ENERGETIC METASTABLE OXYGEN AND NITROGEN ATOMS IN THE TERRESTRIAL ATMOSPHERE

NASA grant NAG5-11857

Annual progress report
For the period 15 March 2002 through 14 March 2003

Principal Investigator
Vasili Kharchenko

January 2003

Prepared for

National Aeronautics and Space Administration

SMITHSONIAN INSTITUTION
ASTROPHYSICAL OBSERVATORY
CAMBRIDGE, MASSACHUSETTS 02138

Director: Irwin I. Shapiro

The Smithsonian Astrophysical Observatory
is a member of the
Harvard-Smithsonian Center for Astrophysics

Energetic Metastable Oxygen and Nitrogen Atoms in the Terrestrial Atmosphere

Grant NAG5-11857

Principal Investigator: V. Kharchenko

Progress report for the period 03/15/2002 through 03/14/2003

We have investigated the energy distributions of the metastable oxygen atoms in the terrestrial thermosphere. Nascent $O(^1D)$ atoms play a fundamental role in the energy balance and chemistry of the terrestrial atmosphere, because they are produced by photo-chemical reactions in the excited electronic states and carry significant translational energies.

1. We have determined the altitude dependence of the thermalization rate of metastable $O(^1D)$ atoms and calculated their energy distributions in the day and night-time atmosphere. Fast atoms lose their kinetic energy in elastic, inelastic, and reactive collisions with atoms and molecules of the atmospheric O, N_2, and O_2 gas. In our new calculations the rate coefficients for the quenching and energy-transfer collisions have been updated with published experimental data [*Matsumi et al. 1994; Matsumi and Chowdhury 1996; Chowdhury 1999; Tanaguchi et al. 2000*]. We have found that the thermalization of the $O(^1D)$ and $O(^1P)$ atoms is modified significantly by quenching collisions of the metastable $O(^1D)$. Non-Maxwellian distributions of the metastable oxygen atoms have been computed self-consistently with the distributions of hot ground state oxygen atoms $O(^3P)$.

The new results on the production rates and energy spectra of the nascent $O(^1D)$ atoms have been obtained for altitudes between 50 and 200 km. We have used the ionic sources of metastable oxygen listed by Hickey et al. (1995) with updated rate coefficients and branching ratios [*Fox and Haćˇ 1997; Vejby-Christensen et al. 1998*]. At lower thermosphere and mesosphere photolysis of the O_2 and O_3 atmospheric gas has been included as an efficient source of metastable oxygen atoms [*Matsumi et al. 2002*]. The energy spectra of the nascent $O(^1D)$ produced by the photodissociation of O_2 molecules have been computed by J. Fox (2000). More than thirty collisions are required for thermalization of the nascent oxygen atoms arising, with the translational energies hundred times larger then thermal energy of the ambient atmospheric gas.

2. Time-dependent and steady state energy distributions of the $O(^1D)$ atoms in the mesosphere and thermosphere have been calculated in different atmospheric conditions. Time-dependent distributions provide an opportunity to analyze the rate of the energy-transfer collisions as well as quenching and reactive collisions of the $O(^1D)$ atoms during the entire thermalization process. A self-consistent solution of the time

dependent Boltzmann kinetic equations for $O(^1D)$ and $O(^3P)$ hot atoms has been carried out using accurate cross sections obtained in recent experiments and calculations [*Balakrishnan et al. 1998, 1999; Kharchenko et al. 2000; Taniguchi et al. 2000; Miura et al. 2002*]. Computational methods for solving the Boltzmann equation beyond the hard sphere approximation, have been developed in our previous projects [*Kharchenko et al. 1997, 1998*]. The fraction of hot atoms in time-dependent distributions of $O(^1D)$ at different atmospheric altitudes has been analyzed. The rate of energy loss and thermalization time has been computed for $O(^1D)$ and $O(^1P)$ atoms, and reported on the AGU2002 Spring and Fall meetings.

3. Calculated steady state distributions of the $O(^1D)$ atoms differ from the Maxwellian by containing a larger amount of hot atoms. The computed values of the average translational energies $< E >$ are significantly larger than the thermal energy of the ambient gas. The characteristics of the steady state distributions of the $O(^1D)$ atoms depend strongly on the relative frequency of the $O(^1D) \rightarrow O(^3P)$ quenching and thermalizing collisions. We have computed steady state distributions of the metastable oxygen atoms in the thermosphere and upper mesosphere above 50 km.

The energy distributions of the $O(^1D)$ atoms at 200 km are shown in Fig.1a for day and night time. The steady state distributions arising due to the photo and ionic sources have been calculated independently.

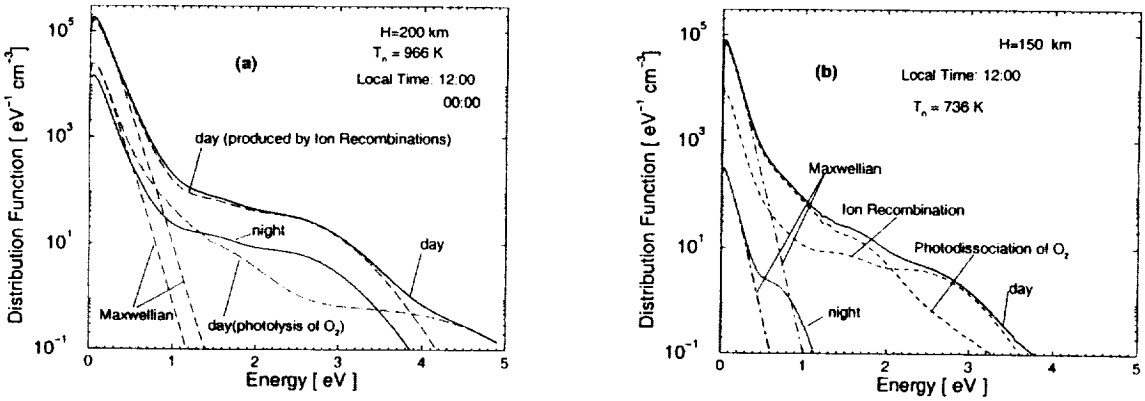

Fig.1 (a) Steady state energy distribution functions of metastable $O(^1D)$ atoms at 200 km for the day and night-time terrestrial atmosphere. (b) The day and night time distribution functions at 150 km.

At noon the total density of metastable oxygen atoms at 200 km is 3.3×10^4 cm^{-3}, and only 12% of them are produced by photo-dissociation. The averaged energy of the metastable oxygen atoms $< E >$ corresponds to the temperature of 1112 K, which is about 15% higher than the temperature of the ambient gas. The high energy tail of the distributions is sensitive to energy spectra of the nascent $O(^1D)$ atoms generated by various mechanisms. Relative contribution of the ionic and photo reactions shows significant diurnal variations. At night time the density of metastable $O(^1D)$ atoms