Appendix E

Diagnostic Sensitivity Test Modeling Results to Achieve Final Base Case Model Configuration for the Continental Divide-Creston O&G EIS

APPENDIX E – DIAGNOSTIC SENSITIVITY TEST MODELING RESULTS TO ACHIEVE FINAL BASE CASE MODEL CONFIGURATION FOR THE CONTINENTAL DIVIDE-CRESTON O&G EIS

INTRODUCTION

The Continental Divide-Creston (CD-C) oil and gas (O&G) development Environmental Impact Statements (EISs) is using the Comprehensive Air-quality Model with extensions (CAMx; ENVIRON, 2009) to estimate ozone and far-field air quality (AQ) and air quality related value (AQRV) impacts due to the proposed project alternatives and cumulative emissions development throughout southwestern Wyoming (SWWY). The first step in the application of CAMx for an air quality analysis is to apply the model using base case year emissions and evaluate the model estimates against available AQ and AQRV measurements in a model performance evaluation (MPE). The MPE includes evaluating the CAMx model performance following EPA guidance metrics and goals (EPA, 1991; 1999; 2007). Once the model has been deemed to meet the established metrics and goals it can then be used to estimate future year AQ and AQRV impacts.

PRELIMINARY CAMX BASE CASE SIMULATION

CAMx has been set up on a 36/12/4 km modeling domain for the 2005 and 2006 calendar years with the 4 km modeling domain focused on SWWY, which includes the location of the proposed CD-C project. A preliminary CAMx base case simulation was performed and an initial MPE conducted under the Hiawatha EIS study (Kemball-Cook, et al., 2009). On August 20, 2009, the CD-C air quality modeling team met with the Cooperating Agencies (BLM, EPA Region 8, NPS, USFS and WDEQ-AQD) to discuss the preliminary CAMx model performance evaluation. The Cooperating Agencies raised concerns over the CAMx model performance. In particular, concerns were raised regarding the summer ozone performance at the SWWY industrial sites (e.g., Boulder, Daniel and Jonah) and the particulate nitrate (NO3) winter overprediction and summer underprediction tendency. The Cooperating Agencies recommended that additional model sensitivity tests be conducted to identify a CAMx base case model configuration with improved ozone and nitrate model performance, with more emphasis on improvements in the ozone than nitrate performance.

DIAGNOSTIC SENSITIVITY MODELING PLAN

Rarely does a photochemical grid model (PGM) meet all model performance evaluation goals in the first base case model simulation. As noted in EPA's latest modeling guidance "By definition models are simplistic approximations of complex phenomena. The modeling analysis … contains many elements that are uncertain (e.g., emission projections, meteorological inputs, model response)" (EPA, 2007, pg. 98). EPA recommends that diagnostic model sensitivity tests be performed to identify an optimally performing model and understand the model uncertainty to key inputs and assumptions. However, care must be taken that any changes in model configuration be scientifically justified and not just based on improved model performance.

Based on discussions with the Cooperating Agencies at the CD-C Air Quality Stakeholders meeting on August 20, 2009 in Cheyenne, the CD-C modeling team identified a set of sensitivity tests that could be conducted with the goal of improving model performance for ozone and nitrate (NO3). These tests were outlined in a Technical Memorandum to the WDEQ-AQD from

ENVIRON and Carter Lake Consulting that was dated September 11, 2009 (Morris, Kemball-Cook and Zapert, 2009a). The CAMx sensitivity tests were divided into three Phases:

- Already Completed Sensitivity Tests: The first set of sensitivity tests were completed before the August 20, 2009 Cooperating Agencies meeting and consisted of the following:
  - Effects of mineral nitrate formation on NO3 model performance; and
  - Updates to the ammonia emissions seasonal distribution based on more recent information.
- Round 1 Sensitivity Test Modeling: The first round of sensitivity tests incorporated an updated version of the CAMx model that includes corrections to the vertical velocity (VV) algorithms and evaluated the following:
  - Effects of CAMx Vertical Velocity update on model performance; and
  - Use of 34 vertical layers with no layer collapsing between the MM5 and CAMx vertical layer structure.
- Round 2 Sensitivity Tests Modeling: Round 2 sensitivity tests were performed using the CAMx VV modeling platform developed under Round 1 and investigated the sensitivity of the CAMx VV model performance to the following:
  - Vertical Mixing – Alternative Kv profiles and minimum Kv;
  - Dry Deposition – use of an update Zhang dry deposition scheme;
  - Horizontal Resolution – use of 4 km resolution grid over portions of SWWY;
  - Aggressive Plume-in-Grid (PiG) – more widespread use of PiG (e.g., compressors, drill rigs, etc.);
  - Horizontal Diffusion – change horizontal diffusion (Kh) coefficients by factor of 3; and
  - Combinations of the above.

The initial sensitivity tests (completed August 2009) and Round 1 sensitivity modeling were documented in a November 19, 2009 Technical Memorandum "Continental Divide-Creston Modeling Preliminary (Round 1) CAMx Sensitivity Test Results for Southwestern Wyoming" (Morris, Kemball-Cook and Zapert, 2009b) and are summarized below.

INITIAL MODEL SENSITIVITY TESTS

Two model sensitivity tests were completed before the August 20, 2009 Cooperating Agencies meeting prior to the beginning of the Round 1 sensitivity modeling:

- Update seasonal adjustments to ammonia emissions.
- Treatment of mineral nitrate formation.

SEASONAL AMMONIA EMISSIONS DISTRIBUTION

Purpose: To determine whether improved representation of the seasonal allocation of ammonia emissions using more recent information would reduce the wintertime NO3 overprediction bias.

APPENDIX E – DIAGNOSTIC SENSITIVITY TEST MODELING RESULTS TO ACHIEVE FINAL BASE CASE MODEL CONFIGURATION FOR THE CONTINENTAL DIVIDE-CRESTON O&G EIS

Approach: Ammonia emissions for the 2005-2006 modeling were generated using the WRAP Ammonia Emissions Model (Mansell, 2005) that accounts for ammonia emissions from livestock, fertilizer usage, domestic sources and wild animals, with livestock and fertilizer usage being by far the two most important source categories in SWWY. The ammonia emissions were updated in this sensitivity test as follows:

- Correct an error in the spatial allocation of fertilizer NH3 emissions in the 12/4 km domain.
- Incorporate new updated monthly ammonia emissions factors for livestock emissions in the WRAP ammonia model:
  - Based on Gilliland et al., (2006).
  - Amplifies seasonal cycle (higher in summer lower in winter).
  - Results in ~25% reduction in livestock NH3 in February.
- Set fertilizer NH3 emissions to zero for grid cells that are covered in snow or where ground is frozen:
  - Fertilizer is generally not applied to frozen or snow-covered ground.
  - Extensive snow cover was present in SWWY during February 2006.
  - Results in ~70% reduction in ammonia emissions due to fertilizer usage in February 2006.

Results: The CAMx NH3 emissions sensitivity test was run for the February 2006 period on the 12/4 km modeling domain. With the updates to the ammonia emissions inventory the total ammonia emissions in the 12/4 domain in the NH3 sensitivity test were approximately half of the base case emissions. Figure E-1 compares the ammonia concentrations at the Boulder site for February 2006 and the Base Case, corrected fertilizer NH3 emissions spatial distribution case (correctedNH3) and NH3 sensitivity test (revisedNH3) with the monthly observed ammonia concentrations in 2007. The February average predicted NH3 concentration is reduced by ~30% in the NH3 sensitivity test simulation at the Boulder monitoring site, but is still higher than what was observed in February 2007. Figure E-2 displays the NO3 fractional bias performance metric in February 2006 across IMPROVE monitoring sites in the 12/4 km domain for the Base Case and NH3 Sensitivity Test. Across all sites the NO3 overprediction bias in February 2006 is reduced from 131% to 126% (Figure E-2). The February 2006 NO3 results for the base case, corrected NH3 spatial distribution and NH3 sensitivity test at Mount Zirkel Wilderness area are shown in Figure E-3 that shows a very slight reduction in NO3 and very minimal improvement in NO3 performance for the NH3 Sensitivity Test.

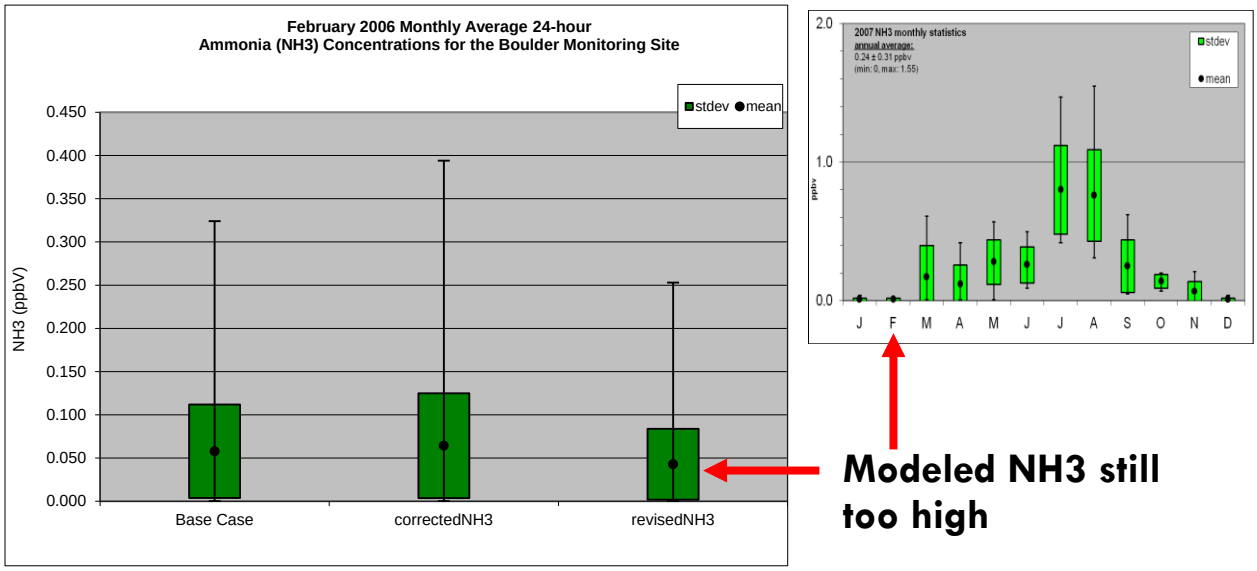


Figure E-1. Comparison of predicted February 2006 ammonia concentrations with observed values in February 2007 for the CAMx base case, corrected NH3 spatial distribution and NH3 sensitivity test.

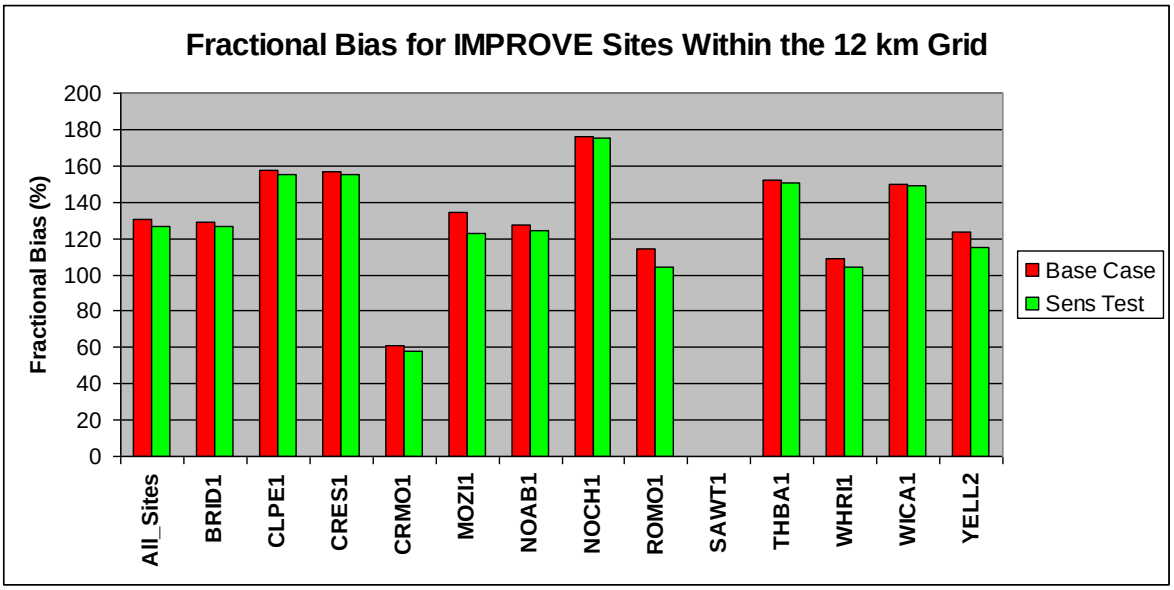


Figure E-2. February 2006 NO3 Fractional Bias at IMPROVE sites in the 12/4 km modeling domain for the CAMx Base Case and NH3 sensitivity test.

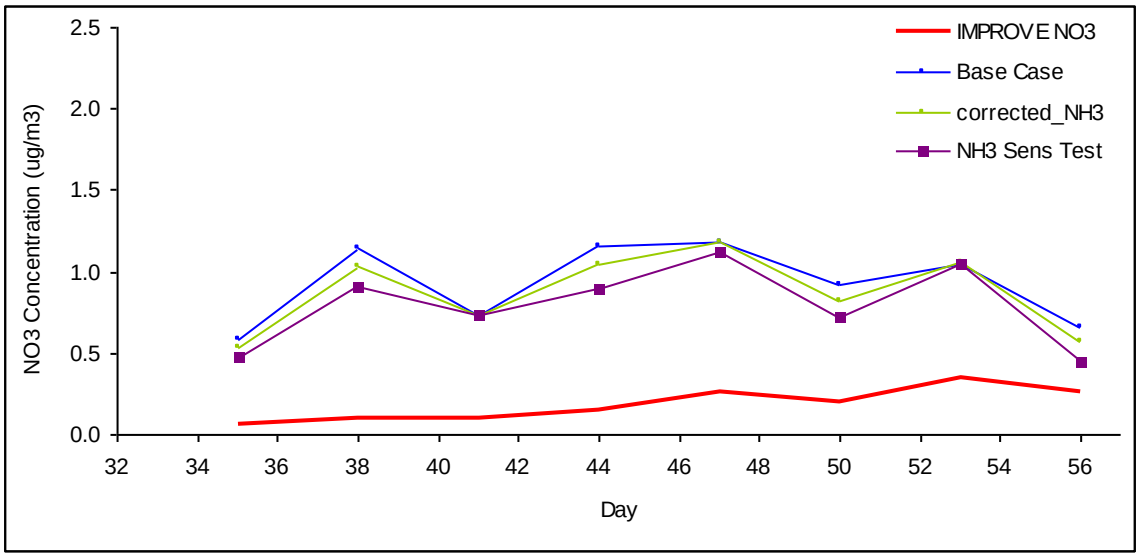


Figure E-3. February 2006 predicted and observed 24-hour average NO3 concentrations at the Mount Zirkel IMPROVE monitoring site for the CAMx base case, corrected NH3 spatial distribution and NH3 sensitivity test.

Recommendation: Although the NH3 temporal allocation sensitivity test has minimal effect on the NO3 model performance, we recommend that the updated ammonia emissions monthly adjustment factors be adopted in the final CAMx base case simulation as it represents more current understanding of ammonia emissions than what was used previously in the WRAP ammonia emissions model (Mansell, 2005).

MINERAL NITRATE SENSITIVITY

Purpose: To account for the effect of the mineral component of crustal PM2.5 emissions (dust) to bind nitrate and convert gaseous nitric acid to particulate nitrate, and determine whether its effect reduces the summer NO3 underestimation bias in CAMx.

Approach: The University of Athens has implemented the capability of simulating mineral nitrate formation in the CAMx model Astitha et al. (2007a,b; 2009a,b). Prior to this, ammonia and sodium were the only basic compounds implemented in CAMx Version 4 that could neutralize gaseous HNO3 to form particulate NO3 [e.g., NH4NO3]. During the warmer summer months, the aerosol thermodynamic properties result in volatilization of particulate NH4NO3 into gaseous HNO3 and NH3. Mineral nitrate, such as Calcium Nitrate, on the other hand, is not volatile so will remain in the particulate phase even under hot conditions. Based on analysis of ambient air quality data, the University of Athens estimated that 6% of the crustal material in their airshed is Calcium and implemented the capability of forming Calcium Nitrate in CAMx assuming that 6% of the crustal material in the model is Calcium. We analyzed IMPROVE measurements in SWWY and nearby regions (e.g., Bridger, Mt. Zirkel and Yellowstone) and found the Calcium to Soil ratio was fairly constant with an average value of also approximately 6%. Thus, we performed a CAMx

sensitivity test in which 6% of the fine and coarse crustal PM species in CAMx were assumed to be Calcium for treatment in the ISORROPIA aerosol thermodynamic model.

Results: The CAMx model was run on the 12/4 km domain for August 2006 using the mineral nitrate algorithm assuming that 6% of the crustal material was Calcium and the modeled NO3 predictions compared against the observed values at the IMPROVE monitoring sites. Figure E-4 displays the NO3 fractional bias performance metric at IMPROVE monitoring sites during August 2006 for the CAMx Base Case and Mineral Nitrate Sensitivity Test. At most of the IMPROVE sites, the CAMx Base Case simulation NO3 fractional bias exhibits an underprediction bias of -60% to -180% during August 2006. The CAMx Mineral Nitrate Sensitivity Test reduces the NO3 underprediction bias slightly, but the CAMx NO3 performance is still characterized by a large underestimation bias (Figure E-4). The fractional bias averaged across IMPROVE monitoring sites in the 12/4 km domain during August 2006 is reduced from -128% in the Base Case to -94% in the Mineral Nitrate Sensitivity Test. Figure E-5 displays predicted and observed time series of 24-hour NO3 concentrations at the Bridger IMPROVE monitor that illustrate the small increases in particulate NO3 due to the inclusion of mineral nitrate in CAMx.

Recommendation: We recommend that mineral nitrate be adopted in the final CAMx Base Case simulation as it represents a real atmospheric constituent that should be accounted for in the modeling.

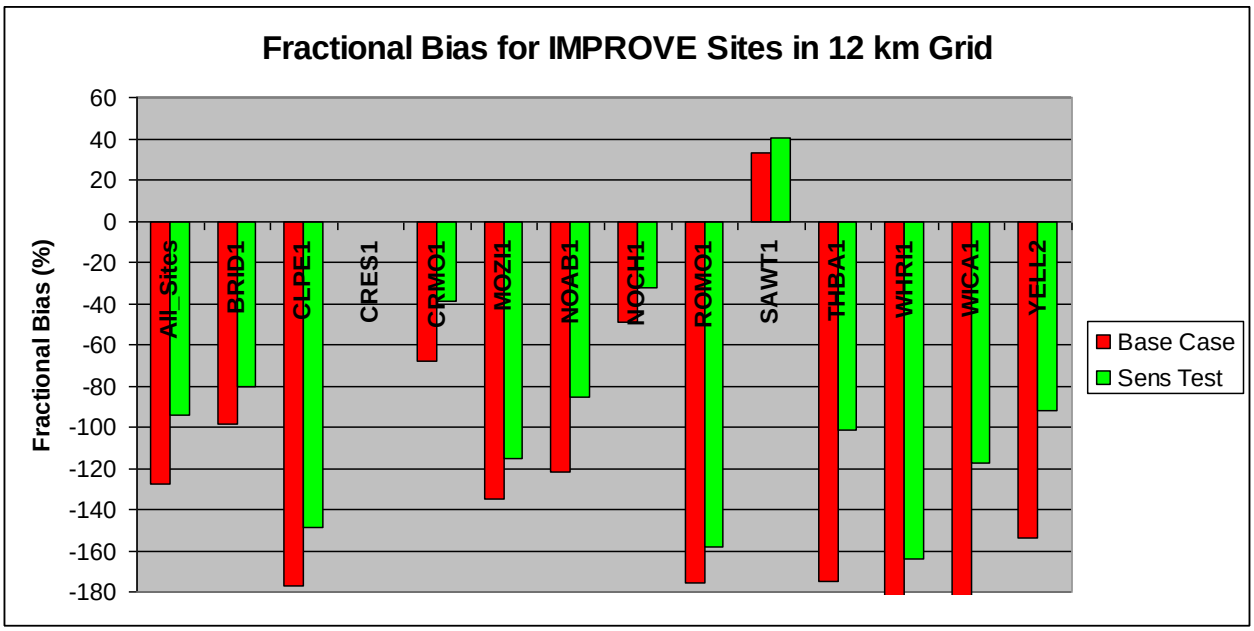


Figure E-4. Fractional bias for NO3 during August 2006 for the CAMx Base Case and Mineral Nitrate Sensitivity test.

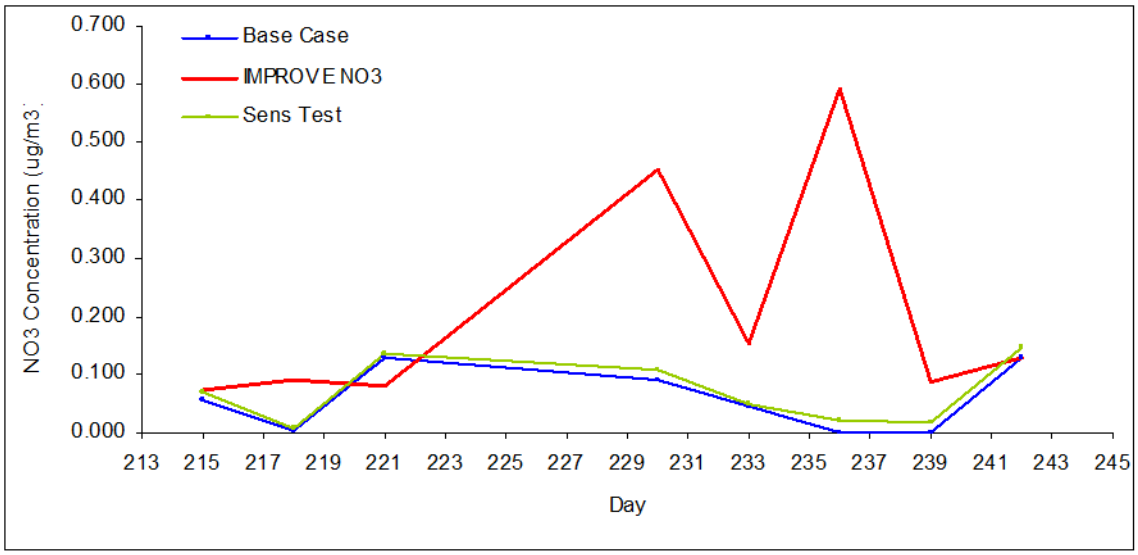


Figure E-5. Time series of predicted and observed 24-hour NO3 concentrations at the Bridger IMPRVE monitoring site for the CAMx Base Case and Mineral Nitrate Sensitivity Test.

ROUND 1 SENSITIVITY MODELING

The Round 1 sensitivity modeling performed under the CD-C EIS focused on the update of the 2005/2006 36/12/4 km CAMx modeling database using a new version of the CAMx model that has corrections to the vertical velocity (VV) algorithm (CAMx VV; Emery et al., 2009a,b)[1] that reduces excessive vertical transport over high terrain. The Western Regional Air Partnership (WRAP) Community Multiscale Air Quality (CMAQ) and Four Corners Air Quality Task Force (FCAQTF) CAMx modeling found that both models generate excessive vertical transport over the highest terrain features. This modeling artifact can bring high ozone concentrations of stratospheric origin from the very top layers of the model (top of model is ~15 km above MSL) to the ground-level over high terrain features, such the Rocky Mountains and the Sierra Nevada Mountains, Cascade Range and Wind River Range. After a focused research effort, the CAMx model was updated with a new vertical velocity algorithm to alleviate this modeling artifact (Emery et al., 2009a,b). EPA has also identified a fix of this modeling artifact (Young, Pleim and Mathur, 2009), but has not released an updated CMAQ code with the correction. Also during Round 1, we evaluated the effects of running with and without vertical layer collapsing between the MM5 meteorological model and the CAMx chemical transport model.

The Round 1 sensitivity modeling incorporated the following updates in the CAMx 2005/2006 36/12/4 km modeling database:

- Use of new lateral boundary conditions (BCs) for the 36 km continental U.S. domain and the 2005 and 2006 modeling periods based on day-specific 2005 and 2006 GEOS-CHEM

[1] http://www.cmascenter.org/conference/2009/slides/emery_reducing_vertical_2009.ppt

global chemistry model output that replaced the monthly average BCs based on 2002 GEOS-CHEM output used in the previous base case simulation[2;]

- Use of higher vertical resolution (22 layers) than used previously (19 layers);
- Use of zero-gradient top BC (i.e., concentrations above the top of the model are assumed to be the same as in the top layer of the model); and
- Use of CAMx VV model version with updated vertical velocity algorithm (Emery et al., 2009a, b).

We also performed one additional sensitivity test with no layer collapsing between the MM5 meteorological model and the CAMx chemical transport model:

- Use of 34 vertical layers in CAMx with no layer collapsing between MM5 and CAMx.

Figure E-6 compares the predicted and observed daily maximum 8-hour ozone concentrations during April 2005 in the western portion of the 36 km domain and the 4 km SWWY domain using the original CAMx model (top) and CAMx VV model with updated vertical velocity algorithm (bottom). Both runs use the new 2005 GEOS-CHEM BCs and have 22 layers in CAMx. The original CAMx model estimates highest daily maximum 8-hour ozone concentrations of 80-95 ppb that occur across the Rocky Mountains from northwest New Mexico stretching northward across Colorado (Figure E-6, top). The observed highest April 2005 daily maximum 8-hour ozone concentrations at four CASTNet sites in these locations (e.g., Mesa Verde, Gothic, Mt. Zirkel) are 10-30 ppb lower ranging from 67 ppb to 73 ppb. In the same locations over the Rocky Mountains, use of the new CAMx VV code results in highest daily maximum 8-hour ozone concentrations during April 2005 that are comparable (65-80 ppb) to the observed values (67-73 ppb). Time series of predicted and observed hourly ozone concentrations were evaluated at the Boulder and Jonah industrial sites during July 7-9, 2005 for the original CAMx base case, the revised CAMx VV, and the 22 and 34 vertical layer sensitivity test runs (Figure E-7). None of these runs reproduce the highest afternoon observed ozone concentrations at the SWWY industrial sites. The CAMx VV simulations run with 22 and 34 vertical layers produce nearly identical results.

Clearly, the overstated ozone over the high terrain produced using the original CAMx model is undesirable so the use of the updated CAMx VV code is recommended for the final CAMx base case configuration. However, it should be noted that both the original CAMx and CAMx VV code still underestimated the summer high afternoon ozone concentrations at the SWWY industrial monitoring sites at the completion of the Round 1 Sensitivity testing.

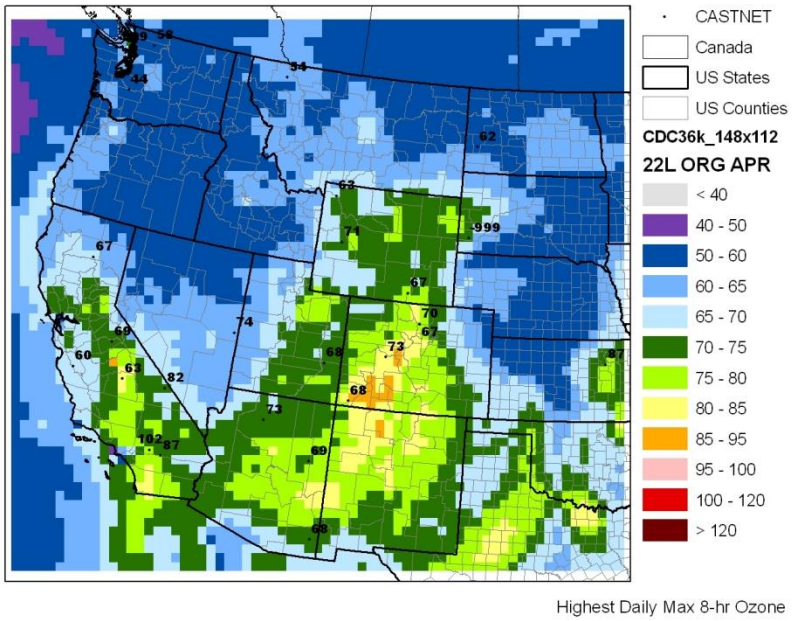
The use of 22 or 34 vertical layers in CAMx is less clear as the two layer configurations produce essentially identical results in SWWY. However, EPA/ORD now recommends that no layer collapsing be utilized with their CMAQ model[3]. A poll of the Cooperating Agencies indicated that

[2] Note that day-specific 3-hour 2005/2006 GEOS-CHEM output were just available for gaseous species and May-September. Particulate species BCs and BCs for other time periods of the 2005/2006 year were still based on the monthly average diurnally varying 2002 GEOS-CHEM results.

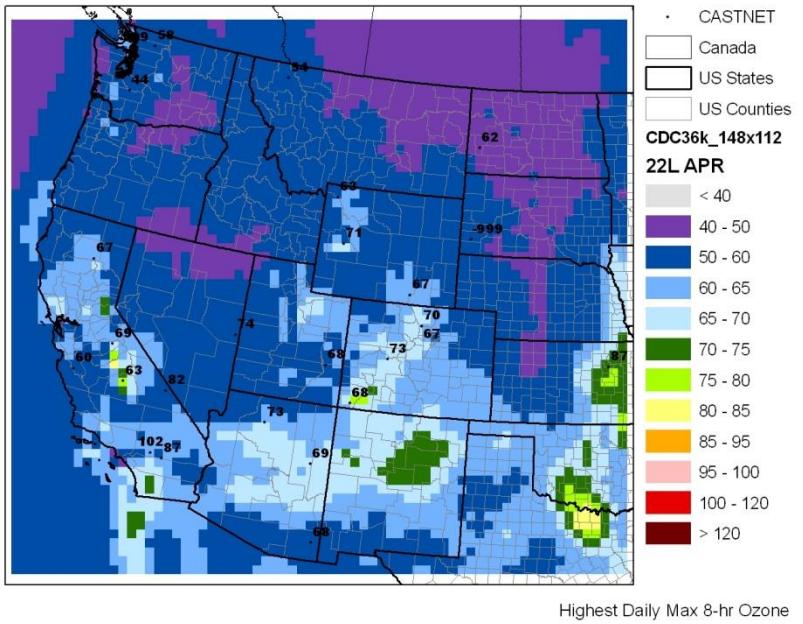
[3] http://www.cmascenter.org/conference/2009/slides/young_mass_consistency_2009.pdf

some had a preference for using a final CAMx base case configuration with no layer collapsing (34 vertical layers), whereas others could go with either 22 or 34 vertical layers in the CAMx modeling. Given this slight preference for using no layer collapsing, the recommended configuration for the final CAMx base case was 34 vertical layers.

Implications of Already Completed and Round 1 Sensitivity Modeling: The use of updated NH3 emissions temporal allocations factors and the mineral nitrate algorithm in CAMx represents better science and has essentially no effect on the CAMx model run times so would not affect schedules associated with the final model base case and future year simulations. Likewise, the original CAMx and CAMx VV codes have similar computation requirements so would also not affect the schedule of the CD-C modeling. Use of the CAMx VV code represents better science. The use of no layer collapsing (34 layers) in CAMx VV produces nearly identical concentrations as using 22 vertical layers with a ~50% increase in model run time for each CAMx simulation.



36 km Grid: New BCs, 22 Layers, and Original CAMx Code



36 km Grid: New BCs, 22 Layers, and New CAMx VV Code

Figure E-6. Comparison of predicted daily maximum 8-hour ozone concentrations (ppb) across the western portion of the 36 km domain during April 2005 using the new 2005 GEOS-CHEM BCs, 22 vertical layers and the original CAMx (top) and updated CAMx VV (bottom) models.

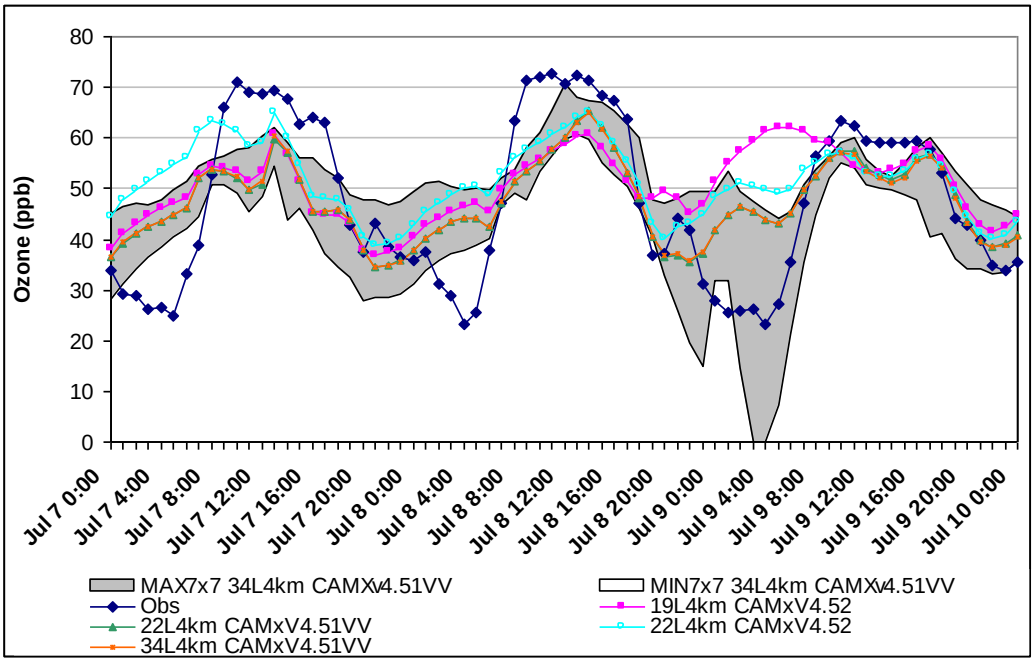


Figure E-7a. Predicted and observed hourly ozone concentrations during July 7-9, 2005 at the Daniel monitoring site for the original CAMx 19 layer base case with 2002 cropped BCs and New 2005 BCs using original CAMx with 22 layers and new CAMx VV with 22 and 34 vertical layers.

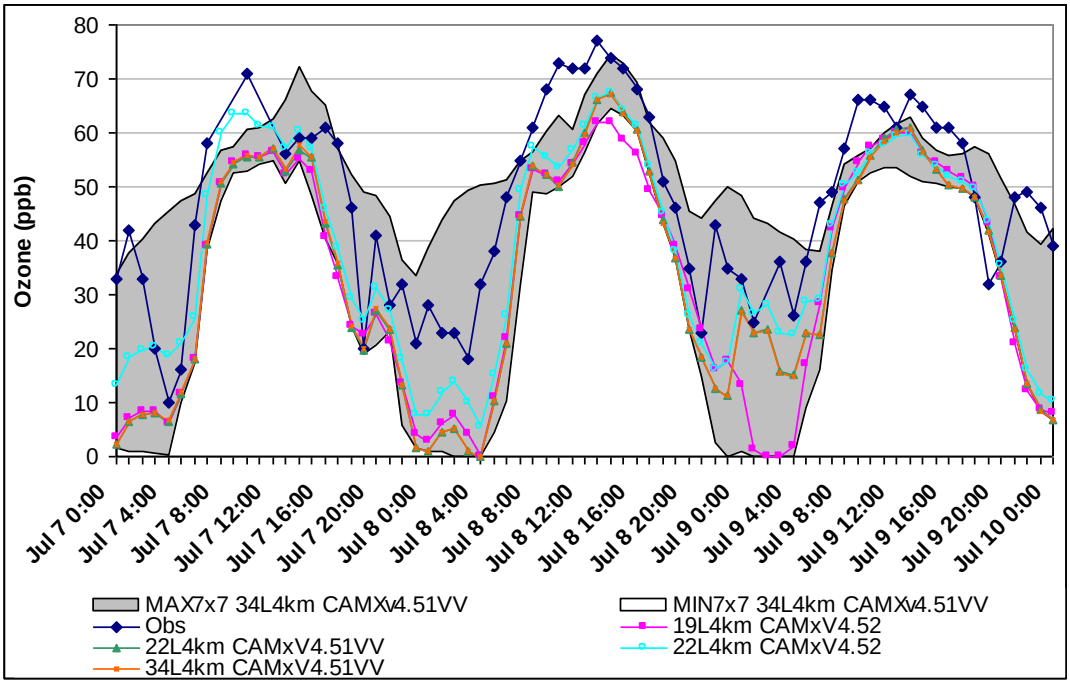


Figure E-7b. Predicted and observed hourly ozone concentrations during July 7-9, 2005 at the Jonah monitoring site for the original CAMx 19 layer base case with 2002 cropped BCs and New 2005 BCs using original CAMx with 22 layers and new CAMx VV with 22 and 34 vertical layers.

ROUND 2 SENSITIVITY MODELING

The original September 11, 2009 Technical Memorandum to the CD-C Stakeholders on the proposed CAMx sensitivity tests contained a list of potential additional CAMx sensitivity tests suggested by the Cooperating Agencies at the August 20th meeting and in follow-up discussions. After discussion among WDEQ-AQD and other Cooperating Agencies, the list of potential sensitivity tests in the September 11, 2009 Technical Memorandum (Morris, Kemball-Cook and Zapert, 2009a) was pared down so that it included only the tests that might lead to changes in the CAMx base case model configuration that would improve ozone and/or nitrate model performance. The following sensitivity tests were performed as part of the Round 2 sensitivity modeling:

- Dry Deposition;
- HONO Emissions;
- Vertical Mixing;
- Horizontal Resolution;
- Aggressive Plume-in-Grid; and
- Horizontal Diffusion.

DRY DEPOSITION SENSITIVITY

Purpose: To determine whether an alternative dry deposition scheme implemented in CAMx would improve ozone and nitrate model performance.

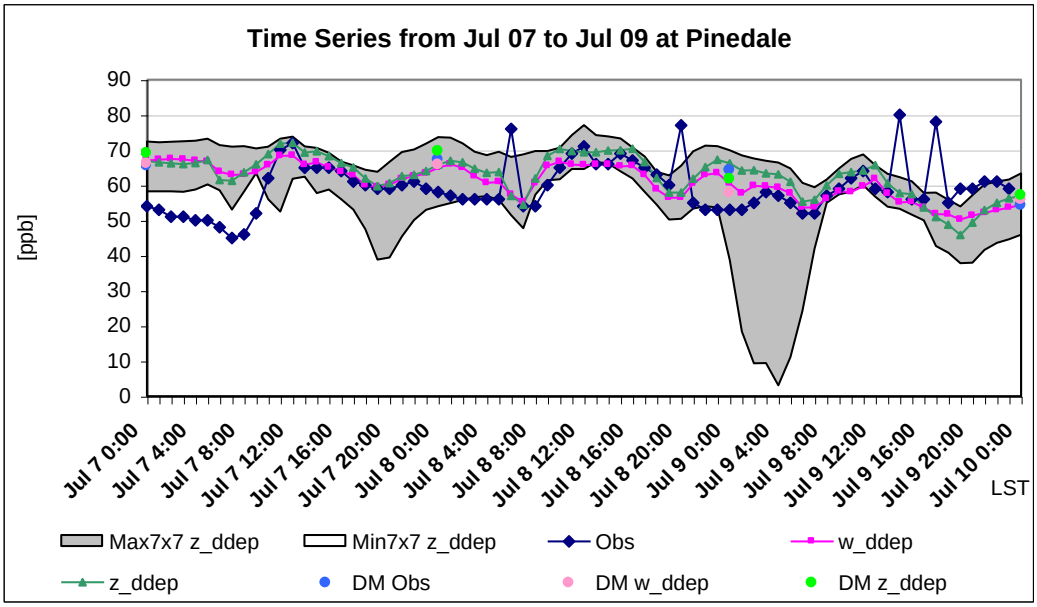
Approach: Dry deposition is an important sink of ozone and its precursors as well as particulate matter. It is active over the entire modeling domain at all times, and the parameterization of dry deposition within a regional model can have a significant impact on model performance. The dry deposition scheme that is currently used in CAMx is based on the Wesely (1989) scheme, which is now rather dated, but still widely used in air quality modeling. Shortcomings of this scheme are that its surface resistances are defined for typical eastern U.S. vegetation types, density, and seasonal conditions and it has a limited representation of atypical conditions (e.g. drought, seasonal transitions). Recently, a new dry deposition scheme (Zhang et al., 2006; 2003) used in the Environment Canada AURAMS air quality model has been incorporated into CAMx. The Zhang scheme is a state-of-the-science algorithm that incorporates recent updates in theory and measurements and has been adapted for use in CAMx to represent atypical conditions through the use of a satellite-derived leaf area index. The Zhang scheme has been used in daily air quality forecasting applications and has been evaluated against recent SO2 and ozone flux measurements. The Zhang algorithm treats deposition of both gases and particles and has a new cuticle and ground resistance formulation for low temperatures and snow-covered surfaces as well as an updated scheme for non-stomatal resistance that accounts for the effects of meteorological conditions. The Zhang scheme uses a more detailed land surface classification scheme than the Wesely scheme (26 land use categories in Zhang versus 13 in Wesely).

The CAMx alternative dry depositions scheme of Zhang and co-workers was used instead of the Wesely (1989) parameterization used in the preliminary and Round 1 CAMx base case simulations to test whether the Zhang parameterization would lead to improved CAMx summer ozone model performance at the SWWY industrial sites.

Results: The Round 1 CAMx 22 layer base case simulation was rerun using the CAMx model with the Zhang dry deposition scheme for the June 15-July 10, 2005 period and the CAMx ozone model performance was evaluated at ozone monitors in SWWY for the July 7-9, 2005 high ozone period. Figure E-8 displays the time series of the predicted and observed hourly and daily maximum (DM) 8-hour ozone concentrations at the Pinedale CASTNet and the Daniel, Jonah and Boulder WDEQ industrial sites for July 7-9. 2005 period and the CAMx model using the Wesely and Zhang dry deposition algorithms. CAMx using the Zhang dry deposition scheme estimates higher ozone concentrations that better matches the observed ozone concentrations at the SWWY WDEQ industrial sites during July 7-9, 2005. Results for the Pinedale CASTNet site are mixed and confounded by the presence of four observed hourly ozone spikes that look like invalid observations.

Figure E-9 displays CAMx estimated daily maximum 8-hour ozone concentrations on July 8, 2005 for the base case (left) and the differences using the Zhang and Wesely (base case) dry deposition algorithms (right). Use of the Zhang dry deposition scheme generally results in daily maximum 8-hour ozone concentrations across SWWY that are 2-6 ppb higher than when the Wesely scheme is utilized. Although increases as high as 8 ppb occur in SWWY and there are even decreases up to -2 ppb on the lee side of the Wind River Range.

At the SWWY WDEQ monitoring sites, CAMx using the Zhang dry deposition algorithms estimates daily maximum 8-hour ozone concentrations that are approximately 3 ppb higher than the CAMx estimates using the Wesely dry deposition scheme. This results in better agreement with the observed daily maximum 8-hour ozone concentrations in SWWY. For example, average across all three WDEQ industrial sites in the Jonah-Pinedale area and the July 7-10, 2005 period the observed average concentrations (63.6 ppb) is underestimated by 11% (-7 ppb) using CAMx with the Wesely dry depositions algorithm (56.7 ppb), but only underestimated by 3% (-2 ppb) when the Zhang dry deposition algorithm is used (61.5 ppb).



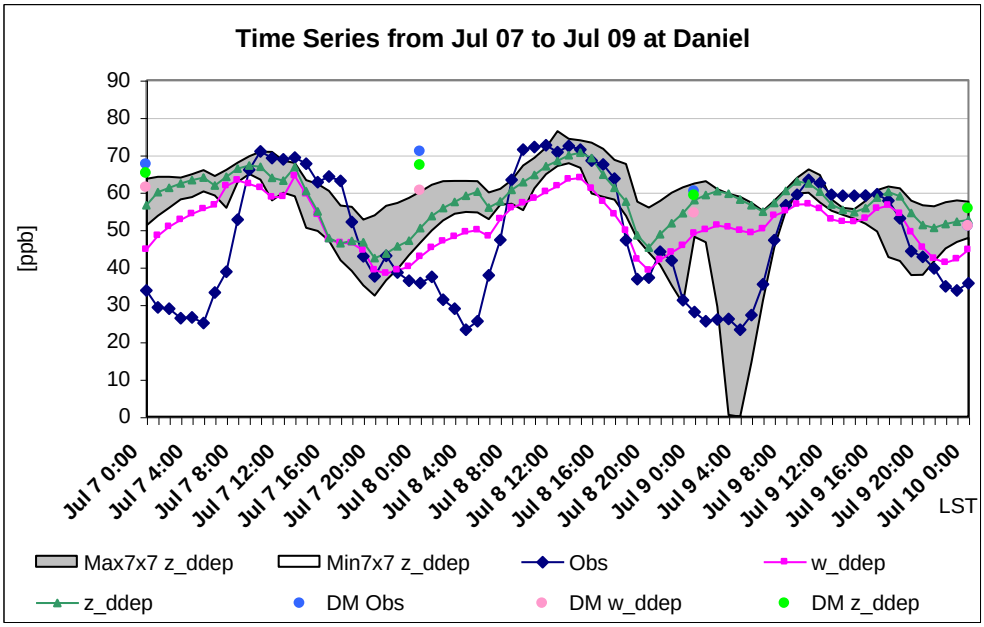
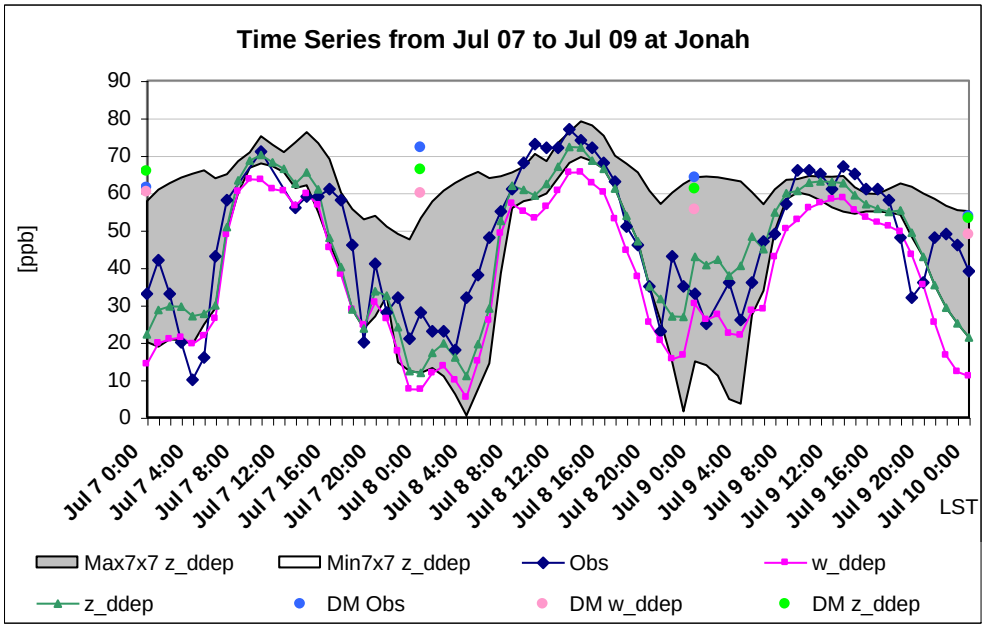


Figure E-8a. Time series of observed (black) and CAMx predicted hourly ozone concentrations (ppb) at the Pinedale CASTNet (top) and Daniel WDEQ industrial (bottom) sites for CAMx using the Wesely (w_ddep; pink) and Zhang (z_ddep; green) dry deposition schemes. Daily maximum (DM) 8-hour ozone concentrations are also shown.



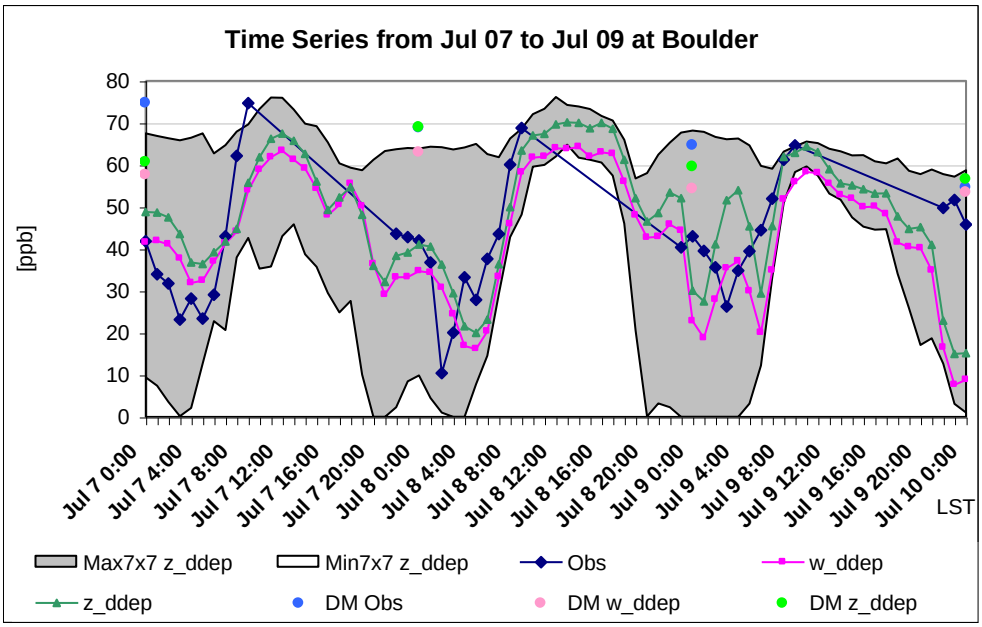


Figure E-8b. Time series of observed (black) and CAMx predicted hourly ozone concentrations (ppb) at the Jonah (top) and Boulder (bottom) WDEQ industrial sites for CAMx using the Wesely (w_ddep; pink) and Zhang (z_ddep; green) dry deposition schemes. Daily maximum (DM) 8-hour ozone concentrations are also shown.

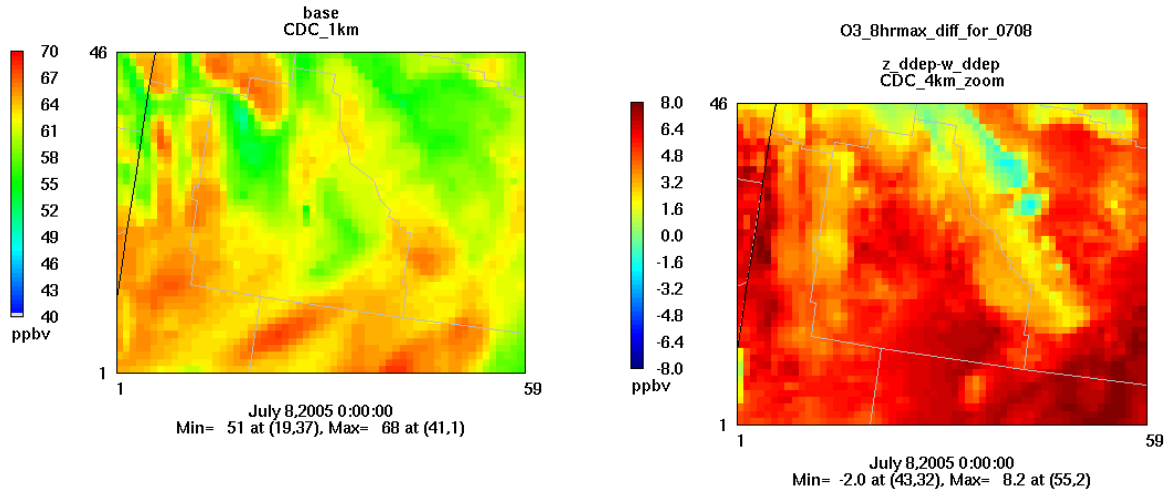


Figure E-9. CAMx estimated daily maximum 8-hour ozone concentrations (ppb) in the Round 1 base case on July 8, 2005 (left) and differences in estimated daily maximum 8-hour ozone concentrations between the Zhang dry deposition sensitivity test with the base case that used the Wesely dry deposition scheme (right; Zhang-Wesely).

HONO EMISSIONS SENSITIVITY (S5)

Purpose: To determine whether the speciation of a small fraction of the NOx emissions into nitrous acid (HONO) would improve summer ozone model performance in SWWY.

Approach: The California Air Resources Board (CARB) performs their PGM modeling assuming that 3 percent of the emitted NOx emissions are HONO. However, when performing PGM modeling outside of California, the EPA and States assume that NOx is emitted as NO and NO2 (typically split as 90% NO and 10% NO2). In this sensitivity test we assumed that all non-biogenic NOx emissions (i.e., combustion NOx emissions including anthropogenic sources and wildfires) in the 12/4 km modeling domain included 3% of the NOx emitted as HONO. The NO and NO2 emissions were adjusted downward so that the HONO sensitivity test included the same amount of total NOx emissions as the original CAMx Round 1 base case simulation.

Results: Assuming that 3% of the NOx emissions are emitted as HONO results in very small increases in the CAMx ozone estimates. This results in a very slight improvement in the CAMx ozone underestimation bias. Figure E-10 displays the CAMx estimated daily maximum 8-hour ozone concentrations non July 8, 2005 for the base case and the differences between the HONO sensitivity test and the base case. The largest increase in daily maximum 8-hour ozone concentrations due to the inclusion of 3% NOx emissions as HONO is 0.6 ppb.

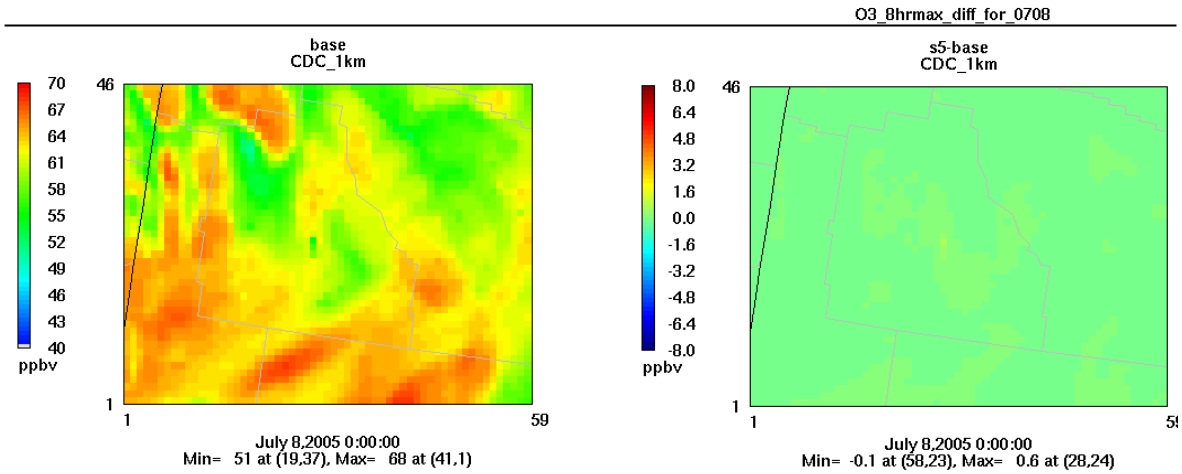


Figure E-10. CAMx estimated daily maximum 8-hour ozone concentrations (ppb) in the Round 1 base case on July 8, 2005 (left) and differences in estimated daily maximum 8-hour ozone concentrations between the HONO emissions sensitivity test with the base case that assumed no HONO emissions (right; HONO-Base).

AGGRESSIVE PLUME-IN-GRID SENSITIVITY (S6)

Purpose: To determine whether aggressive use of the Plume-in-Grid (PiG) module improves ozone model performance in SWWY.

Approach: CAMx includes a subgrid-scale Plume-in-Grid (PiG) module that is used to simulate the near-source plume chemistry and dynamics of point source plumes. Emissions from a point source are initially released as a concentrated point source plume, instead of instantaneously dispersing them across a grid cell (e.g., 4 km or 1 km in SWWY). As the plume moves downwind it expands and entrains concentrations from the grid and performs full chemistry on the plume concentrations. When the size of the PiG plume is commensurate to the size of a grid cell, the emissions from the point source (altered by chemical transformation) are released to the grid model for further simulation.

In a typical CAMx simulation, the PiG module is used to treat the largest NOx point sources. The NOx point sources are ranked in the area of primary interest and the top several hundred NOx point sources are flagged for treatment by the PiG algorithm. For example, in the preliminary and Round 1 CAMx base case simulations the Bridger and Naughton generating stations were treated by the PiG module.

In this sensitivity test we performed aggressive PiG modeling of O&G sources in SWWY. All O&G compressors and drill rigs in SWWY during July 2005 were flagged for treatment by the CAMx PiG module (139 drill rigs operating in SWWY during July 2005). The reasoning behind the PiG sensitivity test is that by treating the O&G NOx sources using the PiG module we may be able to achieve the spatial separation of the O&G VOC emissions (production) from the NOx

emissions (drill rigs and compression) resulting in areas with higher VOC:NOx ratios and potentially higher ozone formation. EPA has performed multi-pollutant and multi-scale modeling of the Detroit area using CMAQ and CAMx and found that, for point sources, much of the benefit from using a high resolution 1 km grid could be realized using a 4 km grid resolution and the PiG module at a fraction of the computer resources.

Results: The more aggressive use of the CAMx PiG module results in areas on ozone increases and decreases. Figure E-11 displays the differences in CAMx-estimated daily maximum 8-hour ozone concentrations between the base case and PiG sensitivity test on July 8, 2005. Ozone increases as high as 2.2 ppb are seen in the center of Sublette County, with more widespread but smaller decreases in ozone also occurring with a maximum decrease of -1.2 ppb. There is essentially no change in the ozone underestimation bias due to the aggressive use of the PiG module. There is also a computational penalty for the aggressive use of the PiG module that approximately doubles the computer time versus the standard PiG configuration.

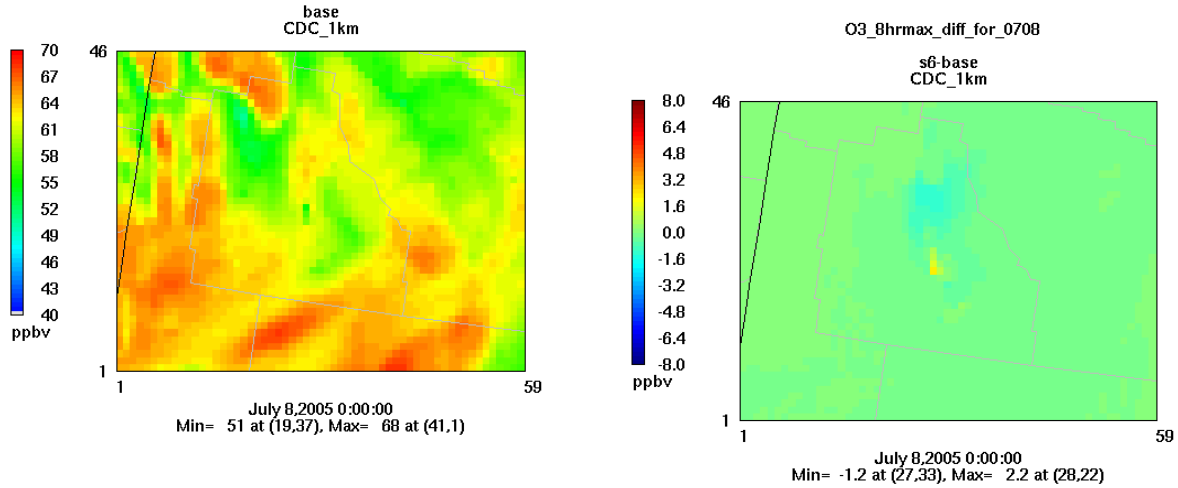


Figure E-11. CAMx estimated daily maximum 8-hour ozone concentrations (ppb) in the Round 1 base case on July 8, 2005 (left) and differences in estimated daily maximum 8-hour ozone concentrations between the aggressive PiG sensitivity test with the base case (right; PiG-Base).

VERTICAL MIXING SENSITIVITY (S7A AND S7B)

Purpose: To determine whether alternative vertical mixing parameterizations can lead to improved ozone and/or nitrate model performance in CAMx.

Approach: Vertical mixing in CAMx is controlled by the vertical turbulent exchange coefficients, which are also called vertical diffusion or eddy coefficients (referred to as Kv or Kz). The Kv values are defined at the interface between two vertical layers in each column of grid cells and are generated by the MM5CAMx processor that converts the MM5 meteorological output data into CAMx meteorological inputs. MM5 does not explicitly simulate Kv values, so they have to be deduced using the MM5 meteorological variables and a parameterization. There are three

Kv parameterizations in MM5CAMx: (1) the O'Brien (OB70) scheme; (2) a scheme similar to the one used in the CMAQ MCIP processor (CMAQ-like); and (3) a scheme used with the Asymmetric Convective Mixing (ACM2) approach. The ACM2 approach has additional code internal to the CAMx model that invokes non-local vertical mixing under convective conditions in addition to the diffusion due to the Kv values. Thus the ACM2 Kv values represent the minimal level of mixing and under unstable convective conditions even more mixing can occur using the non-local mixing.

After one of the three schemes listed above has been used to calculate the Kv, additional post-processing of the MM5CAMx-generated Kv values may be performed to impose a minimal level of mixing in the lowest or lower layers of CAMx to account for mechanical or heat-induced mixing processes not included in MM5 and MM5CAMx. For example, the effects of an urban heat island may not be captured by MM5 so the vertical mixing over an urban area may be too low, trapping the urban NOx emissions in the lowest layer and inhibiting ozone formation within the urban area. The preliminary and Round 1 CAMx base case simulations used the OB70 Kv parameterization.

In this sensitivity test, we examined the sensitivity of the CAMx ozone predictions during July 2005 to an alternative Kv parameterization and typical minimum Kv values. The Round 1 July 2005 12/4 km 34 layer CAMx VV database was used and two vertical mixing sensitivity tests were performed and the resultant ozone predictions compared with the observed values during the July 7-9, 2005 period with high ozone at the SWWY industrial sites. The MM5CAMx processor was rerun to output the CMAQ-like Kv coefficients with a 1.0 m2/s minimum for June-July 2005 and the 12/4 km domains (s7a). A second vertical mixing sensitivity test was performed that ran the kv100 program on the CMAQ-like Kvs that sets the Kvs in the lowest 100 m of the model to the maximum Kv value in that 100 m layer (s7b).

Results: Use of the CMAQ-like Kv (s7a) or CMAQ-like Kv with kv100 (s7b) results in mostly higher estimated ozone concentrations and improved ozone model performance at the SWWY ozone monitors during July 7-9, 2005. Figure E-12 displays the differences in daily maximum 8-hour ozone concentrations on July 8, 2005 between the vertical mixing sensitivity tests and the Round 1 base case simulation. Use of the CMAQ-like Kvs results in mostly increases in daily maximum ozone concentrations on July 8th, with a maximum increase of 4.8 ppb; there are also smaller locations of ozone decreases with the maximum ozone decease (-5.3 ppb) comparable to the maximum ozone increase (Figure E-12, left). The use of the CMAQ-like KVs with kv100 results in even more widespread ozone increases ozone the base case with a maximum ozone increase of 7.3 ppb and even smaller areas of ozone deceases. Both vertical mixing sensitivity tests produce improved ozone bias model performance metrics.

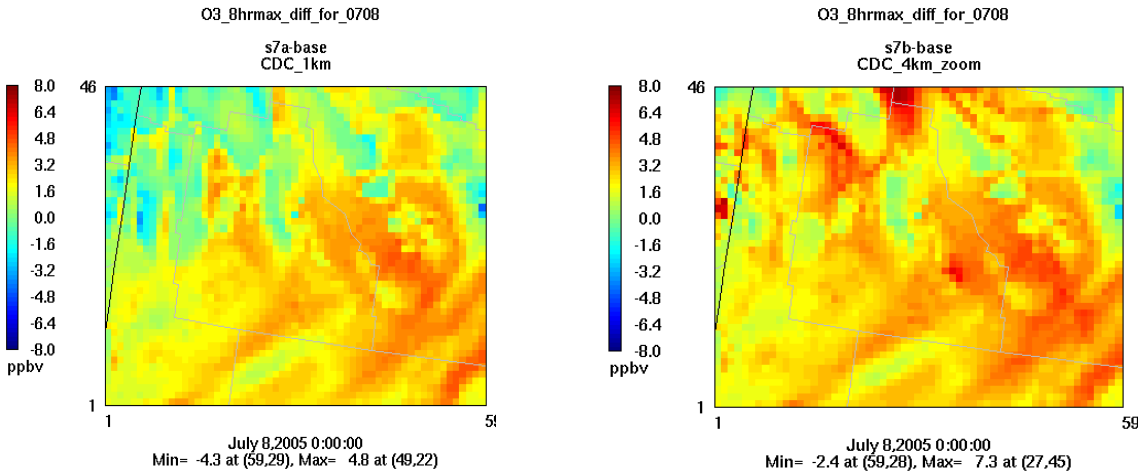


Figure E-12. Differences in CAMx-estimated daily maximum 8-hour ozone concentrations on July 8, 2005 between the CMAQ-like Kv (s7a; left) and CMAQ-like Kv with kv100 (s7b; right) sensitivity tests and the Round 1 base case that used the OB70 Kv parameterization.

HORIZONTAL DIFFUSION SENSITIVITY (S8A & S8B)

Purpose: To determine if increasing or decreasing horizontal diffusion in the CAMx model improves ozone model performance in SWWY.

Approach: Horizontal diffusion in the CAMx and CMAQ models is governed by the 3-D horizontal diffusion coefficients (Kh) that are calculated internally in the two models. Like vertical mixing, the horizontal diffusion coefficient parameterizations are uncertain, although modeled concentrations are believed to be less sensitive to horizontal diffusion than some other meteorological inputs (e.g., vertical mixing, winds, etc.). The horizontal diffusion coefficient sensitivity tests increase and decrease the Kh values by a factor of three and examined their effects on ozone performance in SWWY for July 2005. The reason for performing the Kh reduction sensitivity test (1/3 x Kh) is that it may sharpen the ozone peaks in SWWY and help separate the O&G VOC and NOx emissions resulting in higher VOC:NOx ratios in some locations and consequently greater ozone formation. The reason for the enhanced horizontal diffusion sensitivity test (3 x Kh) is that it may result in more dispersion of the O&G NOx emissions and lessen the NOx inhibition effect on ozone formation.

Results: Figure E-13 displays the differences in estimated daily maximum 8-hour ozone concentrations on July 8, 2005 between the horizontal diffusion sensitivity tests and the Round 1 base case simulations. Again there are areas of ozone increases and decreases in the horizontal diffusion sensitivity tests with most of the ozone changes being within ±2 ppb.

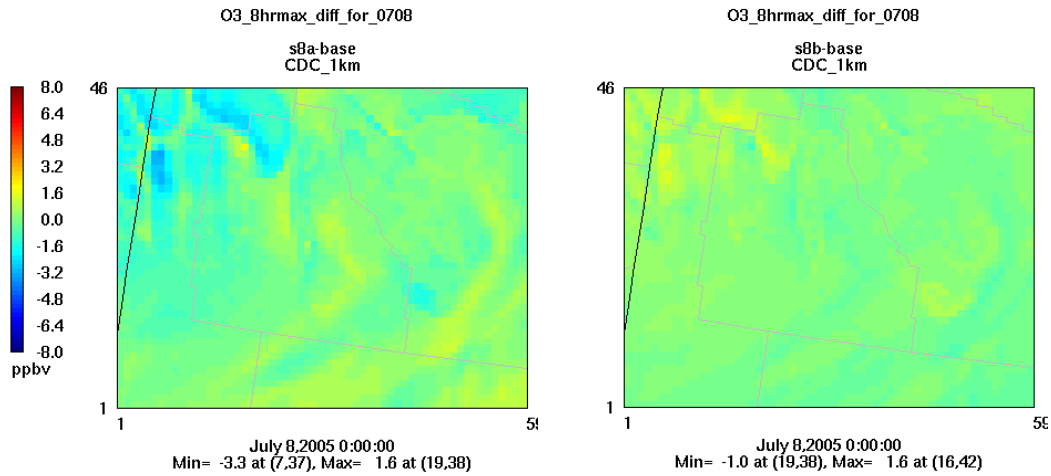


Figure E-13. Differences in CAMx-estimated daily maximum 8-hour ozone concentrations on July 8, 2005 between the Kh × 3 (s8a; left) and Kh ÷ 3 (s8b; right) sensitivity tests and the Round 1 base case.

HIGHER HORIZONTAL RESOLUTION SENSITIVITY

Purpose: To determine whether higher horizontal grid resolution would improve ozone model performance in SWWY.

Approach: A 1 km "flexi-nest" grid was added to the CAMx 12/4 km modeling database that approximately covered Sublette County (Figure E-14). The CAMx flexi-nest feature allows the specification of a two-way nested-grid without having to provide all of the meteorological, emissions and other inputs at the higher resolution by interpolating the inputs from the coarser grid data (4 km in this case). The O&G emissions for SWWY are unique in that all O&G sources (production wells, drill rigs, compression, etc.) are specified as point sources (this is in contrast to O&G emissions in other locations of the western U.S. where the WRAP Phase III inventory is used that is based on county-level emissions data and the spatial distributions of the O&G sources). Thus, the use of a full 1 km flexi-nest in SWWY allows the treatment of the O&G emissions at a 1 km grid resolution. Note that the meteorology and other low-level emissions (e.g., mobile sources, area sources, biogenics, etc.) are interpolated from the 4 km modeling inputs to the 1 km flexi-nest.

One potential reason for the inability of the CAMx model to reproduce the high afternoon ozone concentrations in SWWY is inhibition of ozone formation by the fresh NOx emissions from the drill rigs and compressors. A more refined 1 km grid resolution may allow separation of the NOx (drill rigs/compressor) and VOC (production) O&G sources that would be located in the same grid cell at 4 km resolution. This separation of sources may allow higher VOC:NOx ratios in some regions resulting in higher ozone concentrations and greater horizontal variability in the ozone concentrations.

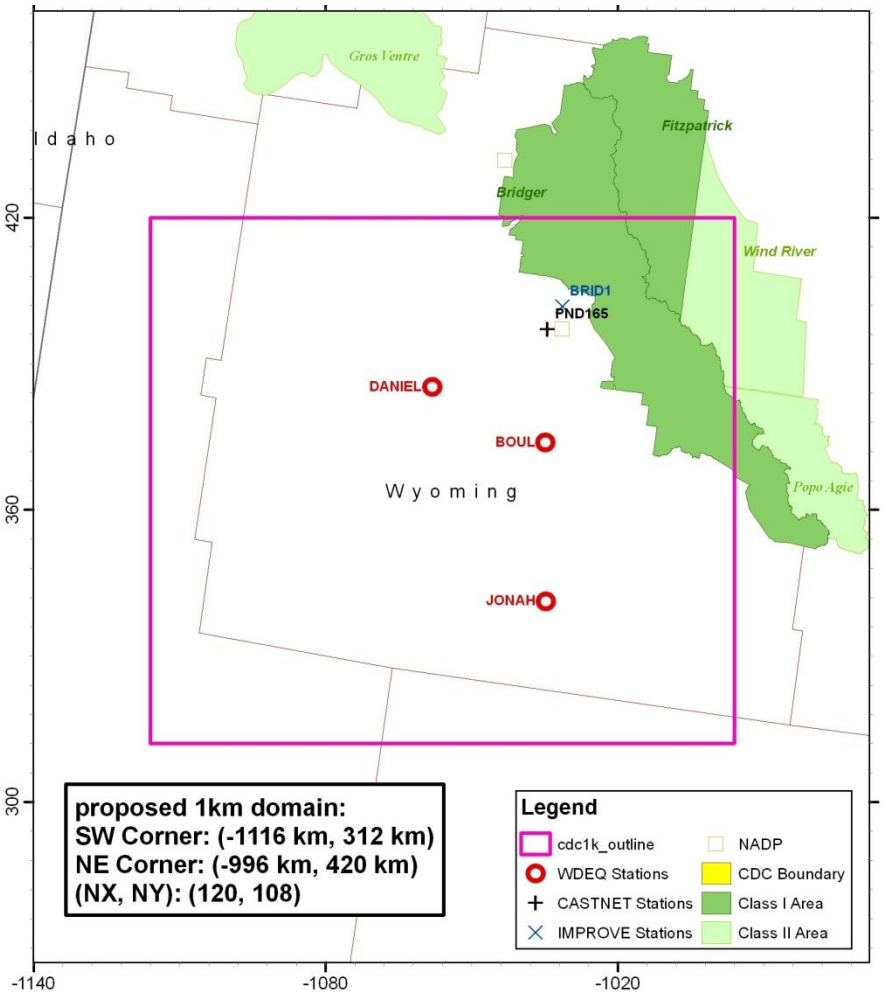


Figure E-14. Location of the 1 km resolution grid used in the s9 high grid resolution sensitivity test.

Results: Figure E-15 displays the CAMx estimated daily maximum 8-hour ozone concentrations ion July 8, 2005 using a 4 km (base case; left) and 1 km flexi-nest (s9; left) grid resolution. As expected, use of the 1 km grid tightens up the peaks and valleys in the modeled ozone concentrations, but doesn't alter their basic features. The overall highest daily maximum 8-hour ozone concentrations on July 8th is the same using either grid resolution (67 ppb). However, as shown in the next section, the use of the 1 km grid resolution actually degrades the ozone model performance measures by increasing the ozone underprediction bias. This is because the 1 km resolution grid not only tightens up the ozone peaks, but also tightens up the ozone valleys as well. There appears to be an area in the central Sublette County where ozone is depressed that is likely due to local NOx emissions. The use of the 1 km grid enhances this ozone depression, which affects ozone at the nearby WDEQ industrial monitoring sites. The use

of the 120 by 108 1 km flexi-nest grid has takes over 3 times longer to run than the 4 km base case, which is a significant computational penalty

---

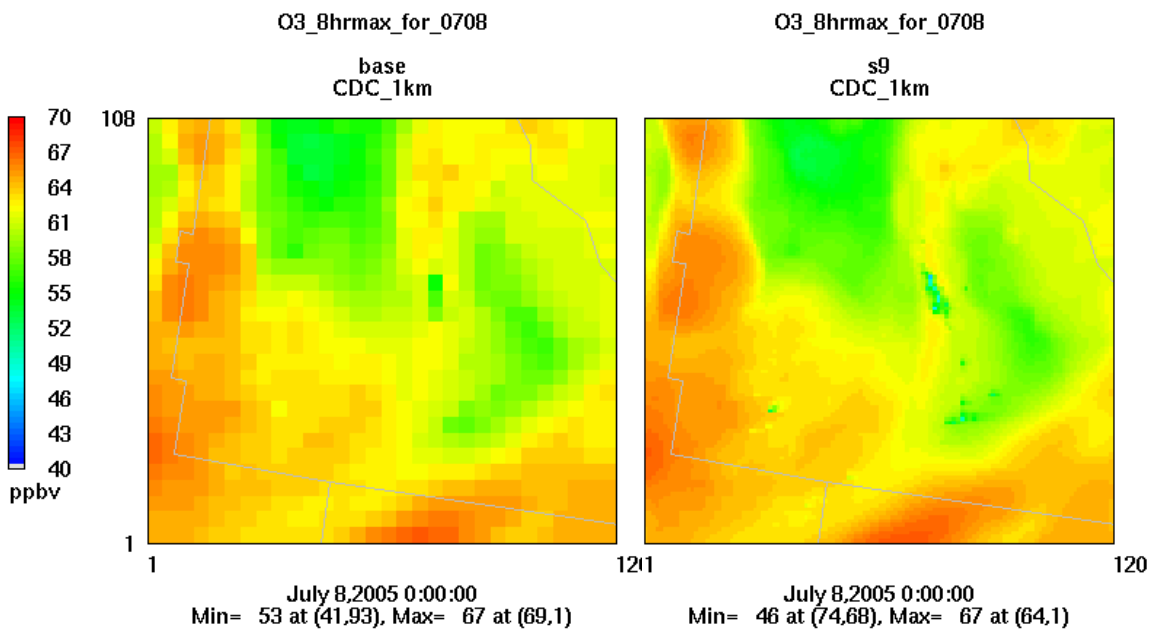


Figure E-15. CAMx estimated daily maximum 8-hour ozone concentrations (ppb) in Sublette County using a 4 km (left) and 1 km (right) grid resolution.

DISCUSSION OF ROUND 2 SENSITIVITY MODELING EFFECTS ON OZONE MODEL PERFORMANCE

EPA has model performance goals for mean normalized bias and gross error of ≤±15% and ≤35%, respectively (EPA, 1991). EPA's original modeling guidance recommended that these performance metrics be calculated for all predicted and observed hourly ozone pairs in which the observed value is greater than 60 ppb (i.e., 60 ppb cutoff). However, EPA's guidance was developed to address the 124 ppb 1-hour ozone NAAQS in urban areas almost two decades ago (EPA, 1991). There have been significant reductions in ozone concentrations over the last 20 years and ozone levels in rural SWWY are usually lower than urban areas. Thus, the mean normalized bias and gross error performance statistics are calculated using a 60, 50 and 40 ppb ozone cutoff concentration. The lower threshold ozone cutoffs are used so that more predicted /observed pairs can be used in the statistical comparisons. Figure E-16 displays these ozone bias and error performance statistics for the July 7-10, 2005 period and SWWY using the three ozone cutoff concentrations and the following CAMx scenarios:

Base – Round 1 base case;
S5 – HONO emissions sensitivity test;
S6 – Aggressive PiG sensitivity test;
S7a – CMAQ like Kv sensitivity test;

S7b – CMAQ-like and kv100 Kvs sensitivity test;
S8a – Kh × 3 horizontal diffusion sensitivity test;
S8b – Kh ÷ 3 sensitivity test; and
S9 – Higher horizontal grid resolution sensitivity test.

All of the sensitivity tests achieve EPA's ≤35% gross error performance goal. Using a 60 ppb ozone cutoff, the CAMx Round 1 base case exhibits a bias of between -16% and -17% so does not achieve EPA's ≤±15% bias performance goal (Figure E-16, top left). The HONO emissions and aggressive PiG sensitivity tests result in small improvements in the bias, but it is still in the -16% to -17% range so still does not achieve EPA's performance goal when a 60 ppb cutoff is used. Similarly, the horizontal diffusion coefficient sensitivity tests (s8a and s8b) also show marginal improvements and degradation in the ozone bias measure with values again in the approximate -16% to -17% range so does not achieve EPA's performance goals. And the higher grid resolution sensitivity test results in a degradation in ozone model performance from the base case with bias metrics using a 60 ppb cutoff in the -17% to -18% range. Only the vertical mixing sensitivity tests (s7a and s7b) result in marked improvements in ozone model performance with the CMAQ-like KVs with kv100 (s7b) producing bias values in the -12% to -13% using a 60 ppb cutoff that achieves EPA's bias performance goal.

Similar improved ozone bias performance statistics for the s7b vertical mixing sensitivity test are seen using 50 and 40 ppb ozone cutoff concentrations. Using a 50 ppb ozone cutoff (Figure E-16, middle left), there is no discernable difference in the bias between the base case (-6.5%) and sensitivity tests except for the s7b (vertical mixing) and s9 (grid resolution) sensitivity tests. The s7b vertical mixing sensitivity test exhibits better bias (-2.5%) than the base case (-6.5%), whereas the s9 grid resolution sensitivity test exhibits degraded ozone bias statistics (-10.6%).

Similarly, using a 40 ppb ozone cutoff concentration (Figure E-16, bottom left) all the sensitivity tests exhibit similar bias values in the -8% to -9.5% range except for the s7b vertical mixing sensitivity test that exhibits much improved bias (-2.6%) and the s9 grid resolution sensitivity test that exhibits degraded bias values (-14.2%).

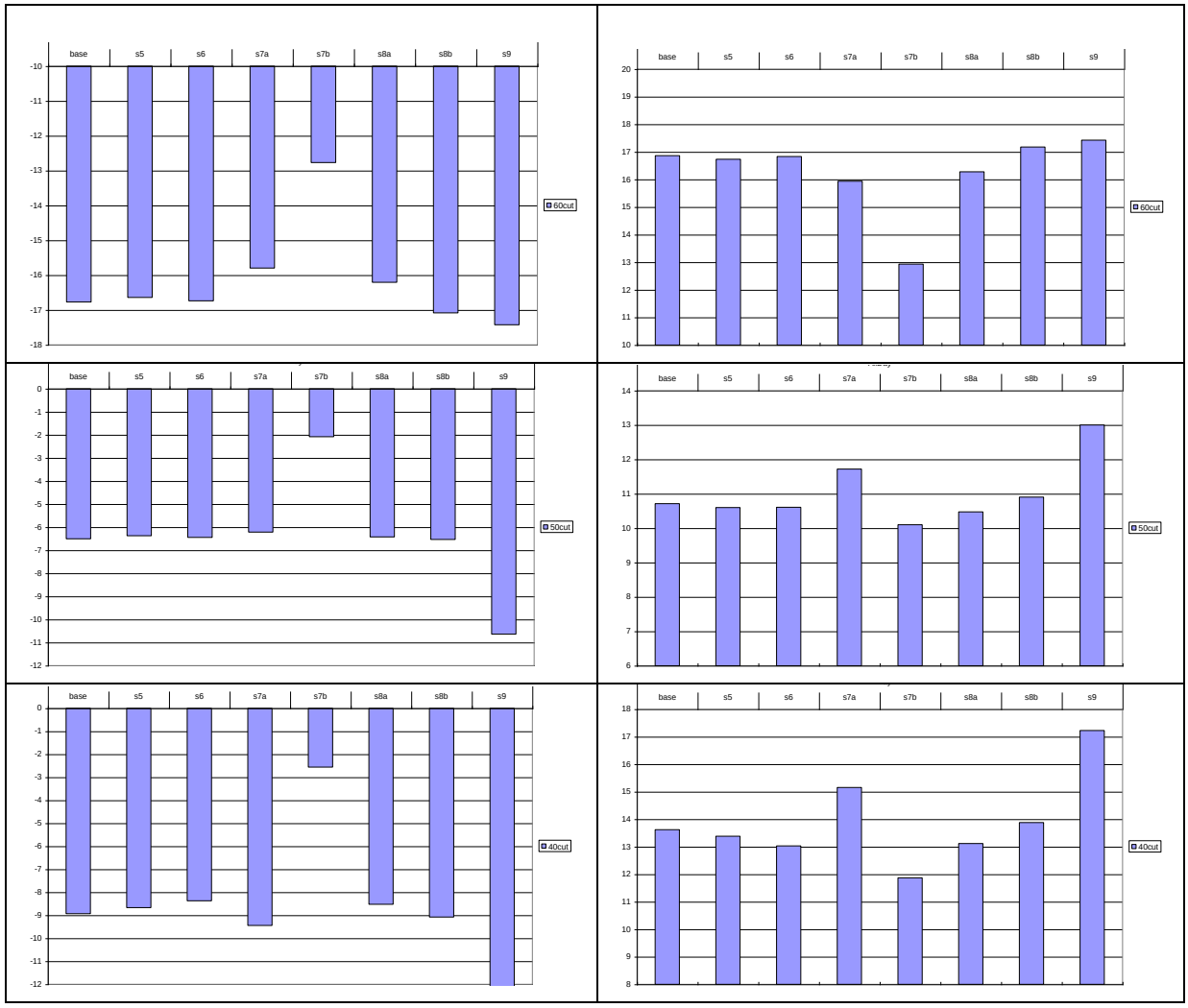


Figure E-16. Ozone model performance mean normalized bias (left) and gross error (right) in SWWY during July 7-10, 2005 using a 60 (top), 50 (middle) and 40 (bottom) ppb ozone cutoff concentrations.

The time series of predicted and observed hourly ozone concentrations during July 7-9, 2005 for the various sensitivity tests are shown in Figure E-17. The time series confirm what the performance statistics indicated in Figure E-16 that the s7b vertical mixing sensitivity test is the best performing with the others not very different from the base case simulation.

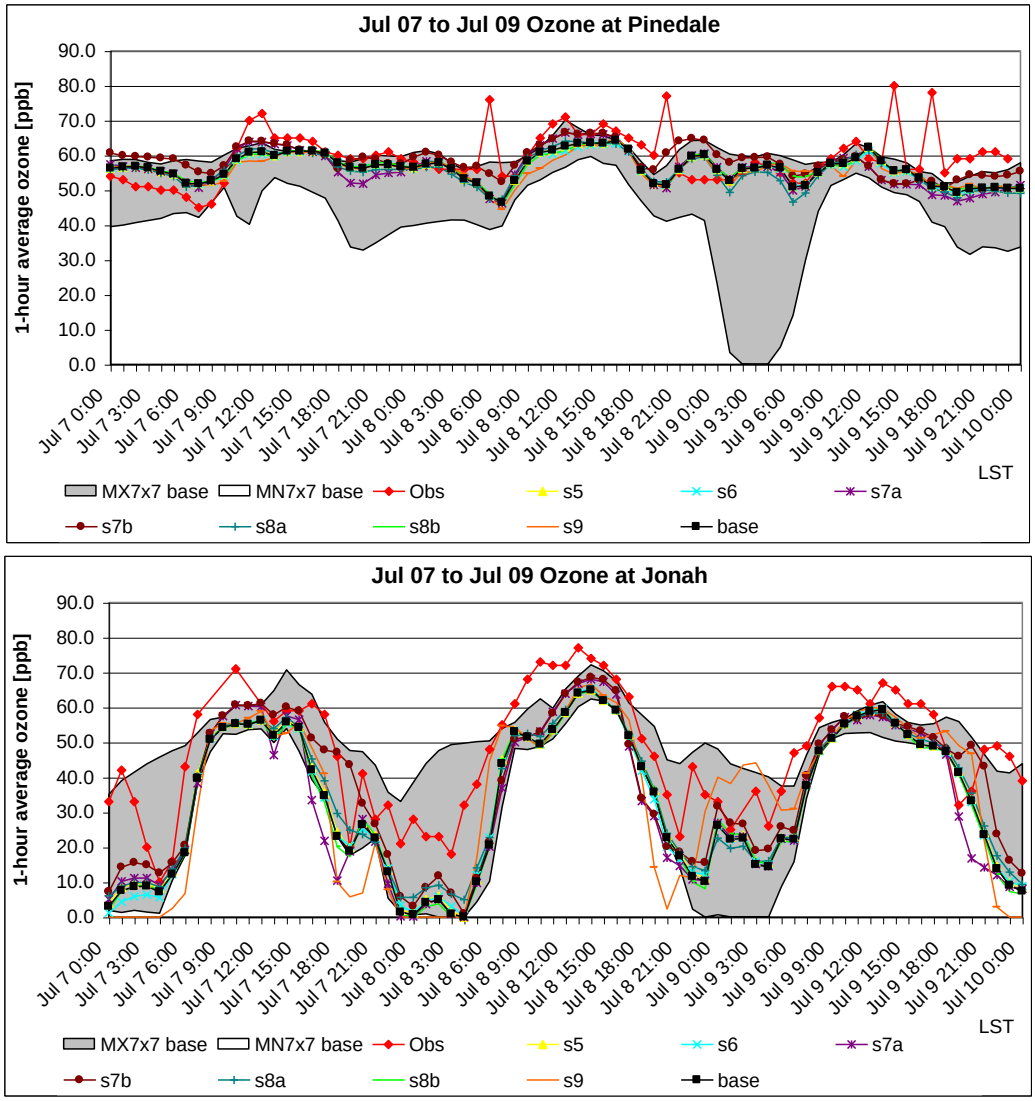


Figure E-17a. Time series of predicted and observed hourly ozone concentrations during July 7-9, 2005 at the Pinedale CASTNet (top) and Jonah WDEQ (bottom) sites for the various CAMx sensitivity tests.

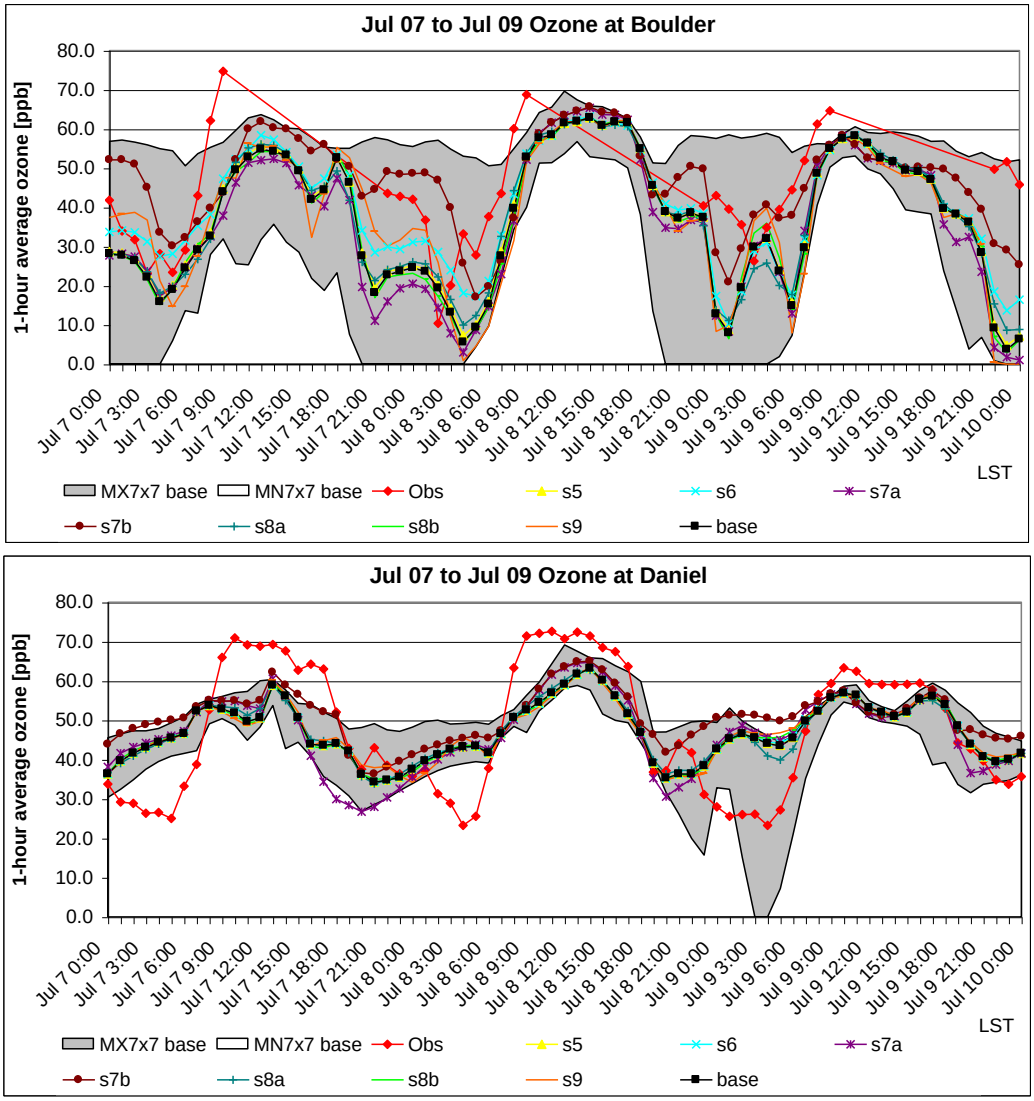


Figure E-17b. Time series of predicted and observed hourly ozone concentrations during July 7-9, 2005 at the Boulder (top) and Daniel (bottom) sites for the various CAMx sensitivity tests.

NITRATE PERFORMANCE EVALUATION

The Round 2 sensitivity tests were focused on improving summer ozone performance in SWWY. The observed and modeled nitrate concentrations are extremely low during the Round 2 July 2005 modeling period so little can be ascertained regarding the sensitivity effects on nitrate performance. The focus on ozone performance in the Round 2 sensitivity modeling was based in part on the conservative nature of the CAMx nitrate predictions for AQRVs in the original (June 2009) CAMx base case simulation. This is shown in Table E-1 that displays the number of predicted and observed days that the visibility impairment due to nitrate exceeds the 0.5 and 1.0 deciview (dv) thresholds at the Bridger and Mount Zirkel IMPROVE monitoring sites during 2005 and 2006 using the 1:3 day sampling frequency. The model is estimating significantly more days in which nitrate visibility exceeds the 0.5 and 1.0 dv thresholds than observed.

The conservative nature of the CAMx nitrate AQRV predictions is also shown in the time series of predicted and observed 24-hour visibility impairment at the Bridger (Figure E-18) and Mount Zirkel (Figure E-19) IMPROVE monitoring sites. Although the modeled nitrate visibility impairment is below the observed value during some summer days, this is when the observed nitrate visibility is extremely low. In the winter when the observed nitrate visibility is more significant the model has an overestimation bias so is conservative.

Table E-1a. Comparison of number days during 2005 that observed and predicted visibility impairment due to NO3 (FLAG Method 6) exceeds the 0.5 and 1.0 deciview thresholds using the 1:3 day sampling frequency and the preliminary CAMx base case simulation (Kemball-Cook et al., 2009).

Site	# Days > 0.5 DV		# Days > 1.0 DV	
	Observed	Modeled	Observed	Modeled
Bridger	43	90	11	78
Mount Zirkel	49	77	21	63

Table E-1b. Comparison of number days during 2006 that observed and predicted visibility impairment due to NO3 (FLAG Method 6) exceeds the 0.5 and 1.0 deciview thresholds using the 1:3 day sampling frequency and the preliminary CAMx base case simulation (Kemball-Cook et al., 2009).

Site	# Days > 0.5 DV		# Days > 1.0 DV	
	Observed	Modeled	Observed	Modeled
Bridger	53	86	24	76
Mount Zirkel	52	67	17	58

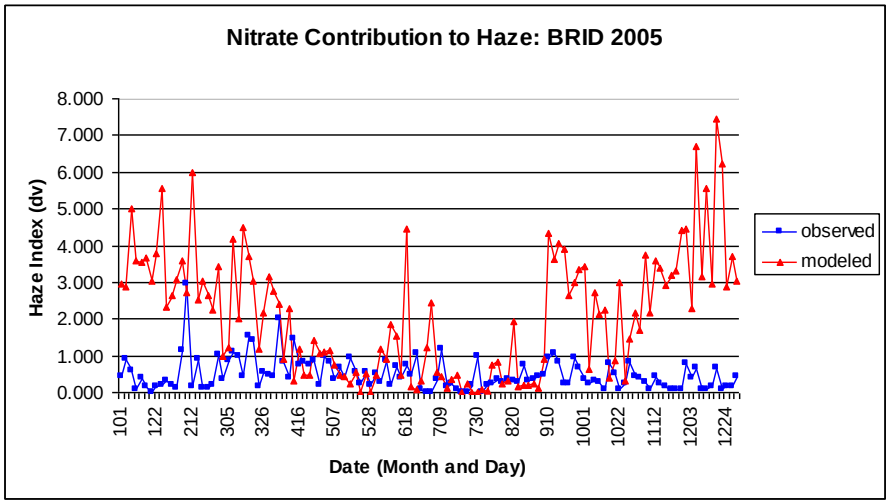


Figure E-18a. Comparison of predicted and observed 24-hour NO3 concentrations at the Bridger IMPROVE monitoring site during 2005 for the preliminary CAMx base case simulation (Kemball-Cook et al., 2009).

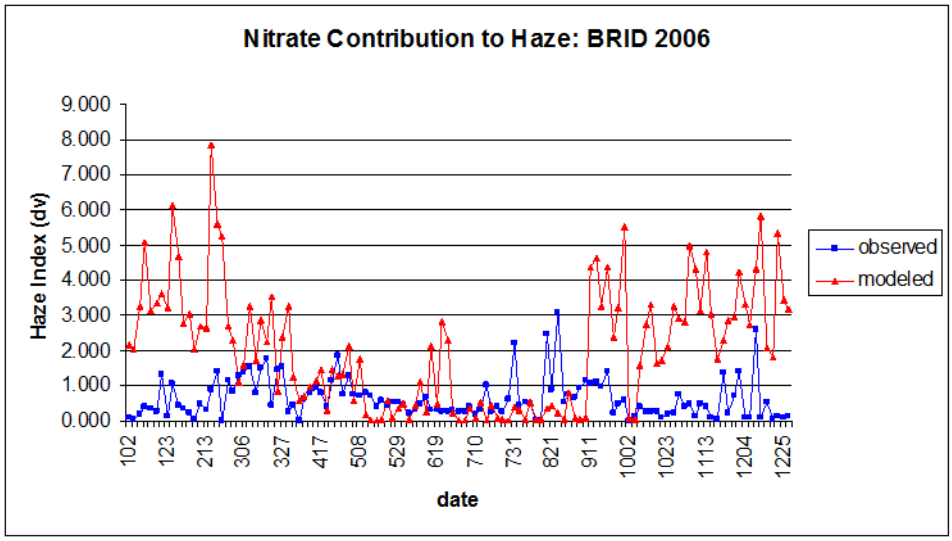


Figure E-18b. Comparison of predicted and observed 24-hour NO3 concentrations at the Bridger IMPROVE monitoring site during 2006 for the preliminary CAMx base case simulation (Kemball-Cook et al., 2009).

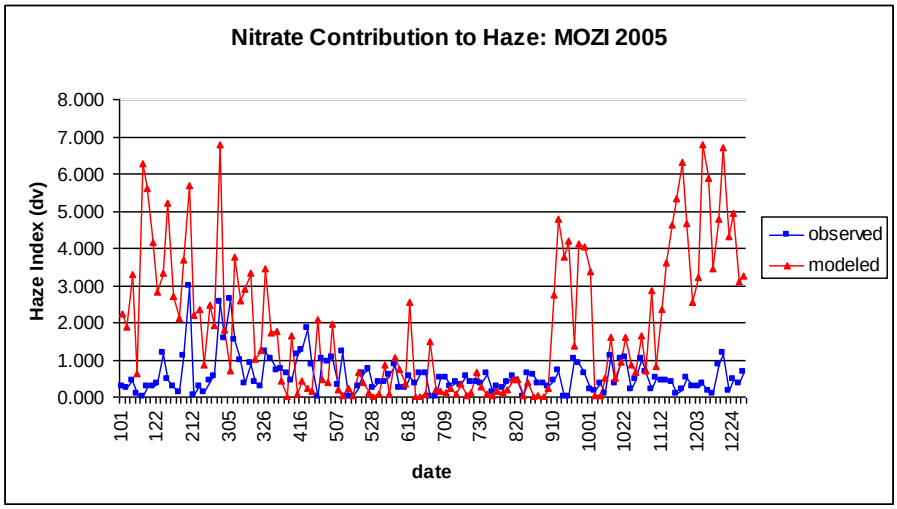


Figure E-19a. Comparison of predicted and observed 24-hour NO3 concentrations at the Mt. Zirkel IMPROVE monitoring site during 2005 for the preliminary CAMx base case simulation (Kemball-Cook et al., 2009).

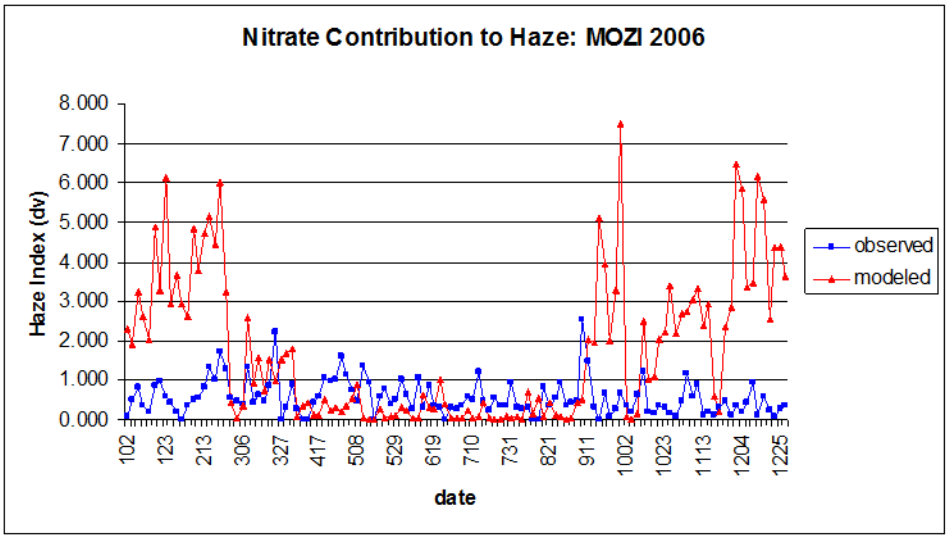


Figure E-19b. Comparison of predicted and observed 24-hour NO3 concentrations at the Mt. Zirkel IMPROVE monitoring site during 2006 for the preliminary CAMx base case simulation (Kemball-Cook et al., 2009).

FINAL BASE CASE MODEL CONFIGURATION

The results of the Round 2 sensitivity tests were presented to the Cooperating Agencies in a meeting January 7, 2010 at WDEQ's office in Cheyenne. The Cooperating Agencies selected the following CAMx model configuration for the revised CD-C 2005/2006 base case simulations:

- CAMx VV model version and Round 1 database updates;
- 34 vertical layers;
- Updated ammonia emission seasonal allocations;
- Include mineral nitrate processes;
- Zhang dry deposition algorithm; and
- CMAQ-like Kvs with Kv100 vertical diffusion.

REFERENCES

Astitha M., 2007a. Characteristic scales of transport and transformation of air pollutants - Impacts on climate. Ph.D. Thesis. University of Athens, School of Physics, Department of Environmental Physics-Meteorology.

Astitha M., Kallos G., Katsafados P., Mavromatidis E., 2007b. Heterogeneous chemical processes and their role on particulate matter formation in the Mediterranean region. 29th NATO/SPS ITM on Air Pollution Modeling and its Applications, September 2007, Aveiro, Portugal.

Astitha and Kallos, 2009a: Gas-phase and aerosol chemistry interactions in South Europe and the Mediterranean Region. Environmental Fluid Mechanics, Vol. 9, Number 1, February 2009.

Astitha M., Spyrou C., Kallos G., Denier Van der Gon HAC, Visschedijk AJH and J. Lelieveld, 2009b: Chemical composition change of aerosols along long-range transport paths. 30th NATO/SPS ITM on Air Pollution Modeling and its Applications, May 2009, San Francisco, USA.

Emery, C., E. Tai, R. Morris and G. Yarwood. 2009a. Reducing Vertical Transport over Complex Terrain in Photochemical Grid Models. Presented at the 8th Annual CMAS Conference, October 19-21, 2009, Chapel Hill, NC. (http://www.cmascenter.org/conference/2009/abstracts/emery_reducing_vertical_2009.pdf)

Emery, C.E., E. Tai, R. Morris and G. Yarwood. 2009b. Reducing Vertical Transport over Complex Terrain in Photochemical Grid Models. AWMA Guideline on Air Quality Models: Next Generation of Models. Raleigh, NC. October 28.

ENVIRON. 2008. "User's Guide Comprehensive Air Quality Model with Extensions (CAMx) Version 4.50." ENVIRON International Corporation, Novato, California. (www.camx.com). September.

ENVIRON and Carter Lake. 2010. Southwest Wyoming Round 2 CAMx Sensitivity Tests. ENVIRON International Corporation, Novato, CA and Carter Lake Consultants, Laramie, WY. PowerPoint presentation to Continental Divide-Creston Cooperating Agencies, Cheyenne, Wyoming. January 7.

EPA. 1991. Guidance for Regulatory Application of the Urban Airshed Model (UAM), Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina.

EPA. 1999. Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for 8-Hour Ozone NAAQS. Draft. U.S. Environmental Protection Agency, Office of Air Quality and Planning Standards, Research Triangle Park, North Carolina.

EPA. 2007. Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze. U.S. Environmental

Protection Agency, Office of Air Quality and Planning Standards, Research Triangle Park, North Carolina. (EPE-454/B-07-002). April.

Gilliland, A., K., K. Appel, R.W. Pinder, and R.L. Dennis, 2006. Seasonal NH3 emissions for the continental United States: inverse model estimation and evaluation. Atmospheric Environment, 40, pp. 4986-4998.

Kemball-Cook, S., R. Morris, J. Johnson, B. Koo, T. Sakulyanontvittaya, L. Parker, T. Shah, U. Nopmongcol, and P. Piyachaturawat, 2009. Draft Report: Hiawatha CAMx 2005-2006 Base Case Model Performance Evaluation, Prepared for SWCA Environmental Consultants, Broomfield, CO. June 26.

Mansell, G. 2005. An Improved Ammonia Inventory for the WRAP Domain. Final Report, Volume I. ENVIRON International, Novato, California. http://pah.cert.ucr.edu/aqm/308/ppt_files/emissions/nh3/Volume_I_FinalReport.3-07.pdf. March 7.

Morris, Ralph, S. Kemball-Cook and J. Zapert, 2009a. Preliminary list of Proposed Sensitivity Tests for the Continental Divide-Creston O&G Development EIS CAMx Base Case, Technical Memorandum. ENVIRON International Corporation, Novato, CA and Carter Lake Consultants, Laramie, WY. Prepared for David Finley, WDEQ/AQD, Cheyenne, Wyoming. September 11.

Morris, Ralph, S. Kemball-Cook and J. Zapert, 2009b. Potential CAMx Sensitivity Tests to Improve Ozone and Nitrate Model Performance under the Continental Divide-Creston Oil and Gas Project, Technical Memorandum. ENVIRON International Corporation, Novato, CA and Carter Lake Consultants, Laramie, WY. Prepared for David Finley, WDEQ-AQD, Cheyenne, Wyoming. September 30.

Wesely, M.L. 1989. Parameterization of Surface Resistances to Gaseous Dry Deposition in Regional-Scale Numerical Models. Atmos. Environ., 23, 1293-1304.

Young, J., J. Pleim and R. Mathur. 2009. Mass Consistency Improvements in CMAQ Advection. Presented at the 8th Annual CMAS Conference, October 19-21, 2009, Chapel Hill, NC. (http://www.cmascenter.org/conference/2009/slides/young_mass_consistency_2009.pdf).

Zhang, L., J. R. Brook, and R. Vet, 2003. A revised parameterization for gaseous dry deposition in air-quality models. Atmos. Chem. Phys., 3, 2067–2082.

Zhang, L., Vet, R., Brook, J.R., Legge, A.H. 2006. Factors affecting stomatal uptake of ozone by different canopies and a comparison between dose and exposure. Science of the Total Environment, 370 (1), pp. 117-132.