Comparison of model estimates of background ozone concentrations based on zero-out and source apportionment modeling

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Introduction / Goal

- It is well-established that background ozone (BGO3) sources and processes can influence surface ozone concentrations over parts of the U.S.
  - Accurate estimates of BGO3 are needed to craft effective control programs
  - Clear example of AQAST success in informing air quality management

- There are several complexities associated with background ozone:
  - Definitions of background can vary
  - Impacts vary greatly across space/time
  - Generated by a variety of processes
  - Difficult to measure. Typically requires air quality modeling.
  - Non-linear ozone chemistry complicates identification of background influence

- Two separate methodologies for estimating background ozone are compared in this analysis:
  - Zero out modeling
  - Source apportionment modeling
EPA has characterized BGO3 for a 2007 simulation using two separate model methodologies which define background differently.

Zero out / emissions perturbation analyses (ZO):
- What would model ozone be in the absence of certain sets of ozone precursor emissions?
- Approach is frequently used to estimate BGO3.
- When coupled with a global model, allows flexibility in defining background (NB, NAB, USB).
- Counterfactual scenario has limited policy application.

Source apportionment analyses (SA):
- How much of the current (modeled) ozone is formed due to emissions from certain sources?
- Approach is widely used in estimating manmade source contributions; less ozone used for BGO3.
- Assessment of BGO3 is limited to influence of boundaries and other specified sources within the domain.
- Potentially more policy-relevant but substantial pressure on model tagging technique.

Combining results from two methodologies may help expand characterization of BGO3.
Two sets of regional-scale (12km) analyses were conducted to estimate BGO3 levels at locations across the U.S.

- Model configurations were similar between the two sets:
  - Meteorological inputs from WRF model.
  - Emissions based on 2008 NEI version 2; climatological-average wildfire emissions.
  - Boundary conditions based on GEOS-Chem 2.0 x 2.5 degree global modeling.

- Four CMAQ zero out runs were completed using four separate boundary conditions
  - Base simulation
  - Natural background: global anthropogenic precursors removed + pre-industrial CH4 levels**
  - N. American background: anthropogenic precursors removed in N. America
  - U.S. background: anthropogenic precursors removed in United States

- One CAMx source apportionment run was completed using the base boundary conditions.
  - 11 categories were tracked: 5 boundaries, U.S. anthropogenic emissions, and 5 in-domain sectors (Can/Mex, fires, biogenics, C3 marine, GoM platforms)
  - The CAMx modeling used the APCA approach which attributes O3 production to manmade sources from combinations of anthropogenic & biogenic emissions

Model performance was evaluated and both models reproduced seasonal mean MDA8 ozone levels with little bias (CMAQ: +3.5, CAMx: +0.5 ppb)
Difference in “USB” estimates:
(as a function of base model ozone level)

**ZO ratios of USB / total O3:**
Proportion of BGO3 drops as base model ozone increases.
Because of non-linear ozone, is possible to have ratios > 1.0

**SA ratios of non US / total O3:**
Proportion of BGO3 drops as base model ozone increases, even more steeply than ZO.
Not possible to have ratios > 1.0
In cases where MDA8 O3 > 70 ppb, typically < 50% of ozone is due to emissions other than US anthro
Model estimates of seasonal mean MDA8 ozone from “USB”

Zero out modeling (CMAQ) estimates of USB
USB ~ 40-45 ppb in WUS
USB ~ 30-35 ppb elsewhere

Source apportionment (CAMx) estimates of apportionment-based USB
USB ~ 35-40 ppb in WUS
USB ~< 30 ppb elsewhere
**Unadjusted** differences between ZO and SA:

ZO model estimates of BGO3 are 5-10 ppb higher than SA estimates over SJV and Great Plains/Midwest. Practical impacts of differences are small.

**Bias-adjusted** differences between ZO and SA

Accounting for model seasonal mean MDA8 O3 biases results in even closer estimates of the influence of non-U.S. sources

**Bias** in the seasonal mean MDA8 is calculated and equally assigned to USB and non-USB portions of total ozone based on USB/total ratio.
Once the bias adjustment is applied to account for base CMAQ and CAMx predictions, the greatest differences between the two estimates occur in urban areas with periodic NOx suppression of ozone (e.g., Los Angeles, Bakersfield).
Conclusions

- Two separate modeling analyses were conducted to estimate the influence of sources other than U.S. anthropogenic emissions across the U.S.

- Defining background as the $O_3$ that would remain after U.S. anthropogenic emissions are removed (zero out) typically results in a higher estimate of USB than when the influence of non-U.S. sources is estimated via source apportionment.
  - Adjusting the results for differences in base model predictions narrowed the differences between the two methodologies.

- Even after bias adjustment, there was a tendency for the zero out approach to estimate higher USB background levels in urban areas with significant NOx.
  - Zero out approach reveals “latent” background

- The use of two separate methods bolsters confidence in the BGO3 estimates, given their generally similar results.
BGO3 recommendations for AQAST
(national AQM perspective)

• Many recent modeling analyses have characterized influence of BGO3:
  o Emery et al., (2012): 2006 CAMx zero out
  o Lin et al., (2012): 2010 GFDL AM3 zero out and tracers
  o WRAP (2013): 2008 CAMx source apportionment
  o Lefohn et al., (2014): 2006 CAMx source apportionment
  o USEPA (2014): 2007 CMAQ zero out and source apportionment

• All confirm the general nature of BGO3 and have informed policy discussion:
  o Mean values of USB range from 25-50 ppb, higher in discrete events
  o BGO3 is particularly problematic in the intermountain WUS in spring/summer
  o BGO3 comprises a larger portion of total ozone as U.S. emissions are (have been) reduced

• Suggestions for focus of next generation analyses:
  o Efforts to quantify individual components of BGO3 (fire, strat, Asia, methane, etc.)
  o Efforts to quantify BGO3 in future years (influence of emissions/climate changes)
  o Look for opportunities to “ground truth” model estimates of BGO3 w/ observations
  o Development of model tools that allow for unified hemispheric/regional modeling