Modeling chemical reactions in the middle atmosphere induced by solar energetic particle events

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Influence of solar energetic particle (SEP) events in the atmosphere has attracted interest of researchers in atmospheric science. In SEP events, copious amounts of X-ray, γ-ray, and protons (also neutrons) come down to the stratosphere. They induce ionization and dissociation of molecules in the air, and subsequent chemical reactions result in changes in chemical compositions. In particular, the concentration changes in odd nitrogen species (NOx) and reactive nitrogen (NOy) are important because they affect short- and long-term change of stratospheric ozone concentration.

We started a simulation study to explicitly deal with many reactions of the chemical species, including ions, produced by protons in SEP events. In our approach, we use two kinds of chemical models. First we simultaneously solve differential equations for both the photochemical reactions and the proton induced reactions, where no transport processes are considered. (Hereafter, this calculation is referred to as BOX-model calculation.) After we estimate values of concentration of NOx from the BOX-model calculation, and we input them into a three-dimensional chemical climate model (CCM) for the instantaneous perturbation as the initial condition, where not only chemical reactions but also the transport of chemical species is included. In the CCM, however, the reactions induced directly by protons are not included. Based on the CCM results, we study the global influence of the SEP events on the distribution of chemical composition on a time scale of several years. Here, we report the results of the BOX-model calculation.

We only took into account of the products from N2 and O2 for the interactions with the SEP protons. The G-values (amount of products per absorbed energy of 100eV) of radiolysis1 was used for estimating the yield of charged products (N', O', N2', O2', and e') and neutral atoms (N(S), N(D), N(P), O(P), and O(D)), under the reasonable assumption that the above products by radiolysis are defined only by the absorbed energy in the air. By considering more than 200 chemical reactions (ion-molecule reactions and neutral chemical reactions including NOx, HOx, and ClOx cycles, etc.), we calculated of temporal variations in the concentrations using a commercial software for complex chemical kinetics (FACSIMILE, mcpa corp.). Fig. 1 shows the temporal behavior of concentrations of chemical species at geometric altitude of 25km. Temperature was set at 216 K during the calculation.

Furthermore, we performed a preliminary calculation for the SEP event that occurred in October 1989 (Fig. 2). The temporal absorbed-energy variation in the air was approximated by a rectangular function with its duration of 8 days2 and the SEP-proton fluence was estimated from the ion-pair production rates by the SEP protons3). W-value (average energy expended in ion-pair formation), and G-values of the air. Climatological temperatures and concentrations of chemical species were used for the initial condition at each geometric altitude between the lower stratosphere (25 km) and upper mesosphere (75 km). The temporal variation during the one-month run for 25km shows that the SEP protons increase the concentrations of NOx and NOy species more than 10%.

Fig. 1. Volume mixing ratio of chemical species in the stratosphere (25 km altitude). Solar photolysis reactions run only during the daytime in this calculation.

Fig. 2. Volume mixing ratio changes of NOx and NOy species for a month including the SEP event period (the first 8 days).

References
2) http://umbra.nascom.nasa.gov/SEP/

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