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Simplification of the reaction mechanism of ozone depletion events in the Arctic spring

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The ozone depletion events (ODEs) in the Arctic spring is found to be influenced by the joint effect of horizontal advection, vertical convection, and local chemistry. However, high-dimensional model studies of ODEs are often computationally demanding, or even infeasible, especially due to the large computing time cost for the calculation of the chemical production and destruction source terms in the governing equations. Thus, it is desirable to reduce the original complex reaction mechanism implemented in these model studies without sacrificing accuracy in describing the chemistry of ODEs.

In order to make simplifications of the ODE reaction mechanism, we applied two different mechanism reduction approaches, namely, the concentration sensitivity analysis and the principal component analysis, on an ODE reaction scheme (39 species and 92 reactions). In the concentration sensitivity analysis, the most influential reactions in different time periods of ODEs were revealed. As a result, eleven redundant reactions with the lowest absolute values of sensitivities were removed from the original reaction mechanism. The temporal behavior of the principal bromine species and the surface ozone during ODEs modeled by the reduced reaction mechanism in a box model are almost identical to the ones using the original reaction scheme.

In the principal component analysis, aside from the 11 reactions identified as unimportant in the concentration sensitivity analysis, additionally nine reactions were indicated to contribute only little to the total response of the system. Thus, a reduced reaction mechanism with a size of 72 reactions among 39 species was obtained. The results computed by applying the reduced reaction mechanism derived after the principal component analysis agree well with those using the original reaction scheme. The maximum deviation of the mixing ratio of principal bromine species is found to be less than 10 %.

The details of the present study can be found in [1], which was recently accepted by Atmospheric Chemistry and Physics.

[1] Cao, L., Wang, C., Mao, M., Grosshans, H., and Cao, N.: Derivation of the reduced reaction mechanisms of ozone depletion events in the Arctic spring by using concentration sensitivity analysis and principal component analysis, Atmos. Chem. Phys., in press, 2016.