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Atmospheric Chemistry and Physics Discussions

Interactive comment on "3D simulations of tropospheric ozone depletion events using WRF-Chem" *by* Maximilian Herrmann et al.

Anonymous Referee #1

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1 general comments

`evaluating the overall quality of the discussion paper`

- The manuscript is presenting an extension of halogen chemistry in the regional model WRF-chem and an implementation of a bromine release mechanism from ice and snow based on the work of ().
- The authors study bromine explosions and ozone depletion events (ODEs), respectively. They focus on one spring season (2009) at two sites, Utiqiaġvik, Alaska and Summit, Greenland. They discuss spatial extends (3 dimensions) as

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Discussion paper

well as temporal course (+1 dimension) of the events. The title of this manuscript is not reflecting this. A better title might be: *Spatio-temporal WRF-Chem simulations of ozone depletion events in the Arctic troposphere*.

- The authors use in situ measurements of O_3, temperature, wind speed, ozone sonde profiles, as well as GOME2 satellite retrievals of tropospheric BrO to valid their model results.
- The manuscript is well structured.
- The scientific content of the manuscript is sound, there are only a few minor remarks.
- The language is overall concise but needs some refinement where the statements are not entirely clear.

2 specific comments

`individual scientific questions/issues`

Abstract

- L1–2: *"Tropospheric bromine release and ozone depletion events [...] are studied using the regional software WRF-Chem."* The term "regional software" is rather uncommon. It should either read as "regional model" or "mesoscale numerical weather prediction system with atmospheric chemistry module" based on the description given on the WRF web page (https://www.mmm.ucar.edu/weather-research-and-forecasting-model).

- L13: *"Meteorological nudging is found to be essential for a good prediction of ODEs [...]"* This finding is central to the manuscript. Given the close connection of the bromine release mechanism to weather conditions, this is not unexpected (). The verb "found" in this context, however, might have such a connotation. Maybe change "found" → "confirmed" to circumvent this interpretation.

Section 1

- L83–88: *"The salinity of the sea ice is also an important factor. [...]* Br_2 *emissions directly from the sea ice were not observed [...]."* There seems to be a contradiction in this paragraph. If no direct emission of bromine from sea ice is observed, how does its salinity affect emissions from a snow pack on top of it? The authors should elaborate on the logic of this paragraph as there seems to be a confusion between the roles of ice and snow in the release of bromine.

- L106–110: OASIS data is not mentioned any other place than here. If not used for the present model evaluation, what is the purpose of mentioning it? Are you intending to use them in follow-up studies as mentioned later on? You should make this clear, e.g. in Section 4.

Section 2

- L189: The authors state the use of ERA-interim. Why this choice? Other reanalysis data exists and in the meanwhile a global reanalysis of higher resolution ERA5 has been released, though there might be issues with these data especially in the Arctic. Taking into account the importance of nudging for predicting ODEs as one of the main points in this manuscript, could higher resolution ERA5 improve the model performance with respect to observations?

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- L204–205: *"The initial mixing ratio of* HBr *and* Br_2 *are set to 0.3 ppt [...]. The mixing ratio of* $CHBr_3$ *is fixed to 3.5 ppt."* How sensitive is the model to the choice of these values? How well are they constrained by observations? Could actual heterogeneities in space and time explain the mismatch with observed ODEs? Have you considered oceanic emissions of very short-lived brominated species (CH_2Br_2, CH_3Br) as source terms in the model ()?

- *"Nudging is [...] inactive inside the boundary layer."* As nudging is one of the main points in this manuscript, this paragraph on nudging is a stub. How is the inactivity in the boundary layer realized (fixed height)? How strong is the nudging (nudging coefficients)? Is there a sharp transition between nudged and unnudged regimes of the atmosphere or is there a gradual relaxation of nudging towards the boundary layer? Are there systematic differences in boundary layer height between ERA-I and WRF which would affect the model results?

Section 3

- L221–232: The paragraph about the retrieval of BrO from GOME2 is too detailed for the purpose of this study – unless performed exclusively for this study. It should be shortened.

Section 4

- L247–251: *"The NOAA and ESRL Global Monitoring Division Surface Ozone measurements near UtqiaÄąvik and Summit [...]"* Are these observations independent or have they been assimilated into ERA-I?

- L267-278: *"[...] there is an overestimation of the temperature when it is cold, which is likely due to the lowest temperatures occurring during the spin-up time."* Unclear how these relate. May the authors elaborate on this?

- L277-278: *"Both wind speed and direction are predicted less accurately, which might result in wrong source locations or times of the occurrence of ODEs; this is likely to explain some of the differences between simulations and observations."* In other words, for a near real time prediction of ODEs one would need to assimilate observations. How large are the uncertainties on observed wind?
- L315–319: If lower latitude intrusion of polluted or ozone enriched air is a limiting factor, would nesting within a larger outer domain help improve the simulation result? Are there observations of "arctic haze" during these particular episodes available? Could these be used to improve the boundary conditions for the regional simulation?
- L353–355: *"[...] the time period with the highest ozone level is also found by the model which is due to stratospheric ozone, [...]"* The sentence is unclear and needs to be rewritten and probably split. Do the authors intend to say that the highest observed values of ozone at Summit are due to intrusion of stratospheric air masses in the course of tropopause folding events. This is correctly reproduced by the model?
- L374–375: *"[...] very small-scale structures such as open leads [...]"*Open leads could also lead to local emissions of brominated VSLS from the ocean.
- L375–376: *"[...]an accurate modeling of surface inversions might require very high vertical resolutions which are difficult to obtain in a synoptic scale simulation."* Could you achieve this by nesting?
- L406–409: *"Some of the differences might be explained by a higher model resolution [...] resulting in more detailed structures in the model. Other differences [...] errors in the meteorology [...]."* How does the uncertainty from satellite retrieval compare to the magnitude of divergence with modeling results?

- L503–505: *In a follow-up study it is planned to simulate ODEs in the year 2019 for which the new TROPOMI BrO VCDs with a high resolution of 5.5 km x 3.5 km are available. For this purpose, the grid resolution will be increased in order to allow for a comparison of the more refined observation data.* You should connect this statement with the earlier introduction of the OASIS dataset.

3 technical corrections

`purely technical corrections`

- L58: *"A further* Br_2 *release mechanism [...] was suggested, this was also found in a laboratory study [...]"* It would be better to split this sentence at the comma: "A further Br_2 release mechanism [...] was suggested. Evidence for this mechanism was found in a laboratory study [...]."
- L80: *"Temperatures [...] are likely to favour the occurrence of ODES [...]"* typo "ODES" → "ODEs"
- L104: *"[...] 3D air quality model GEM-AQ. [...] the EMAC model [...]* These acronyms may need more explanation. For clarification: What are the major differences/improvments by using WRF-chem compared to the above mentioned models/simulations? GEM-AQ is much like WRF-Chem a weather prediction model with chemistry and aerosols able to run on different scales, while EMAC is a global chemistry climate model with a focus on middle atmosphere chemistry and dynamics.

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- L232: *"[...] above a chosen sensitivity threshold of 0.5 are used."*. Units?
- L425: typo "weighs" → "weights"
- Fig. 6: Rainbow color color maps are generally depreciated for various reasons. First, it implies a distinct visual divergence of data at the edge between blue and green/yellow. This may lead to unintended misinterpretation() in some cases. Second, it is not colorblindness friendly. As the figure is purely used for illustration, chances of misinterpretations are low. Therefore, the authors may consider changing the color map, but it is not a must scientifically.

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