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# Molecular escape of $H_2$ from Titan's atmosphere: kinetic Monte Carlo simulations

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## Abstract

A molecular model of $H_2$ diffusion through a static background gas of $N_2$ and $CH_4$ in Titan's upper atmosphere and subsequent escape is compared to Cassini density measurements and continuum model results. Normalizing the densities and temperatures at the lower boundary of the simulation region ($r_o$ = 3685 km, $T_o$ ~ 132 K & $T_o$ ~161 K) to recent INMS data [3] we found that the increase in the $N_2$ densities measured when Titan is in Saturn's plasma sheet results in a decrease in the $H_2$ densities above the exobase and a 10% decrease in the escape rate compared to simulations using $N_2$ densities measured when Titan is outside the plasma sheet.

## 1. Introduction

A wealth of measurements on the structure of Titan's upper atmosphere has been provided by the Cassini spacecraft during its several flybys. However interpreting the globally averaged densities of the major atmospheric components, $N_2$, $CH_4$ and $H_2$, remains the subject of much discussion, e.g. Ref. 1. Continuum models of hydrodynamic escape and models the diffusion of $CH_4$ and $H_2$ through a static $N_2$ background gas require significant escape fluxes to match the Cassini data [1]. In contrast molecular models of thermal escape have reproduced Cassini density measurements of $N_2$ and $CH_4$ without requiring large escape rates [2]. In this study a similar molecular model to that discussed in Ref. 2 is used to consider the diffusion and escape of $H_2$ in a static background gas of $N_2$ and $CH_4$ and the results are compared with Cassini density measurements and the continuum models of diffusion and escape.

## 2. Escape and Jeans flux

A molecule has the highest probability to escape from a planet in the exosphere region where molecular collisions are rare. The lower boundary to this region is the exobase which is defined as the radial distance where molecules can travel an atmospheric scale height without suffering a collision. At the exobase distance $r_x$ the theoretical Jeans escape flux $F_J$ is evaluated as a function of temperature $T_x$ and density $n_x$ where $\lambda_x$ is the Jeans parameter at the exobase. The Jeans parameter is the ratio of the gravitational energy ($GMm/r_x$) to the thermal energy ($kT_x$) at the exobase where G is the gravitational constant, $M$ is the planet mass, $m$ is the molecular mass and $k$ is the Boltzmann constant. At Titan the exobase distance derived from $N_2$ is $r_x$ ~ 4075 km and the Jeans parameters are ~ 50, 30 and 4 for $N_2$, $CH_4$ and $H_2$ respectively.

$$\lambda_x = GMm/kT_x r_x \quad (1)$$

$$F_J = \tfrac{1}{4} n_x \left(\tfrac{8kT_x}{\pi m}\right)(1+\lambda_x)\exp[-\lambda_x] \quad (2)$$

## 3. Cassini density data

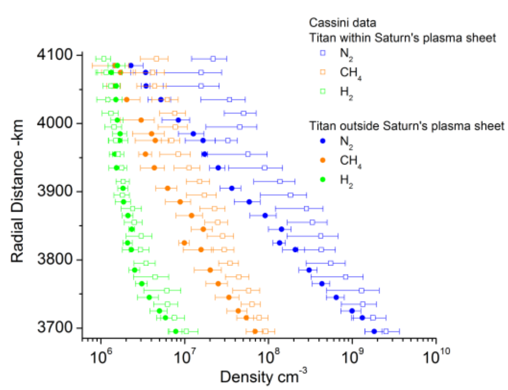


Figure 1: Globally averaged INMS density data for Titan when located within and out of Saturn's plasma sheet.

The Cassini density data obtained by the Ion Neutral Mass Spectrometer (INMS) in Titan's upper atmosphere is considered most accurate for radial distances between ~3500 km and 4075 km (Fig 1). In addition the density data is highly variable. For example, enhancements seen in the $N_2$ densities measurements vs. r when Titan orbits within Saturn's plasma sheet are suggestive of non-thermal heating processes occurring in the upper atmosphere [3]. Earlier we showed the continuum models of orbitally averaged data sets required escape rates that were much too large for $N_2$ and $CH_4$ [2] for a specific $n_o$ and $T_o$ at the lower boundary $r_o$.

## 5. Summary and Conclusions

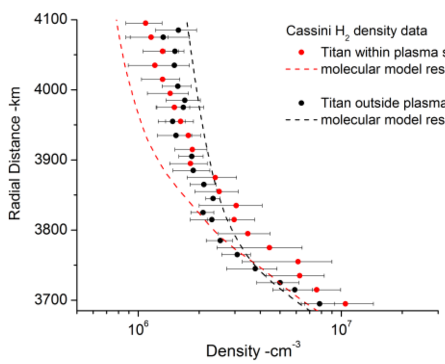


Figure 2: Comparison of molecular simulation results (dashed lines) to averaged INMS density data for $H_2$ for Titan orbits within (open red triangles) and outside (open black circles) of Saturn's plasma sheet.

A set of molecular simulations are performed for the diffusion and escape of $H_2$ from Titan's atmosphere using hydrostatic density profiles of $N_2$ and $CH_4$ for $r_o$ = 3685 km and $T_o$ = (132 & 165) K from fits to the INMS density data obtained while Titan orbited within and outside Saturn's plasma sheet (Fig. 2). The molecular simulations describe collisions with variable cross section sizes based on the relative velocity between molecules, and allow for the exchange of rotational energy with translation energy. For the temperatures given above $T_o$ the molecular model obtains $H_2$ escape rates of ~1.1 x$10^{28}$ $s^{-1}$ and 1.0 x$10^{28}$ $s^{-1}$, ~1.5·$F_J$ and 1.4·$F_J$ respectively. The above molecular simulations do not fit the averaged INMS data points, however the simulation for conditions when Titan is outside the plasma sheet obtains $H_2$ densities roughly within the variations of the data. Furthermore $H_2$ is produced by $CH_4$ photo-dissociation on the sunlit side of Titan therefore a globally averaged data set of $H_2$ densities for day and night flybys may underestimate the $H_2$ densities at the upper most altitudes. While the INMS averaged densities for $N_2$ and $CH_4$ increase when Titan orbits in the plasma sheet the $H_2$ densities are indistinguishable. Roughly consistent with the INMS data the molecular simulations show a decrease in $H_2$ densities with an increase in temperature and density of the $N_2$ background gas (Fig. 2).

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