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Chemical Reactions in the Stratosphere Induced by Transient Astronomical Ionizing Events

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Issues on terrestrial consequences of astronomical ionizing events (such as solar energetic particle events or supernovae) have motivated researchers both in astronomy and aeronomy. We focus especially on the influences of such events on the concentration change of nitric oxides (NOx) and ozone in the stratosphere, and start to do a new simulation study at the frontier of atmospheric chemistry, chemical physics, astronomy, and climate-change research. In this research area, Thomas et al. recently performed a two-dimensional photochemical transport model calculation and reported that gamma-ray bursts could induce ozone depletion (at most 20 - 30 % depletion) in the stratosphere [1,2]. In their photochemical model, they did not explicitly consider intermediate ions to avoid heavy calculations of the ion-molecule reactions. Instead, they used reported parameters of initial nitric oxide (NOx) increase per ion pairs generated by the irradiation.

In our approach, first we directly solve differential equations of ion-molecule reactions and analyze the influence of each reaction on the concentration change of NOx species. After we find adequate values of NOx concentration change we use them as input parameters for large-scale simulation. In the future we plan to realize a three-dimensional large-scale simulation with a chemistry climate model that is more advanced than the simulation by Thomas et al. For the first step of our study, we build a zero-dimensional model where the geographical height (altitude) is the only parameter (so-called BOX model).

Due to solar energetic particle events, showers of photons (X ray and gamma ray) and high energy ($>$100 MeV) particles (protons, neutrons) come down to the atmosphere, and due to near-earth supernovae, showers of photons (X ray and gamma ray whose energy are less than about 1 MeV) come. These high-energy particles/photons ionize and dissociate N_2 and O_2 in the stratosphere. On this radiolytic processes of N_2 and O_2, we used the G values of radiolysis [3] to obtain the yield of product ions (N^+, O^+, $N_2{}^+$, $O_2{}^+$, e^-) and radicals ($N(^4S)$, $N(^2D)$, $N(^2P)$, $O(^3P)$, $O(^1D)$). G value is the number of product atoms or molecules per 100eV energy absorbed by the reactant system. We can roughly say that the product species generated by radiolysis of light atoms are defined only by the absorbed energy, which allow us to use G values. With this treatment we can estimate rate constants without considering the details of initial multi-step scattering processes. The ions and radicals generated by the radiolytic process react and form positive and negative ions for example, NO^+, $O_4{}^+$,O^-, and $O_2{}^-$. We include more than 100 chemical reactions (including ozone-destroying NOx, HOx, and halogens) at this stage and used the software for complex chemical kinetics, FACSIMILE (mcpa corp.)

In the present study, we assumed large solar-proton events (for example, see [4]) as input irradiation of the astronomical events, and represented the temporal variation of the irradiation with a step-function as Thomas et al. did in their calculations. We set the values of the fluence and duration at $1.0*10^9$ cm^{-2} and 24 hours, respectively. We did calculations with parameters (temperature and initial concentrations of chemical species) corresponding to altitudes between upper (50 km) and lower (25 km) stratosphere.

We discuss NOx concentration change and primary reaction paths, and their altitude dependence.

References

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