

Interactive comment on “Derivation of the Reduced Reaction Mechanisms of Ozone Depletion Events in Polar Spring by Using Concentration Sensitivity Analysis and Principal Component Analysis” by Le Cao et al.

Anonymous Referee #2

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“Derivation of the Reduced Reaction Mechanism of Ozone Depletion Events in Polar Spring by Using Concentration Sensitivity Analysis and Principal Component Analysis,” by Cao et al applies concentration sensitivity analysis (CSA) and principal component analysis (PCA) to a reaction scheme representative of the chemical reaction scheme that may govern Arctic ozone depletion events. CSA enables quantification of the dependence of species concentration on varied reaction rate constants while PCA flags unimportant reactions from a complex chemical scheme. These techniques also allows for the reduction of computational effort to complete simulations.

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Through the CSA approach, they find that the original (92 reactions) and reduced reaction mechanism (81 reactions) both produce identical onsets of each time period of ODEs; simultaneously, the maximum deviation of bromine mixing ratios between the original and reduced reaction mechanisms is less than 1%. CSA also revealed 11 unimportant reactions. Applying PCA to the original reaction mechanism revealed the dependence on species on concentration on varied reaction rates and identified an additional 9 unimportant reactions (yielding 72 reactions for the reduced reaction mechanism from both CSA and PCA). PCA also revealed that the maximum deviation of the principal bromine species (Br, HBr, HOBr, BrO, and Brtot) between the original and reduced reaction mechanism was less than 10%. Overall, the original and reduced chemical mechanism for Arctic ODEs produced analogous model results via the box model KINAL.

I highly recommend this paper for publication. I enjoyed reading this manuscript given its robust and quantitative nature. Cao et al’s aims to elucidate a fundamental query (what reaction mechanism quantitatively and explicitly governs polar tropospheric ODEs?) that still – that is, in the most explicit manner – via multiphase modeling – is still unanswered. This manuscript makes great strides at identifying (as a function of species concentration, reaction rates, and temporally) the dominant 72 reactions that may govern Arctic ODEs. This work is significant as it pinpoints the dominant reactions (in a multiphase fashion) that governs Arctic ODEs. The study is also important as it provides greater constraints on ice/snow reactions to investigate further in the lab/snowpack simulation chamber. I recommend that the authors refine the paper by emphasizing in a more transparent manner the key findings of the study – that is, identification of a concise reaction mechanism that may govern Arctic ODEs (from a more complex reaction mechanism) via a multiphase/box model approach, which in turn saves computational time. I can see this statistical approach becoming more valuable and applicable in the geosciences.