Sensitivity of Northeast U.S. surface ozone predictions to the representation of atmospheric chemistry in CRACMMv1.0

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Equations used for calculating site-specific statistics reported in Table S1

Equation 1. $$MB = \frac{1}{S}\sum_{j=1}^{S}\left[\frac{1}{T}\sum_{i=1}^{T}\left(p_{i,j} - o_{i,j}\right)\right]$$

Equation 2. $$r = \frac{1}{S}\sum_{j=1}^{S}\left[\frac{\sum_{i=1}^{T}(p_{i,j}-\overline{p_j})(o_{i,j}-\overline{o_j})}{\sum_{i=1}^{T}(p_{i,j}-\overline{p_j})^2 \sum_{i=1}^{T}(o_i-\overline{o_j})^2}\right]$$

Equation 3. $$NMB = 100\% \times \frac{1}{S}\sum_{j=1}^{S}\left[\frac{\sum_{i=1}^{T}(p_{i,j}-o_{i,j})}{\sum_{i=1}^{T}(o_{i,j})}\right]$$

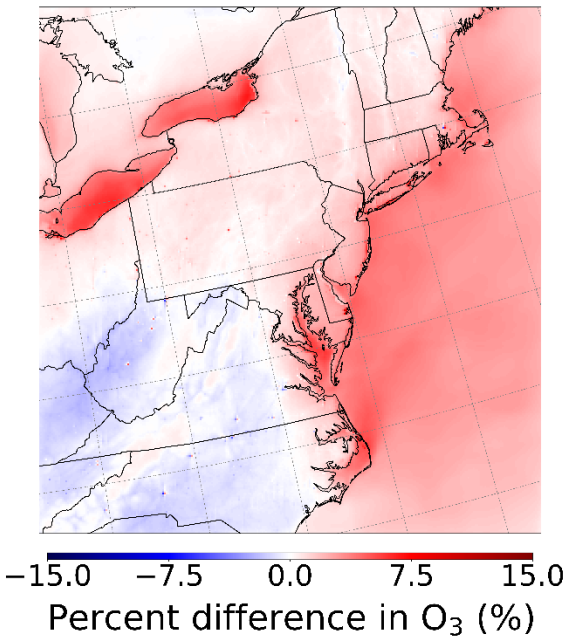
Equation 4. $$NME = 100\% \times \frac{1}{S}\sum_{j=1}^{S}\left[\frac{\sum_{i=1}^{T}(|p_{i,j}-o_{i,j}|)}{\sum_{i=1}^{T}(o_{i,j})}\right]$$

Where S is the number of sites, T is the number of time periods (number of 1-hour or MDA8 values), $p_{i,j}$ and $o_{i,j}$ are the model predicted and observed values over a specific time period, *i*, at site, *j*, and $\overline{p_j}$ and $\overline{o_j}$ are the mean predicted and observed values over all times at a site, *j*.

Table S1: Mapping from CRACMMv0.21 to CRACMMv1.0 and RACM2_ae6 emissions for use in CMAQ. The mechanism number changed from v0.21 (an interim version used to create CMAQ-ready CRACMM emissions) to v1.0 in the final version used in the study. RACM2_ae6 mappings are approximate based on the major contributors in each CRACMM category and information from William P.L. Carter (https://intra.engr.ucr.edu/~carter/emitdb/).

CRACMMv0.21 species	**CRACMMv1.0 species**	**RACM2_ae6 Species**
ACRO	ACRO	MACR
BDE13	BDE13	DIEN
BEN	BEN	BENZENE
FURAN	FURAN	HC8
HC8	HC10	HC8
NAPH	NAPH	XYM
PROG	PROG	HC8
TOLUENE	TOL	TOL
XYOP	XYE	XYO*0.5+XYP*0.5
ROCIOXY	VROCIOXY	NA

a) (CRACMMv1.0-CB6r3_ae7)/CRACMMv1.0 *100%



b) (CRACMMv1.0-RACM2_ae6)/CRACMMv1.0 *100%

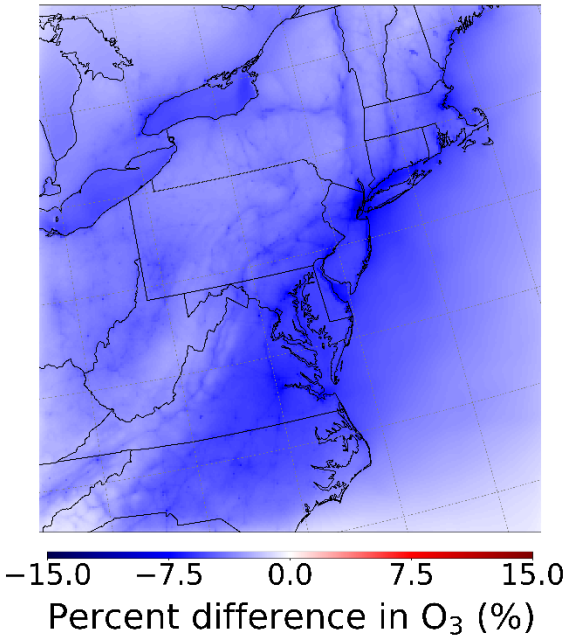


Figure S1. Percent difference in average O_3 between a) CRACMMv1.0 and Cb6r3_ae7 and b) CRACMMv1.0 and RACM2_ae6.

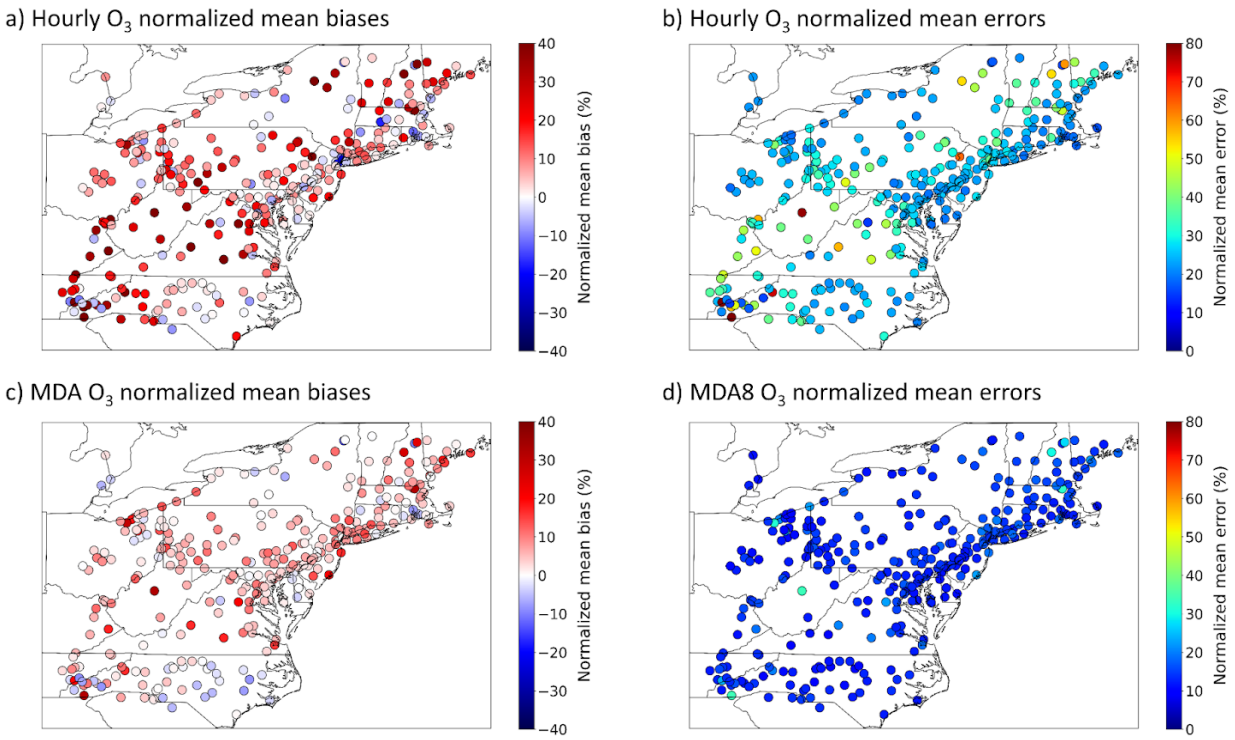


Figure S2. CRACMM hourly and MDA8 O_3 NMB and NME site statistics.

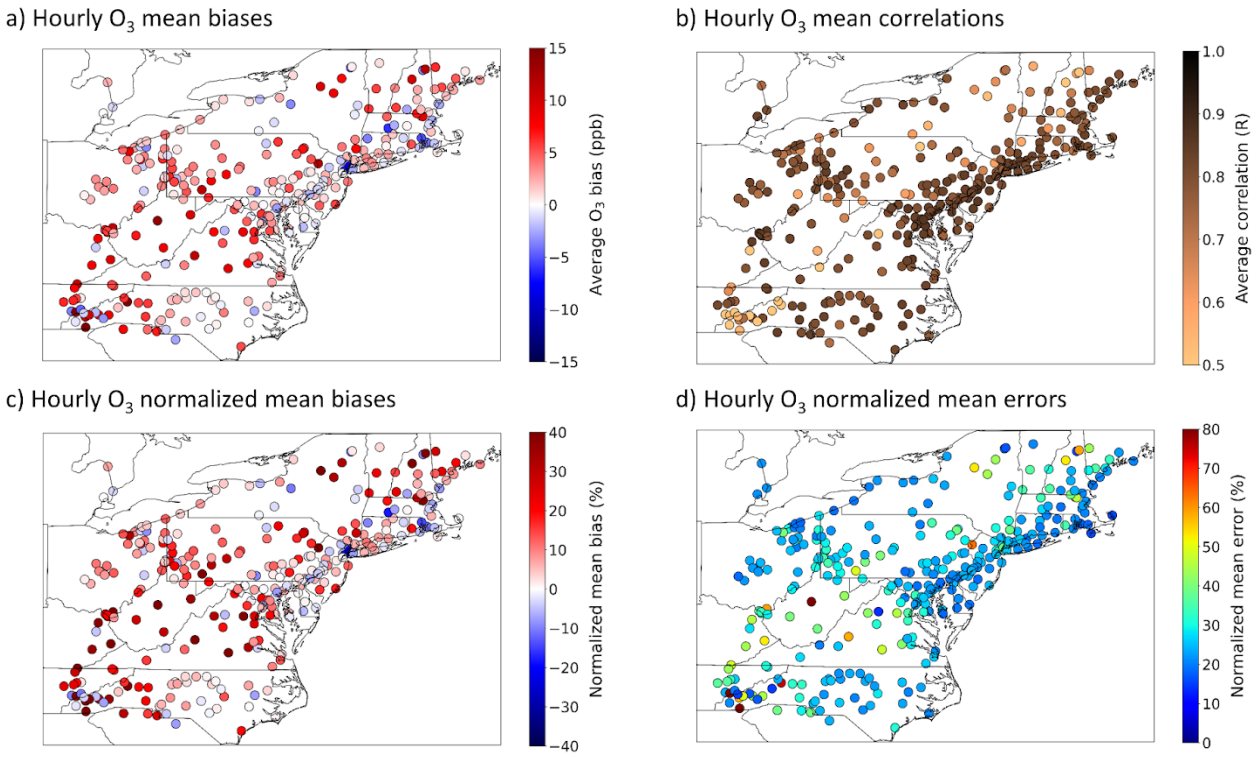


Figure S3. CB6r3_ae7 all hour site statistics.

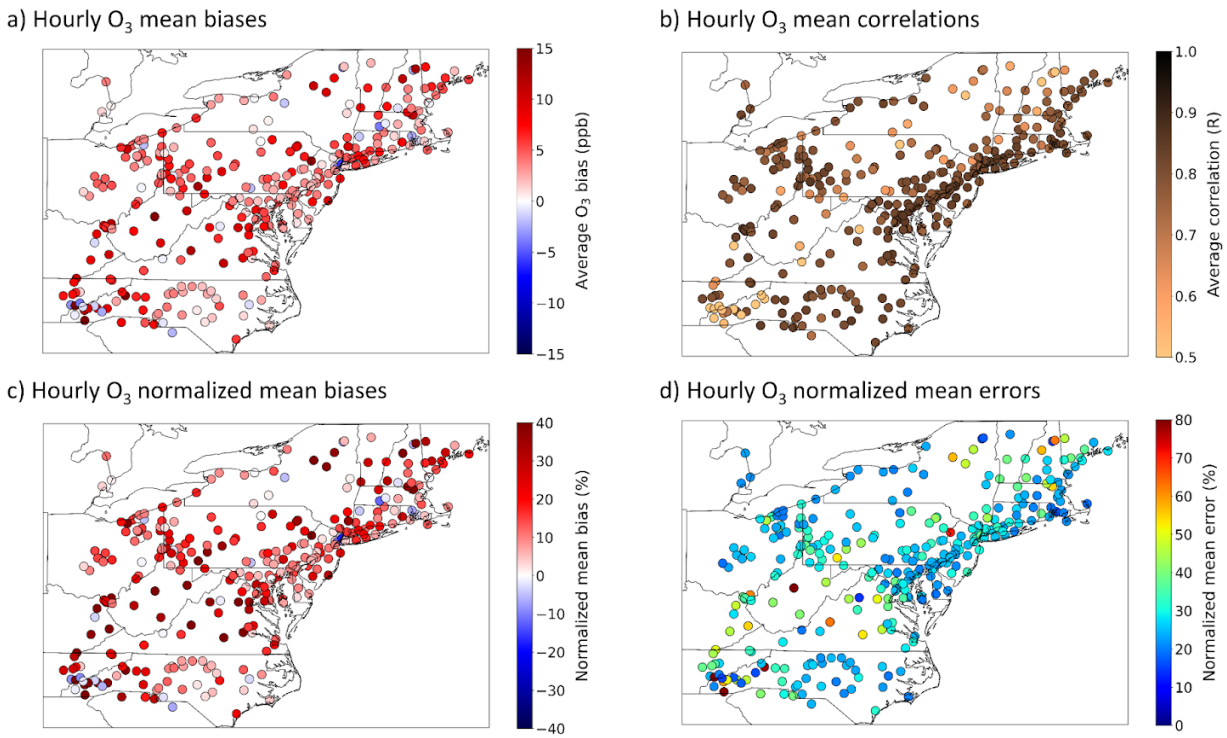


Figure S4. RACM2_ae6 all hour O_3 site statistics.

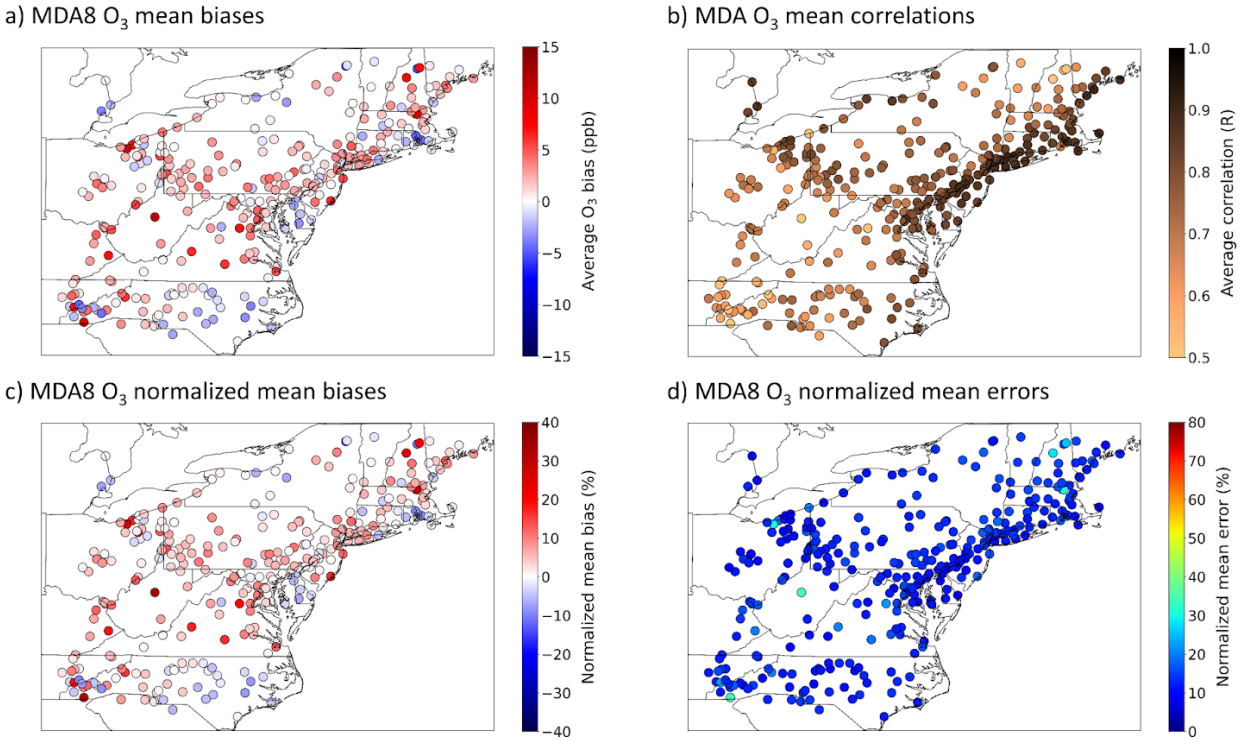


Figure S5. CB6r3_ae7 MDA8 O_3 site statistics.

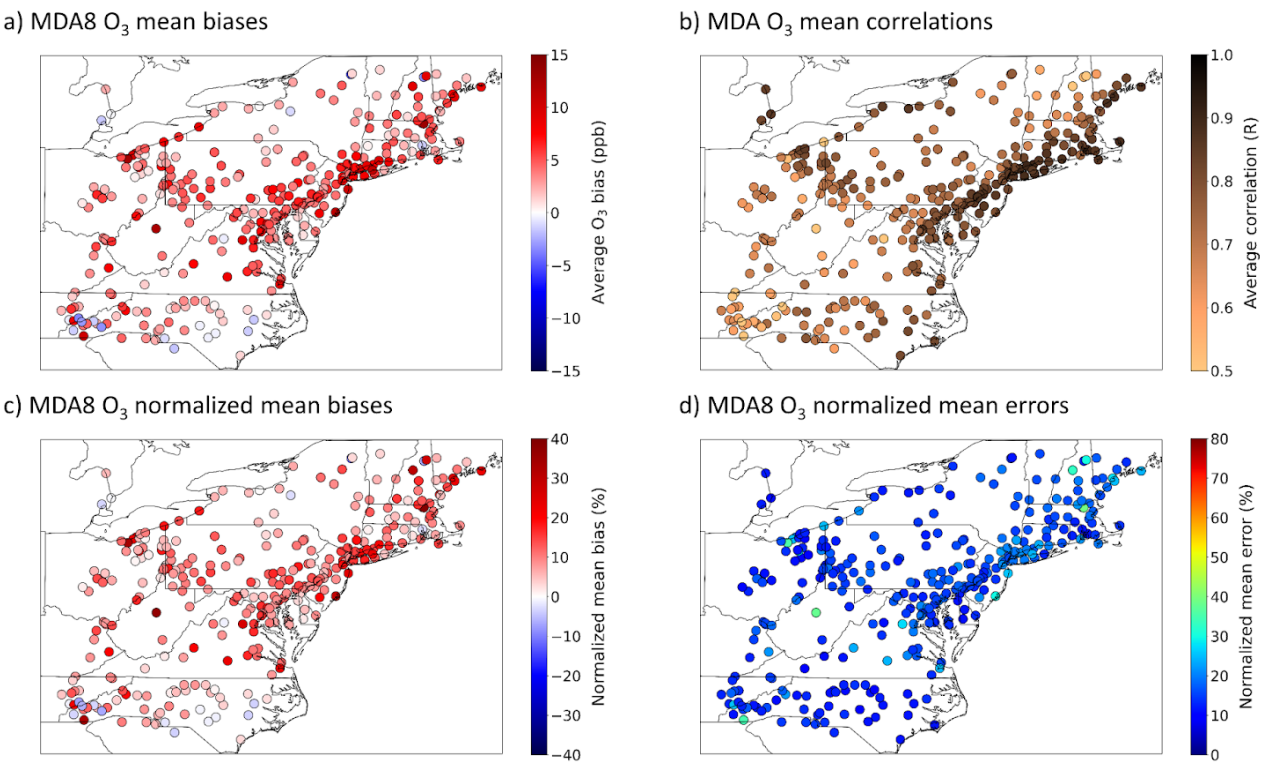


Figure S6. RACM2_ae6 MDA8 O_3 site statistics.

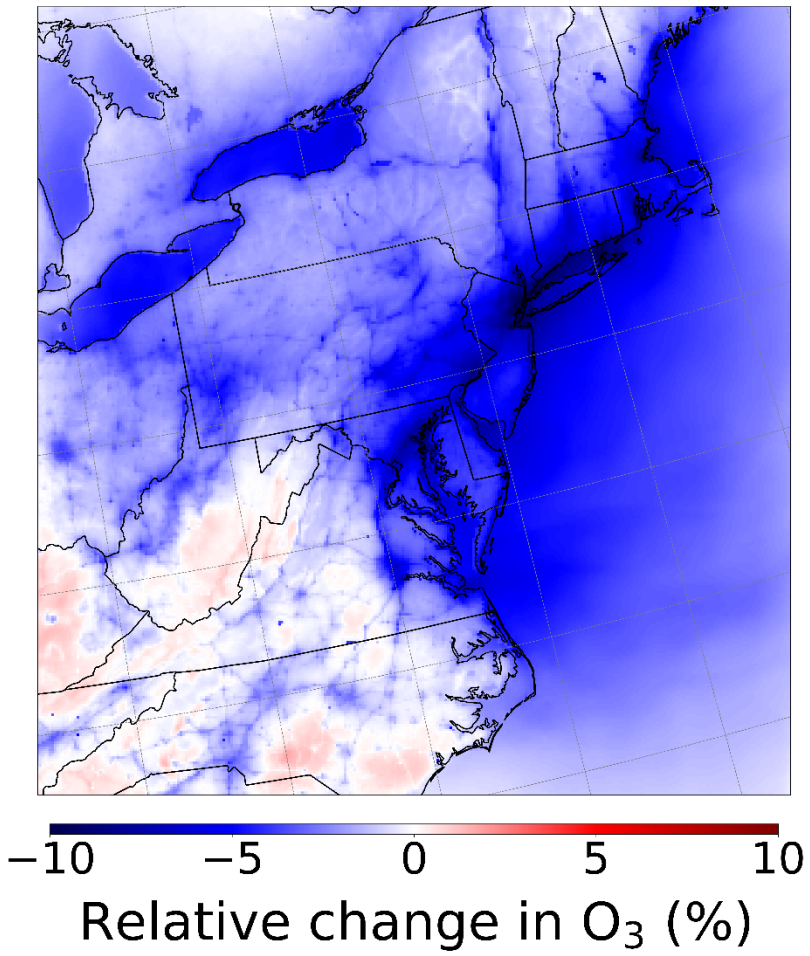


Figure S7. RACM2_ae6 biogenic zero-out percent change in O_3.

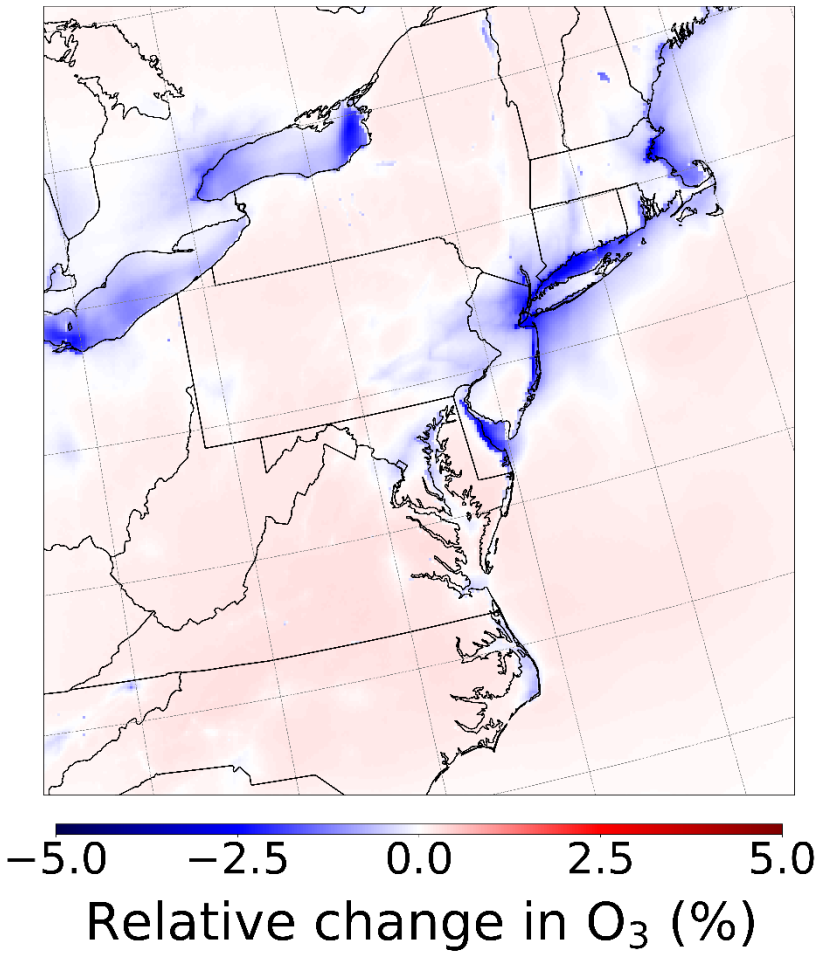


Figure S8. RACM2_ae6 BTX zero out percent change in O_3.

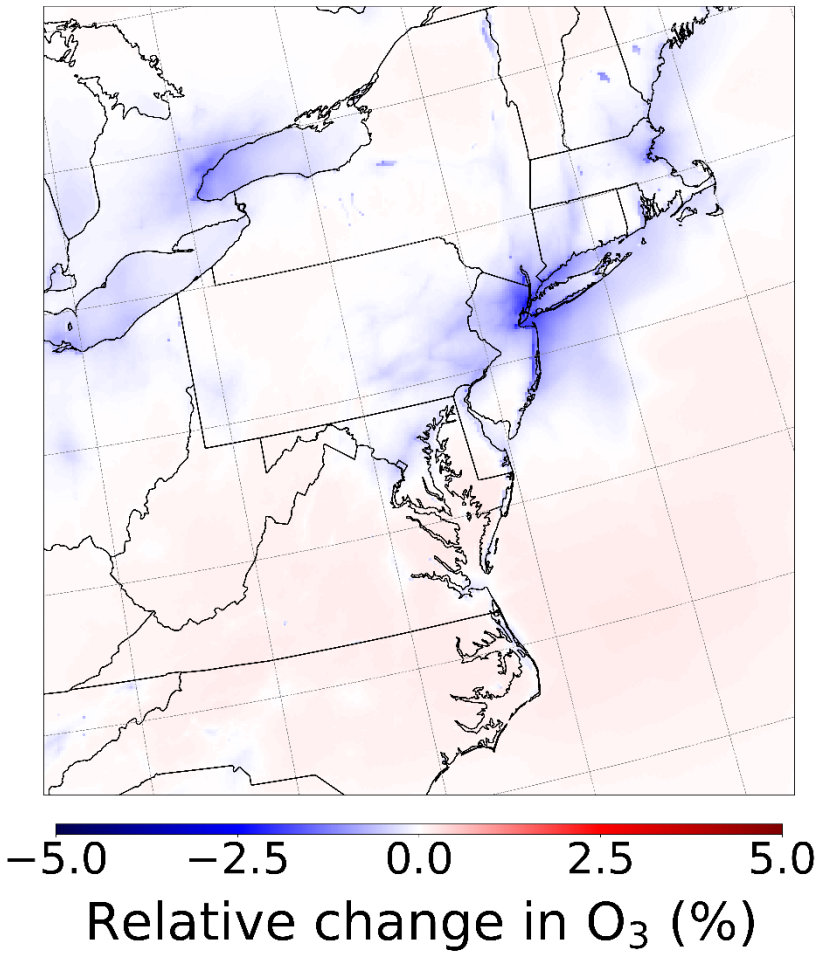


Figure S9. CB6r3_ae7 BTX zero out percent change in O_3.

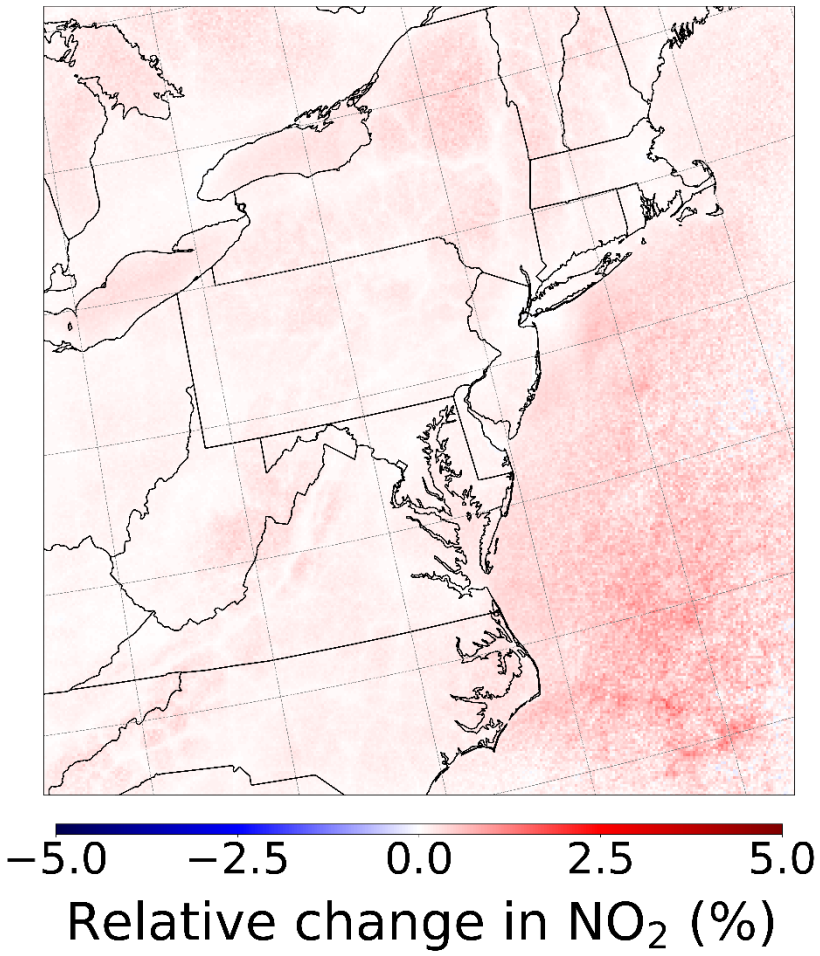


Figure S10. CRACMM HC10 zero out percent change in NO_2.

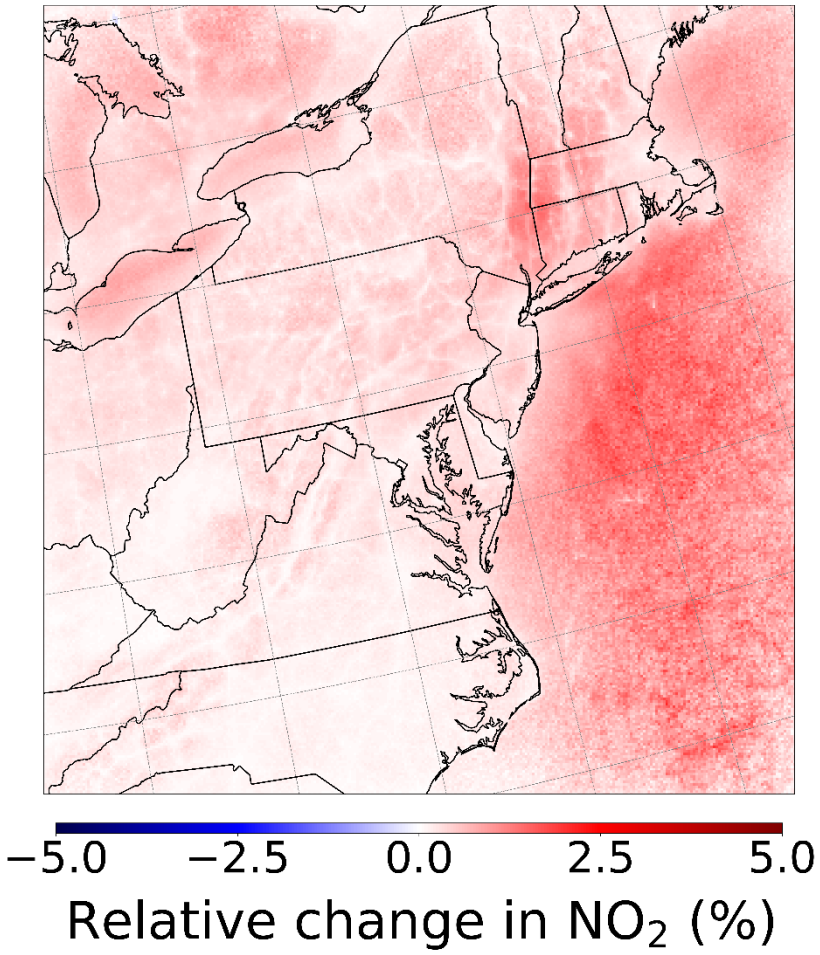


Figure S11. CRACMM SVOC zero out percent change in NO_2.

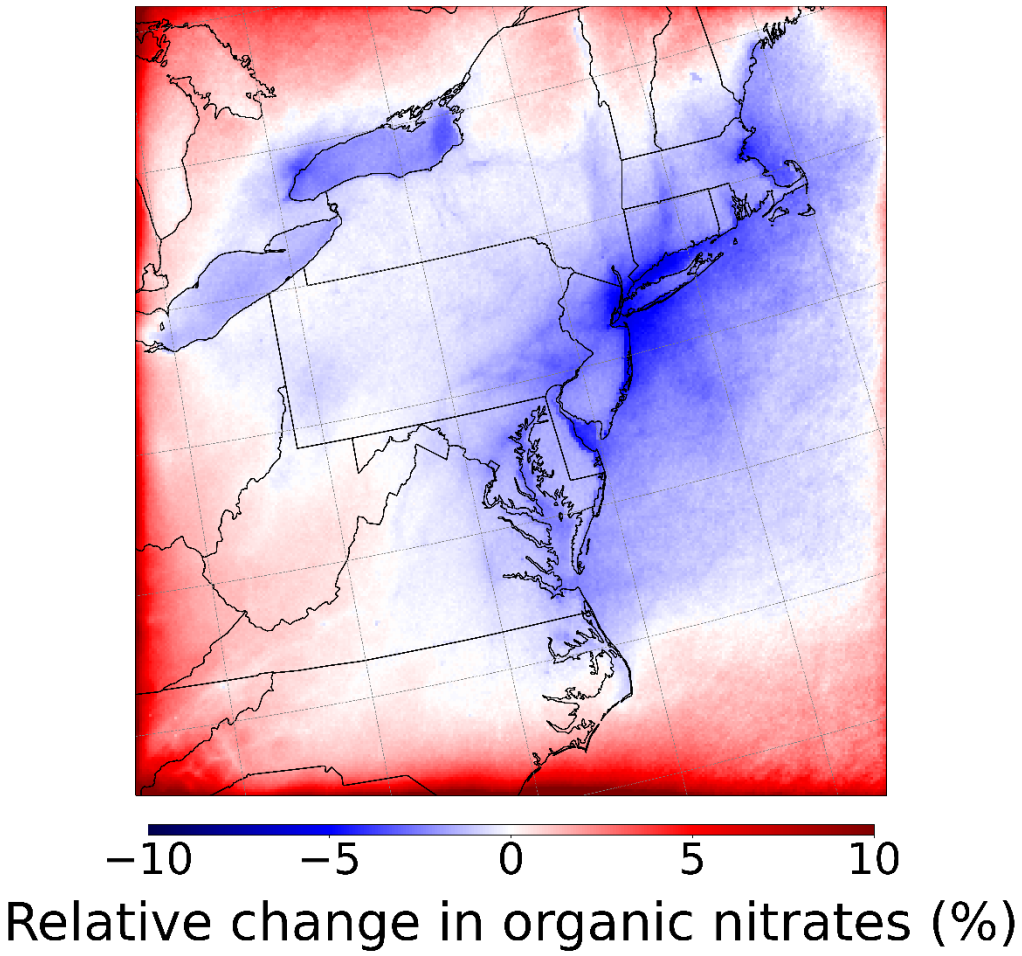


Figure S12. CRACMM HC10 zero out percent change in organic nitrates.

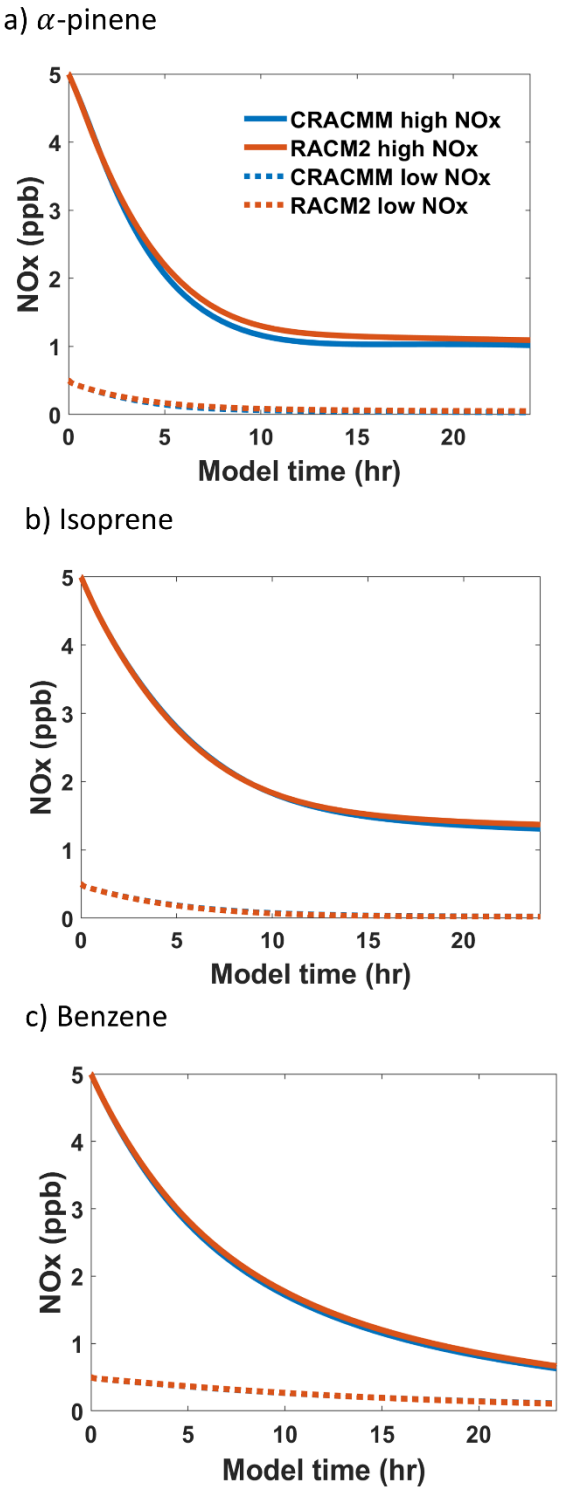


Figure S13. Evolution of NO_x from photochemical oxidation simulations in the F0AM box model simulations using a) α-pinene and b) isoprene and c) benzene as ROC precursors under high NO_x (5ppb) and low NO_x (0.5 ppb) conditions.