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A Three-Dimensional Model Study of Ozone Depletion and Bromine Explosion in Polar Spring

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Since the 1980s, it has been reported that in spring season, the amount of ozone in the polar troposphere drops from tens of ppb to a near zero value within a few days or even hours[1]. Satellite observations[2,3] show that tropospheric ozone depletion is strongly correlated to enhanced chemical reactions including halogen species. The reactive halogen species are involved in an autocatalytic chemical reaction cycle, leading to ozone depletion. Due to increased air pollution, ozone concentration is also affected by the presence of NO_x species. In the present study, a detailed chemical reaction mechanism is identified and analyzed using the chemical kinetic software KINAL[4]. It is found that NO_x may lead to either enhancement or retardation of ozone depletion, and the conditions for this effect are identified. The heterogeneous reactions leading to bromine explosion are included through the effective ice surface area and aerosol particle properties[5,6].

Moreover, a three-dimensional model is developed using the open-sourced software OpenFOAM. The reaction mechanism identified and reduced through KINAL is implemented into the advanced model. Navier-Stokes equations account for the horizontal and vertical transport of air parcels. In particular, a large eddy simulation (LES) is performed for modeling the turbulent diffusivity, and the Monin-Obukhov similarity[7] is applied at the surface boundary.

The numerical results show that the vertical turbulent mixing of air parcels is constrained below the height of polar boundary layer. The active halogen flux generated at the surface by the heterogeneous activation processes leads to a non-uniform vertical distribution of chemical species. Complete ozone destruction and large enhancement of halogen species concentrations in the boundary layer are captured. The temporal evolution of species concentrations shows that the ozone depletion process in the boundary layer lasts for two days in the case of a tropospheric boundary layer with 200 meters height, and the total ozone depletion time increases as the boundary layer grows higher. Due to the increased bromine concentration in the air during the depletion process, the most dominant NO_x reaction cycle is related to the $BrONO_2$ hydrolysis. The study reveals that in polar spring, the tropospheric ozone depletion rate is influenced by the heterogeneous reaction rate, wind speed, boundary layer stability, air composition and aerosol particle properties. The simulation is currently extended to include the real topography of mountains.

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