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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Combined Impacts of Nitrous Acid and Nitryl Chloride on Lower Tropospheric Ozone: New Module Development in WRF-Chem and Application to China" *by* Li Zhang et al.

Anonymous Referee #1

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General comments The authors previously expanded the gas-phase CBMZ mechanism in WRF-Chem model to include comprehensive sources of HONO. Here, they update the CMBZ mechanism by incorporating HONO and chlorine chemistry including the heterogeneous ClNO2 formation. They perform four different model simulations over China for a 12-day period using a 27-km horizontal grid resolution, describe impact of the chemistry, compare model results with observed data and suggest that the additional chemistry increases HONO, ClNO2, and ozone and improves model performance. Overall, the article is written clearly and merits publication. However, several issues need to be addressed before publication.

Specific comments

Introduction, line 12-13 While chlorine atoms react with hydrocarbons, the reactions of NO2 with hydrocarbons are generally negligible. Clarifications are needed.

Heterogeneous formations, line 16-18 Foley et al. (2010) article does not provide any reaction rates for R5–R7. Correct reference is needed. It will be convenient to readers to include the reaction rates for R5–R7 in this article.

Direction emissions, line 20-23 HONO emissions prescribed as 1.6% of NO2 emissions appear to be too high. Generally, HONO emissions are prescribed as a function of NOx emissions. A reference is needed.

Model configurations, line 17-19 The Model for Ozone and Related Chemical Tracers likely did not contain any ClNO2 and/or additional HONO sources. The authors may include a sentence to clarify the issue.

Model configurations, line 24-25 The spin-up time of 24 h appears to be too small.

Emission data, line 3-6 SO2, NOx, CO, CO2, NH3, PM2.5, PM10, BC, OC are not defined anywhere.

Spatial and vertical distributions of N2O5 and ClNO2, line 30-31 A plot of chloride distribution will be helpful to readers.

Model performance of HONO and N2O5/ClNO2 NOx emissions affect HONO, ClNO2, as well as O3 production. Thus, NOx emissions are critical for this study. Authors present a qualitative comparison of observed and measured NO2 in Figure S1. Is it possible to calculate model performance for NO2 and present a table similar to Table 5?

Enhancements in regional ROX and O3 levels over polluted regions, line 11-12 ROx is defined in line 12 but used in line 10 prior to defining. It is good to define it at the time of first introduction.

Summary and conclusions, line 1-15 HONO production is related to the prescribed NOx emissions while ClNO2 production is related to the prescribed NOx and chloride emissions. A very brief discussion on the uncertainty of NOx and chloride emissions is needed.

Summary and conclusions, line 1-8 Simulations were conducted for a 12-day period, not for the entire summer. Thus, it is I suggest adding the first sentence as follows (or something similar it):

In this study, we incorporated comprehensive processes of HONO and chlorine chemistry into a new chemical mechanism option, CBMZ_ReNOM, in the WRF-Chem model and applied the new model to simulating the spatial distribution of HONO, ClNO2, and N2O5 and their impact on O3 in China during the 12-day simulation period in summer.

NCP, YRD, PRD have already been defined earlier; no need to redefine them.

Summary and conclusions, line 12-13 Model performance improved at NCP, PRD, and China but deteriorated at YRD (Table 5). Thus, some caveat is needed. Perhaps, the authors may revise the sentence as follows (or something similar): With current emissions estimates, the revised WRF-Chem generally improved O3 prediction across China.

Table 1 It appears that some of the references are not correct. For example, reaction 18 (Cl + NO2 = ClNO2 is not included in IUPAC). Please check all references and update as appropriate.

It appears that rate constant for reaction 12 (ClO + NO2 = ClONO2) is not taken from IUPAC. IUPAC recommends a pressure dependent rate constant.

All symbols need to be defined.

Figure S2. It will be helpful to readers to define eastern China. Perhaps, the authors can mark “eastern China” in Figure S1 or other figures.

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