.

The exobase distances for these simulations range from \( r_e \sim 3900–4300 \text{ km} \). For simplicity we take the exobase distance as \( r_e \sim 4150 \text{ km} \) when calculating the theoretical Jeans rates. These are compared with the DSMC-H₂ escape rates in Table 3. Over this range of temperatures the simulated H₂ density profiles are very different, as seen in Fig 5a. At \( r = 4150 \text{ km} \), the simulation using \( T_{N₂} = 200 \text{ K} \) resulted in a density approximately one order of magnitude smaller than that in the simulation using \( T_{N₂} = 100 \text{ K} \). In addition, as shown by the production of escaping molecules in Fig. 5b, with increasing temperature the background gas is denser and the subsequent upward flow of H₂ is increasingly impeded. This result is qualitatively consistent with the concept of diffusion limited escape. Over the simulated temperature range there is a

### Table 2

<table>
<thead>
<tr>
<th>Lobe</th>
<th>( n_e ) (cm⁻³)</th>
<th>( T_e ) (K)</th>
<th>( \phi_L ) (molecules/s)</th>
<th>( \phi_{DSMC} ) (molecules/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂</td>
<td>1.55 × 10³</td>
<td>113.9</td>
<td>64</td>
<td>2100</td>
</tr>
<tr>
<td>CH₄</td>
<td>4.67 × 10⁴</td>
<td>113.5</td>
<td>37</td>
<td>4.2 × 10¹⁴</td>
</tr>
<tr>
<td>H₂</td>
<td>2.86 × 10⁵</td>
<td>111.2</td>
<td>46</td>
<td>9.0 × 10⁷</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Plasma</th>
<th>( n_e ) (cm⁻³)</th>
<th>( T_e ) (K)</th>
<th>( \phi_L ) (molecules/s)</th>
<th>( \phi_{DSMC} ) (molecules/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂</td>
<td>1.48 × 10³</td>
<td>153.6</td>
<td>46</td>
<td>8.9 × 10¹⁰</td>
</tr>
<tr>
<td>CH₄</td>
<td>4.93 × 10⁴</td>
<td>153.2</td>
<td>27</td>
<td>9.9 × 10¹⁰</td>
</tr>
<tr>
<td>H₂</td>
<td>1.22 × 10⁵</td>
<td>148.5</td>
<td>3.3</td>
<td>1.3 × 10⁰</td>
</tr>
</tbody>
</table>

The simulations were performed using lower boundary conditions given Table 1. The exobase distances are located \( r_e \sim 4000 \text{ (1425) km} \) and \( ~4100 \text{ (1525) km} \) for the lobe and plasma sheet respectively.

### Table 3

<table>
<thead>
<tr>
<th>( T_{N₂} )</th>
<th>( \phi_{DSMC} \times 10^{-28} \text{ H}_2/\text{s} )</th>
<th>( n_e \times 10^{14} \text{ cm}^{-3} )</th>
<th>( \phi_{DSMC} )</th>
<th>( \phi_{DSMC}/\phi_L )</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 K</td>
<td>1.24</td>
<td>4.5</td>
<td>0.80</td>
<td>0.80</td>
</tr>
<tr>
<td>125 K</td>
<td>1.48</td>
<td>2.5</td>
<td>0.93</td>
<td>0.93</td>
</tr>
<tr>
<td>150 K</td>
<td>1.48</td>
<td>1.4</td>
<td>0.95</td>
<td>0.95</td>
</tr>
<tr>
<td>175 K</td>
<td>1.45</td>
<td>0.84</td>
<td>1.03</td>
<td>1.03</td>
</tr>
<tr>
<td>200 K</td>
<td>1.35</td>
<td>0.62</td>
<td>1.03</td>
<td>1.03</td>
</tr>
</tbody>
</table>

* The Jeans rates for all simulations were evaluated at \( r_e = 4150 \text{ (1575) km} \) using the \( N₂ \) temperature for qualitative comparisons.
small variance in the escape rate \((1.24–1.48 \times 10^{28} \text{H}_2/\text{s})\), and the simulations appear to exhibit a slight maximum in the escape rate for \(T_0 = 150 \text{K}\). As seen in Eq. (4b), the diffusion limited escape rate slightly decreases with increasing temperature. However, as discussed below there are quantitative differences between results obtained from the DSMC simulations and the diffusion equation.

The averaged INMS data sets obscure the fact that the \(\text{H}_2\) densities obtain diffusive equilibrium at lower altitudes for lower temperatures, e.g., Fig. 1. However, in an investigation of individual INMS passes, Cui et al. (2011) concluded that the \(\text{H}_2\) exospheric density showed temporal variations with the changing plasma environment. Since the variation of the \(\text{H}_2\) densities versus altitude are averaged over in the data sets used above, below we examine individual data sets (Table 4) to determine if the individual flybys exhibit the trend of \(\text{H}_2\) obtaining diffusive equilibrium at lower altitudes for lower temperatures.

The inbound T18 flyby (\(T_{N_2} \sim 130 \text{K}\)) and T19 flyby (\(T_{N_2} \sim 140 \text{K}\)) occurred approximately 1 Titan day apart, with plasma conditions for the T18 flyby classified as lobe and conditions for the T19 flyby as plasma sheet. The \(N_2\) and \(\text{H}_2\) densities versus altitude for these flybys are shown in Fig. 5a. We see the same trend in these individual INMS data sets as in the DSMC simulations: molecular hydrogen diffusively separates from \(N_2\) at lower altitudes for lower temperatures. However, this pattern is not obvious in the entire INMS data set. For example, the T36 flyby (\(T_{N_2} \sim 188 \text{K}\)) and T39 flyby (\(T_{N_2} \sim 120 \text{K}\)) (e.g., Cui et al., 2011) both classified as plasma sheet, show only a slight difference in the \(\text{H}_2\) density profiles even though the temperature difference between these flybys is suggested to be more than 60 K Fig. 5b.

We carried out DSMC-\(\text{H}_2\) simulations for the T41 and T29 flybys classified as lobe and plasma sheet respectively (Fig. 7). The \(\text{H}_2\) densities from these passes are very different. Again \(\text{H}_2\) appears to separate at lower altitudes for T41 flyby, qualitatively consistent with the DSMC simulations, but the simulations do not reproduce the INMS densities. The simulated escape rates are \(1.8 \times 10^{28} \text{H}_2/\text{s}\) and \(4.4 \times 10^{28} \text{H}_2/\text{s}\) for the T29 and T41 respectively. Therefore, additional effects must be occurring, such as ballistic redistribution of \(\text{H}_2\) discussed in Section 5.4.

### Table 4

<table>
<thead>
<tr>
<th>Flyby</th>
<th>Classification</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>T18</td>
<td>Lobe</td>
<td>23, September 2006</td>
</tr>
<tr>
<td>T19</td>
<td>Plasma sheet</td>
<td>09, October 2006</td>
</tr>
<tr>
<td>T36</td>
<td>Plasma sheet</td>
<td>02, October 2007</td>
</tr>
<tr>
<td>T39</td>
<td>Plasma sheet</td>
<td>20, December 2007</td>
</tr>
<tr>
<td>T29</td>
<td>Plasma sheet</td>
<td>26, April 2007</td>
</tr>
<tr>
<td>T41</td>
<td>Lobe</td>
<td>22, February 2008</td>
</tr>
</tbody>
</table>

* The Flyby information is taken from Westlake et al. (2011).
To summarize, we find fits to the averaged INMS data obtained with the molecular diffusion equation disagree with our DSMC simulation results. For example, the averaged plasma sheet density profile can be fit using the diffusion equation by assuming an escape rate of $\varphi_{D} \approx 6.89 \times 10^{-7} \text{H}_2/\text{s}$ (Fig. 8a). This rate is approximately ~97% of the diffusion limited escape rate $\varphi_{DL} = 7.05 \times 10^{-7} \text{H}_2/\text{s}$. On the other hand, the DSMC simulations reproduce the observed density profile, but with a larger thermal escape rate of $\varphi_{DSMC} = 1.4 \times 10^{-9} \text{H}_2/\text{s}$. This is the case even though the effective diffusion coefficient, estimated from our cross section, $D_{H2} = \frac{T_{L}}{(1.5) \times \sigma_{H2-H2} \times \omega_{H2}}$, with $\sigma_{H2-H2} = 3.95 \times 10^{-15} \text{cm}^2$, $\omega_{H2} = 0.705$, $\omega_{L} = 3.28 \text{km/s}$ and $m_{H2}$, is the reduced mass, are similar to those used in the diffusion equation (e.g., Bird, 1994). Written in the more typical form, $D_{H2}(\text{cm}^2/\text{s}) = b_{H2} \omega_{H2}^{2}/m_{H2}$, we have $b_{H2} = 2.9 \times 10^{-17}$.

In using the diffusion equations to fit the density data, the gas is assumed to have a Maxwell–Boltzmann velocity distribution at all altitudes. In addition, the temperature of the diffusing species is typically assumed to be equal to that of the background gas, and escape is assumed to occur from a well defined altitude. Even at altitudes well below the nominal exobase the DSMC distribution of radial velocities for H$_2$ is enhanced in upward velocities and depleted in downward velocities for speeds larger than the escape speed Fig 8b: see also Volkov et al. (2011b). Furthermore, we have shown that H$_2$ escape, its heating by, and cooling of the background, occurs over a broad range of altitudes. Other studies have shown such differences can lead to discrepancies between results obtained with kinetic models from those obtained from a diffusion model (e.g., Chamberlin and Smith, 1971 and Cui et al., 2008). Therefore, escape rates obtained using Eq. (3b) can be inaccurate.

5.4. Ballistic redistribution of H$_2$

Due to the small value of the Jeans parameter in the exobase region, not only does H$_2$ escape efficiently, but typical angular excursions of returning molecules are large. For example, it may be shown analytically that on average H$_2$ molecules at ~160 K are most likely to return ~80° from their source. Therefore, there is considerable redistribution of H$_2$ not accounted for in the 1D DSMC simulations. In addition, since steady state takes ~1/2 Titan day, there is considerable temporal averaging in the H$_2$ corona. Clearly a coupled 3D DSMC/ballistic transport model is needed to account for the spatial morphology of the upper thermospheric temperature profile. Preliminary to such a simulation, we modeled a ballistic corona in which we chose an average exobase at 4150 km and let the temperature vary across the globe in an azimuthally symmetric way from 160 K to 120 K. Assuming, for the purpose of this test, a Maxwellian flux distribution at the local exobase $T_v$, we tracked the H$_2$ from its source to where it returned to the exobase. We found that the spatial distribution of the return flux and the vertical column density, not surprisingly, differed from that expected when using a globally uniform exobase temperature. For the non-uniform temperature profile used, these quantities were found to vary by less than ~5% across the globe. Therefore, the similarity between the INMS averaged H$_2$ density profiles for the lobe and the plasma is due, at least in part, to ballistic transport in the corona. Based on this finding, a coupled DSMC/ballistic Monte Carlo model of the upper thermosphere and corona is being developed which can account for this transport along with diffusion, escape and cooling of the background gases.

6. Discussion and summary

We present here the first 3-component DSMC simulations of thermal escape from Titan’s upper atmosphere. Many of the results obtained here are similar to those described in the exobase region of Mars by Boqueho and Blelly (2005) using a 13 moment method, but the DSMC technique can more accurately describe the details of atmospheric escape. Prior to these simulations, several fluid/continuum models used to fit the highly variable CH$_4$ density profiles infer escape rates ranging from Jeans-like to hydrodynamic-like. Consistent with our earlier DSMC studies, it is confirmed here.
that thermal escape is essentially Jeans-like for temperatures characteristic of Titan's upper atmosphere. When fitting the measured CH₄ density profiles, continuum models, which have upper boundary conditions that assume escape is occurring, have suggested large CH₄ loss rates. We showed here that this is at least in part explained by the fact that H₂ escape cools CH₄ so that the DSMC densities differ from a simple isothermal profile without requiring significant escape. We find that, although the simulated CH₄ densities are within the variation of the collective INMS data set, at the higher altitudes they are, on average, somewhat larger than the averaged INMS data points. This suggests that non-thermal escape processes must be contributing. Since a rough bound on the methane escape has been suggested by very low densities of carbon bearing ions observed by the Cassini Plasma spectrometer a few Saturn radii about Titan (e.g., Crary et al., 2010), simulations are needed in which non-thermal processes are included. In addition, introducing eddy mixing at high altitudes could make the lobe simulations methane densities agree better with the average INMS data and horizontal transport of H₂ occurring by thermospheric winds or by ballistic transport in the corona can spatially average the density profiles. Eddy mixing has been suggested to be an important processes in the upper atmosphere up to distances r ~ 3575 km by Bell et al. (2011), this distance is 100 km below the lower boundary used in our 3-component DSMC simulations (Bell et al., 2011). Additional 3-component DSMC simulations performed for greater depths in Titan's atmosphere would be helpful but would require including eddy diffusion and thermospheric heating processes.

The DSMC simulations reproduce the effect of the background N₂ density in limiting the upward flow of H₂ as also suggested by the INMS data for individual encounters. This interaction affects the radial depth from which H₂ molecules are able to escape. That is, we find the H₂ molecules begin escaping from a column of N₂ atmosphere ~3-4 x 10¹⁶ N₂/cm², and with increasing temperature this N₂ column density occurs at higher altitudes. However, the simulated H₂ densities versus altitude for the lower temperature flybys are larger than that indicated by the INMS data. Below we consider reasons for the discrepancy between the simulated H₂ density profiles and the INMS data.

Since our results depend on the value of the N₂–H₂ collision cross-sections, if underestimated, it would produce the lower altitude seen in our lobe simulations for the onset of diffusive separation. Since Cui et al. (2011) suggested the H₂ densities in Titan's exosphere exhibit temporal variations on timescales less than a Titan day, comparisons to time dependent results would be insightful. Related to this, global transport has been suggested to be important in the thermosphere (e.g., Müller-Wodarg et al., 2008). Here we also show that steady state for the H₂ corona profile takes of the order of a half a Titan day, suggesting considerable temporal averaging is occurring and ballistic transport of H₂ acts to produce a more uniform global coronal column density. Finally, Michael et al. (2005) showed that sputtering of N₂ by pickup ions produces a cascade of non-thermal collisions. Although this only produced a modest change in the exobase temperature in the background gas (AT ~ 5 K), above the exobase the H₂ densities eventually are comparable or dominate N₂. Therefore, a detailed simulation of the direct plasma interaction with the extended H₂ density profile is needed. For instance, rapid removal of H₂ at high altitudes by direct collisions, ionization and sweeping, or dissociation would also affect the comparison with the INMS data.

Acknowledgments

This research was supported by the NASA Planetary Atmospheres Program and the NSF Astronomy Program. The authors are grateful for discussions with J. Erwin and comments provided by Dr. J. Bell, Prof. D. Strobel, and an anonymous reviewer.

References


