

**Supplement to:**

**Examining the impact of heterogeneous nitryl chloride production on air quality across the United States**

**G. Sarwar<sup>1</sup>, H. Simon<sup>2</sup>, P. Bhave<sup>1</sup>, G. Yarwood<sup>3</sup>**

<sup>1</sup> National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, USA

<sup>2</sup> Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, USA

<sup>3</sup> ENVIRON International Corporation, Novato, California, USA

Figure S1. September 2006 8-hr max O<sub>3</sub> mean bias (for days when obs > 65 ppbv) in the simulation without heterogeneous ClNO<sub>2</sub> formation (top) and change in absolute value of 8-hr max O<sub>3</sub> mean bias with the implementation of ClNO<sub>2</sub> chemistry (bottom). Negative values in bottom plot denote improvements in performance and positive values denote degradations in model performance due to ClNO<sub>2</sub> chemistry.

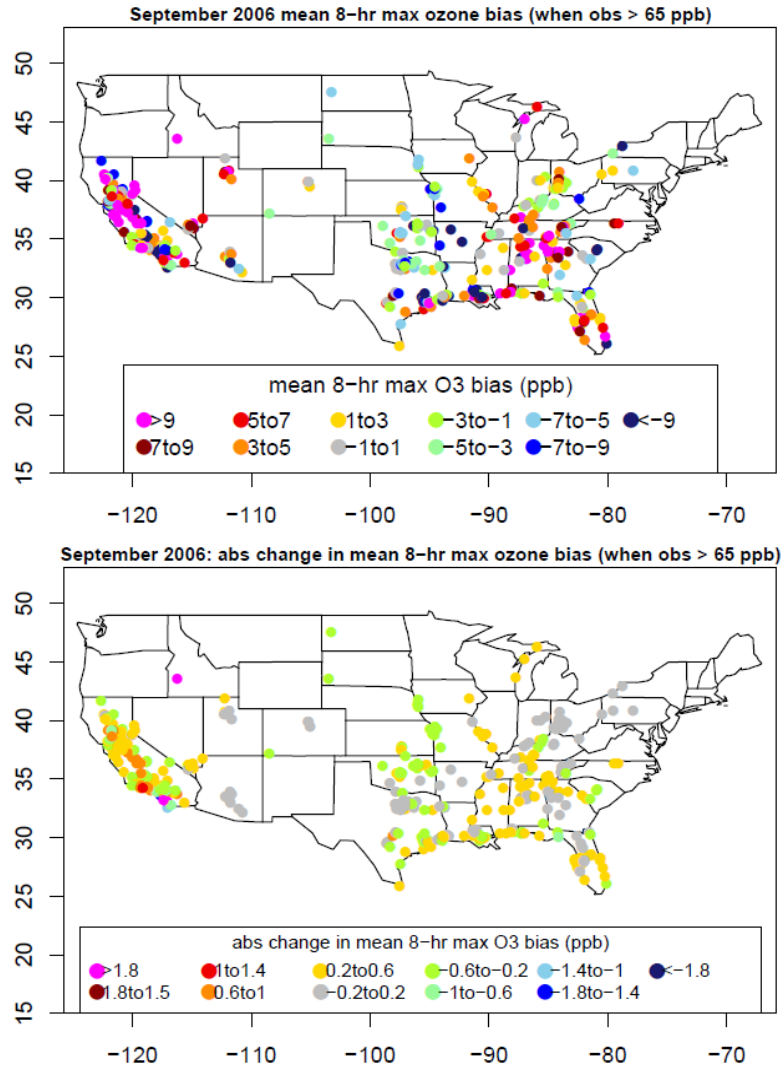


Figure S2. TNO<sub>3</sub> mean observed concentration (top), TNO<sub>3</sub> mean bias in the simulation without heterogeneous CINO<sub>2</sub> formation (middle) and change in absolute value of TNO<sub>3</sub> mean bias with the implementation of CINO<sub>2</sub> chemistry (bottom). Negative values in bottom plot denote improvements in performance and positive values denote degradations in model performance due to CINO<sub>2</sub> chemistry. All plots show comparisons of weekly average values at CASTNet monitoring sites during the month of February 2006.

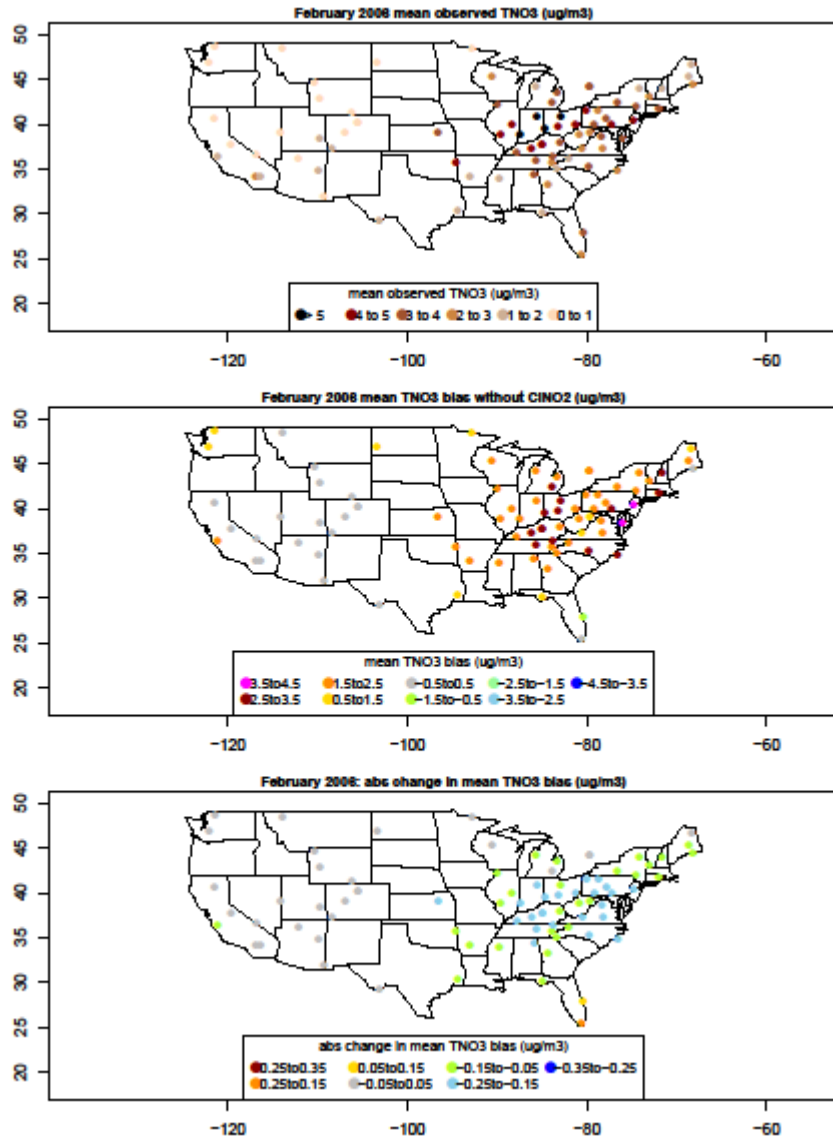


Figure S3. TNO<sub>3</sub> mean observed concentration (top), TNO<sub>3</sub> mean bias in the simulation without heterogeneous CINO<sub>2</sub> formation (middle) and change in absolute value of TNO<sub>3</sub> mean bias with the implementation of CINO<sub>2</sub> chemistry (bottom). Negative values in bottom plot denote improvements in performance and positive values denote degradations in model performance due to CINO<sub>2</sub> chemistry. All plots show comparisons of weekly average values at CASTNet monitoring sites during the month of September 2006.

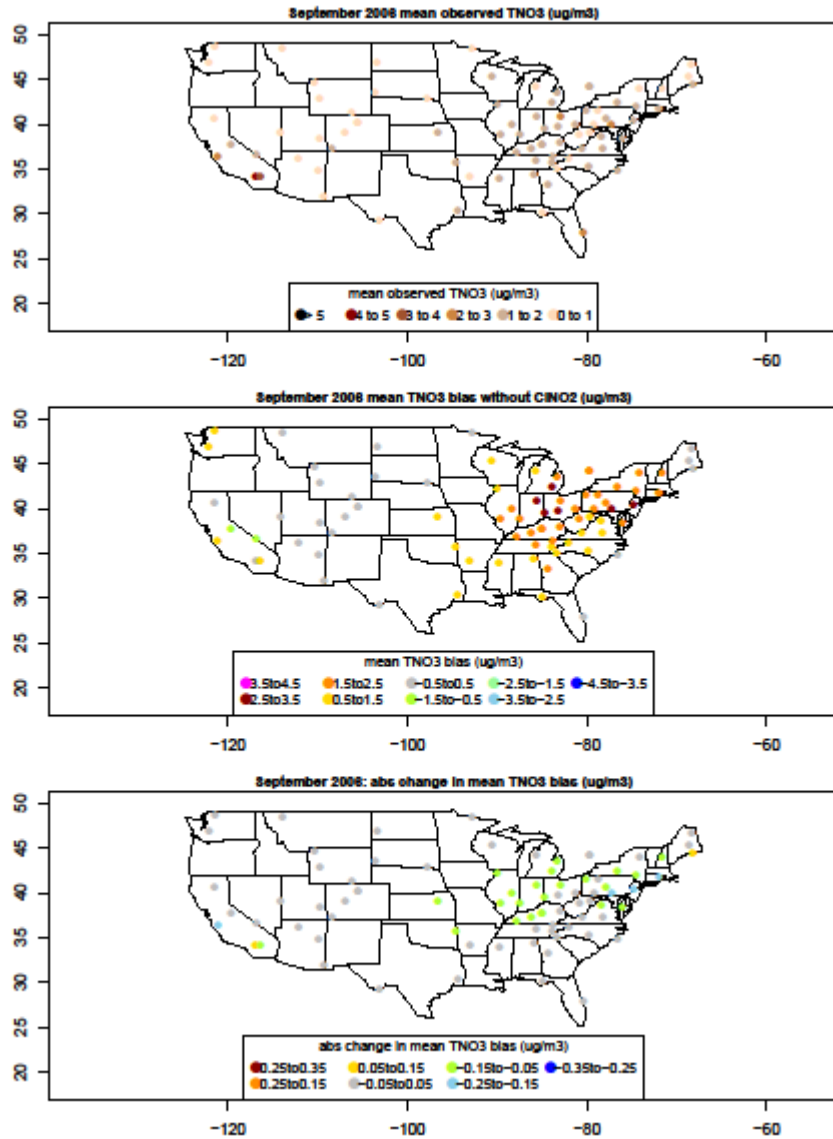


Figure S4. Particulate NO<sub>3</sub> mean observed concentration (top), Particulate NO<sub>3</sub> mean bias in the simulation without heterogeneous CINO<sub>2</sub> formation (middle) and change in absolute value of Particulate NO<sub>3</sub> mean bias with the implementation of CINO<sub>2</sub> chemistry (bottom). Negative values in bottom plot denote improvements in performance and positive values denote degradations in model performance due to CINO<sub>2</sub> chemistry. All plots show comparisons at CASTNet, CSN, IMPROVE, and SEARCH monitoring sites during the month of February 2006. Note: CASTNet comparisons are made for weekly average concentrations while IMPROVE, CSN, and SEARC comparisons are made for 24-hr average concentration.

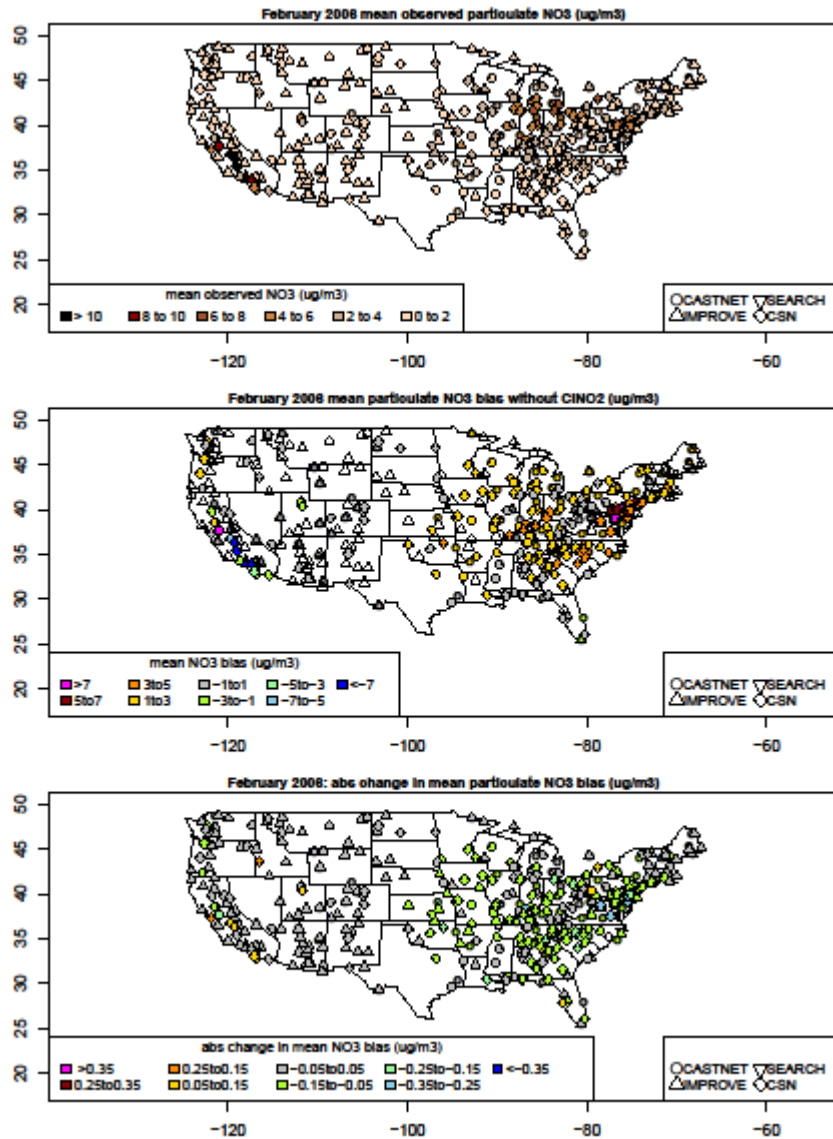


Figure S5. Particulate NO<sub>3</sub> mean observed concentration (top), Particulate NO<sub>3</sub> mean bias in the simulation without heterogeneous CINO<sub>2</sub> formation (middle) and change in absolute value of Particulate NO<sub>3</sub> mean bias with the implementation of CINO<sub>2</sub> chemistry (bottom). Negative values in bottom plot denote improvements in performance and positive values denote degradations in model performance due to CINO<sub>2</sub> chemistry. All plots show comparisons at CASTNet, CSN, IMPROVE, and SEARCH monitoring sites during the month of September 2006. Note: CASTNet comparisons are made for weekly average concentrations while IMPROVE, CSN, and SEARC comparisons are made for 24-hr average concentration.

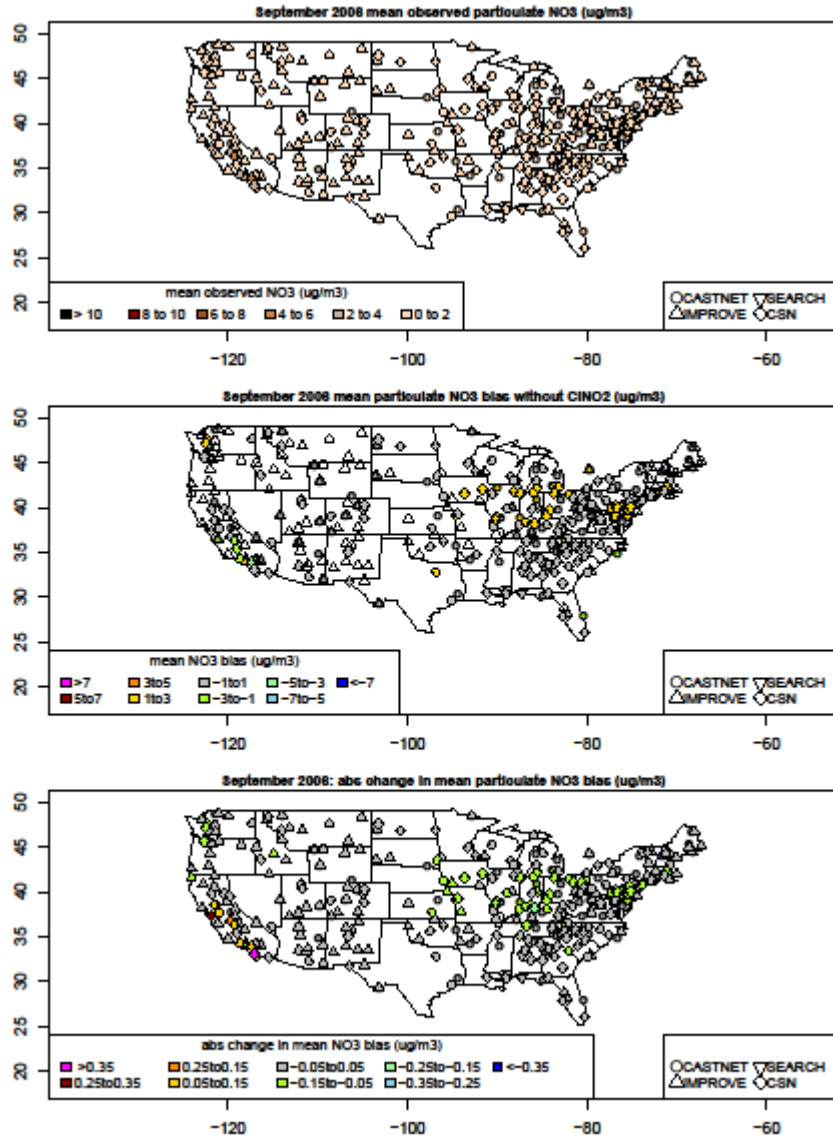


Figure S6: Impact of  $\gamma_{\text{N}_2\text{O}_5}$  parameterization on  $\text{TNO}_3$  in February (10-days) (a) mean  $\text{TNO}_3$  with  $\gamma_{\text{A}}$  (b) mean  $\text{TNO}_3$  with  $\gamma_{\text{B}}$  (c) changes in mean  $\text{TNO}_3$  with  $\gamma_{\text{A}}$  due to heterogeneous production of  $\text{ClNO}_2$  (d) changes in mean  $\text{TNO}_3$  with  $\gamma_{\text{B}}$  due to heterogeneous production of  $\text{ClNO}_2$ .  $\gamma_{\text{A}} = \gamma_{\text{N}_2\text{O}_5}$  of Davis et al. (2008) on fine particles and  $\gamma_{\text{N}_2\text{O}_5}$  of Bertram and Thornton (2009) on coarse particles and  $\gamma_{\text{B}} = \gamma_{\text{N}_2\text{O}_5}$  of Bertram and Thornton (2009) on fine as well as coarse particles.

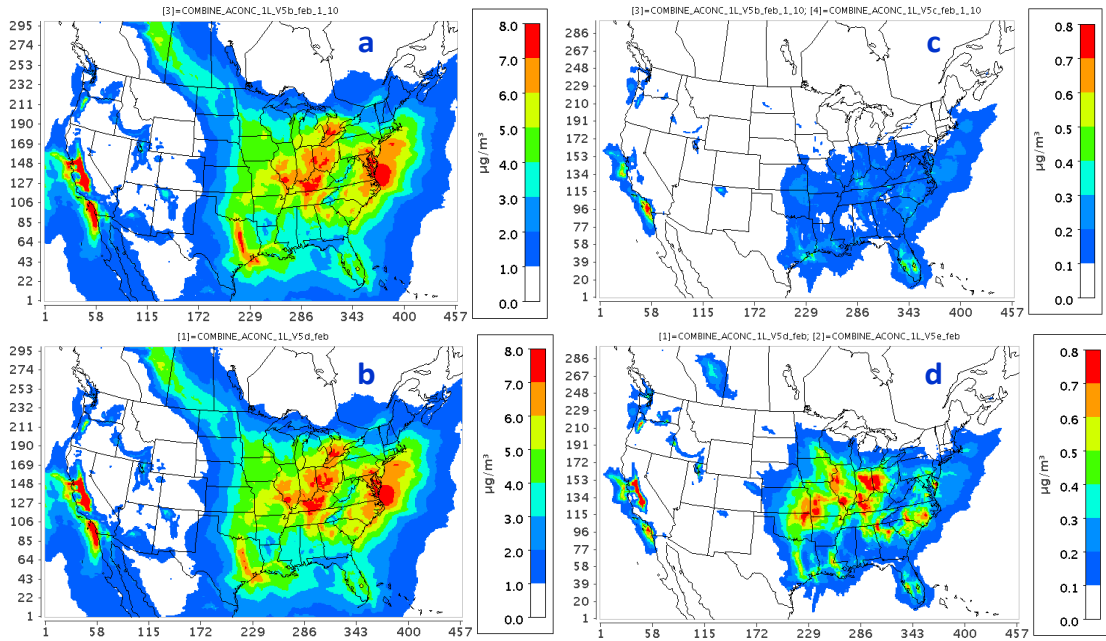


Figure S7: Impact of  $\gamma_{\text{N2O5}}$  parameterization on  $\text{TNO}_3$  in September (10-days) (a) mean  $\text{TNO}_3$  with  $\gamma_A$  (b) mean  $\text{TNO}_3$  with  $\gamma_B$  (c) changes in mean  $\text{TNO}_3$  with  $\gamma_A$  due to heterogeneous production of  $\text{ClNO}_2$  (d) changes in mean  $\text{TNO}_3$  with  $\gamma_B$  due to heterogeneous production of  $\text{ClNO}_2$ .  $\gamma_A = \gamma_{\text{N2O5}}$  of Davis et al. (2008) on fine particles and  $\gamma_{\text{N2O5}}$  of Bertram and Thornton (2009) on coarse particles and  $\gamma_B = \gamma_{\text{N2O5}}$  of Bertram and Thornton (2009) on fine as well as coarse particles.

