Development of the daytime model of electronic-vibrational kinetics for excited products of photodissociation of O_2 and O_3 in the mesosphere and lower thermosphere

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The first in the USSR Department of Atmospheric Physics was founded in Saint-Petersburg State University in 1932. In 1970 Dr. Khvorostovskaya L. E. together with her pupils Yankovsky V. A, Potekhin I. Yu. and Divin D. V. established the laboratory for study of the rate constants of aeronomic processes with applications to kinetics of electronic and vibrational molecular states and the airglow of the middle and upper atmosphere of the Earth, Venus, and Mars. Unique techniques for measuring the rate constants in plasmas of gas discharges have been devised with the use of emission and absorption spectroscopic measurements in the range from the near UV to the IR and the probe techniques. The glow discharge in O_2 was used to study the kinetics of negative ions and metastable states of the oxygen atoms and molecules. In result the rate constants of several quenching reactions including $\mathbf{O^-} + O_2(a^1\Delta_g, v=0) \rightarrow O_3 + \mathbf{e}$ for overthermal ion energies and $O(^1S) + O_3 \rightarrow 2O_2$ for the temperature range of T = 300 - 445 K were measured at first time by Khvorostovskaya and Yankovsky (1991).

Beginning with the 1990s, the experimental studies were carried out in two directions: a) measurements with the hollow-cathode discharge have made it possible for the first time to determine the rate constant of quenching the $CO_2(01^10)$ state by $O(^3P)$ atoms for the temperature range 200 - 300 K as were reported by Khvorostovskaya L. E. et al. (2002); b) the kinetics of production and quenching of $O_2(b^1\Sigma_g, v = 0 – 2)$ and $O_2(a^1\Delta_g, v=0)$ molecules in O_2 discharge plasma were presented by Yankovsky (1992). On the basis of these studies the model of electron-vibrational kinetics of excited products of photodissociation of O_2 and O_3 in mesosphere and lower thermosphere were designed and were represented by Yankovsky and Manuilova (2006) in which the populations of 44 electronic-vibrational excited states of the O_2 molecule (three states of $O_2(b^1\Sigma_g, v = 0 - 2)$, six states of $O_2(a^1\Delta_g, v = 0 - 5)$ and 35 states of $O_2(X^3\Sigma_g, v=1 - 35)$ as well as the first excited state of atomic oxygen $O(^1D)$ can be calculated from solution of the system of 45 kinetic balance equations for arbitrary dayglow conditions (the latest version of the program is called as YM2011).

Among the results obtained by the YM2011 model, there are two most important: (i) the methodology of simple yet accurate calculations of $H_2O(v_2)$ vibrational levels pumping from the collisions with vibrationally excited $O_2(X^3\Sigma_g, v = 1)$ molecules, which is required for correct retrievals of H_2O volume mixing ratios from the 6.3 μm band radiance were represented by Yankovsky et al. (2011), (ii) the emissions $O_2(b^1\Sigma_g, v = 2)$ or $O_2(b^1\Sigma_g, v = 0)$ molecules can be employed as proxies for retrievals of altitude profile of $[O(^3P)]$ at the altitudes nearly 90-120 km and the emission $O_2(b^1\Sigma_g, v = 1)$, $O_2(a^1\Delta_g, v = 0)$ can be used as proxies for retrievals of altitude profile of $[O_3]$ at the altitudes 50-100 km, and self-contained $[O_3]$ and $[O(^3P)]$ could be retrieved simultaneously.

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