Comments to
EPA Clean Air Scientific Advisory Committee, Ozone Review Panel
1st External Review Draft
Risk and Exposure Assessment for Ozone
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Use of Rollback and Other Means in the Assessment of Risk

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My comments focus of the approach to project urban air quality data for the purposes of calculating city/population-specific health risks, as described in the First External Draft of the Health Risk and Exposure Assessment (REA), as well as in supporting documentation on the quadratic rollback technique (Wells et al., 2012) and the proposed model-based rollback technique (Simon et al., 2012). Overall, the first draft REA is difficult to follow given omissions to be completed in later drafts, several mislabeled references to other sections and appendices, the reliance on references to external documentation, and inconsistencies in various details between the REA and referenced supporting documentation. After carefully reviewing all three cited documents, I believe that I have a basic understanding of the techniques employed for the first draft REA and the proposed model-based rollback to be employed for future drafts. Comments below reflect my current general understanding of the process and may be subject to inaccuracies in certain details.

An expanded set of written comments will be submitted to the REA Docket by the October 12, 2012 deadline.

Air Quality Data

Section 4 of the REA describes the preparation and use of urban-oriented hourly ozone monitoring data from the Air Quality System (AQS) database. Ultimately data from 16 cities will be used in the assessment of health risk over the years 2006-2010. Section 4 states that for the epidemiological analyses using BenMAP in 12 cities, missing data for 1-2 hours were filled in by interpolation, but longer periods of missing data were not replaced. For the exposure/clinical analyses using APEX in 4 cities, a much more complex filling procedure was employed to practically remove all missing data. Section 4 references Appendix 4-B (I believe the correct reference should be Appendix 5-B) for additional information on the filling procedure. Wells et al. (2012) references “Section 5” of the REA for the same information (again, I assume that should be Appendix 5-B). A clarifying discussion should be included in Section 4 of the REA on why there are such major differences in data preparation between the epidemiological and exposure analyses. I can only surmise that it is because hourly area-wide averages representing a “composite monitor” are provided to BenMAP while site-specific data are provided to APEX.

The 2007 REA (EPA, 2007) describes the previous fill-in procedure that included a 75% data completeness criterion to accept or reject a site for exposure calculations. The current REA does not mention this specific criterion, but states that "… all monitors lacking sufficient data to calculate a valid 3-year design value were excluded (see 40 CFR Part 50, Appendix P)." This criterion is more lax than the previous requirement of 75% data completeness because it is plausible that a valid design value could be calculated for sites with significantly less data. Furthermore, the approach described in Appendix 5-B does not include cases when all monitors in an urban area are missing data for more than 6 consecutive hours (such occurred in 2008, when 34 consecutive hours were missing from all monitors in Houston). My concern is that extensive data-gap filling for extended periods (greater than 6 hours), especially by assignment from other sites, can result in a skewing of the hourly ozone frequency distribution, thereby misrepresenting the chemical conditions of the monitored area. Applying rollback, either quadratic or model-based, will further degrade the assumed ozone distribution supplied to APEX. The specific site acceptance/rejection criteria and a more complete description of the specific fill-in methods used for the current REA needs to be explicitly described.

Quadratic Rollback

Section 4 of the REA describes the quadratic rollback technique that is applied to just meet the current 75 ppb 8-hour ozone standard. Background "floor" values were set using a relative response factor (RRF) technique that yields a set of monthly-averaged 24-hour diurnal factors for each city (i.e., spatially averaged) that are applied to the hourly rolled-back concentrations throughout any year. The factors are based on GEOS-Chem simulations for 2006 (Zhang et al., 2011), and are specifically defined as the ratio of simulated US background (0% emissions) to simulated "base case" (100% emissions). ENVIRON provided the 2006 CAMx results from Emery et al. (2012) to EPA staff, who further analyzed and compared CAMx and GEOS-Chem simulation results (Henderson et al., 2012). This comparison is summarized in the third draft of the Integrated Science Assessment. EPA found that while substantial uncertainty exists in both modeling applications, CAMx tended to perform slightly better than GEOS-Chem and CAMx-estimated background ozone was consistently higher in most areas of the US. Background estimates from both models should be used in the calculation of risk as a means toward characterizing sensitivity to background uncertainties, and that sensitivity should be documented in the next draft of the REA.

The quadratic rollback technique is too simplistic. Rollback coefficients are determined to just achieve the 75 ppb standard at the single site in each city with the maximum design value. Then these coefficients are used for all other sites in the area, which is a necessity specific to the quadratic rollback technique, and it does not account for different chemical conditions in various locations within each city. The proposed model-based rollback will be a much better approach by projecting concentrations at each site individually based on local chemical conditions (to the extent that it is characterized in the chemical transport model).

Then the background "floor" is applied at each site using the RRF technique, but RRF values above 1 are truncated to 1 (i.e., only ozone reductions, no ozone increases). Then, the lower of the original ozone measurement and the background-scaled value is used as the final rolled-

back value. **The entire approach biases the outcome to minimize ozone across the entire frequency distribution.** This is a major limitation to the quadratic rollback method: low hourly ozone values below background levels that result from NO suppression cannot be rolled upward in response to NOx controls, as realistically occurs. Neither is the application of background scaling allowed to increase low ozone upward toward background levels. The REA includes some comments on the limitations of this approach for urban areas with wide differences in chemical regimes and with many hours of low to zero ozone due to NO titration. Wells et al. (2012) also correctly state that all monitors should not shift equivalently as they do with quadratic rollback. However, such comments are buried deep in the body of the approach and in the report by Wells et al. (2012). Such important limitations need to be expressed up front when introducing the quadratic rollback approach.

Figures 4-3 and 4-4 in the REA show clear examples of the flaws associated with quadratic rollback: **low measurements that are clearly below background (0-20 ppb) receive downward scaling.** Table 4-2 shows that the use of monthly-average background RRFs lead to adjustments that are infrequent and small; usually (95% of the time) the final value is set to the original (lower) value and **not any level remotely resembling a "background floor"**. The REA states that "In conclusion, the U.S. background adjustment procedure had little effect on the rollback concentrations." That statement must be recognized to result from a flawed technique.

In Section 7, on page 7-17, the REA again discusses the use of models to develop background concentration estimates. However, it refers to a blend of GEOS-Chem and EPA's CMAQ regional chemical transport model. In several instances the REA refers to these models being run at approximately 70 km resolution. This is rather confusing, since it is the first and only mention of CMAQ as a source of background ozone estimates and the several statements referring to 70 km resolution may be to the GEOS-Chem results from Zhang et al. (2011). A clarification or correction to this section is needed.

Model-Based Rollback

The REA and Simon et al. (2012) describe EPA's plans to institute a new model-based approach to roll back observation data in response to controls that meet alternative levels of the ozone standard. We are encouraged that EPA is developing a viable technique similar to the approach we discussed with EPA earlier this year. Since that meeting, ENVIRON has conducted similar modeling for the entire year of 2006 using the datasets described by Emery et al. (2012).

The new technique involves the EPA's CMAQ chemical transport model equipped with the higher-order decoupled direct method (HDDM) of sensitivity analysis. Simon et al. (2012) describe an initial scoping application of CMAQ/HDDM over the eastern US for June-July 2005 and the approach to develop scaling factors in the form of RRFs to apply to observational data in other years. Overall, the approach to apply scaling factors is similar to the quadratic rollback in that monthly-average hourly diurnal RRFs are applied to the observational data. The improvements offered by HDDM are in (1) using high-resolution simulations with a state-of-the-science regional modeling system, where site-specific rollback can be applied that reflects specific chemical conditions; and (2) retrieving high-order sensitivity output leading to more

appropriate non-linear responses to precursor reductions under all conditions, including individual sensitivity to NOx, VOC, and NOx+VOC reductions. The approach lends itself well to the need to evaluate risk under alternative ozone standards.

ENVIRON has run CAMx, equipped with HDDM, for the entire year of 2006. HDDM sensitivity output was extracted for all CASTNET sites and for all AQS sites in 23 cities (represented as combined statistical areas) across the US. A spreadsheet-based tool was developed that allows a user to select a site and NOx/VOC control level, and the tool will report hourly time series for a selected period of time, frequency distributions of 1-hour and 8-hour ozone, and time-averaged diurnal ozone profiles. A technique is applied within the tool to adjust HDDM predictions to actual observation data (when available) that results in an exact replication of hourly observational data when the full (100%) NOx/VOC emissions are selected. Predictions for both full precursor emissions and the chosen NOx/VOC control level are reported to clearly indicate the effect of controls.

Figures 1 through 4 present examples of CAMx/HDDM results for single sites in Atlanta and Detroit reported by Simon et al. (2012). These results are specific to the respective 2006 ozone monitoring periods in each city and results are shown for the full (100%) emissions case (observations) and a control case with NOx and VOC emissions reduced by 50%. These sites are classic examples of NOx-influenced locations, with a wide range of 8-hour ozone spanning 0-100 ppb. The Atlanta site exhibits a large frequency of near zero ozone. Note that controls reduce ozone frequency distributions at both high and low ends, while increasing mid-range frequencies in the range of background (15-40 ppb). Diurnal profiles show that low nighttime ozone levels are increased while daytime levels are reduced. These responses are entirely reasonable and agree with early results reported by Simon et al. (2012) using CMAQ/HDDM but differ with the frequency distributions obtained with quadratic rollback techniques as shown in Section 2.3.1.2 of the REA for reasons discussed above. A report on these HDDM analyses is forthcoming.

While the application of CMAQ/HDDM and the calculation of ozone response to various NOx and VOC precursor changes are relatively straightforward, there remain many issues related to the projection of those sensitivities to observational data in other years. In EPA's preliminary approach, days were grouped into 5 or 6 "types" based on observed and simulated maximum daily 8-hour (MDA8) ozone as well as high and low nighttime ozone. Average 24-hour diurnal profiles of HDDM sensitivity calculated were calculated for each day type, and applied via an RRF approach to the typed observation days in 2006-2008. This approach appears to be appropriate and consistent with EPA's modeling guidance for attainment demonstrations of ozone and PM standards. But other options may need to be considered and developed to reduce uncertainties associated with RRF scaling.

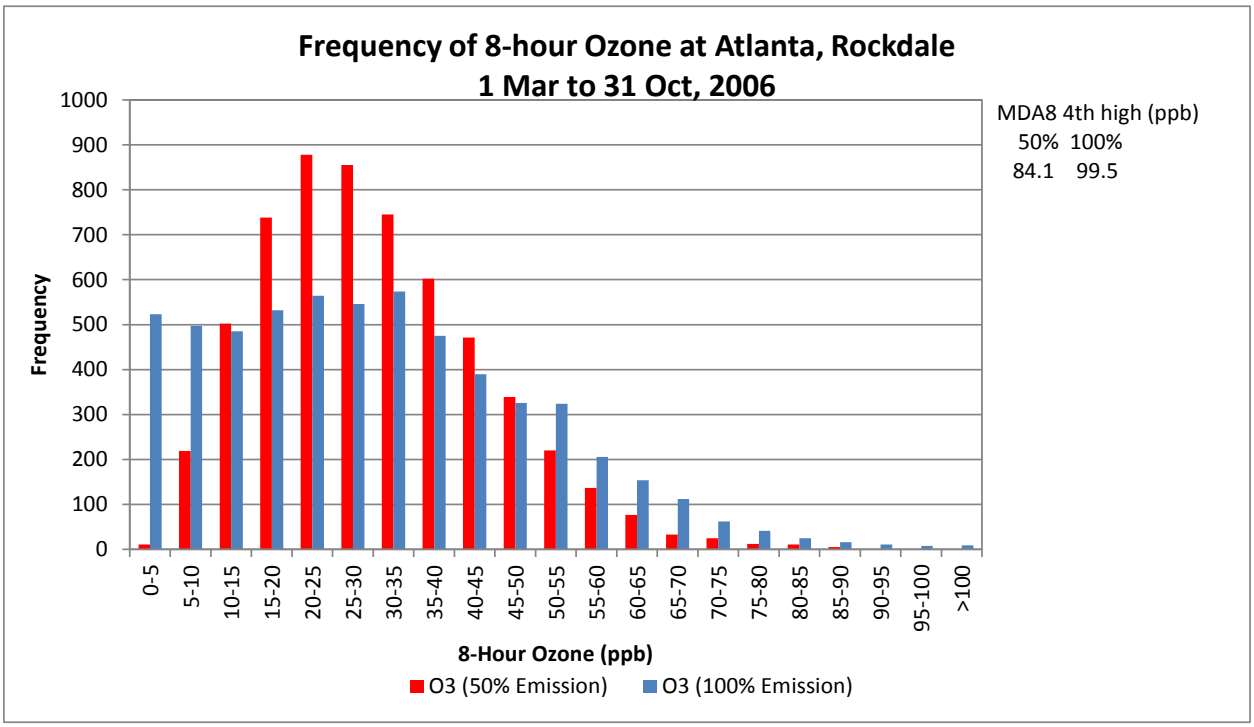

Figure 1. CAMx/HDDM ozone-season 8-hour ozone frequency distribution at the Atlanta Rockdale site (AQS ID 132470001). Blue bars are the full (100%) emissions case (observations) and red bars are the 50% emissions reduction case. 4th highest maximum daily 8-hour ozone values are given on the right.

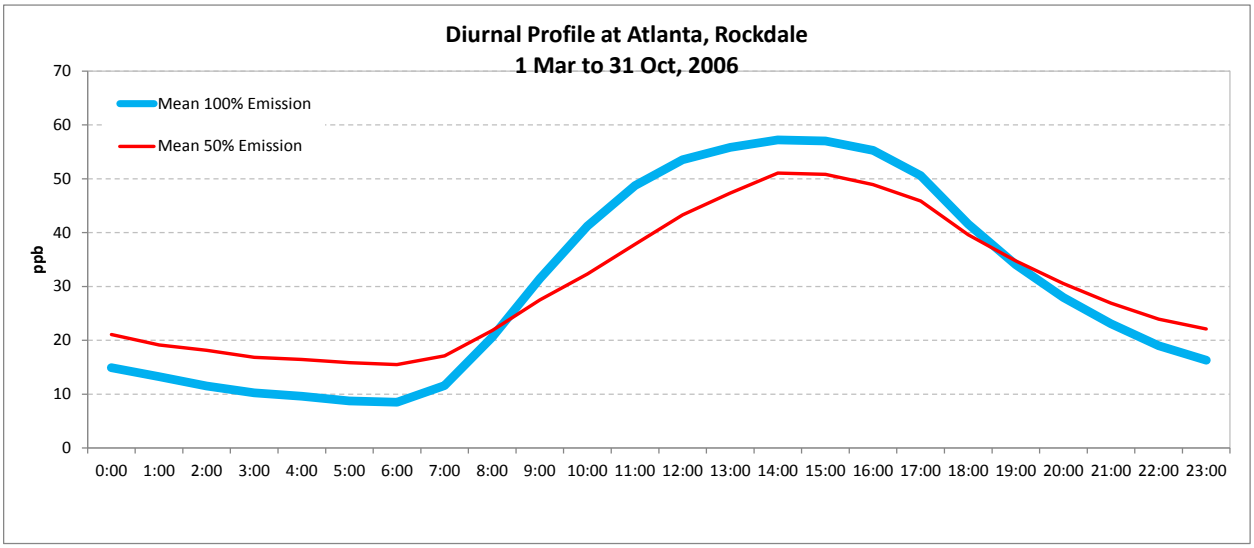

Figure 2. CAMx/HDDM ozone-season mean diurnal ozone profile at the Atlanta Rockdale site (AQS ID 132470001). Blue line is the full (100%) emissions case (observations) and red line is the 50% emissions reduction case.

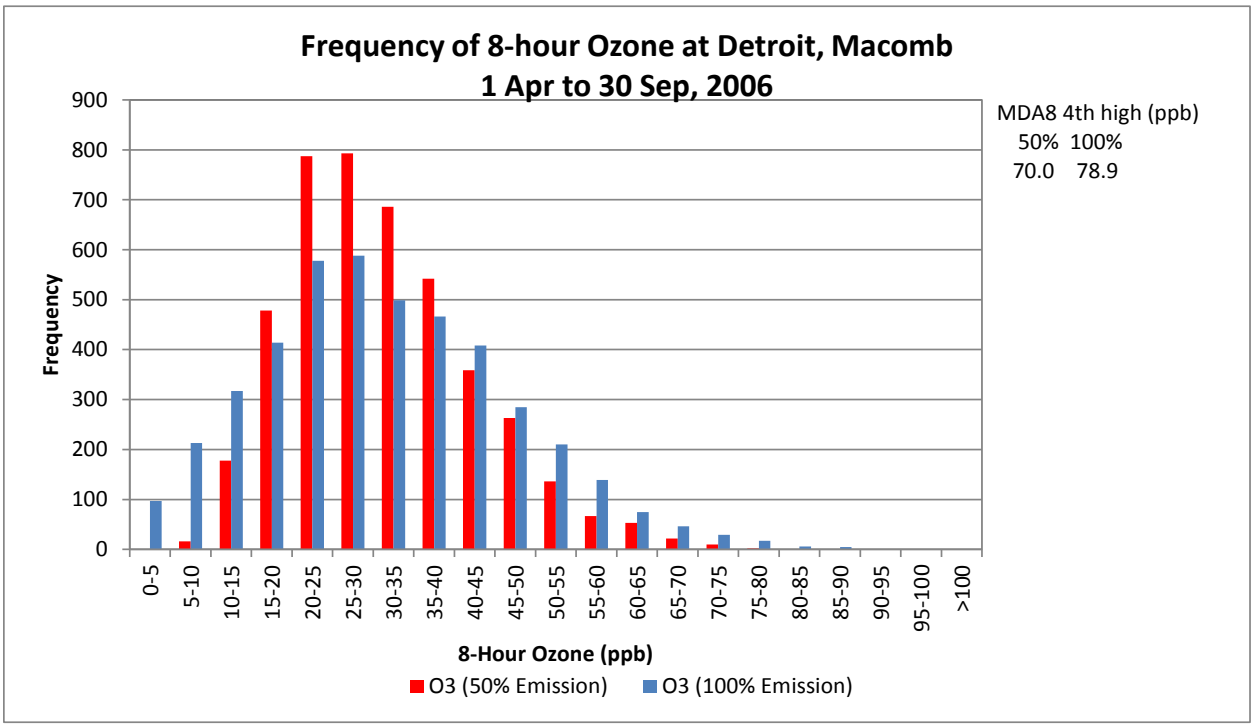

Figure 3. CAMx/HDDM ozone-season 8-hour ozone frequency distribution at the Detroit Macomb site (AQS ID 260990009). Blue bars are the full (100%) emissions case (observations) and red bars are the 50% emissions reduction case. 4th highest maximum daily 8-hour ozone statistics are given on the right.

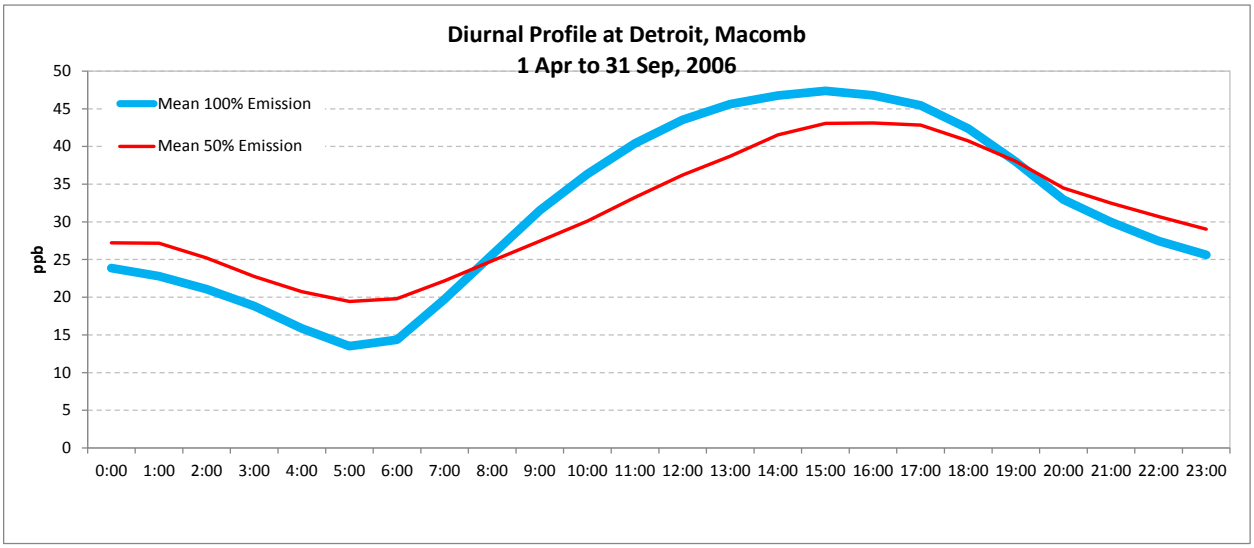

Figure 4. CAMx/HDDM ozone-season mean diurnal ozone profile at the Detroit Macomb site (AQS ID 260990009). Blue line is the full (100%) emissions case (observations) and red line is the 50% emissions reduction case.

HDDM modeling, especially employing high resolution over the entire US, is very time-consuming and requires significant computer resources. Given the strong non-linear response of ozone to NOx, EPA found that multiple CMAQ/HDDM runs were necessary to adequately address the full range of NOx reductions. We arrived at a similar conclusion based on our HDDM modeling. Nevertheless, simulations of the majority or entirety of a year during the 2006-2010 analyses period would improve the model-based rollback technique. It might even be necessary to simulate a high ozone year and a low ozone year to represent the range of chemical conditions and emission responses under such conditions, or to simulate an early year and a late year to include effects of on-going emission reductions over the five year analysis period.

The REA and Simon et al. (2012) correctly state that the explicit specification of a background "floor" is not necessary for the HDDM-based rollback technique because background contributions (e.g., boundary conditions representing global transport, stratospheric influences, and natural emissions) are directly included in the simulation as a systemic component of the model solution. However, as a model, it is subject to uncertainties associated with complex input datasets, resolution employed, and internal physics and chemistry modules. Therefore it is imperative that EPA rigorously evaluate the performance of the model in replicating observed total ozone, calculate model estimates of background ozone through zero-out runs, determine contributions from various background contributors via source apportionment techniques, and compare those results against existing model estimates of background. As indicated by HDDM and source apportionment modeling being conducted by ENVIRON using the datasets of Emery et al. (2012), as well as the analyses reported by Henderson et al. (2012), uncertainties associated with background contributions remain very large in all chemical transport models and these have potentially large impacts on background ozone estimates (and ultimately risk calculations) throughout the US and throughout the year. A report on those analyses is forthcoming.

ENVIRON looks forward to sharing our mutual HDDM modeling results and experiences with EPA to further develop details of the model-based rollback approach.

References

Emery, C., J. Jung, N. Downey, J. Johnson, M. Jimenez, G. Yarwood, R. Morris, 2012. Regional and global modeling estimates of policy relevant background ozone over the United States. *Atmospheric Environment*, doi:10.1016/j.atmosenv.2011.11.012.

Henderson, B., N. Possiel, F. Akhtar, H. Simon. 2012. "Regional and seasonal analysis of North American background ozone estimates from two studies." Prepared by the US Environmental Protection Agency, Office of Research and Development. EPA Docket #EPA-HQ-OAR-2012-0699.

Simon, H., K. Baker, N. Possiel, F. Akhtar, S. Napelenok, B. Timin, B. Wells. 2012. "Model-based rollback using the higher order decoupled direct method (HDDM)." Prepared by the US

Environmental Protection Agency, Office of Air Quality Planning and Standards. EPA Docket #EPA-HQ-EPA-2008-0699.

Wells, B., K. Wesson, S. Jenkins. 2012. "Analysis of recent US ozone air quality data to support the O_3 NAAQS review and quadratic rollback simulations to support the first draft of the risk and exposure assessment." Prepared by the US Environmental Protection Agency, Office of Air Quality Planning and Standards. EPA Docket #EPA-HQ-EPA-2008-0699.

Zhang L., Jacob D.J., Downey N.V., Wood D.A., Blewitt D., Carouge C.C., van Donkelaar A., Jones D.B.A., Murray L.T., Wang Y., 2011. Improved estimate of the policy-relevant background ozone in the United States using the GEOS-Chem global model with 1/2°×2/3° horizontal resolution over North America. *Atmospheric Environment*, doi:10.1016/j.atmosenv.2011.07.054.