APPENDIX B. ESTIMATION OF UNCERTAINTY IN EMPIRICAL COUNTERFACTUALS

This Appendix was reviewed solely for spelling, grammar, and cross-references to the main text. It has not been formatted or fully edited by HEI. This document was reviewed by the HEI Review Committee.

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The models for counterfactual concentrations have two major sources of uncertainty: the sensitivities of concentrations to emissions and the estimate of emissions changes from actual to counterfactual. Estimates from the distributions of each of these will feed into the model to create different realizations of the counterfactuals. This appendix describes how the distributions are estimated and sampled.

Previous attempts to estimate uncertainty included input from Community Multiscale Air Quality-modeled (CMAQ*) sensitivities. This approach was insufficient for a few reasons. First, CMAQ sensitivities are not directly comparable to empirical sensitivities — CMAQ sensitivities (as calculated) represent the total contribution from a source, and empirical sensitivities are source- and species-specific. While it is possible to produce species-based sensitivities with CMAQ, the empirical sensitivities are estimated using emissions that are highly correlated within source and between species; therefore, the total sensitivity from each source is more informative. However, combining CMAQ sensitivities with empirical sensitivities requires splitting CMAQ sensitivities by species using the empirical fraction, which leads to counterfactuals that do not intuitively match expectations.

* A list of abbreviations and other terms appears at the end of this appendix.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Name</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i$</td>
<td>Ambient concentration species</td>
<td>–</td>
</tr>
<tr>
<td>$j$</td>
<td>Emissions source-species</td>
<td>–</td>
</tr>
<tr>
<td>$J$</td>
<td>Emissions source</td>
<td>–</td>
</tr>
<tr>
<td>$C_i$</td>
<td>Concentration of species $i$</td>
<td>ppb, $\mu g m^{-3}$</td>
</tr>
<tr>
<td>$\beta_{j,i}$</td>
<td>Empirical sensitivity of species $i$ to source-species $j$</td>
<td>ppb ton$^{-1}$, $\mu g m^{-3}$ ton$^{-1}$</td>
</tr>
<tr>
<td>$S_{j,i}$</td>
<td>Empirical total sensitivity of species $i$ to source-species $j$</td>
<td>ppb, $\mu g m^{-3}$</td>
</tr>
<tr>
<td>$S_{J,i}$</td>
<td>Empirical total sensitivity of species $i$ to source $J$</td>
<td>ppb, $\mu g m^{-3}$</td>
</tr>
<tr>
<td>$S_{j,i}^*$</td>
<td>Monte Carlo sampled total sensitivity of species $i$ to source $J$</td>
<td>ppb, $\mu g m^{-3}$</td>
</tr>
<tr>
<td>$S_{j,i}^*$</td>
<td>Fractioned sample sensitivity of species $i$ to source-species $j$</td>
<td>ppb, $\mu g m^{-3}$</td>
</tr>
<tr>
<td>$\beta_{j,i}^*$</td>
<td>Fractioned sensitivity of species $i$ to source-species $j$</td>
<td>ppb ton$^{-1}$, $\mu g m^{-3}$ ton$^{-1}$</td>
</tr>
</tbody>
</table>

Table B.1. Definitions of variables used in the models

* A list of abbreviations and other terms appears at the end of this appendix.
Statistical Pollutant Sensitivity Models

In the model used to relate pollutant concentrations to emissions, after controlling for meteorology, each ambient pollutant concentration ($C_i$, where $i$ is $O_3$, $PM_{2.5}$ etc.) is modeled as a function of source-specific species emissions (e.g., $E_{EGU}^{NOx}$, $E_{EGU}^{SO2}$, $E_{MOB}^{NOx}$, etc., where $EGU$ is electricity generating unit and $MOB$ is mobile):

$$C_i = \beta_0 + \beta_{EGU NOx,i} f_{EGU NOx,i}(E_{EGU}^{NOx}) + \beta_{EGU SO2,i} f_{EGU SO2,i}(E_{EGU}^{SO2})$$

$$+ \beta_{MOB NOx,i} f_{MOB NOx,i}(E_{MOB}^{NOx}) + \cdots + \alpha M$$

Where $\beta_{0,i}$ is the intercept, $\beta_{j,i}$ is the sensitivity of $C_i$ to each function $f_{j,i}()$ of source-specific species emissions, $E$:

$$f_{j,i}() = E_j(a + bPS^*)$$

$PS^*$ is the metric for atmospheric photochemical state, $a$ and $b$ are determined in the regressions, and $b$ is equal to zero for many of the pollutants. $\alpha M$ is the contribution of daily meteorology. One exception for the definition of $f_{j,i}()$ is the interaction of mobile oxides of nitrogen (NOx) and volatile organic compound (VOC) emissions ($E_{MOB}^{NOx}$ & $E_{MOB}^{VOC}$) in the regression for ozone:

$$f_{MOB NOx MOB VOC,i}() = E_{MOB NOx} E_{MOB VOC}(a + bPS^*)$$

Empirical Source-Specific Sensitivities

Source-specific sensitivities are estimated by multiplying each $\beta_{j,i}$ by the associated emission term and summing the results, giving units of concentration (keep in mind the distinction between the sensitivity to a source $S_{j,i}$ and the sensitivity to a source-species $s_{j,i}$ — see Table B.1). For instance, the sensitivity of $C_i$ to all EGU emissions (we consider EGU NOx and SO2 emissions) is:

$$S_{EGU,i} = s_{EGU NOx,i} + s_{EGU SO2,i} = \beta_{EGU NOx,i} f_{EGU NOx,i}(E_{EGU}^{NOx}) + \beta_{EGU SO2,i} f_{EGU SO2,i}(E_{EGU}^{SO2})$$

Counterfactual concentrations are estimated using the $s_{j,i}$’s and counterfactual emissions. The uncertainty in counterfactual concentrations, therefore, comes from both $s_{j,i}$ and emissions.
Estimating Uncertainty in Sensitivities

Each regression parameter in Equation 1 has an associated distribution, and these distributions were sampled simultaneously using information in the variance–covariance matrix of the regression.

Uncertainty in Emissions

The estimate of the change in emissions for each intervention is the other source of uncertainty in the final model. This is separate from (though not completely independent of) an estimate in the uncertainty in total emissions. Uncertainty in total emissions comes from uncertainty in instrument measurements for in EGUs and parameterizations in MOVES2010b, which was the model for MOB emissions (U.S. EPA 2012). Uncertainty in the change in emissions comes from our method to estimate the counterfactuals.

EGU Emissions

Uncertainty is estimated from the estimate of standard error in the mean load-based emissions factor at the beginning of the period.

Our estimate of uncertainty in $\Delta E_{\text{EGU}}$ will come, primarily from two sources: the estimate of the 1995 emissions factor used to estimate the counterfactual, and uncertainty in attributing reductions to specific control and/or regulatory program. Uncertainty in the 1995 emissions factor (EF$_{1995}$) for NO$_x$ and SO$_2$ will come from sampling a distribution around the mean. This distribution (Figure B.1 for NO$_x$) will be sampled from when estimating the 5,000 realizations of the counterfactuals for use in the health analysis. The approach is identical for SO$_2$.

Mobile Emissions

Uncertainty in mobile emissions is more difficult to estimate than in EGU emissions. The approach up to this point has been to sample a ±50% uncertainty around the original estimate of $\Delta E_{\text{MOB}}$. However, this estimate is likely too high based on emissions-concentration estimates in prior work at Georgia Tech and others (Blanchard et al. 2012; Pachon 2011), and we are investigating alternative estimates of the change in mobile emissions over time.
Figure B.1. NOx emissions. Counterfactual emissions are estimated by multiplying the mean emissions factor in 1995 (EF$_{1995}$) by the daily load. A 95% confidence interval around the mean EF$_{1995}$ produces the above distribution of counterfactuals. Note: 2015 data is only through March.

Monte Carlo Sampling

The two distribution groups — the first from $\Delta E$ and the second from the sensitivities — were sampled 5,000 times and used in each of the species models in a Monte Carlo approach to estimate 5,000 alternative counterfactual outcomes for the EGUMOB. The approach allows for uncertainty distributions to be estimated for counterfactuals relating to any combination of regulatory programs.
Figure B.2. Monthly-averaged observed and distributions of counterfactual O₃ for three scenarios.
Figure B.3. Monthly-averaged observed and distributions of counterfactual NO$_2$ for three scenarios.
Figure B.4. Monthly-averaged observed and distributions of counterfactual CO for three scenarios.
Figure B.5. Monthly-averaged observed and distributions of counterfactual SO\textsubscript{2} for three scenarios.
Figure B.6. Monthly-averaged observed and distributions of counterfactual PM$_{2.5}$ for three scenarios.
Figure B.7. Monthly-averaged observed and distributions of counterfactual SO$_4^{2-}$ for three scenarios
Figure B.8. Monthly-averaged observed and distributions of counterfactual NH$_4^+$ for three scenarios.
Figure B.9. Monthly-averaged observed and distributions of counterfactual NO$_3^-$ for three scenarios.
Figure B.10. Monthly-averaged observed and distributions of counterfactual OC for three scenarios.
Figure B.11. Monthly-averaged observed and distributions of counterfactual EC for three scenarios.
References


Abbreviations and Other Terms

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>CMAQ</td>
<td>Community Multiscale Air Quality</td>
</tr>
<tr>
<td>EGU</td>
<td>electricity generating unit</td>
</tr>
<tr>
<td>MOB</td>
<td>on-road mobile</td>
</tr>
<tr>
<td>MOVES</td>
<td>U.S. EPA MOtor Vehicle Emissions Simulator</td>
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