Comments to
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2nd External Review Draft
Integrated Science Assessment for Ozone and Related Photochemical Oxidants
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Modeling Uncertainties Related to Estimates of North American Background Ozone

Christopher Emery (cemery@environcorp.com)
ENVIRON International Corporation

The EPA has relied on global modeling to establish the range of North American Background (NAB) ozone. Global models have improved greatly over the years, with advancements in spatial resolution, emission estimates, tropospheric chemistry, and the driving meteorological analyses. According to the current ISA draft, recent high-resolution versions of GEOS-Chem are predicting higher NAB estimates than older low-resolution versions. But while monthly means and unpaired (in time) frequency distributions of daily maximum 8-hour ozone are shown to be fairly well replicated across the US, observed ozone levels greater than 60 ppb continue to be consistently under predicted and time-paired comparisons show low correlations (Zhang et al., 2011). Observational research has routinely reported more natural short-term variability than global modeling predicts, with higher background ozone events (often exceeding 50 ppb) and more evidence of stratospheric intrusion in the winter and spring seasons (Yienger et al., 1999; Lefohn et al., 2001; Cooper et al., 2005; Hocking et al., 2007; Oltmans et al., 2008; Langford et al., 2009).

ENVIRON has recently completed 2006 annual modeling of North America using the CAMx and CMAQ regional transport models at 12 km resolution, with GEOS-Chem providing boundary conditions (Emery et al., 2012). Compared to previous GEOS-Chem runs, our regional modeling showed improved paired performance in replicating ozone measurements, particularly at the upper end of the frequency distribution, and predicted higher NAB ozone. Together with the results of Zhang et al. (2011), our analyses have demonstrated that simulated NAB levels are strongly influenced by model resolution – it is a source of first-order uncertainty. Earlier research with GEOS-Chem suggested little sensitivity to resolution, but that conclusion was likely clouded by compensatory errors and a tendency to focus on seasonal means. Higher resolution directly impacts the characterizations of complex terrain; regional weather features that drive deep three-dimensional circulations; and the distribution of natural sources (e.g., fires and lightning NOx). Furthermore, higher temporal resolution needs to accompany higher spatial resolution to adequately characterize the evolution of the more spatially resolved circulations systems. One-hour frequency used in the regional models is superior to the six-hourly frequency used in global models.

NAB estimates from global and regional models are increasing and converging to a more credible characterization, and there is a point of diminishing returns; but we have yet to reach it. Further refinement is limited by higher order sources of model uncertainties that have become increasingly evident with higher resolution applications. These issues are not all separable, as many are inter-dependent across models and processes. Today I will discuss some of the major modeling uncertainties that need to be addressed to close toward an improved characterization of NAB ozone.

First, vertical resolution is just as important as horizontal resolution, as appropriately mentioned in the current ISA draft. While stratosphere-troposphere exchange is often associated with highly localized and transient events, it can influence tropospheric ozone levels over large spatial and temporal scales, so it needs to be accurately modeled. Poor vertical resolution adds significant uncertainty to model estimates of stratospheric ozone contributions to the NAB. Indeed our modeling has demonstrated a need to maintain high vertical resolution near the tropopause (8-11 km altitude) to properly treat this exchange throughout the year, and specifically to better capture tropopause folding events. Additionally, higher resolution reduces numerical diffusion, which we show is rather problematic in artificially transporting large stratospheric ozone gradients into the troposphere, particularly over high terrain. The vertical transport algorithms in both CAMx and CMAQ have been improved recently to dramatically reduce numerical diffusion, but our modeling shows that it continues to be an issue when traditional layer structures are employed with layers 2-4 km thick spanning the tropopause.

Second, regional models do not contain stratospheric chemistry mechanisms, and thus cannot chemically maintain a stratosphere. The stratosphere in these models is defined by lateral boundary conditions from global models. In our modeling we have seen instances of spurious evacuation or buildup of ozone in the topmost layers, usually associated with tropopause folding events. This is related to several issues: (1) use of a simple top boundary condition treatment; (2) lateral fluxes that cannot balance the vertical transport; and (3) use of just a few thick layers that cannot adequately resolve the dynamics around the tropopause and result in excessive numerical diffusion. These issues can be mostly alleviated by explicitly accommodating top boundary conditions from global models, and employing higher layer resolution. For much larger domains, such as hemispheric CMAQ applications, an explicit stratospheric chemistry mechanism is needed.

My third and final point relates to two natural sources of ozone that are increasingly recognized as imparting a significant influence on NAB ozone: wildfires and lightning NOx. Fires have had an insufficient effect in GEOS-Chem because they are not well resolved in space and time and do not include all of the VOC chemistry. The regional models resolve the fires and associated chemistry much better, but simply account for fire plume rise by injecting emissions according to a highly parameterized vertical profile. The models themselves do not account for fire convection nor smoke shading, and we believe this can lead to large over predictions of boundary layer ozone.

Lightning NOx is based on simple parameterizations, usually keyed to some type of meteorological evidence for convective activity to specify location, timing, and flash rates, while constraining NOx yields according to gross observational evidence. This highly uncertain process needs refinement, preferably through reconciliation with event-specific data from lightning detection networks or other commonly available sources. Additionally, meteorological models output very limited information on convective activity and so such conditions need to be re-diagnosed within the air quality models. It is important to note that meteorological models such as MM5 and WRF have been shown to consistently over predict convective activity throughout the US, especially in the southwest and southeast. If such information were passed directly to the regional models, it would be important to limit the influence of any over predicted activity. Besides impacting lightning NOx estimates, convection contributes to vertical transport of ozone between the upper troposphere and the boundary layer.

Model evaluations to date have appropriately focused on comparisons of total ozone against surface observations in rural areas across the US. While such comparisons can shed some light on uncertainties in modeled NAB estimates, we are unable to discern the extent to which compensating errors may affect various processes important to NAB concentrations and their variability. Focused, process-oriented analyses help to answer the following questions:

- How well does modeling represent each process (emissions, transport, stratospheric intrusion, chemistry, and removal)?
- How well does the model reproduce natural ozone events according to conceptual models derived from observational analyses?
- How do the largest model uncertainties each impact total ozone, NAB, and source attribution estimates?

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