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## New sources for the hot oxygen geocorona

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**Abstract.** This paper investigates new sources of thermospheric non thermal (hot) oxygen due to exothermic reactions involving numerous minor (ion and neutral) and metastable species. Numerical calculations are performed for low latitude, daytime, winter conditions, with moderately high solar activity and low magnetic activity. Under these conditions we find that the quenching of metastable species are a significant source of hot oxygen, with kinetic energy production rates a factor of ten higher than those due to previously considered  $O_2^+$  and  $NO^+$  dissociative recombination reactions. Some of the most significant new sources of hot oxygen are reactions involving quenching of  $O^+(^2D)$ ,  $O(^1D)$ ,  $N(^2D)$ ,  $O^+(^2P)$  and vibrationally excited  $N_2$  by atomic oxygen.

### Introduction

The possibility of a hot atomic oxygen geocorona was first discussed theoretically by *Rohrbaugh and Nisbet* [1973] who calculated the flux of energetic atoms resulting from the dissociative recombination of  $O_2^+$  and  $NO^+$  in the F region of the Earth's ionosphere. They found that the hot atoms can ascend to altitudes of several thousand kilometers and can travel horizontally to distances of the order of the Earth's radius.

The existence of a substantial hot oxygen geocorona is of importance to our understanding of the Earth's atmosphere for several reasons including the maintenance of the nighttime ionosphere, the escape flux of He, and energetic ion populations in the plasmasphere. The hot O could help to explain the maintenance of the nighttime ionosphere by increasing the rate of conversion of plasmaspheric  $H^+$  into  $O^+$ . Current model calculations, which include ionosphere-plasmasphere coupling, indicate that the flux from the plasmasphere is not sufficient to maintain the ionospheric densities at the observed levels [*Richards et al.*, 1994].

Another possible effect of the hot O geocorona could be to enhance the escape of light atoms from the atmosphere by increasing the population of the high energy tail of the light ion distribution through collisional energy exchange. Thus, hot O could help to explain the well known discrepancy between the He outgassing rate and the Jeans escape flux. Finally, the existence of a significant hot O population in the plasmasphere coupled with charge exchange with  $H^+$  could enhance the population of plasmaspheric  $O^+$  and also the heating of plasmaspheric ions.

Experimental evidence for the hot oxygen geocorona has been presented by *Yee et al.* [1980] who made twilight measurements of the  $O^+(^2P)$  7320 Å emission. Their measurements indicated a hot oxygen density of up to  $10^6 \text{ cm}^{-3}$  at 550 km altitude. Further

experimental evidence was supplied by *Hedin* [1989]. He inferred hot oxygen densities of 1 to  $3 \times 10^4$  at 1100 km for low to moderate solar activities by comparing the satellite drag based (*Jacchia*) model and the mass spectrometer based (MSIS) model. More recently, *Cotton et al.* [1993] have inferred a substantial hot O population from a sounding rocket measurement of the ultraviolet atomic oxygen dayglow.

The only sources of hot O that were considered by *Rohrbaugh and Nisbet* [1973] were electron recombination of  $O_2^+$  and  $NO^+$ . However, there are a large number of other possible sources of hot oxygen atoms that have not been considered previously [Table 1]. Most of these reactions were not considered by *Rohrbaugh and Nisbet* [1973] because they involve metastable species whose importance was only established later, mainly through the Atmosphere Explorer program [*Torr and Torr*, 1982]. Metastable species contain electronic energy that can be transferred to translational energy in quenching processes. For example, the metastable  $N(^2D)$  which has an electronic energy of 2.4 eV is produced very efficiently in the thermosphere through direct photodissociation and numerous chemical reactions and is quenched efficiently by atomic oxygen. When  $N(^2D)$  is quenched, the electronic energy is made available to the translational energy of the two atoms which would then both be hot.

### Model

The hot oxygen production rates are calculated using the Field Line Interhemispheric Plasma (FLIP) transport model [*Richards et al.*, 1994]. This model solves the coupled time dependent energy, momentum, and continuity equations for the major ions ( $O^+$ ,  $H^+$  and  $He^+$ ), and photoelectron transport equations, from 80 km in one hemisphere, along a field line to 80 km in the other hemisphere. The concentrations of the major neutral species are provided by the MSIS-86 model [*Hedin*, 1987]. The main outputs of the FLIP model include ion densities ( $O^+$ ,  $O^+(^4S)$ ,  $O^+(^2D)$ ,  $O^+(^2P)$ ,  $H^+$ ,  $He^+$ ,  $N^+$ ,  $NO^+$ ,  $N_2^+$ ,  $N_2^{+*}$ ), neutral densities ( $N(^4S)$ ,  $N(^2D)$ ,  $N(^2P)$ ,  $NO$ ,  $O(^1D)$ ,  $O(^1S)$ ,  $N_2(A^3\Sigma_u^+)$ ,  $N_2^*$ ), electron and ion temperatures and flow velocities, the photoelectron flux, and a large number of emissions. A recent summary of the FLIP model is provided by *Torr et al.* [1990].

We have identified a total of twenty six possible sources of hot oxygen. They are listed in Table 1 and are taken from *Rees* [1989]. Note that reactions 1, 2 and 3 have been previously examined as a source of hot oxygen by *Rohrbaugh and Nisbet* [1973]. In this paper we make no attempt to decide the partitioning of energy amongst the products of the reactions. This partitioning can be complex depending on the pathways for the reactions. In reactions involving atomic species of similar masses (O and N) it is probably reasonable to assume that the electronic energy is shared equally by the resulting products, whereas in reactions involving molecules, the energy partitioning is complicated by possible electronic and vibrational excitation of the molecule. For example, reaction 10 ( $O^+(^2D) + N_2 \rightarrow O + N_2^+$ )

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**Table 1.** Potential sources of hot oxygen and their exothermicities ( $\Delta E$ )

No.	Reaction	Reaction Rate ( $\text{cm}^3 \text{s}^{-1}$ )	$\Delta E$ (eV)
1	$\text{NO}^+ + e \rightarrow \text{N} + \text{O}$	$4.3 \times 10^{-7} (T/300)^{-1}$ (22%)	2.75
2	$\text{NO}^+ + e \rightarrow \text{N}(^2\text{D}) + \text{O}$	$4.3 \times 10^{-7} (T/300)^{-1}$ (78%)	0.38
3	$\text{O}_2^+ + e \rightarrow \text{O} + \text{O}$	<i>Torr et al.</i> (1990)	4.42
4	$\text{O}^+ + \text{N}(^2\text{D}) \rightarrow \text{N}(^4\text{S}) + \text{O}$	$\sim 7 \times 10^{-13}$	2.38
5	$\text{O} + \text{O}(^1\text{D}) \rightarrow \text{O} + \text{O}$	$8 \times 10^{-12}$	1.96
6	$\text{O} + \text{O}^+(^2\text{P}) \rightarrow \text{O}^+ + \text{O}$	$4 \times 10^{-10}$	5.00
7	$\text{O} + \text{O}^+(^2\text{D}) \rightarrow \text{O}^+ + \text{O}$	$5 \times 10^{-12}$	3.31
8	$\text{N}(^2\text{D}) + \text{O}^+ \rightarrow \text{N}^+ + \text{O}$	$5 \times 10^{-11}$	1.46
9	$\text{O}_2 + \text{O}^+ \rightarrow \text{O}_2^+ + \text{O}$	$2.1 \times 10^{-11} \{T_n + 2T_i/3 \times 300\}^{-0.763}$	1.55
10	$\text{N}_2^+ + \text{O}^+(^2\text{D}) \rightarrow \text{N}_2^+ + \text{O}$	$8 \times 10^{-10}$	1.33
11	$\text{O}(^1\text{D}) + \text{N}_2 \rightarrow \text{O} + \text{N}_2$	$2.0 \times 10^{-11} \exp(107.8/T)$	1.96
12	$\text{O}^+ + \text{H} \rightarrow \text{O} + \text{H}^+$	$2.2 \times 10^{-11} T^{0.5}$	$kT_i$
13	$\text{N}(^2\text{D}) + \text{O}_2 \rightarrow \text{NO} + \text{O}$	$6 \times 10^{-12}$	3.76
14	$\text{N}(^2\text{P}) + \text{O}_2 \rightarrow \text{N} + \text{O}$	$1.7 \times 10^{-11}$	3.58
15	$\text{NO} + \text{N} \rightarrow \text{N}_2 + \text{O}$	$3.4 \times 10^{-11}$	3.25
16	$\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$	$4.4 \times 10^{-12} \exp(-3220/T)$	1.385
17	$\text{N}^+ + \text{O}_2 \rightarrow \text{NO}^+ + \text{O}$	$2 \times 10^{-10}$	6.67
18	$\text{O}^+(^2\text{D}) + \text{O}_2 \rightarrow \text{O}_2^+ + \text{O}$	$7 \times 10^{-10}$	4.865
19	$\text{O}^+(^2\text{P}) + \text{N}_2 \rightarrow \text{N}_2^+ + \text{O}$	$4.8 \times 10^{-10}$	3.02
20	$\text{O}(^1\text{D}) + \text{O}_2 \rightarrow \text{O}_2 + \text{O}$	$2.9 \times 10^{-11} \exp(67.5/T)$	1.96
21	$\text{O}_2^+ + \text{N} \rightarrow \text{NO}_2^+ + \text{O}$	$1.2 \times 10^{-10}$	4.2
22	$\text{NO} + \text{N}(^2\text{D}) \rightarrow \text{N} + \text{O}$	$7 \times 10^{-11}$	5.63
23 - 26	$\text{N}_2^*(v=i) + \text{O} \rightarrow \text{N}_2(v=i-1) + \text{O}$	<i>McNeal et al.</i> (1974)	0.3v

may result in the excitation of the  $\text{N}_2^+(A)$  state [Omholt, 1957], in which case most of the energy will be radiated. Alternatively, the reaction may produce  $\text{N}_2^+(X)$  in vibrational levels up to  $v = 5$ . Spectroscopic measurements made on the ATLAS 1 mission indicate significant production of  $\text{N}_2^+(X)$ , with little or no production of  $\text{N}_2^+(A)$  (Torr et al., 1993). In this case, O quenching of the vibrational levels may lead to a significant source of hot O. However, the chemistry of vibrationally excited  $\text{N}_2^+$  has not yet been fully quantified. Reaction 12 ( $\text{O}^+ + \text{H} \rightarrow \text{O} + \text{H}^+$ ) would only be a significant source of hot O for  $T_i \gg T_n$ , which only occurs above  $\sim 500$  km where  $\text{O}^+$  densities are low. It is not likely to be a significant source of hot O on Earth. Reaction 12 is only a candidate for oxygen ion temperatures exceeding 3000 K. Reactions 23 to 26 correspond to  $\text{N}_2^+$  vibrational levels ( $v$ ) ranging from 1 to 4, respectively. In this study we are primarily interested in comparing the new sources of hot oxygen with the previously known sources (reactions 1, 2 and 3) in order to demonstrate the potential importance of these new sources. We emphasize that it is the local production of hot oxygen that is calculated here. The final distribution of hot oxygen atoms will depend on collisions and transport, and is beyond the scope of this paper. Transport will become important above 300 - 400 km and will be primarily responsible for populating the exosphere.

## Results

The FLIP model was run for different seasons and different levels of solar activity. It was discovered that the new sources of hot oxygen favored conditions of high solar activity ( $F_{10.7} = 200$ ) during winter (day 1). It is these results that we have chosen to describe here. A more detailed analysis involving seasonal and solar cyclical variations of these sources is the subject of a paper in preparation. A low level of magnetic activity ( $A_p = 12$ ), a low latitude ( $23^\circ\text{N}$ ), and a local time of 12.9 hours were used. The

model was run for an initial period of 24 hours prior to this time, in order to reduce dependence on initial conditions.

The hot O number density production rates derived from the set of chemical reactions given in Table 1 are plotted as a function of altitude in Figure 1. For clarity of presentation, the results have been separated into two groups, the first containing reactions 1 to 11 and the second containing reactions 13 to 26 (reaction 12 did not contribute to the production of hot O for the results considered here). The hot O number density production rate is dominated by quenching of  $\text{N}_2^+(v=1$  and 2) by atomic oxygen (reactions 23 and 24) at all but the highest altitudes (Figure 1b). At the highest altitudes, the hot oxygen number density production rates are predominantly produced by (in decreasing order of importance) reactions 10, 5, 7 and 4 (Figure 1a), with smaller production rates being due to the dissociative recombination reactions 2 and 3.

While the number density production rates are useful indicators of which sources may be of significance to the hot O population, the kinetic energy production rates are of greater interest because they are a direct measure of the available kinetic energy for the product oxygen atom. These kinetic energy production rates (Figure 2) were obtained by multiplying the number density production rate by the exothermicity for each reaction in Table 1. In general, the energy imparted to the atomic oxygen will only be half of the total energy.

The results shown in Figure 2a demonstrate that dissociative recombination of  $\text{NO}^+$  (reaction 1) and  $\text{O}_2^+$  (reactions 2 and 3) are not the most significant sources of hot oxygen at high altitudes. Atomic oxygen quenching of  $\text{O}^+(^2\text{D})$  (reaction 7) is a large source of hot oxygen at high altitudes, but a minor source at low altitudes. At high altitudes, the kinetic energy production rate due to  $\text{O}^+(^2\text{D})$  quenching exceeds that due to the dissociative recombination reactions by a factor of eight. Quenching of the metastable states  $\text{N}(^2\text{D})$  (reactions 4),  $\text{O}(^1\text{D})$

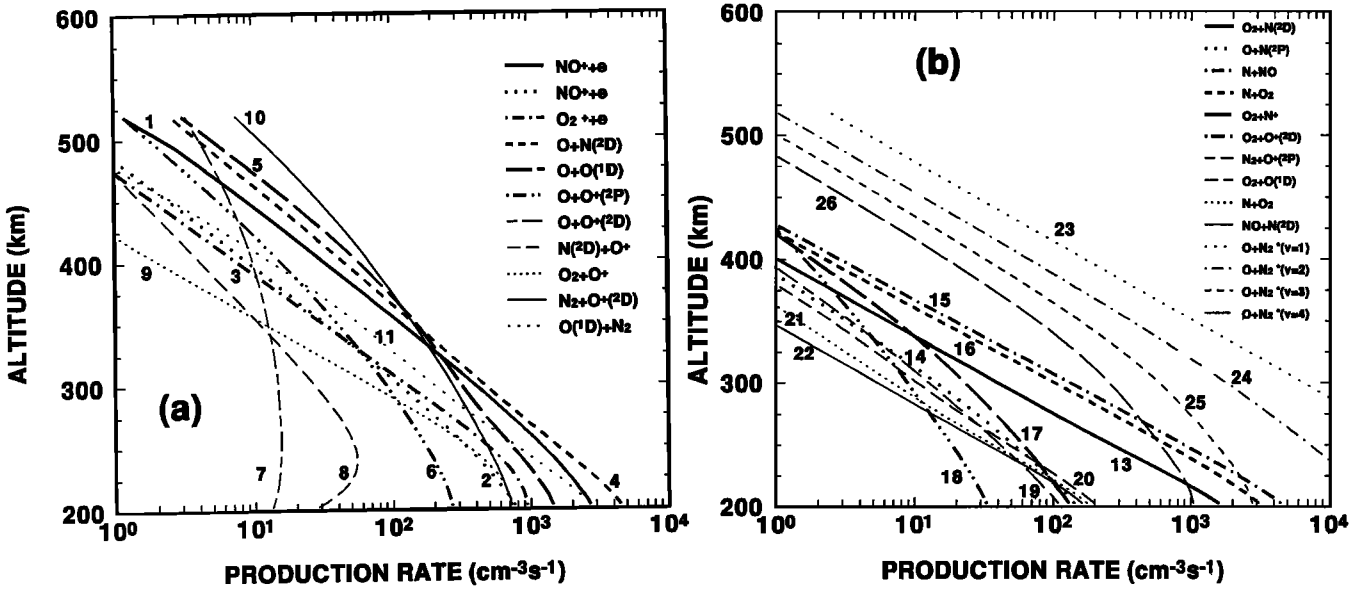


Figure 1. Hot O number density production rates for reactions (a) 1 to 11, and (b) 12 to 26.

(reaction 5) and  $O^+(^2P)$  (reaction 6) by atomic oxygen are also large sources of hot oxygen at high altitudes. The fact that reactions 1 to 7 all produce atoms of similar mass means that the partitioning of energy between the two reaction products will be similar for these reactions. Therefore, the kinetic energy production rates due to these reactions can be compared directly. Reaction 10 is potentially a very large source of hot oxygen at high altitudes, although the uncertainty associated with the energy partitioning must not be overlooked. Quenching of  $O^+(^2D)$  by  $O_2$  (reaction 18), and quenching of  $N_2^+(v=1$  to 3) by atomic oxygen (reactions 23, 24, and 25) (Figure 2b) are sources of hot oxygen that are comparable to those due to reactions 1, 2 and 3 at high altitudes. We note that there is some uncertainty regarding the values of some of the reaction rates, particularly those for reactions 5, 6 and 7.

**Conclusion**

We have found that the quenching of metastable species is a significant source of hot oxygen for the exosphere. For the geophysical conditions employed here (winter, high solar activity), the kinetic energy production rates due to some of these new sources exceeded, by a factor of ten, those due to the previously considered  $O_2^+$  and  $NO^+$  dissociative recombination reactions. Some of the most significant new sources of hot oxygen found in this study are due to reactions involving quenching of  $O^+(^2D)$ ,  $O^+(^1D)$ ,  $N(^2D)$ ,  $O^+(^2P)$  and vibrationally excited  $N_2$  by atomic oxygen. These additional sources of hot oxygen may help to explain the maintenance of the nighttime ionosphere, the escape flux of helium, and energetic ion populations in the plasmasphere.

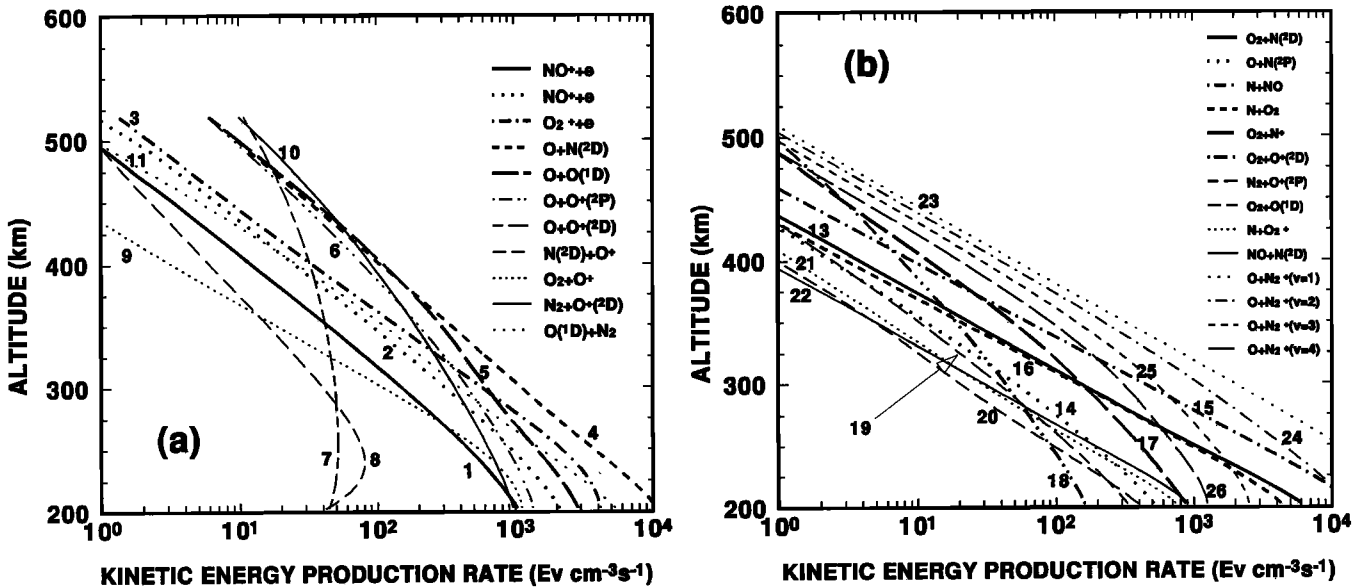


Figure 2. Hot O kinetic energy production rates for reactions (a) 1 to 11, and (b) 12 to 26.

A detailed study is now under way to ascertain the diurnal, seasonal, and solar cyclical variations of the main sources of hot O. Further work is also needed to determine the partitioning of energy between the products of the reactions that may produce energetic O atoms.

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