Photochemical escape of O and C from Mars: the impact of collisional cross sections

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Introduction:

Recent estimates based on Ar isotope fractionation in the upper atmosphere suggest that Mars has lost at least 66% of its original atmosphere to space, including most of its initial water inventory. In the current epoch, the photochemical escape is considered responsible for much of the loss of atomic oxygen and carbon, while Jeans escape remains the dominant escape mechanism of hydrogen. The classical picture is that H and O escape from Mars in 2:1 ratio when averaged over time periods longer than about 10^5 years, with H escape responding to O loss. Thus, the physical processes governing the O escape effectively determine the overall escape rate, while the variations due to seasonal effects and climate cycles average out.

More recently, NASA's Mars Atmosphere and Volatile EvolutioN (MAVEN) mission detected seasonal variations of hydrogen escape in excess of an order of magnitude, in contrast to the predictions of the classical picture. Here, the leading hypothesis is that these variations occur due to the enhanced vertical transport of water to higher altitudes than previously thought possible because of stronger coupling of the lower and middle atmospheres during the Martian summers[3]. The dust storms may also play a role in enhancing the transport: the atmospheric water vapor on Mars at altitudes as high as 80 km has been observed during global and regional dust storms[1,2]. During the regional 2019 C-storm, the hydrogen corona reconstructed from measurements of the hydrogen Ly α line brightness implied that enhanced water transport from mid-altitudes (60-80 km) took place. The ExoMars Trace Gas Orbiter (TGO) observation of HDO during the 2018 global dust storm arrived at the same conclusion.

Quantitative characterization of these loss processes and their role in the past epochs requires an accurate description of the physical mechanisms involved, including collisional cross sections between the escaping energetic atoms and atmospheric atomic and molecular species, as well as accurate global models of the atmospheric escape to guide the interpretation of the observations.

Results and Discussion:

Here, we present new calculations of scattering cross sections for C-CO2 elastic and inelastic collisions, as well as preliminary full-dimensional O-CO2 cross sections. These two scattering processes play a major role in the atmospheric escape due to the abundance of CO2 in the Martian atmosphere. The C-CO2 state-to-state velocity-dependent cross sections were computed using a modified Arthurs-Dalgarno quantum-mechanical rigid rotor model, whereas the O-CO2 cross sections were constructed using the Multi Configuration Time Dependent Hartree (MCTDH) formalism on a new full-dimensional potential energy surface capable of correctly describing the vibrational and bending modes of CO2.

We estimated the impact of the new cross sections on the atmospheric escape rates using a 1-D column escape model and compared them to the results obtained using a global 3-D model[4] (3D Mars Global Ionosphere Thermosphere Model coupled with the Adaptive Mesh Particle Simulator; M-GITM+AMPS; see Y. Lee *et al.*[5] for a detailed description of the model setup and parameters). The resulting difference coronae for three scenarios[5] considered are given in Fig. 1 while the total O escape rates are summarized in Table 1.

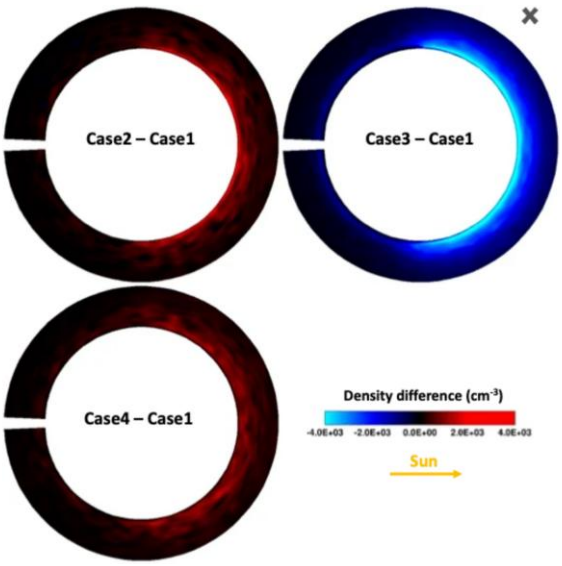

Figure 1: Difference hot O corona of Mars (meridional plane view) calculated for three scenarios: Case 2 includes O-CO2 cross sections[6] at a single energy (2.5 eV), Case 3 includes O-CO2 cross

sections with the full energy dependence[6], and Case 4 includes both O-CO2 and newly calculated energy-dependent O-CO cross sections. All cross sections are taken as total (elastic + inelastic) cross sections. The color indicates hot O density difference between the reference Case 1 (previous study) and three considered scenarios.

Table 1: Total escape rates for Cases 1 through 4 calculated using the global 3D model[5].

Escape rate (s^{-1})			
Case 1	Case 2	Case 3	Case 4
4.1×10^{25}	4.8×10^{25}	4.7×10^{25}	5.4×10^{25}

The most realistic scenarios (Case 3 and Case 4) predict about 15% and 30% greater O escape rate than previously used Case 1, respectively.

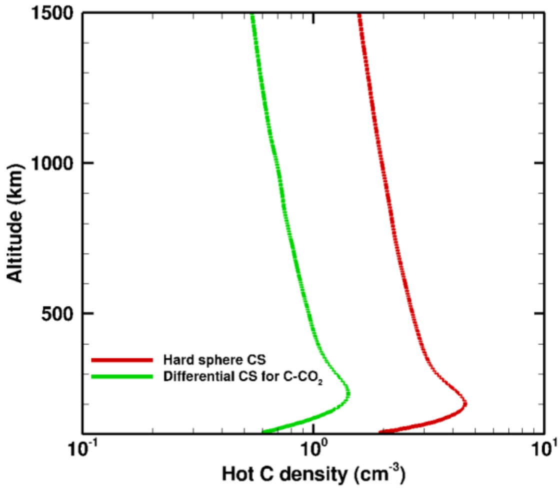

Figure 2: Hot C density at Mars modeled using the new C-CO2 cross sections in comparison to hard sphere cross sections.

In contrast, our preliminary calculation of hot C escape rate[5], shows about 60-70% reduction when the new C-CO2 cross sections are used in place of the hard sphere cross sections (Fig. 2). Another notable result is that O-CO cross sections significantly affect the thermalization of hot O and the total escape rate (Case 4).

The studied scenarios clearly illustrate the importance of using accurate collision cross sections, as well as their angular (differential cross sections) and velocity dependence, in a global 3D simulation for quantitative characterization of the escape of neutral O and C from Mars.

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