Supplementary materials

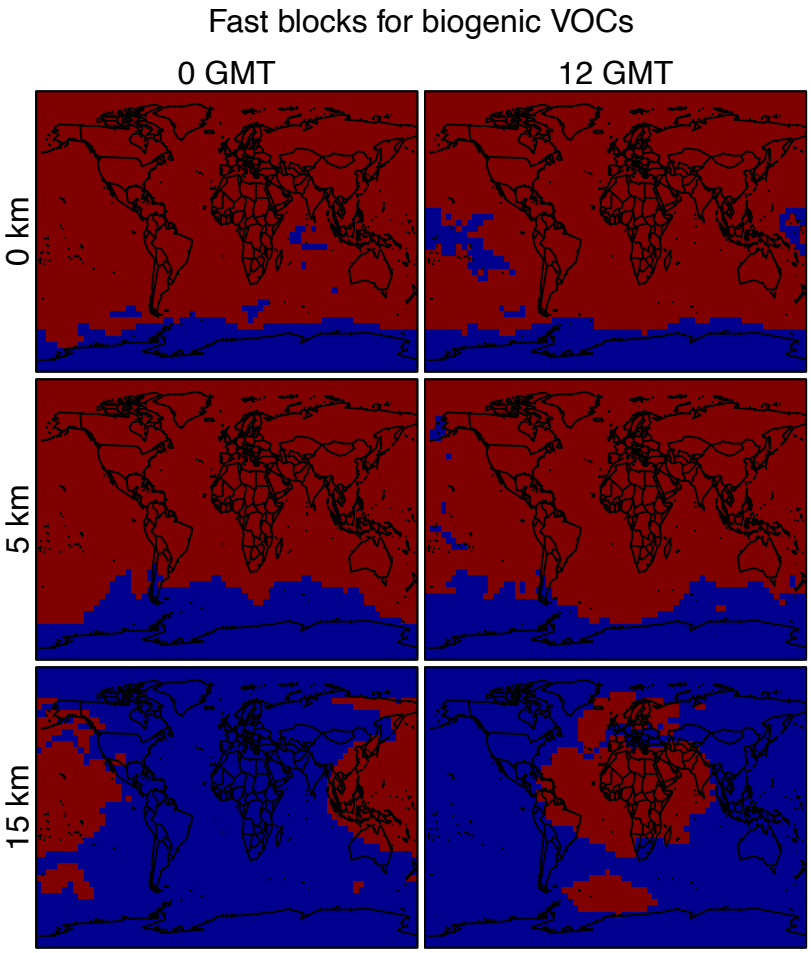


Fig. S1. Locations of anthropogenic blocks (block 5-7) that need to be solved as fast (red color). If any of block 5-7 is fast, the gridbox will be labeled as red. Results are shown on August 1 2013 at 0 and 12 GMT using a threshold δ of 500 molecules cm^{-3} s^{-1} to define the fast and slow species, and a lifetime of 10 days to define the short-lived and long-lived species.

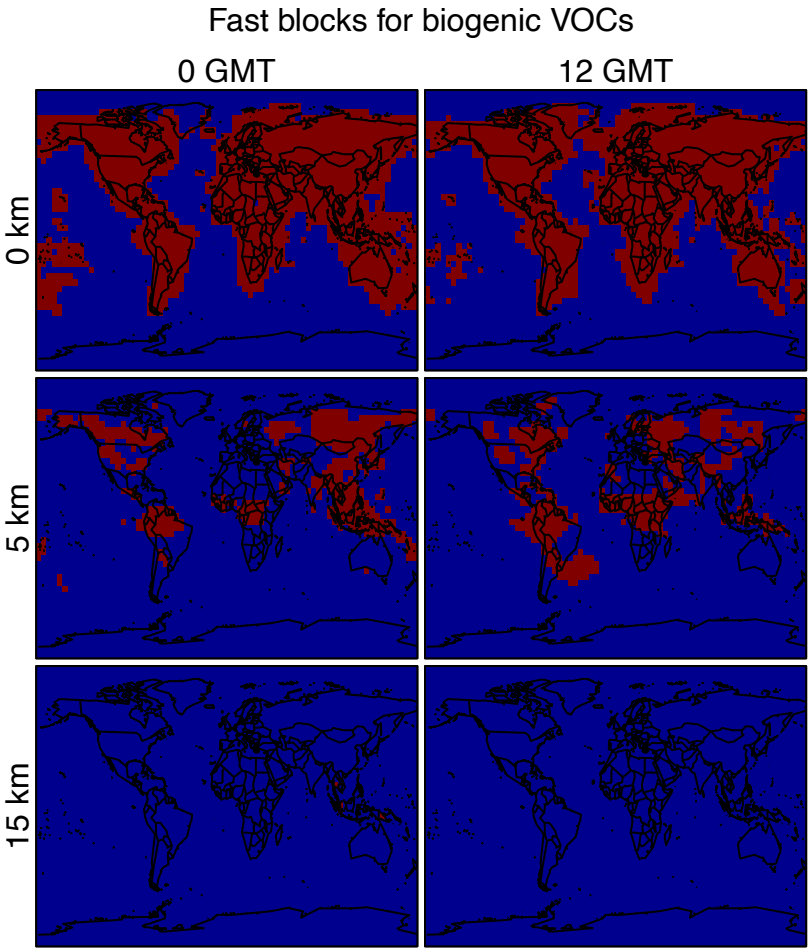


Fig. S2. Locations of biogenic blocks (block 8-11) that needs to be solved as fast (red). If any of block 8-11 is fast, the gridbox will be labeled as red. Results are shown on August 1 2013 at 0 and 12 GMT using a threshold δ of 500 molecules cm^{-3} s^{-1} to define the fast and slow species, and a lifetime of 10 days to define the short-lived and long-lived species.

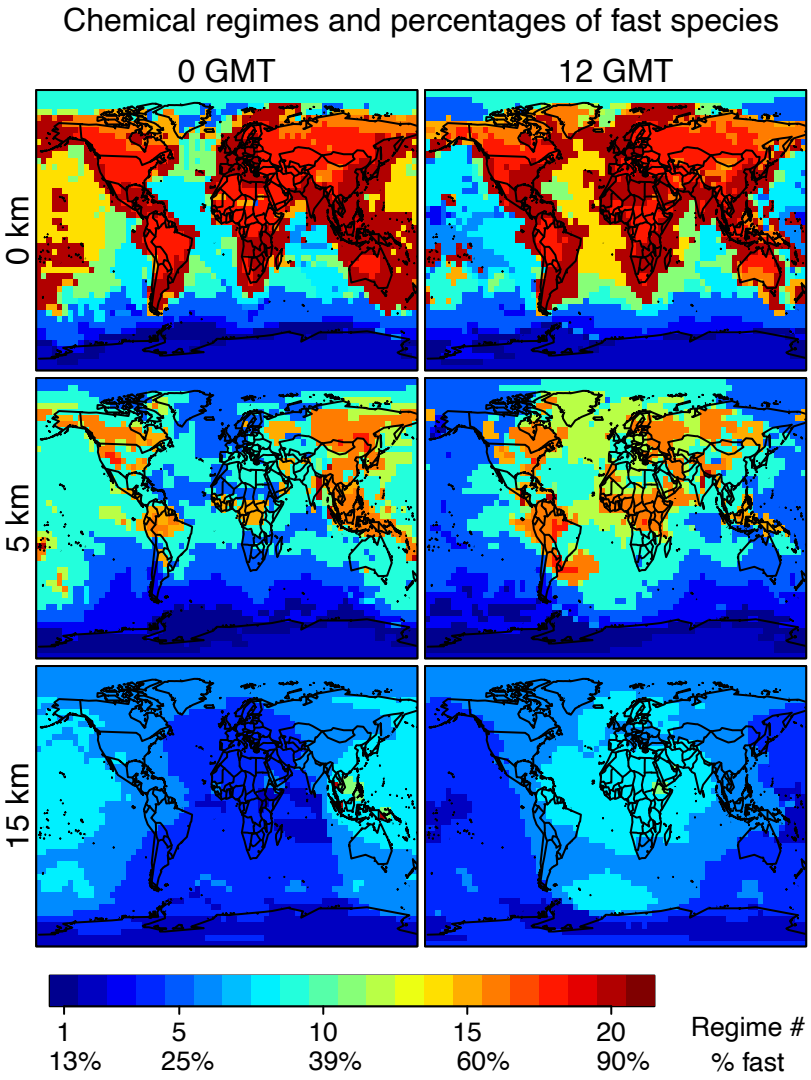


Fig. S3. Chemical mechanism complexity used in the adaptive chemical mechanism in different regions of the atmosphere. The Figure identifies the submechanism from Fig. 5 needed to simulate a given GEOS-Chem gridbox on August 1 2013 at 0 and 12 GMT. The percentage of species treated as fast in that chemical regime is shown on the colorbar and more details are in Table 1. The 21st chemical regime is the full chemical mechanism. We use a threshold δ of 500 molecules cm^{-3} s^{-1} to partition the fast and slow species.

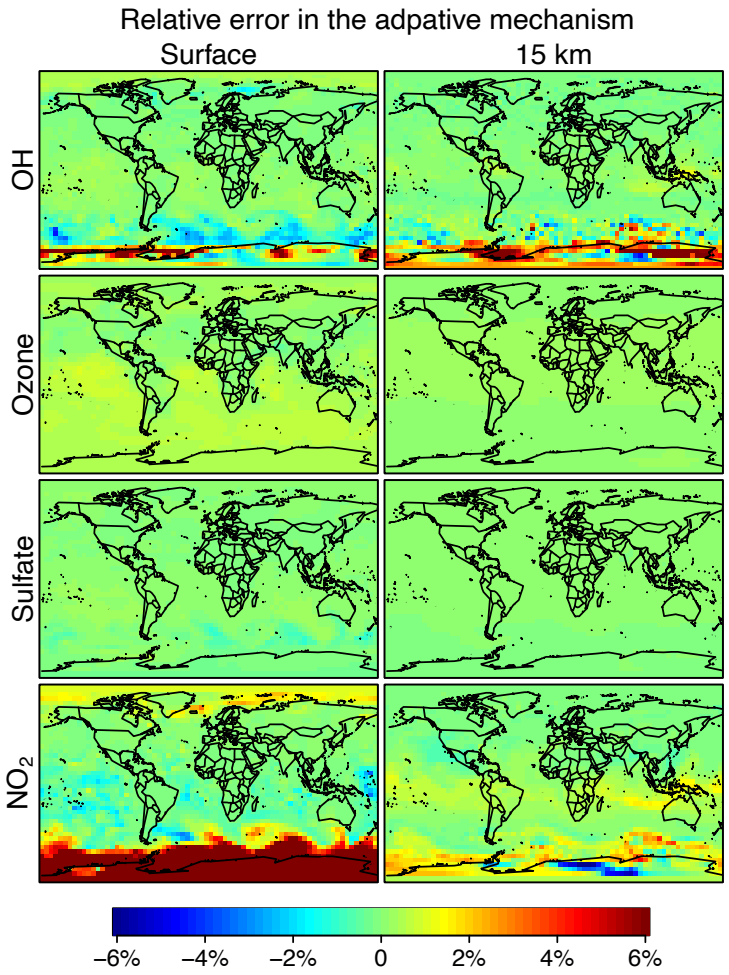
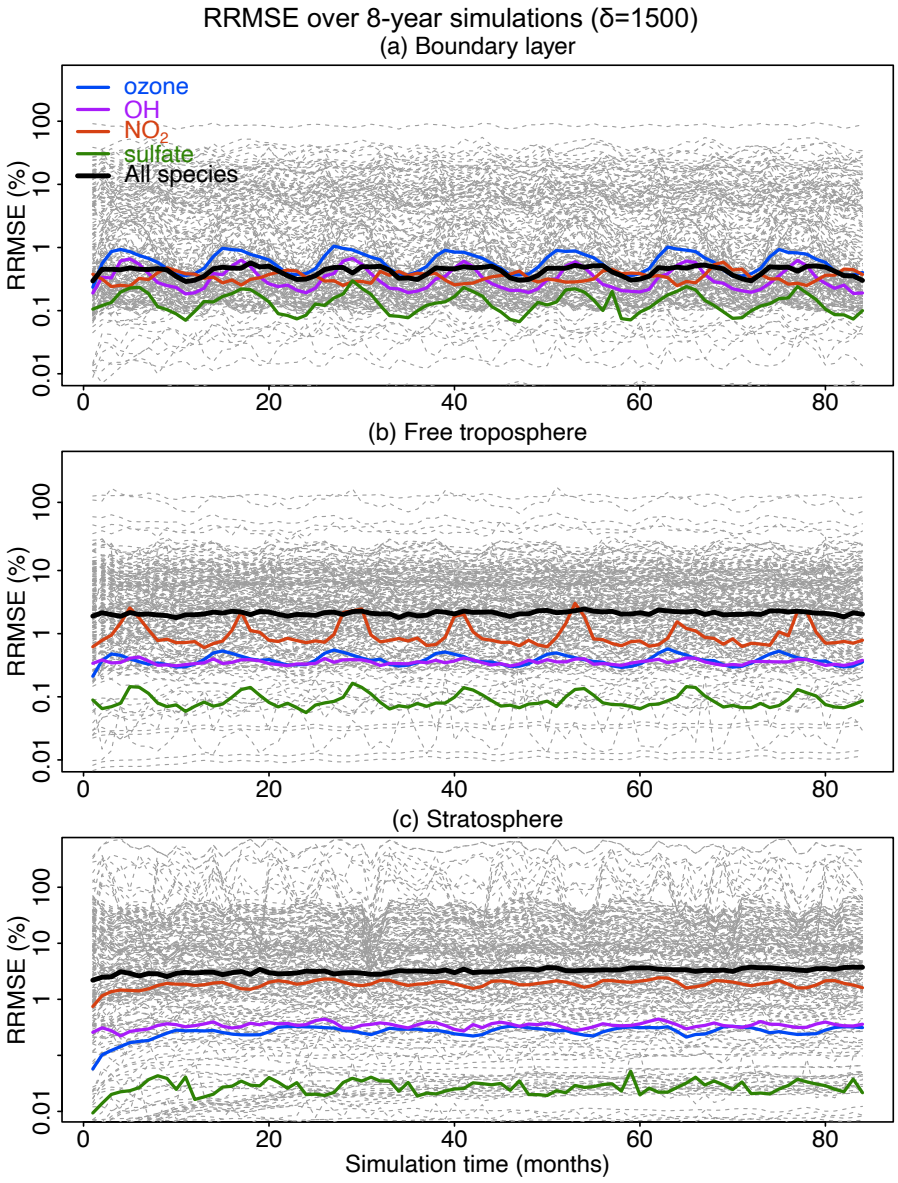


Fig. S4. Relative error from the adaptive mechanism reduction method after three years of simulation in the GEOS-Chem global 3-D model for tropospheric-stratospheric chemistry. The figure shows relative differences of 24-h average OH, ozone, sulfate and NO_2 concentrations relative to the full-chemistry simulation on the last day of the three-year simulation. The calculation removes slow (P and L < 1500 molecules cm^{-3} s^{-1}) and slow reactions (rate < 10 molecules cm^{-3} s^{-1}). The number of blocks (*N*) is 13 and the number of chemical regimes (*M*) is 20.



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25 **Fig. S5.** Same as Figure 7 but we calculate the RRMSE by accounting for gridboxes that can comprise 99% mass in each
26 atmospheric domain (the 99% thresholds are different in different domains in this case), including the (a) boundary layer, (b)
27 free troposphere, and (c) stratosphere.

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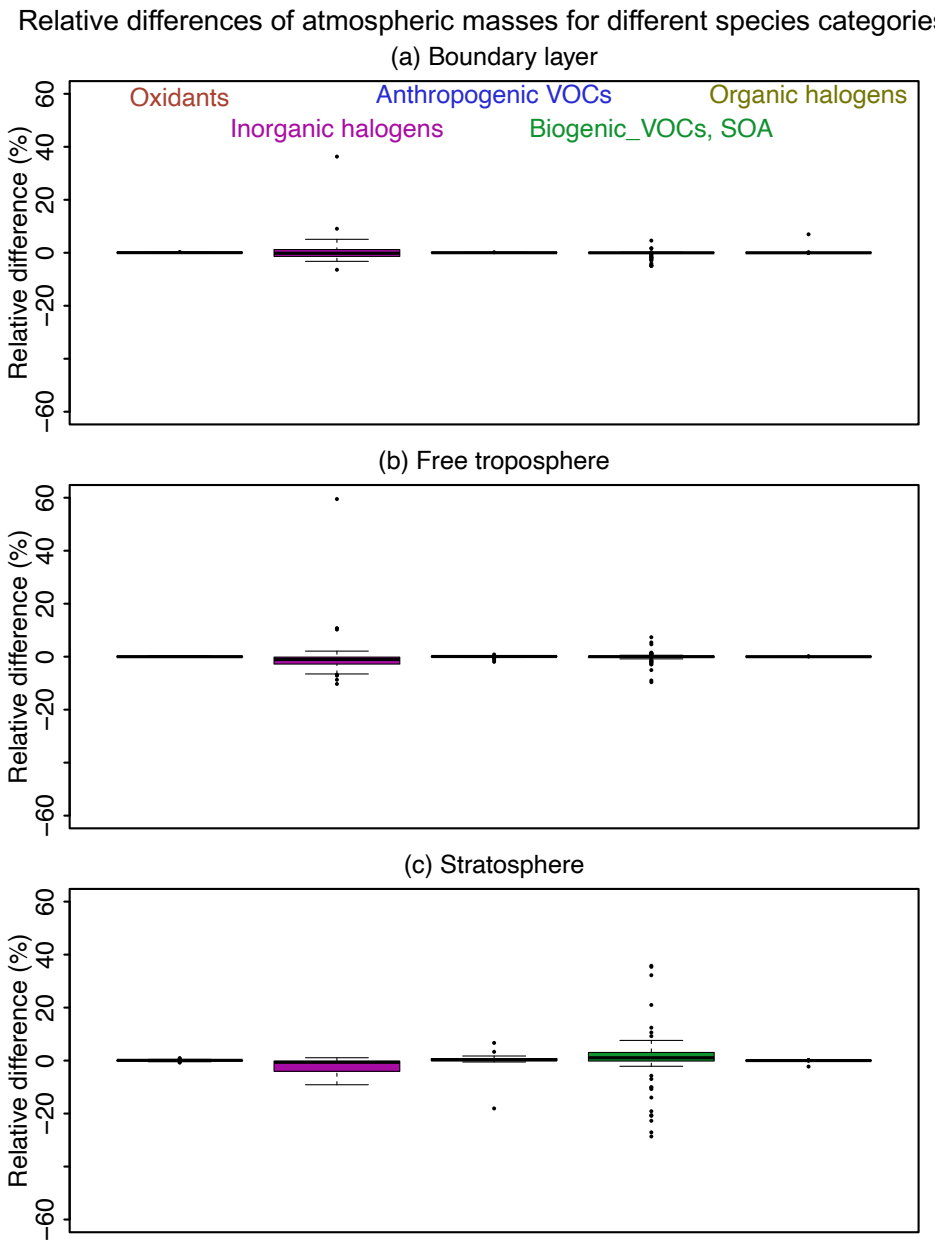


Fig. S6. The relative differences of atmospheric mass (averaged in the 8-year simulations) in the adaptive reduced chemistry mechanism for different species categories in the (a) boundary layer, (b) free troposphere, and (c) stratosphere. The top and bottom of each box are the 25th and 75th percentile, and the centerline is the 50th percentile. We use a threshold δ of 1500 molecules cm^{-3} s^{-1} to separate fast and slow species here.

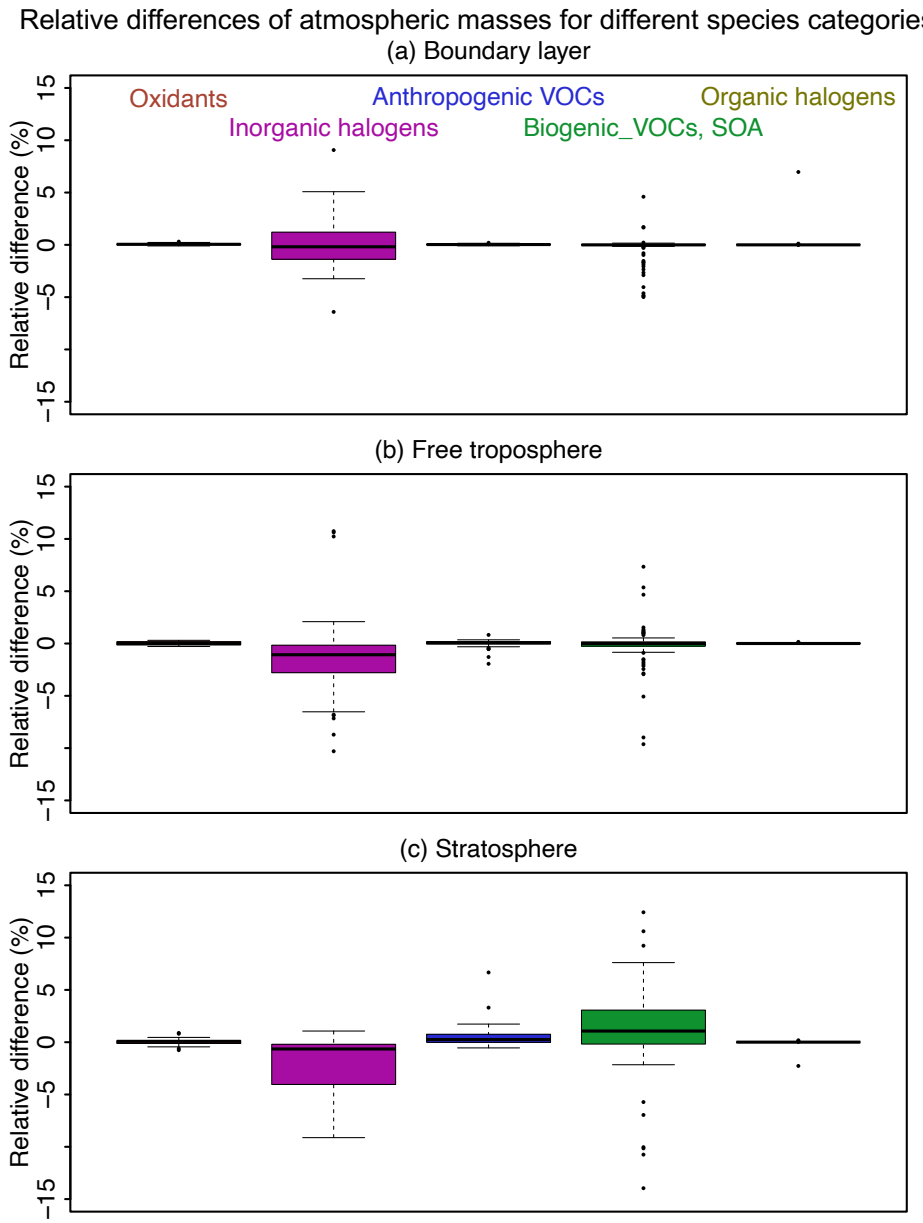
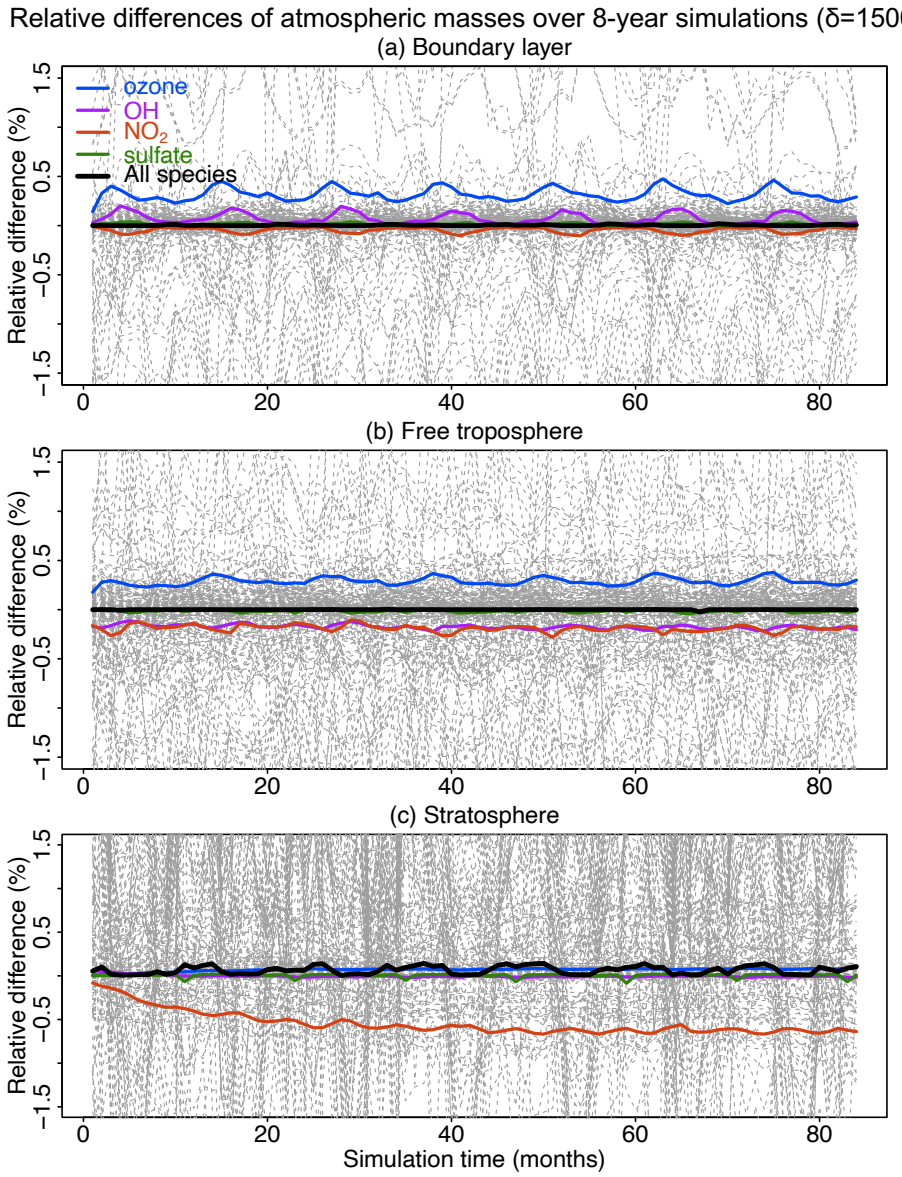


Fig. S7. Same as Fig. S6 but we present more details for the data from -15% to 15%.



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39 **Fig. S8**. Same as Figure 8 but for more details in the range between -1.5% and 1.5%. Results are also shown for the median
40 relative difference across all species in the mechanism and more specifically for ozone, OH, NO_2, and sulfate.

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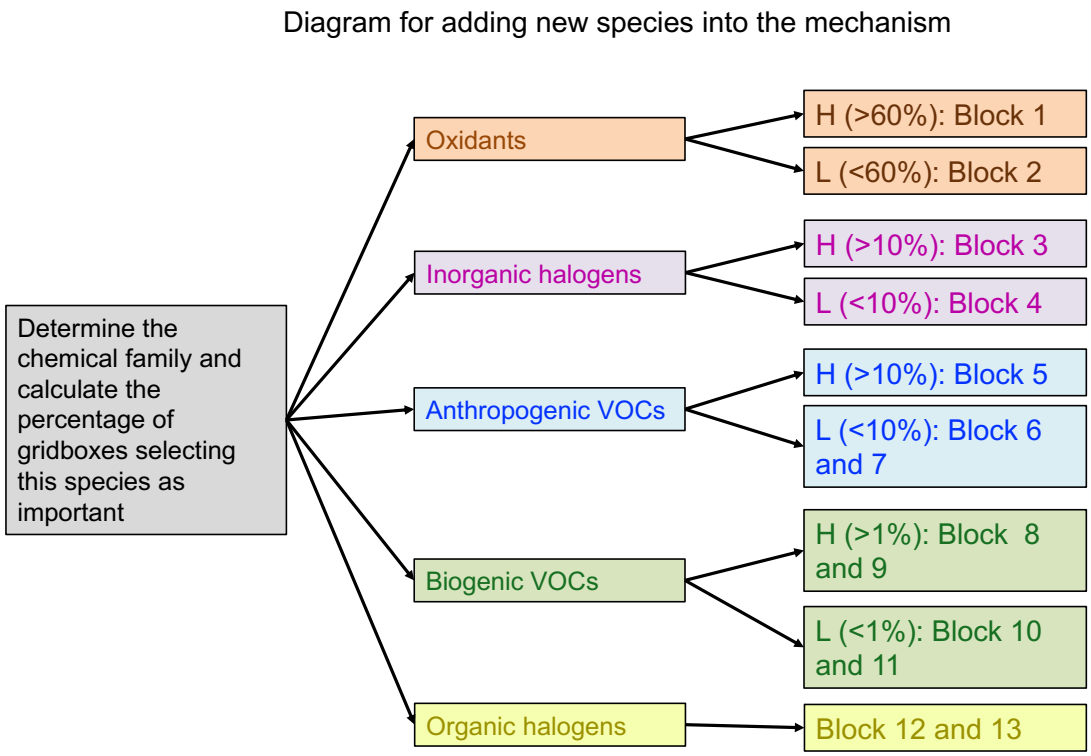

Fig. S9. Diagram of adding a new species to the mechanism. The location of the species is determined by its chemical family and the percentage of gridboxes (in parentheses in the last column) that select this species as fast. 'H' ('L') means higher (lower) percentage of gridboxes that consider this species as fast. We use a threshold of 500 molecules cm^{-3} s^{-1} to partition fast and slow species.

Table S1. Top 10% Species with highest RRMSE and relative mass bias in the boundary layer, free troposphere and stratosphere*.

	RRMSE	Relative mass bias
Boundary layer	I2O4, I2O2, I2O3, IBr, INO, ICl, IONO, OIO, PRPN, HOI, BrSALC, BrSALA, ISNOHOO, IONO2, ISNOOB, I2, PRN1, MAN2, MACRN, MAOPO2, IO	I2O2, I2O3, INO, TRO2, N, XRO2, Cl2O2, IONO, OIO, PRPN, Br2, BrSALC, BrSALA, ISNOHOO, IONO2, ISNOOB, I2, Cl2, PRN1, MAN2, MACRN, MAOPO2
Free troposphere	ISN1OG, I2O4, I2O2, I2O3, INO, ICl, OIO, PRPN, BrSALA, MAOP, ISNOHOO, ISNOOB, I2, PRN1, MAN2, ISNOOA, MACRN, MAOPO2, I, IO, NMAO3, INO2	AERI, ISN1OG, I2O4, I2O2, I2O3, INO, HI, IONO, OIO, HOI, BrSALC, BrSALA, ISNOHOO, ISNOOB, I2, Cl2, PRN1, MAN2, MACRN, I, IO, NMAO3
Stratosphere	ISN1OA, ISN1OG, LVOC, PMNN, MRP, IPMN, MACRNO2, MONITS, GAOO, MVKN, MGLYOO, GLYX, MGLOO, MAN2, MACRN, HCOOH, KO2, MGLY, RIO2, INO2, MRO2	ISN1OA, ISN1OG, DHDC, PRPN, DHPCARP, ISNOHOO, ISNOOB, INPN, I2, PRN1, PROPNN, MAN2, ISNOOA, MACRN, MAOPO2, OLND, OLNN, KO2, NMAO3, ISN1, RIO2, INO2

*The full GEOS-Chem mechanism has 228 species. The full names of these acronyms can be found at http://wiki.seas.harvard.edu/geos-chem/index.php/Species_in_GEOS-Chem.