A Simulation Study of Stratospheric Chemical Reactions Induced by Astronomical Ionizing Events

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Introduction
Chemical kinetic studies of astronomical ionizing events at the stratosphere

Terrestrial consequences of astronomical transient events, such as solar proton events and supernovae, have attracted researchers both in astronomy and aeronomy. Introducing a chemical kinetic approach where radiolysis of gases induced by high-energy protons/photon is explicitly included, we performed a simple calculation as the first step with selected ion-molecule reactions to see the formation of NOx (reactive nitrogen) in the N₂-O₂ atmosphere.

Solar Proton Events
High-energy protons as the reaction trigger

Solar proton events (SPEs) are those where high-energy particles (mostly protons of energies from 10 - 500 MeV) are emitted from the surface of the sun during large solar flares. It is known in the >30 MeV energy range that the most commonly occurring SPEs have an omnidirectional fluence in the 10¹⁰ to 10¹¹ cm⁻² range. Very large SPEs exhibit 3 orders of magnitude larger fluence of >1 x 10¹⁰ cm⁻². These very large events only occur a few times in a single 11-year solar cycle.

Assumptions for simplified SPE spectrum:
As the 1st step simulation, we used a step-function following the treatment by Thomas et al. [1].
- Omnidirectional solar proton fluence
- Typical duration time: 1 day
- Typical energy of solar protons: 30 MeV

Simulation Method
Starting with the simplest case
Homogeneous Chemical Kinetics

BOX model with 53 reactions
We used an Integrator (FACSIMILE, mcpa corp.) to solve differential equations.

Simulation Results
Preliminary results obtained by FACSIMILE

O₃, NO, NO₂, NO₃ and N₂O

Positive and Negative Ions

In the duration of the energy-input pulse, O₃, NO₂, NO₃, NO₂ increase monotonically and rapidly.

Density of N₂⁺ and N⁺ are extremely small due to the fast reactions. (See the reaction rates shown in the right.)

Initial Radiolytic Reactions
Production of ions and radicals from N₂-O₂ atmosphere

NOx formation
Chemical reaction scheme

Chemical Reactions and Rates
As the 1st step of the calculation

Electron and NO radicals are produced.

N₂ → N + N
N₂ + e⁻ → N₂ + e⁻
N₂ + N⁺ → N₂ + N + e⁻
N₂ + e⁻ → N₂ + e⁻
N₂ + H → N₂ + H⁺ + e⁻
N₂ + e⁻ → N₂ + e⁻
N₂ → N₂ + e⁻
N₂ → N₂ + e⁻
N₂ + N⁺ → N₂ + N + e⁻
N₂ + e⁻ → N₂ + e⁻
N₂ + H → N₂ + H⁺ + e⁻
N₂ + e⁻ → N₂ + e⁻
N₂ → N₂ + e⁻

In the presence of N₂, N₂ + e⁻ → N₂ + e⁻

Density of N₂⁺ and N⁺ are extremely small due to the fast reactions. (See the reaction rates shown in the right.)