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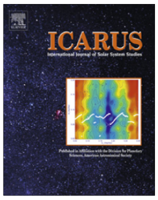

The escape of O from Mars: Sensitivity to the elastic cross sections

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A B S T R A C T

We have predicted the escape fluxes of energetic O from Mars for high and low solar activity models of the martian thermosphere, using a Monte Carlo code to determine the escape probabilities as a function of altitude and energy. Among the most important inputs to this code are the integral and differential elastic cross sections for hot O with various target species in the background atmosphere. In previous studies, we assumed that the integrated elastic cross section for each target species was 3×10^{-15} cm^2. Here we adopt more realistic elastic cross sections for O with each target species. We have identified calculations or measurements of such cross sections as a function of energy for O with seven of the twelve background species in our models. We adopt as constant a value that is appropriate to the 2–3 eV energy range, which is just above the escape energy of O. For the five background species for which there are no data, we estimate the elastic cross sections as similar to those of a species of approximately the same size. The most important species for which there are no reported cross sections for elastic interactions with O is CO_2, which is the major species in the martian thermosphere below about 200 km. For our nominal model we adopt an elastic cross section that is slightly larger than that for O with N_2. We then test the sensitivity of the model to the O–CO_2 cross section by adopting values that are smaller or larger than this value. We report O escape probabilities for four cases, and the resulting escape fluxes and rates. There are small but not insignificant differences between the escape probabilities and fluxes for these cases. For low solar activity there is a factor of 2–3 range in the computed escape fluxes; for high solar activity, the factors are smaller, of the order of 1.5 or less. We compare these results with those of our previous calculations for a common constant collision cross section. We find that the O escape fluxes for the latter case, which are of the order of $(2\text{–}4) \times 10^8$ cm^{-2} s^{-1}, are larger by factors of 9–28 than those of the four test cases here, which are in the range $\sim(1\text{–}6) \times 10^7$ cm^{-2} s^{-1}.

1. Introduction

The non-thermal escape of O from the martian atmosphere at the present epoch appears to be dominated by ionospheric production of hot O atoms in dissociative recombination (DR) of O_2^+, which may proceed via five energetically allowed channels with exothermicities in the center-of-mass (c-o-m) frame as shown below:

$$\begin{aligned} O_2^+ + e &\rightarrow O(^3P) + O(^3P) + 6.99\ \text{eV} && (1a)\\ &\rightarrow O(^1D) + O(^3P) + 5.02\ \text{eV} && (1b)\\ &\rightarrow O(^1D) + O(^1D) + 3.06\ \text{eV} && (1c)\\ &\rightarrow O(^1D) + O(^1S) + 0.83\ \text{eV} && (1d)\\ &\rightarrow O(^1S) + O(^3P) + 2.77\ \text{eV}. && (1e) \end{aligned}$$

The exothermicities shown above are for zero relative collision energies of the ion and electron in the center-of-mass (c-o-m) frame, and do not include the vibrational and rotational energies of the reactant $O_2^+(X^2\Pi_g)$. Guberman (1983, 1987) first showed theoretically that the branching ratio for channel (1e) should be negligible for the first few vibrational levels of $O_2^+(v)$. Since the escape energy of O is about 1.97 eV near 200 km at midlatitudes, the O atoms produced in O_2^+ DR have enough energy to escape only in channels (1a) and (1b). The branching ratios for channels (1a)–(1e) have been measured in ion storage rings and have been found to depend upon the relative collision energy of the reactants (e.g., Peverall et al., 2001; Petrignani et al., 2005a), and upon the vibrational energy level of the $O_2^+(v)$ ion (Petrignani et al., 2005b).

In recent investigations (Fox and Haćˊ, 2009, 2010; hereafter FH09 and FH10, respectively), we have computed the escape fluxes of ^{16}O and ^{18}O from the martian atmosphere due to DR of O_2^+ using a Monte Carlo escape model. This model is based on the well-known kinematics of two-body collisions, which is discussed in any of numerous textbooks on classical dynamics (e.g., Marion, 1970). We have described our method, including the parameters that are determined with random numbers, thoroughly in the Appendix to FH09.

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Using this model we determine the escape probabilities of hyperthermal O atoms initially produced at altitudes from 130 to 350 or 400 km on a 1 km grid, with energies ranging from 1.8 eV to 6.27 eV on a 0.03 eV grid. We track the test particles from their altitude of origin from collision to collision in spherical geometry until their energies drop below the escape energy or they reach 700 km with enough energy to escape. The initial angular distribution of the hot O atoms produced in DR is assumed to be isotropic. The model is three-dimensional only in the sense that the velocities of the projectile O in the c-o-m frame and the velocities of the center of mass have *x*, *y* and *z* components. The neutral density profiles of the background atmosphere are, however, assumed to depend only on altitude.

The advantage to computing escape probabilities as a function of altitude and energy of initial production is that the Monte Carlo code only needs to be run once for a given background atmosphere and set of assumptions about the differential and integral elastic scattering cross sections for the projectile with each target species. This allows us to use a very large number of test particles, in this case $\sim(2–3)\times10^6$ O atoms at each altitude. Any mechanism for production of hot O atoms that are distributed on the same energy and altitude grid may then be convolved with the escape probabilities, and the total O escape fluxes may be determined.

In FH09 and FH10, we assumed that the elastic cross sections of O with thermospheric neutrals were energy-independent, and we adopted the "traditional" value for the collision cross section of 3×10^{-15} cm^2 for elastic collisions of O with all 12 species in the background atmosphere. Many previous calculations of the density profiles of the martian O corona and of O escape from the martian atmosphere have employed collision cross sections in the range $(1.2–3)\times10^{-15}$ cm^2 for both O–O and O–CO_2 collisions (e.g., Ip, 1988, 1990; Nagy and Cravens, 1988; Lammer and Bauer, 1991; Kim et al., 1998; Lammer et al., 2000; Hodges, 2000, 2002; Kaneda et al., 2009; Valeille et al., 2009, 2010). Most of these studies included only O and CO_2 as components of the thermosphere, although Hodges (2000, 2002) included collisions of O with ions as well as neutrals. Krest'yanikova and Shematovich (2005) used the measured O–O elastic cross sections of Kharchenko et al. (2000) for both O–O and O–CO_2 collisions. Krest'yanikova and Shematovich (2006) included vibrational and rotational excitation of CO_2 in collisions with energetic O, but did not describe in detail either the processes or the cross sections that they employed in this calculation.

In this study, we adopt different integral elastic cross sections for interactions of hot O with each of the species in the background atmosphere, and compare the results to those that were predicted previously by FH09 and FH10. Computed or measured elastic cross sections are apparently available for interactions of hyperthermal O with only seven of the twelve background species that are in our model, including Ar, N_2, O, N, He, H, and H_2. For the species for which there are no measurements or calculations available, we adopt the cross sections for a species of similar size. The values and references for the adopted elastic cross sections are shown in Table 1. The most important target species for which there are no elastic cross section data is CO_2, which is the dominant species in the martian thermosphere below ~200 km.

To test the sensitivity of the model to the adopted value for the O–CO_2 cross section, we construct here four models. In Model 1, we first adopt a nominal cross section of 2.0×10^{-14} cm^2 for O–CO_2 collisions; this is slightly larger than the adopted value for O interactions with N_2 (Balakrishnan et al., 1998a). In Models 2 and 3, we carry out calculations for smaller values of this cross section of 0.6×10^{-14} cm^2 and 1.2×10^{-14} cm^2, respectively. The former fairly small value is tested because it has been used by previous investigators. In Model 4, we increase the O–CO_2 cross section to 2.4×10^{-14} cm^2. We report here the escape probabilities, escape fluxes, and escape rates of hyperthermal O atoms for these four sets of assumptions, and compare them to the escape fluxes computed by FH10, in which the elastic cross section for each species pair was assumed to be 3×10^{-15} cm^2. We refer to the latter case as Model 5.

Table 1
Assumed values for the elastic cross sections for O with various target species.

Species	Cross section[a]	Reference
CO_2	2.0(−14)[b]	Estimated (see text)
Ar	1.2(−14)	Braunstein et al. (2004)
N_2	1.8(−14)	Balakrishnan et al. (1998a)
O_2	1.8(−14)	Assumed similar to O–N_2
NO	1.8(−14)	Assumed similar to O–N_2
CO	1.8(−14)	Assumed similar to O–N_2
O	6.4(−15)	Kharchenko et al. (2000)
N	9.0(−15)	Kharchenko et al. (1997)
C	9.0(−15)	Assumed similar to O–N
He	3.5(−15)	Bovino et al. (2011)
H	4.2(−15)	Zhang et al. (2009)
H_2	2.3(−15)	Gacesa et al. (2012)

[a] Units are cm^2.
[b] Read as 2.0×10^{-14}.

2. Thermosphere and ionosphere models

To facilitate comparison with our previous work, we determine here the escape fluxes and rates for the same thermosphere/ionosphere models that were used by FH10. We briefly describe them here. The models for the low and high solar activity thermospheres include 12 species: CO_2, Ar, N_2, O, CO, O_2, NO, N, C, He, H, and H_2; the altitude range is 80–700 km and the altitude grid size is 1 km. The densities of the major species of the low solar activity model are based on the Viking neutral density profiles (e.g., Nier and McElroy, 1977), and those of the high solar activity model are based on the MTGCM of Bougher et al. (2000, 2009). We have multiplied the high solar activity O densities by a factor of 2, so that the resulting O mixing ratio is larger than that at low solar activity. The density profiles of the minor species, including NO, N, C, He, H, and H_2 are computed self-consistently in the models. The neutral densities are extrapolated from the top altitude of the measurements or calculations to 700 km by assuming that the scale height for each species is constant.

We compute the density profiles of 13 ions and 9 minor neutral species from 80 to 400 km on a 1 km grid. The model includes more than 200 reactions, most of which are listed by Fox and Sung (2001), although there have been some updates and additions to the reaction list since then. The solar photon fluxes for the wavelength range 18–2000 Å were taken from the S2K v1.24 models of Tobiska (2004). Those for low solar activity were adopted for day 200 of 1976 when the $F_{10.7}$ index was 76; and those for high solar activity were adopted for day 178 of 1999 when the $F_{10.7}$ index was 214. The photon fluxes were adopted in "Hinteregger" format, that is, at 1 Å resolution in the continua and as delta functions at the strong solar lines. For X-rays with wavelengths from 3 to 17 Å, the photon fluxes are taken from Ayres (private communication, 1996; cf., 1997). The photon fluxes shortward of 100 Å in the 76,200 model have been found to be significantly larger than those of the low solar activity TIMED/SEE XPS level 4 spectrum for 21 June 2008 (e.g., Woods et al., 2008). This difference has little effect on the topside of the ion peak. The solar zenith angle was assumed to be 60°, and the Sun–Mars distance was assumed to be the average value over the orbit.

The upper boundary conditions are diffusive equilibrium for most of the neutral species, except for H and H_2, for which the Jeans effusion velocities are imposed at 400 km. We apply a