HOT H ESCAPE AT MARS: AN ASSESSMENT OF THE IMPORTANCE OF PHOTOCHEMICAL H LOSS MECHANISMS

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Introduction:

The loss of hydrogen to space has played an important role in the desiccation of Mars, which has lost most of its initial water. Hydrogen escape is therefore important for understanding the planet's atmospheric evolution. This process has been largely attributed to thermal escape, in which the high-energy tail of H atoms in a Maxwell-Bolzmann velocity distribution may have sufficient energy to be irreversibly removed from the upper atmosphere. However, a smaller population of higher-temperature H atoms is also expected to be present, indicated by modelling studies (e.g. Nagy et al., 1990) and inferred by observations (e.g. Chaufray et al., 2008; Bhattacharyya et al., 2015; Chaffin et al., 2018). These "hot" or nonthermal hydrogen atoms are those that are either produced by photochemical reactions which may give them a large initial kinetic energy, or those that gain additional energy through charge or momentum transfer processes with other particles.

Here, we present escape estimates for 45 photochemical mechanisms that produce hot H, in order to compare the importance of these mechanisms for nonthermal H loss from Mars and direct future lines of enquiry.

Escape probability profiles:

We use a new Monte Carlo model based on those of Deighan (e.g. Lillis et al., 2017) and Gröller (Gröller et al., 2010, 2012, 2014) to produce an escape probability profile. The model simulates a distribution of hot H particles and tracks them as they move through the atmosphere and collide with background species. The simulation ends when the particles a) undergo sufficient collisions such that their energies drop below the escape energy (~0.05-0.13 eV, dependent on altitude), b) hit the lower boundary of the model (~80 km) or c) move with more than escape energy beyond the upper boundary (~5000 km). We count the number of test particles in category (c) in the simulation in order to calculate an escape rate.

For two different energies (5 eV and 0.2 eV), we choose a series of altitudes between 80 and 400 km and produce 1000 test particles at each altitude. We count the number of test particles that escape, and repeat the simulation three further times for each altitude in order to take the mean. We do this for both low and high solar activity models (as defined in Fox (2015)), using background species density profiles from Fox (2015).

We find that escape probabilities are very small below ~130-140 and ~140-150 km for low and high solar activity model atmospheres, respectively, and as large as 0.92 and 0.84 at 400 km (our highest production altitude; Figures 1c and 1g). The latter are much larger than the maximum escape probabilities for hot oxygen atoms on Mars (Lillis et al., 2017). Even though the directions of the initial velocities of the H atoms are uniformly-distributed, with 50% of the population moving upward initially and the other half moving downward toward the planet, the comparatively low mass of H atoms means that the number of collisions required to turn the downward-directed particles around is less than that required to thermalise the particles.

Estimates of nonthermal H escape:

We calculate the total background column density above each chosen altitude (N), and fit curves of the form $p = Ae^{-a\sigma N}$, where p is the escape probability and σ is the cross-section. The constants a and A are both between 0 and 1: a is a transparency coefficient to account for the insufficiency of single collisions to prevent escape, while A is the escape probability at which N is zero.

Using reactant density and temperature profiles (Fox, 2015) and rate coefficients (Rodriguez et al., 1984; Fox, 2015 and references therein), we calculate production rate profiles. The escaping H production rate is equal to the production rate multiplied by the escape probability at each altitude. We integrate the escaping H production rate profile over altitude to obtain a hot H escape flux for each mechanism, for each of the two example energies. This method is summarised in Figure 1.

We find that for both the low and high solar activity cases, for both energies, the dissociative recombination of HCO^+ (HCO^+ DR) is the most important nonthermal mechanism producing escaping H. For low solar activity conditions, HCO^+ DR contributes 52% and 42% of the total nonthermal H escape for the 5 eV and 0.2 eV distributions, respectively. For both low and high solar activity, other important mechanisms include $CO_2^+ + H_2 \rightarrow OCOH^+ + H$, $O^+ + H_2 \rightarrow OH^+ + H$, and $OH^+ + O \rightarrow O_2^+ + H$. We find that $CO_2 + H^+ \rightarrow CO_2^+ + H$ is also within the top five most important mechanisms for

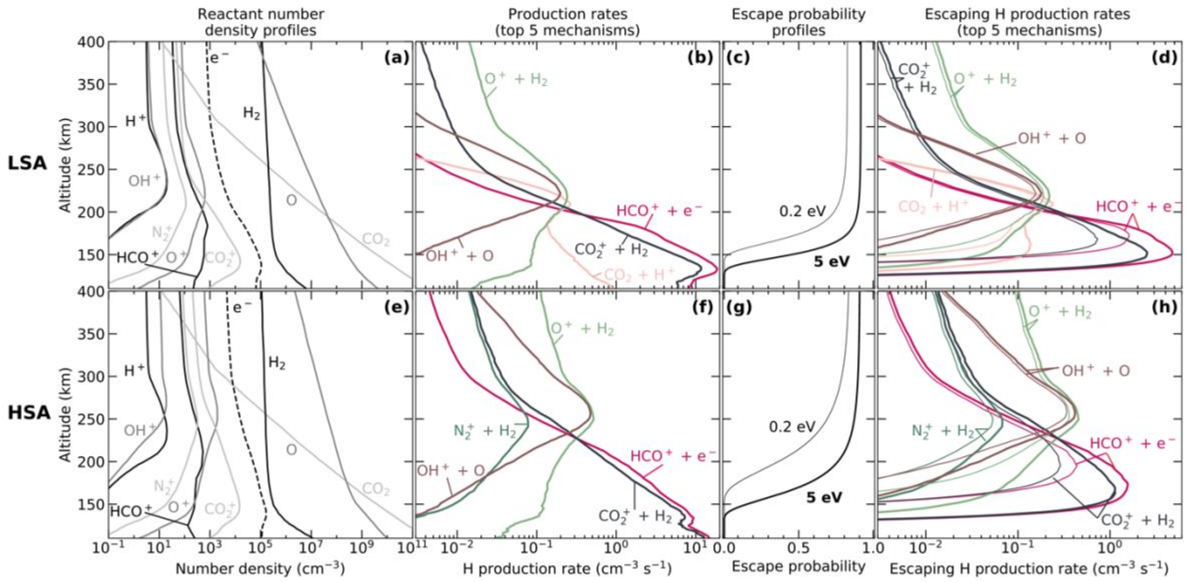

Figure 1: Illustration of escaping H production rate calculation method and preliminary results. Panels (a) and (e) show number density profiles for the reactants of the top 5 photochemical mechanisms in both the low (LSA) and high (HSA) solar activity models in our study. Panels (b) and (f) show the hot H production rate profiles for the top 5 mechanisms, for low and high solar activity, respectively. Panels (c) and (g) show the escape probability profiles for two kinetic energies for low and high solar activity, respectively. Panels (d) and (h) show the calculated escaping H production rate profiles, which are the product of the production rate and escape probability at each altitude. Thicker lines show escape rate results for 5 eV particles, while thinner lines show escape rate results for 0.2 eV particles.

low solar activity conditions and $N_2^+ + H_2 \rightarrow N_2H^+ + H$ is within the top five most important mechanisms for high solar activity conditions. The top five mechanisms contribute 90-94% and 88-91% of the total nonthermal H escape for low and high solar activity, respectively. For each of the top mechanisms, the reactant number density, H production rate, escape probability and escaping H production rate profiles are shown for low and high solar activity in Figure 1.

Applications and future work:

Our escape probability curves are independent of reactant number density, background number density and temperature profiles, so are flexible for use with different model or observational output profiles, including temporally-varying profiles. We have performed detailed Monte Carlo model calculations for HCO^+ DR (Gregory et al., *in prep*), and will carry out more detailed modelling of the subsequent four most important mechanisms shown here, for both low and high solar activity conditions, in a future study. The detailed modelling will allow for better predictions of nonthermal H escape, as the particle energies given by each mechanism will be properly accounted for. Though shown to be less important than other mechanisms here, we will also examine resonant charge exchange (H + H+), as it is known to be important on Venus.

Conclusion:

Here we show new escape probability profiles for nonthermal H, of up to more than 90%, which is higher than that for nonthermal oxygen (Lillis et al., 2017). Since our escape estimates are independent of density and temperature profiles, they are flexible for use with different inputs. We produce escape estimates for 45 photochemical H-producing mechanisms, and show that the most important, for both low and high solar activity model atmospheres and particle energies of 5 eV and 0.2 eV, is the dissociative recombination of HCO^+. Our preliminary results give a total nonthermal escape flux of 11-13% and 5% of the canonical thermal H escape flux (2.4×10^8 cm^{-2} s^{-1}; McElroy, 1972) for 5 eV and 0.2 eV populations, respectively. We are currently working on detailed Monte Carlo modelling of the five most important mechanisms, as well as resonant charge exchange, in order to obtain more comprehensive escape rates for the most significant nonthermal H escape sources.

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