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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 #2

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Zhang et al. describe an updated WRF-Chem model with a new chemical mechanism (CBMZ_ReNOM) developed to improve predictions of photochemical O3 production in Eastern China, incorporating revised source chemistry of HONO and photolyzable chlorine species.

The paper is written well and is publishable. Ultimately, I wasn't sure how much an improvement this work actually represents. One might hope that a more explicit representation of chemistry within a model does improve its accuracy. Perhaps this part of the manuscript could be strengthened, for instance, through a more reasonable

comparison of predicted with observed concentrations: instead of comparing averages (Tables 4 and 5), why not compare selected time series of measurements and model predictions, in particular for transient species such as HONO and ClNO2 whose concentrations are highly variable.

Specific comments

pg 3 line 17 "To the best of our knowledge, no global or regional models, however, have simultaneously considered the sources/processes of HONO and ClNO2 and evaluated their regional impacts on the formation of O3 pollution in the boundary layer of the atmosphere." I am not sure the statement as written is true. Many studies have simultaneously considered HONO and ClNO2 as radical sources and showed how these species affect O3. For instance, Sarwar et al 2004 [GRL, 2014] studied O3 formation using CMAQV5.02 which contains the RACM2 mechanism [Goliff et al., AE 2013] and HONO chemistry. Also, Ahmadov et al. [ACP, 2015] and Edwards et al. [Nature, 2014] used models and HONO/ClNO2 data to investigate high wintertime ozone pollution events in an oil- and natural gas-producing region of the western US. There have also been numerous papers using 0D box models examining this chemistry.

pg 4 line 9 "reproduced the observed HONO by 85% on average" Not sure what this means.

pg 5 line 17. What is FMCl? A fluorine-metal compound?

pg 7 line 7. "has been proved" A model cannot be proven, at least not in a mathematical sense. Why not simply say that this model has made reasonable predictions of PM2.5 and O3?

pg 7, section "2.2.3 O3 and NO2 measurement data" Please state how accurate these measurements are.

pg 7, last line. The Mo converter also "detects" NO3, 2N2O5, HONO, ClNO2, PAN, and HNO3 to some degree as if it were NO2. The model should give some indication

as what fraction of NOy is in the form of NOz (as a function of time of day); consider a sensitivity run in which the NO2 reported by the routine measurements is scaled down by this factor.

pg 8 " 3.1.2 Spatial and vertical distributions of N2O5 and ClNO2 ". These predicted concentrations are considerably lower than recent measurements in the HK area (see sections further down).

pg 9, line 11 "The model very well captured the measured HONO at Wangdu in the NCP region during a matching simulation period, reproducing 86% of the observations (0.81 vs. 0.94 ppb)" I don't understand this sentence. How does a model reproduce 86% of observations? Consider instead a scatter plot of model concentrations vs observations.

pg 9, line 25 onward. Brown, S. S., et al. (2016), Nighttime chemistry at a high altitude site above Hong Kong, J. Geophys. Res.-Atmos., 121(5), 2457-2475, doi: 10.1002/2015jd024566 observed much higher concentrations than the model predicts. Please discuss.

pg 18, Table 1. Please state the units of the reaction rates.

rxn 7. Water should have a subscript.

rxn 26. What are PAR and X? Also, define the other terms, such as OLI, ALD2 etc.

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