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Note

Evolution of an early Titan atmosphere

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ABSTRACT

Rapid escape from a proposed early CH_4/NH_3 atmosphere on Titan could, in principle, limit the amount of NH_3 that is converted by photolysis into the present N_2 atmosphere. Assuming that this conversion occurred, a recent estimate of escape driven by the surface temperature and pressure was used to constrain Titan's accretion temperature. Here we show that for the range of temperatures of interest, heating of the surface is not the primary driver for escape. Atmospheric loss from a thick Titan atmosphere is predominantly driven by heating of the upper atmosphere; therefore, the loss rate cannot be used to easily constrain the accretion temperature. We give an estimate of the solar driven escape rate from an early atmosphere on Titan, and then briefly discuss its relevance to the cooling rate, isotope ratios, and the time period suggested to convert NH_3 to the present N_2 atmosphere.

1. Introduction

The evolution of, and escape from, Titan's atmosphere is still debated in spite of the large amount of Cassini data: >100 passes through Titan's upper atmosphere (e.g., Mandt et al., 2014, 2015; Glein, 2015). There is agreement that the present H_2 loss rate (e.g., Tucker et al., 2013) is roughly consistent with the rate of photolysis of CH_4 and the subsequent precipitation of larger carbon-containing molecules (e.g., Atreya et al., 2006). However, the present escape rate for carbon and nitrogen containing molecules is small and still being studied (e.g., Tucker et al., 2013, 2016; Snowden and Yelle, 2014). Therefore, not much light has been shed on the early evolution of Titan's atmosphere or on the possibility that nitrogen was initially present as NH_3 and was subsequently converted to its present form N_2 (e.g., Atreya et al., 1978; Strobel, 1982). Because the surface temperature following accretion (>~300 K: Kuramoto and Matsui, 1994) was much higher than that at present (~94 K), it was suggested that this parameter might determine the escape rate from an early Titan atmosphere (Gilliam and Lerman, 2014). Here we show that although the atmospheric temperature is important for the proposed nitrogen chemistry, the range of accretion temperatures of interest is a secondary effect in determining the escape rate, which is primarily driven by the solar energy absorbed in the upper atmosphere. We first give an estimate of the escape rate due only to the heating of Titan's surface. We then discuss the heating of the upper atmosphere and give a new estimate of nitrogen loss from an early CH_4, NH_3 atmosphere.

2. Escape driven by surface heating

Molecular kinetic simulations have shown that the escape from a *thick* atmosphere can be simulated reasonably well by applying the Jeans escape rate iteratively as an upper boundary condition in a fluid dynamics simulation. This procedure is often referred to as a fluid-Jeans simulation (e.g., Erwin et al., 2013; Johnson et al., 2015). The Jeans escape rate in molecules per second (s^{-1}) can be written as

$$\Phi_J = \pi r^2 n(r) \langle v \rangle [1 + \lambda(r)] \exp[-\lambda(r)] \quad (1)$$

where $n(r)$, $\langle v \rangle$, and $\lambda(r)$ are the molecular density, mean thermal speed and Jeans parameter in the atmosphere at a radius r from the center of the planet. The Jeans parameter is $\lambda(r) = U(r)/kT(r)$, the ratio of the gravitational binding energy of a molecule, $U(r)$, to a measure of its thermal energy, $kT(r)$, with k the Boltzmann constant and $T(r)$ the local temperature. Here $U(r) = GMm/r$ with G the gravitational constant, M the planet's mass and m the molecular mass. By using Eq. (1) to calculate the escape rate, one assumes that molecular collisions, which might affect the escape rate, can be ignored above r. Therefore, it is typically evaluated at the nominal exobase ($r = r_x$). Since the surface temperature may be known but the exobase altitude and temperature require a detailed calculation, the escape rate is sometimes approximated by replacing

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r_x by the surface radius, r_0 (e.g., Schaller and Brown, 2007). This is referred to as the surface-Jeans (SJ) approximation, which is appropriate for very thin atmospheres. A thick atmosphere heated only by the surface temperature typically decreases in temperature and pressure with altitude in the absence of upper atmosphere heating. Therefore, the SJ estimate can be orders of magnitude larger than the correct escape rate (e.g., Volkov et al., 2011a, 2011b; Volkov, 2015; Johnson et al., 2015).

Escape driven only by the surface temperature and pressure has been simulated using the fluid-Jeans (FJ) model in which the escape rate in Eq. (1) is evaluated at the exobase with r_x found iteratively. FJ simulations, which are accurate for large column densities, can be supplemented by molecular kinetic simulations for the lower column densities. Such simulations were recently carried out for atmospheres spanning a range of surface Jeans parameters [$\lambda(r_0)=\lambda_0=10$ to 30] and column densities [$N(r_0)=N_0=10^{18}$ to 10^{31} molecules/m^2] as shown in Fig. 2 of Johnson et al. (2015). Here $N_0=P_{vap}/mg_0$, with P_{vap} the vapor pressure and $g_0=U(r_0)/r_0$ the surface gravity. In that paper the ratio, R, of the simulated escape rate to the SJ rate was roughly fit using the Knudsen number evaluated at the surface, Kn_0, defined in this paper as $Kn_0=(\lambda_0 N_0\sigma_{eff})^{-1}$ with σ_{eff} the effective collision cross section between the atmospheric molecules. [1] The fit to that ratio is

$$R^{-1}\sim R_1^{-1}+R_2^{-1}, R_1\sim 1/Kn_0^{0.09},\ R_2\sim 70[Kn_0\exp(\lambda_0)]/\lambda_0^{2.55} \quad (2)$$

where R_1 applies at small N_0 (large Kn_0) calculated using a molecular kinetic model and R_2 applies at large N_0 (small Kn_0). A roughly equivalent theoretical equation for R_2 was derived in Volkov (2015, Eq. (25)). One such result, relevant to the discussion below, is given in Fig. 1. This was calculated using parameters for an N_2 atmosphere. Using Kn_0 and λ_0, Eq. (2) can be scaled to approximate other compositions (Volkov et al., 2011b).

Because the photolytic conversion of NH_3 into N_2 has been suggested to be efficient only if Titan's atmospheric temperature is greater than ~150 K (Atreya et al., 1978; Strobel, 1982) the post-accretion cooling rate of Titan's surface is critical. Therefore, it is of concern whether or not the loss of NH_3 occurred more rapidly than either the cooling to below 150 K and/or the conversion to N_2. With this in mind Gilliam and Lerman (2014) estimated simultaneous cooling and escape rates. Their suggested initial inventories of NH_3 and CH_4 are $\sim 1.62\times10^{21}$ kg and $\sim 0.75\times10^{21}$ kg with a small fraction in the atmosphere as determined by the surface vapor pressures. In their first model the surface starts with a post-accretion temperature of 355 K producing 5.8 bar of atmospheric NH_3 (0.38×10^{20} kg) with $\lambda_0=20.3$ and 19.6 bar of CH_4 (1.2×10^{20} kg) with $\lambda_0=19.1$. The total escape rate was then estimated as the surface cooled using a model roughly equivalent to Eq. (1).

Applying Eq. (1) at Titan's surface ($r_0=r_T=2576$ km) for an atmosphere in equilibrium with the suggested 355 K surface temperature gives an upward flux of molecules with sufficient energy to escape of $\sim 0.65\times10^{35}$ NH_3/s and $\sim 6.8\times10^{35}$ CH_4/s which is the SJ estimate discussed above. The initial loss rate in Gilliam and Lerman (2014), applied at one scale height above the surface, is about a factor of two larger, $\sim 1.4\times10^{35}$ NH_3/s and 15×10^{35} CH_4/s, and is, therefore, roughly consistent with the SJ estimate. As the surface and, hence, the atmosphere cools, the estimated rate drops rapidly as indicated by the exponential dependence on $\lambda(r)$ in Eq. (1). They note that for an initial 355 K surface the loss of the initial atmosphere is much faster than the NH_3 to N_2 conversion rate, so not enough NH_3 could be converted into the amount of N_2 required for the present atmosphere unless there was a continuous surface source of NH_3. Therefore, they suggested the initial accretion temperature might be lower, ~300 K, significantly reducing their estimated loss rate. However, their estimates of the escape rate driven only by the surface temperature are much too large.

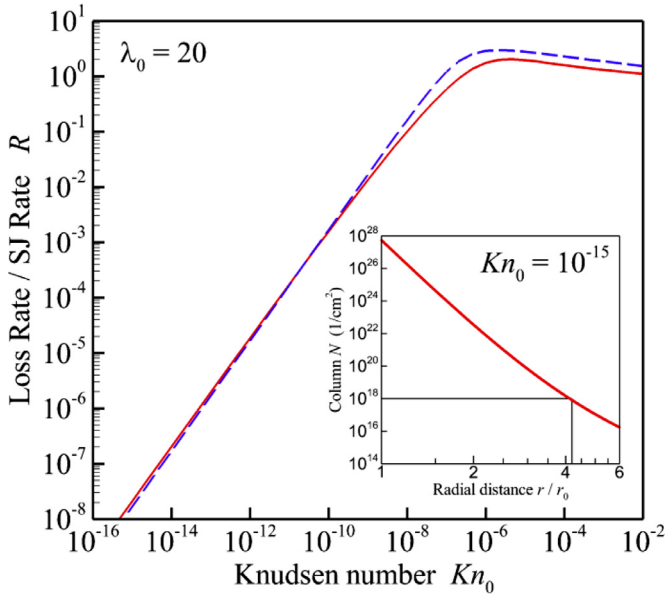

Fig. 1. Escape driven by the surface temperature and pressure: R is the ratio of the simulated loss rate to the SJ estimate shown for $\lambda_0=20$ vs. $Kn_0=(\lambda_0 N_0\sigma_{eff})^{-1}$ with $\sigma_{eff}=10^{-14}$ cm^2. Solid lines: FJ simulations for a diatomic gas with the viscosity index equal to 1; dashed line: approximate fit in Eq. (2); the difference at larger Kn_0 (smaller N_0) is estimated from molecular kinetic simulations which give a more accurate description of the exobase region (Johnson et al., 2015). Insert: column density N_0 vs. r/r_0 for $\lambda_0=20$ and $Kn_0=10^{-15}$, close to the conditions in GL for a 355 K early atmosphere: lines indicate a column $N=10^{18}$/cm^2 which gives a rough estimate of the absorption peak ($r_a\sim 4.3r_0$) *prior* to the atmospheric expansion due to UV/EUV absorption; the nominal exobase, r_x, at $N(r_x)\sim 10^{14}$cm^{-2}, is seen to be $r_x\gg 6r_0$. Results can be very roughly scaled to Titan's atmosphere using λ_0 and Kn_0 (Volkov, 2011b).

Titan's present exobase is well above Titan's surface ($\sim 1.6r_T$) and was even higher for the proposed early Titan atmosphere. Therefore, applying a surface or near surface approximation for escape is incorrect. A good estimate for the escape rate driven by the surface pressure can be obtained using the ratio, R, in Eq. (2). Based on their NH_3 and CH_4 vapor pressures for the proposed 355 K early atmosphere, the average molecular mass is ~16.2 amu giving $\lambda_0=19.3$, close to the case shown in Fig. 1 for which $r_x\gg 6r_T$. For the initial column density, $N_0=7\times10^{27}$ molecules/cm^2 and a collision cross section of $\sigma_{eff}\sim 10^{-14}$ cm^2 we obtain $Kn_0=7.5\times10^{-16}$. The resulting ratio of the simulated rate to the SJ rate using Eq. (2) is $R\sim 10^{-8}$. Therefore, their *initial* loss rate is almost eight orders of magnitudes too large. In addition, the net escape rate integrated over the cooling process is also orders of magnitude too large as shown in Table 1. Their estimated net loss rate from their preferred atmosphere, having initial surface temperature of 300 K, is also many orders of magnitude too large. Therefore, such rates cannot be used to constrain Titan's accretion temperature.

3. Escape driven by heating of the upper atmosphere

Although the escape rate from an early Titan atmosphere is likely large, it is not driven by the near surface atmospheric temperature. Rather, as assumed in most studies, the energy deposited in the upper atmosphere dominates the loss rate. Escape due to heating of the upper atmosphere was recently modeled using

[1] The Knudsen number in a 1D atmosphere varying only with the radius, r, is the ratio of the mean free path for molecular collisions, l_c, to the length scale over which the molecular density, n, changes, $\sim|n/(dn/dr)|$. Here we use $Kn=l_c/r$; in other papers the atmospheric scale height, H, has been used.