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UNCERTAINTY IN OZONE CHANGES FROM CONTROL STRATEGY IMPLEMENTATION

Executive Summary

January 2021

COORDINATING RESEARCH COUNCIL, INC.

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The objectives of this study were:

- Estimate the uncertainty in modeled ozone (O_3) changes (ΔO_3) from 2012 to 2020 in eastern Texas due to uncertainty in boundary concentrations (BCs), deposition velocities, emissions, and chemistry.
- Estimate the uncertainty in Relative Reduction Factors (RRFs) for monitoring sites in Dallas-Fort Worth (DFW), Houston-Galveston-Brazoria (HGB), and San Antonio (SAN).

We used the Comprehensive Air Quality Model with Extensions (CAMx) and the Carbon Bond 6 revision 4 (CB6r4) chemical mechanism to simulate O_3 formation in eastern Texas in June 2012 and 2020. (Results for 2020 do not consider the impact of the pandemic.) The input data sets for CAMx were those developed by the Texas Commission on Environmental Quality (TCEQ) for the Texas State Implementation Plan. We also calculated sensitivities to 11 model inputs: O_3 BCs, dry deposition velocities of O_3 and of all other species, DFW anthropogenic nitrogen oxides (NO_x) and volatile organic compound (VOC) emissions, DFW biogenic NO_x and VOC emissions, anthropogenic and biogenic VOC and NO_x emissions outside DFW, all anthropogenic CO emissions, and all inorganic iodine emissions from the ocean. Lastly, we simulated O_3 in 2012 and 2020 using six variations of the CB6r4 chemical mechanism developed in a prior project for TCEQ. Three of these alternative mechanisms represent higher (+1 standard deviation or +1σ) and three represent lower (-1σ) O_3 formation than the standard mechanism.

We estimated uncertainty factors for the 11 model inputs and used these factors plus the sensitivities and results of the simulations with the alternative chemical mechanisms to estimate the uncertainty in the maximum daily average 8-h (MDA8) O_3 concentrations in 2012 and 2020 and the uncertainty in ΔO_3 between these years. The methodology employed builds on previous published work that estimated the uncertainty in 2012 O_3 concentrations.

Some model inputs, e.g. deposition velocities, are the same for both years, and hence we assumed that errors in these inputs are correlated between years, either an over-estimate or an under-estimate by the same percent. For anthropogenic emissions, however, it is not clear to what extent errors are correlated between the two years. E.g., projected anthropogenic emissions for a future year can have errors independent of the errors in the base year due to over- or under-estimating the effects of new emission controls on some sources. Because the amount of correlation is difficult to determine, we considered two cases: Case A, full correlation of errors between years; Case B, no correlation of errors (independent errors). The true situation lies between these extremes.

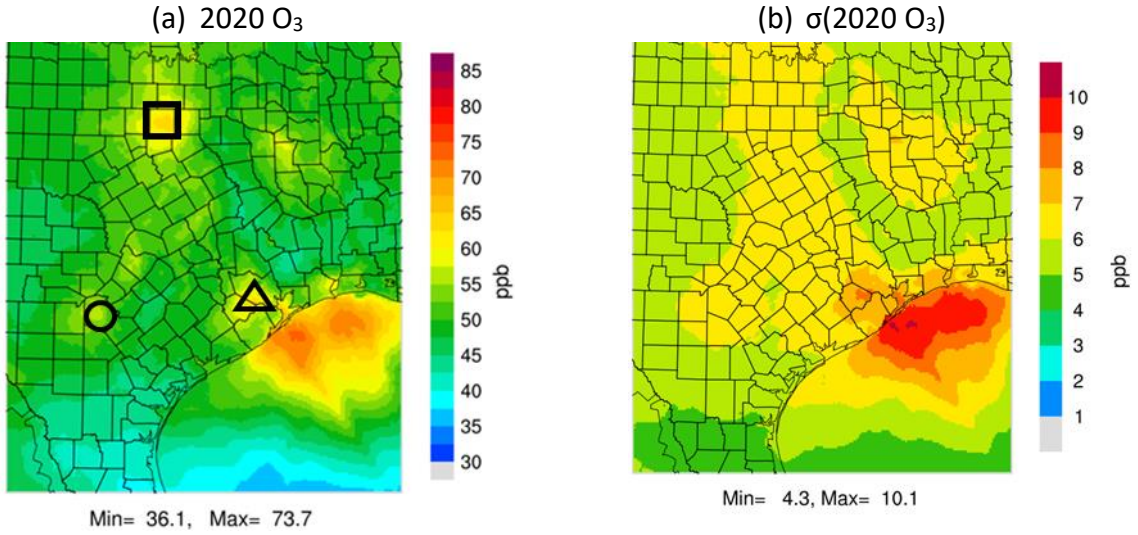

Figure ES-1. (a) MDA8 O_3 concentration in 2020 averaged over the top 10 days in June 2012 and (b) the uncertainty (1σ) in this averaged O_3 concentration. The square, triangle, and circle indicate the locations of Dallas-Fort Worth, Houston-Galveston-Brazoria and San Antonio, respectively. Results do not include the impact of the pandemic.

Figure ES-1 gives the MDA8 O_3 projected for 2020 and the 1σ uncertainty in the concentration. This concentration is an average over the 10 days in June 2012 with the highest observed MDA8 O_3 in eastern Texas (top 10 days). Figure ES-2 displays the ΔO_3 averaged over the top 10 days and the uncertainty in this change assuming Case A or Case B for the anthropogenic emissions. For both Case A and Case B, the uncertainty in ΔO_3 is less than the uncertainty in O_3 because O_3 responds similarly in the two years to input parameter changes and all (Case A) or some (Case B) of the errors are correlated between years. However, the ΔO_3 uncertainty for Case B is larger than that for Case A by a factor of >3, and for Case B, the uncertainties in the anthropogenic emissions dominate the uncertainty in ΔO_3.

An RRF for a monitoring site is defined as $RRF = C_f/C_b$, with C_b and C_f being averages of model results for MDA8 O_3 in the base and future years, respectively. The days and grid cells used for the averages are determined separately for each monitoring site using a procedure defined by the Environmental Protection Agency. The design value for a future year, DVF, is determined from $DVF = RRF \times DVB$. The design value for the base year, DVB, is an average over five years of MDA8 O_3 concentrations measured at the site. We estimated the uncertainty in an RRF by a procedure analogous to that used for ΔO_3 and calculated DVFs for 2020 for all the monitoring sites in DFW, HGB, and SAN. Figure ES-3 presents a comparison of three projections of MDA8 O_3 for 2020 at selected monitoring sites: modeled O_3; DVF; DVB + ΔO_3. The monitoring sites chosen have the largest DVB for 2012 in a city or the second largest. The 2020 O_3 concentrations generally follow the ranking DVF ~ DVB + ΔO_3 > modeled O_3, with some

exceptions for sites not shown. The uncertainties for the DVFs and the DVBs + ΔO_3 obtained with the Case B assumption (shown in the figure) are similar in magnitude for all sites and always smaller than the uncertainties for the modeled O_3. The uncertainties obtained with the Case A assumption are smaller than those for Case B by factors of 3 - 8 for the DVBs + ΔO_3 and by factors of 5 - 33 for the DVFs.

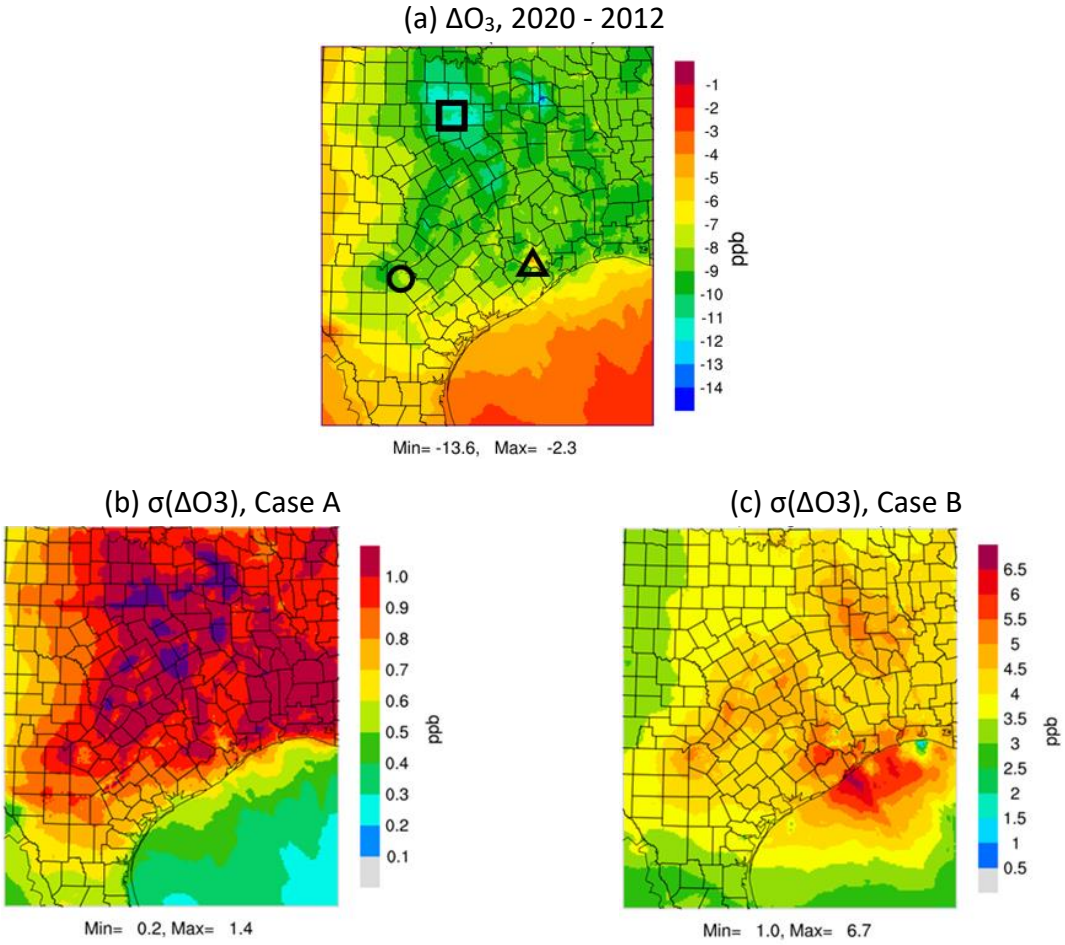

Figure ES-2. (a) MDA8 O_3 change from 2012 to 2020; (b) and (c) uncertainty (1σ) in the O_3 change for Cases A and B. The scales for (b) and (c) differ. Results are for the O_3 change averaged over the top 10 days in June 2012.

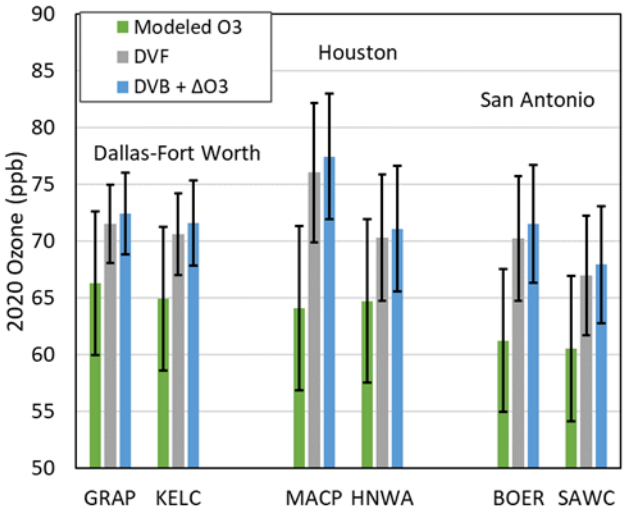

Figure ES-3. MDA8 O_3 at monitoring sites projected to 2020 by three methods: modeled O_3 with 2020 emissions; DVF = relative reduction factor × 2012 base-year design value (DVB); 2012 DVB plus modeled O_3 change. Uncertainty limits are ±1σ and are derived with the Case B assumption for the anthropogenic emissions.

There are some important uncertainties not included in our work. First, there is inherent variability in the meteorology from year to year, but we used the same meteorological inputs for 2012 and 2020, as is standard practice. Based on a recent estimate in the literature, this variability results in an uncertainty of 2 - 5 ppb in the modeled future MDA8 O_3. Second, climate change can cause longer-term changes in the temperature and other features of the meteorology during O_3 episodes. Third, there can be a shift between years to or from drought conditions in different areas of the modeling domain, which can affect biogenic and wildfire emissions and the deposition of O_3 and other species.

The major conclusions of our study are:

- O_3 responds similarly in 2012 and 2020 to changes in model inputs and chemistry. If there is an increase (decrease) in O_3 in the base year for a specific change, there is also an increase (decrease) in O_3 in the future year by a similar amount.
- The uncertainty in ΔO_3 is less than the uncertainty in O_3; in Case A it is 10-20% of the uncertainty in O_3 over most of the domain and in Case B it is 45-75%.
- Over most of eastern Texas, the uncertainty (1σ) in ΔO_3 is 0.6 - 1.4 ppb (Case A) or 3.5 – 6.0 ppb (Case B).
- For monitoring sites in the three cities, the uncertainty in the RRFs is 0.2 - 1.0% of the RRFs (Case A) or 4.8 - 8.5% (Case B).

- The DVF = RRF × DVB and the DVB + ΔO_3 estimates give similar projected 2020 O_3 for the monitoring sites, with the DVFs having smaller uncertainties for Case A and the two estimates having similar uncertainties for Case B.
- The results for Case A and Case B indicate that using DVFs or DVBs + ΔO_3 are likely to produce more accurate predictions of future O_3 than the modeled O_3 itself.
- Improved estimates of the uncertainties in emission inventories and the correlation of uncertainties between years are needed. In particular, determining whether the emission uncertainties are closer to Case A or B is important because with Case A the ΔO_3 and DVF uncertainties are smaller than the estimated uncertainty from the year-to-year variation in meteorology but with Case B they are comparable.

The method developed here can be applied to other regions of the U.S. The important emission sectors would need to be identified, uncertainty factors assigned to them, and, ideally, the degree of correlation of the factors between years estimated. Uncertainty factors for the BCs and deposition velocities might also need to be updated, especially if these model inputs are obtained from new sources. Then, sensitivities to the model inputs would need to be calculated and the model run with alternative chemical mechanisms representing the uncertainty in O_3 resulting from uncertainties in rate constants and stoichiometric coefficients. (Such alternative mechanisms are documented for the CB6r4 mechanism). Lastly, the sensitivities and results from the alternative chemical mechanisms can be processed using straightforward formulas to yield estimates of the standard deviation of O_3 and ΔO_3.