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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Examining the impact of heterogeneous nitryl chloride production on air quality across the United States" *by* G. Sarwar et al.

Anonymous Referee #1

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In response to the recent observation of prominent levels of nitryl chloride (ClNO2), the goal of the work by Sarwar et al. is to develop a chemical mechanism suitable for regional air quality models that takes into account the production of ClNO2 through the heterogeneous hydrolysis of N2O5. The new mechanism expands upon the existing CB05TU mechanism for gas-phase reactions and now includes chlorine-related reactions. As for the heterogeneous reactions, the existing CMAQ configuration is augmented with added yields for ClNO2 production, which in turn reduce HNO3 production. The newly developed chemical mechanism is tested through the implementation in the Community Multiscale Air Quality (CMAQ) modeling system (version 5.0 beta) for a modeling domain that spans the whole United States. Two simulation periods

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are considered: February and September 2006. The model performance of the new parameterizations and relevant chemical mechanism updates is evaluated based on ClNO2 predictions as well as predictions for secondary pollutants, ozone and particulate nitrates.

Overall, the manuscript provides a comprehensive overview of the methodology for the development of the new mechanisms to account for ClNO2 production through heterogeneous N2O5 hydrolysis. Sufficient background of the scenario development, from emission inventory to meteorological conditions, is presented in the manuscript. The conclusions drawn from the analysis of the simulation results indeed demonstrate the importance to include the new mechanism for the improvement of air quality model performance. However, there are several questions that the authors should address, which would require some revisions to the manuscript:

- In section 2.3, what is the motivation behind the decision to use the Davis et al. (2008) parameterization for fine particles and the Bertram and Thornton (2009) for coarse particles? - In section 3.2, the statement "all current γN2O5 parameterizations, available in the peer-reviewed literature, produce higher γN2O5 values" is made without any reference. What about γN2O5 values for organic particles? They have been shown to have significantly lower γN2O5 compared to inorganic particles, see for example Chang et al., Aerosol Science and Technology, 45:655–685, 2011. - The discussion in section 3.6 mentioned that the enhancement of O3 obtained with the different γN2O5 value varied occasionally by 1-2 ppbv, and it is concluded that this is not much of an impact on O3. However, this seems to be on the same order of magnitude as the change in O3 between the base case and the heterogeneous ClNO2 production case (section 3.4.2). Please clarify why the differences due to γN2O5 are deemed to be negligible. - In Table 4, while the observed and modeled levels of ClNO2 are in reasonable agreement, model results seem to be consistently over-predicting ambient levels. Could this be quantified by the over-estimation of γN2O5? A discussion of this should be added to the manuscript.

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Interactive Comment

Minor points: - Citation Davis et al. (2008), not (2010). - page 6153, l.4: variable d has a tilde in the equation, but not in the explanatory text.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 6145, 2012.