Escape of atoms from Mars: A comparison of the exobase approximation to a Monte Carlo method

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Mars Thermosphere

12 Background species: CO₂, O, N₂, Ar, CO, O₂, NO, N, C, He, H, H₂
O photochemical escape: mostly $O_2^+$ DR
O escape energy 1.98 eV

1. $O_2^+ + e \rightarrow O(^3P) + O(^3P) + 6.95 \text{ eV}$
2. $O_2^+ + e \rightarrow O(^1D) + O(^3P) + 4.98 \text{ eV}$
3. $O_2^+ + e \rightarrow O(^1D) + O(^1D) + 3.02 \text{ eV}$
4. $O_2^+ + e \rightarrow O(^1S) + O(^3P) + 2.76 \text{ eV}$ (branching ratio=0)
5. $O_2^+ + e \rightarrow O(^1D) + O(^1S) + 0.83 \text{ eV}$

Branching ratios depend on vibrational level of $O_2^+$ ($v$) and $E_{\text{coll}}$
(e.g., Petrignani et al., 2005a,b; Peverall et al., 2000, 2001)

No simultaneous measurements of $v$ dependence and $T_e$
dependence of branching ratios or rate coefficients.
Energy distributions of $^{18}$O and $^{16}$O in O$_2^+$ DR in the lab frame
Monte Carlo calculations of escape probabilities

- Follow the atoms from collision to collision in space until their energy drops below escape energy or they reach 700 km with energy above escape energy
- Atoms are allowed to travel at any angle in spherical geometry to any altitude (i.e. they are not binned)
- Details in Fox and Hać (2009, 2010).
- First use $3 \times 10^{-15}$ cm$^2$ for elastic $\sigma$ for all species pairs
- Then use different cross sections for different species pairs
- O- CO$_2$ elastic $\sigma$ unknown but very important!! HELP!!!!
- We adopt $1.2 \times 10^{-14}$ cm$^2$
- equal to O-Ar; similar to O-N$_2$ $1.8 \times 10^{-14}$ cm$^2$ )
Escape probability as a function of energy and altitude

Left: 2009, constant $\sigma$  
Right: 2012 different $\sigma$ for each species pair
Monte Carlo calculations of production rates of escaping O and total O$_2^+$ DR rates
Compare Fluxes for Monte Carlo to those for Exobase approximation ($\text{cm}^{-2}\text{s}^{-1}$)

- High solar activity, Non-eroded model: (old)
  - Exobase: $6.7 \times 10^7$; Monte Carlo: $4.4 \times 10^8$
  - New: Exobase: $3.4 \times 10^7$; Monte Carlo $1.2 \times 10^8$

- High solar activity, eroded model (old):
  - Exobase $2.4 \times 10^7$; Monte Carlo $3.6 \times 10^8$
  - New: Exobase $1.1 \times 10^7$; Monte Carlo $6.9 \times 10^7$
Improvements to be made

• Add inelastic scattering $\text{O-CO}_2(\nu_2)$
• Differentiate between $\text{O}$ and $\text{O}^{(1}\text{D})$
• Include quenching of $\text{O}^{(1}\text{D})$, excitation of $\text{O}^{(3}\text{P})$
• Include transformations between $\text{O}^{(3}\text{P})$ and $\text{O}^{(1}\text{D})$
Table of Escape Rates for Monte Carlo and Exobase approximation

<table>
<thead>
<tr>
<th>Model</th>
<th>Low Solar Activity</th>
<th>High Solar Activity</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>non-eroded</td>
<td>eroded</td>
</tr>
<tr>
<td>Isotropic$^a$</td>
<td>2.1(7)$^d$</td>
<td>1.2(7)</td>
</tr>
<tr>
<td>Forward$^b$</td>
<td>2.5(8)</td>
<td>2.2(8)</td>
</tr>
<tr>
<td>Exobase$^c$</td>
<td>2.9(7)</td>
<td>1.2(7)</td>
</tr>
</tbody>
</table>

$^a$ Isotropic scattering model

$^b$ Forward scattering model

$^c$ Exobase model

$^d$ The numbers in parentheses represent uncertainties.
The Exobase Approximation: RIP