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Supplementary Information

Implementation and Evaluation of the Automated Model Reduction (AMORE) Version 1.1 Isoprene Oxidation Mechanism in GEOS-Chem

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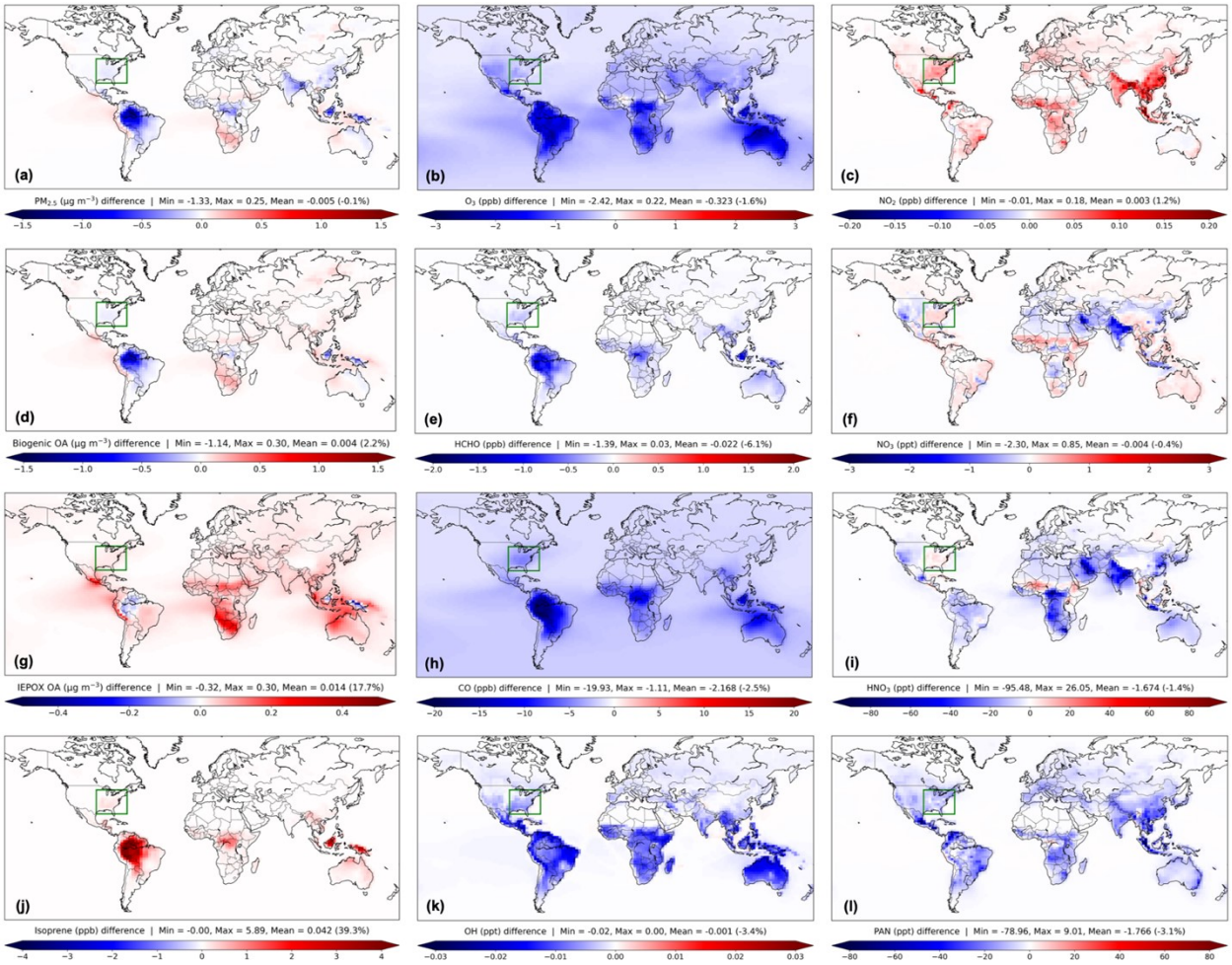

Figure S1. Global difference (AMORE - BASE) maps of 2° x 2.5° GEOS-Chem simulated surface (a) $PM_{2.5}$ (μg m^{-3}), (b) O_3 (ppb), (c) NO_2 (ppb), (d) biogenic OA (μg m^{-3}), (e) HCHO (ppb), (f) NO_3 (ppt), (g) aerosol-phase IEPOX (μg m^{-3}), (h) CO (ppb), (i) HNO_3 (ppt), (j) isoprene (ppb), (k) OH (ppt), and (l) PAN (ppt) averaged over June 2018 – May 2019. Blue and red denote grid boxes where concentrations were lower and higher, respectively, in AMORE than BASE. Minimum, maximum, and mean global differences are shown above the color bars. Our primary study area is the eastern US (green boxes).

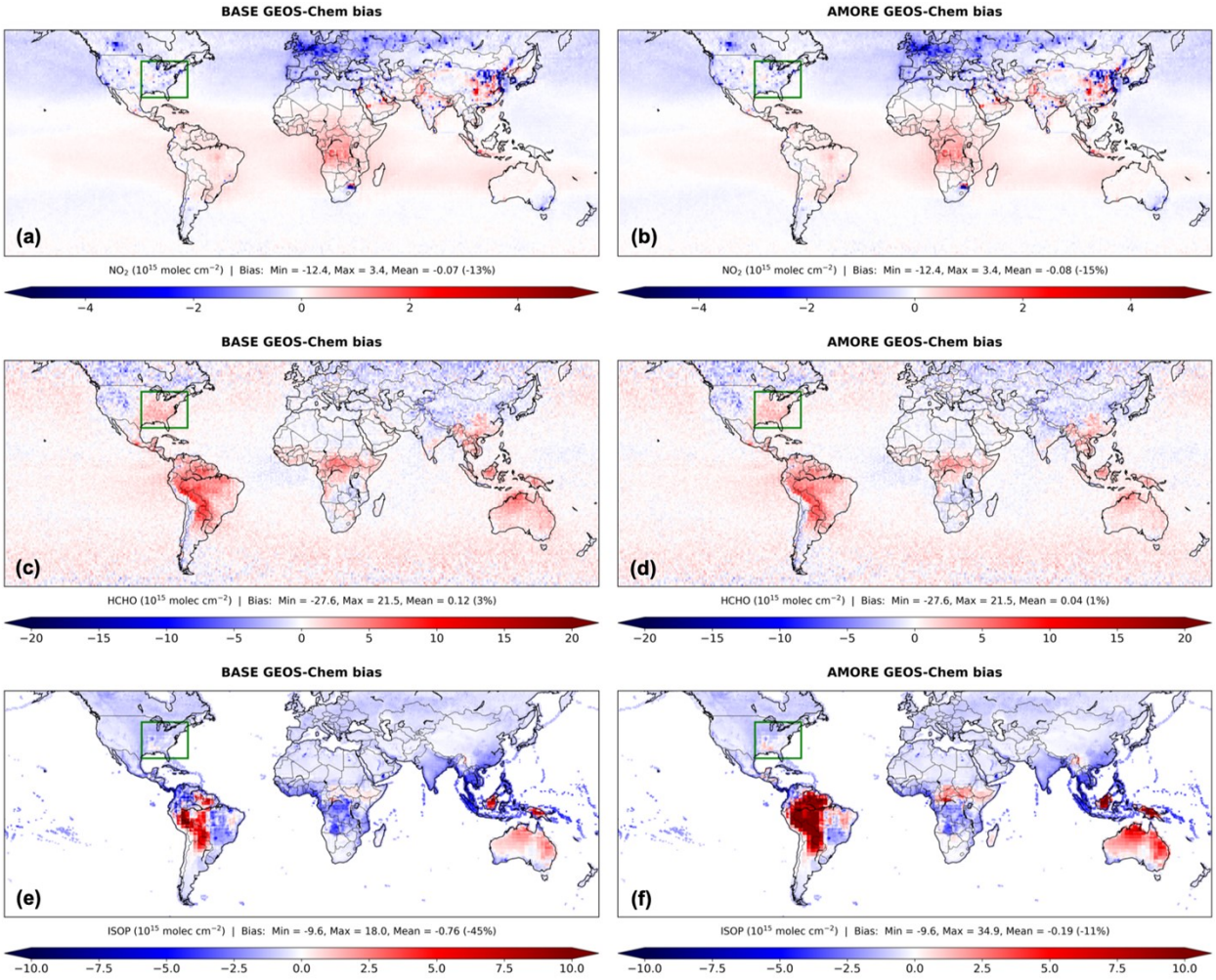

Figure S2. Global model biases (modeled - observed) of the 2° x 2.5° GEOS-Chem simulations evaluated against TROPOMI/CrIS observations for annual (June 2018 – May 2019) mean (a-b) NO_2 tropospheric VCD, (c-d) HCHO tropospheric VCD, and (e-f) isoprene total VCD, all in units of 10^{15} molecules cm^{-2}. BASE (left column) and AMORE (right column) biases indicate either overprediction (red) or underprediction (blue).

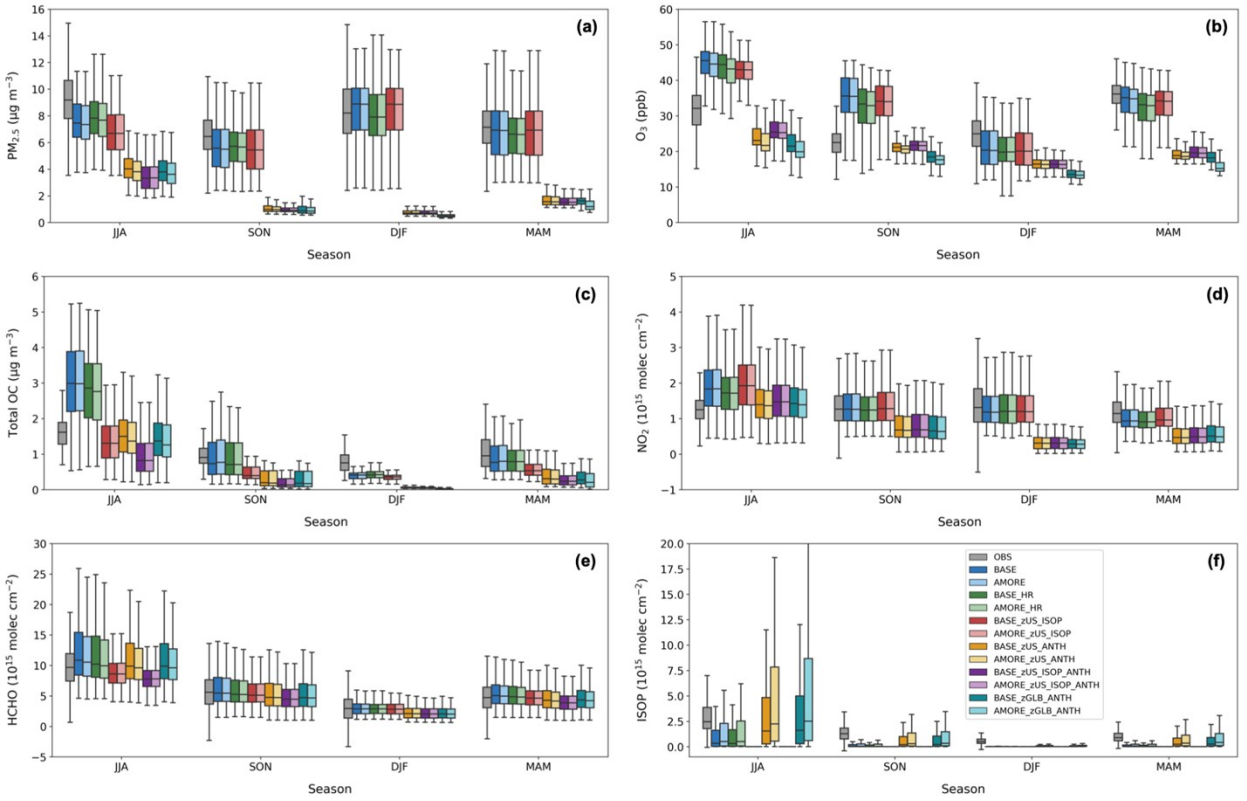

Figure S3. Seasonal distributions of monthly (a) surface $PM_{2.5}$ (μg m^{-3}), (b) surface O_3 (ppb), (c) surface total OC (μg m^{-3}), (d) NO_2 tropospheric VCD (10^{15} molecules cm^{-2}), (e) HCHO tropospheric VCD (10^{15} molecules cm^{-2}), and (f) isoprene total VCD (10^{15} molecules cm^{-2}) at AQS/IMPROVE sites (a-c) or TROPOMI/CrIS grid boxes (d-f) across the EUS for observations (gray box plots) versus all 12 GEOS-Chem simulations (other box plots). BASE (dark colors) and AMORE (light colors) mechanism sensitivity simulations are paired. The order of seasons is summer (JJA), fall (SON), winter (DJF), and spring (MAM). Each box plot shows the standard interquartile range (IQR) from the 25th (Q1) to 75th (Q3) percentiles, with whiskers extending to Q1 - (1.5 × IQR) and Q3 + (1.5 × IQR).

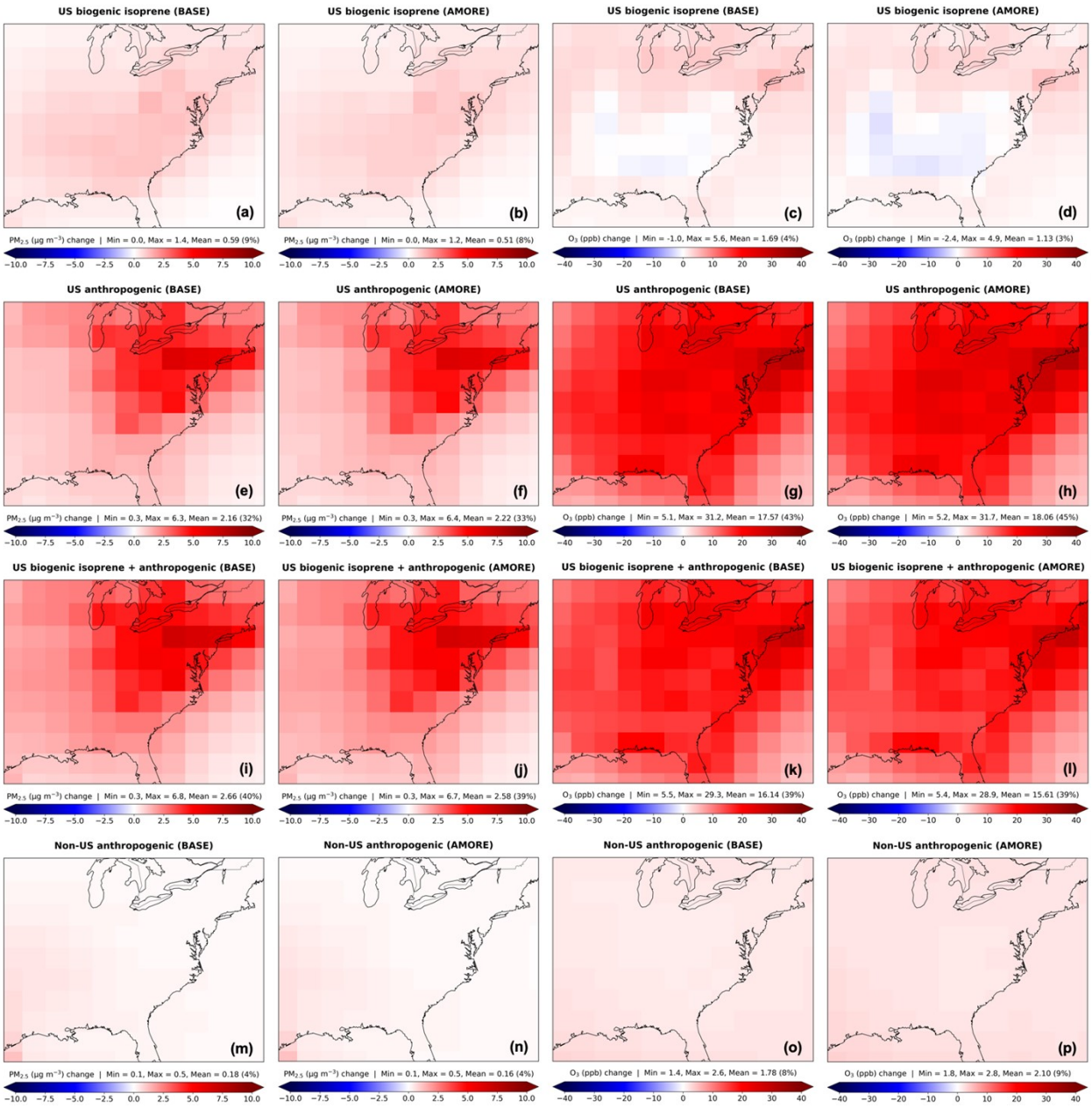

Figure S4. EUS maps of summer average (June–August 2018) sensitivities of surface $PM_{2.5}$ (μg m^{-3}, columns 1-2) and O_3 (ppb, columns 3-4) to "adding in" different emissions across the EUS domain at 2° x 2.5° resolution. Concentration changes are BASE minus BASE zero emissions or AMORE minus AMORE zero emissions (rows 1-3). Non-US anthropogenic (row 4) represents zUS_ANTH minus zGLB_ANTH.