An Approach for Determining Optimal Control Strategies for Energy System Emissions of Ozone Precursor Gases


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Objective

Optimize *ozone benefits* to human health & ecosystems of potential *energy systems emissions reductions* which could achieve regulatory endpoints through *efficient sensitivity analysis*.
Method

Create base case
(2007 12-km CONUS, 2007 NEI emissions)

Execute CMAQ
(6 mn ozone concentrations)

Calculate exposure effects
(health, ecological)

Calculate change of impact with concentration
($\partial J/\partial C$)

Optimize emissions weighted by effects

$\partial J/\partial (\text{emissions})$

$\text{emissions, met}$

concentration (C)

cost function ($J$)

$\text{largest } \Delta J/\Delta (\text{emissions})$
Method

1. Create base case (2007 12-km CONUS, 2007 NEI emissions)
2. Execute CMAQ (6 mn ozone concentrations)
3. Calculate exposure effects (health, ecological)
4. Calculate change of impact with concentration (∂/∂O\textsubscript{3})
5. Execute CMAQ adjoint
6. Optimize emissions weighted by effects
7. Calculate change of impact with concentration (∂/∂(emissions))

largest ∆J/∆(emissions)

cost function (J)

concentration (C)
Quantifying Ozone Disbenefits

Agricultural

Estimate reduced productivity of five crops from cumulative exposure of crops to ozone, expressed as W126.

Ecosystems

Evaluate biomass reduction from exposure of timber to ozone, expressed as W126, for eleven species.

Human Health

Approximate mortalities attributable to ozone through population-weighted exposure metric.

MARKAL

CMAQ adjoint

Ozone Effects
Estimating Premature Mortality

\[ \Delta M = M_0 P \left( 1 - e^{-\beta \Delta C} \right) \]

where \( M_0 \) is the baseline mortality, \( P \) is the exposed population over 30 years old, \( \beta \) is 0.0427% per ppb \( O_3 \), and \( C \) is the 6-month mean of hourly maximum \( O_3 \).

(BenMAP, Jerrett et al., 2009)
Ecosystem Ozone Exposure Metric

Relative yield loss (RYL) as a function of the W126 ozone exposure metric has been empirically determined for 5 crops and 11 tree species.

Multiplying RYL by the productivity determines the potential productivity loss (PPL) of each species.

The formula for W126 is:

$$W_{126,90\text{ day}} = \left[ \sum_{i=1}^{90} \left( \frac{[O_3]}{1 + (4403e^{-126[O_3]})} \right) \right]_{i,8\text{am}-8\text{pm}}$$

$$R\text{YL} = 1 - \exp \left[ - \left( \frac{W_{126}}{A_i} \right)^{B_i} \right]$$

Legend:
- Red: Cotton
- Orange: Maize
- Blue: Potato
- Green: Soybean
- Brown: Wheat

AOT40

- Red: Cotton
- Orange: Maize
- Blue: Potato
- Green: Soybean
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W126

- EPA (2007)
- Mills et al. (2011)
Crop Degradation by Ozone Exposure

Crop Production

USDA National Agricultural Statistics Survey (NASS) 2007 crop production distributed in accordance with the Biogenic Emissions Landuse Database (BELD) v.4

Degradation Rate

Time-averaged degradation rate over the 3-month growing period.
Timber PPL by Ozone Exposure

Tree Biomass Distribution

USDA Forest Inventory Analysis tree biomass distributed in accordance with the National Land Cover Database; MODIS-derived image composites and percent tree cover; and other geographic and climatological parameters.

Potential Productivity Loss (PPL) Rate

Time-averaged degradation rate over the 3-month growing period.

Blackard et al., 2008, Remote Sensing of the Environment
Connecting Ozone Effects to Emissions with CMAQ adjoint

\[ \frac{\delta(O_3 \text{ effect})}{\delta(\text{emissions})} = \frac{\partial}{\partial (\text{emission} \ \text{parameters})} \left( \frac{\partial}{\partial (\text{modeled} \ \text{concentrations})} \right) \]

\[ \delta \bar{x} = (F')^T(x, \delta y) \]

- MARKAL
- CMAQ adjoint
- Ozone Effects

\[ \delta(\text{Health Disbenefit}) \]
\[ \delta(\text{Crop Yield Losses}) \]
\[ \delta(\text{Ecosystem Service Losses}) \]
Proof of Concept Scenario

Ozone Concentration

June 11-24, 2007
CMAQ 4.7.1 adjoint
WRF meteorology
2007 National Emissions Inventory
Sensitivity of Mortality to Emissions

\[ \Delta M = M_0 P (1 - e^{-\beta \Delta C}) \]

\[ \partial J = \left[ \frac{\partial (\text{mortality})}{180} \right]_{\max \ 1\text{-hr} [O_3]} \]
Emissions Influences on Mortality

Urban nature of the cost function leads to negative influence of NOx and positive influence of VOCs on mortality.
Emissions Influences on Corn PPL

Small VOC-limited regime near Chicago leads to negative influence of NOx emissions from this location. Otherwise, NOx contributes to the ozone that reducing biomass yield of corn.

Isoprene & ethane have similar levels of influence on corn degradation.
Emissions Influences on Tulip Poplar PPL

More rural nature of cost function leads to positive contributions for NOx & VOCs. Isoprene & ethane differ by orders of magnitude in influence.
Health & Ecosystem Responses to NOx Differ Significantly

Mortality

Tulip Poplar

\[ \frac{\delta [\text{Tulip poplar PPL}]}{\delta [\sigma_{\text{emis, NOx}}]} \text{ (tons %)} \]

Corn

\[ \frac{\delta [\text{Corn PPL}]}{\delta [\sigma_{\text{emis, NOx}}]} \text{ (bu %)} \]
Capabilities & Next Steps

- Assessed the rate of degradation of human mortality, crop productivity, and timber biomass with O$_3$ exposure.
- Determined relative influence of NOx and various VOC emissions on these end points for a brief episode in June 2007.
- Confirmed hypothesis that emissions controls can benefit human health differently than ecosystems.

- Complete the modeling of May-August 2007.
- Connect the NOx emissions influences to the MARKAL framework for propagating the influence of energy sector emissions changes on ozone benefits.
Based on W126 calculated from summer 2007, potential productivity loss rates can be applied for each specific day of the early June episode.

Through the adjoint, these are related to the influence of emissions of each species.
Emissions Influences on Red Maple Biomass PPL

\[ \frac{\delta \text{[Red Maple PPL]}}{\delta \text{[NOx emis]}} \text{ (tons tons}^{-1}) \]

\[ \frac{\delta \text{[Red Maple PPL]}}{\delta \text{[toluene emis]}} \text{ (ton ton}^{-1}) \]

\[ \frac{\delta \text{[Red Maple PPL]}}{\delta \text{[isoprene emis]}} \text{ (ton ton}^{-1}) \]
Connecting Ozone Effects to Emissions with CMAQ adjoint

Spatial Distribution of Relative Contributions

\[ \frac{\partial (\{O_3, \text{exposure}\})}{\partial (\text{emissions})} \]

Modeling domain: Continental US

2007

image credit: Google Earth; adapted from Daven Henze’s representation of sensitivity methods
USDA National Agricultural Statistics Survey (NASS) 2007 crop production distributed in accordance with the Biogenic Emissions Landuse Database (BELD) v.4
Effects of Ozone Exposure on Crops

\[ \partial J = \frac{\partial W_{126}}{\partial C_{O_3}} \frac{\partial Y_{RL}}{\partial W_{126}} \frac{\partial Y_{L}}{\partial R_{YL}} \]