10.5 DEVELOPMENT OF A WRF-AERMOD TOOL FOR USE IN REGULATORY APPLICATIONS

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ABSTRACT

The Tennessee Valley Authority (TVA) has developed a WRF-AERMOD tool which transforms the Weather Research and Forecasting (WRF) model output into the meteorological input needed by AERMOD (AERMAP/AERMET/AERMOD), the EPA-recommended model for short-range dispersion modeling. The tool was used to model 2002 emissions from TVA's Allen Fossil (ALF) Plant in Memphis, Tennessee. Modeling using NWS data was also performed and results were compared. Analyses of modeling results showed several differences between the two approaches, with much of the inconsistencies attributed to four main findings. First, the NWS-AERMOD approach tended to stay more unstable in the summer and stable in the winter with unrealistically high mechanical boundary layer (MBL) heights. Second, user-estimated (or AERSURFACE-derived) surface parameters - Bowen ratio, albedo, and surface roughness - in the NWS approach were substantially different from WRF-estimated values which led to significant differences in the derived boundary layer parameters. Third, the considerable percentage of calms in the NWS dataset affected NWS-AERMOD results as boundary layer parameters and estimated concentrations were not calculated during calm conditions. Finally, when 24-hour SO_2 concentrations from both approaches were compared to the onsite ALF SO_2 monitor, WRF-AERMOD estimated values much closer to observed. The WRF tool had several advantages over NWS as it was able to directly output more land use and boundary layer parameters needed by AERMOD than NWS, it had a more representative upper air profile, it contained no missing data, and it was able to provide comprehensive data at the precise location of the source.

1. INTRODUCTION

For short-range regulatory dispersion modeling (less than 50km), the U.S. Environmental Protection Agency (USEPA) recommends use of the AERMOD modeling suite[1]. The meteorological data preprocessor AERMET incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts and requires representative National Weather Service (NWS) surface and upper air data as well as onsite data, if available. For rural sources, the closest representative NWS station may be greater than 50-100 kilometers away. Furthermore, NWS data limitations - instrumentation limits, missing data, and lack of surface parameters required by AERMET - have motivated the EPA to explore the use of prognostic meteorological models, specifically MM5 (Brode 2008), which can provide a timely and spatially comprehensive meteorological dataset for input to AERMOD. The EPA has been testing an in-house MM5-AERMOD tool for possible use in future regulatory applications. However, since MM5 is no longer supported by its developers and the WRF (Weather Research Forecasting) model is now considered the state-of-the-art meteorological model to replace it, TVA developed a WRF-AERMOD tool that takes WRF three-dimensional meteorological output (surface and upper air) and transforms it into the AERMET-ready surface and profile files for use in AERMOD. The tool was used to model 2002 emissions from TVA's Allen Fossil Plant in Memphis, Tennessee.

2. WRF-AERMOD SETUP

The WRF meteorological model is a mesoscale numerical weather prediction system that has been designed to be a flexible, state-of-the art atmospheric simulation system, suitable for use in a broad range of applications across scales ranging from meters to thousands of kilometers (Michalakes et al 2004). The WRF model was set up using one course domain at 12 kilometer resolution and with 27 vertical sigma-pressure levels. The major physics options included the YSU PBL (Planetary Boundary Layer) scheme, the NOAH LSM (Land Surface Model), the RRTM (Rapid Radiative Transfer Model) scheme for long-wave radiation, the Dudhia scheme for shortwave radiation, the KF (Kain and Fritsch) cumulus scheme, and the WSM (WRF Single-Moment) 3-class simple ice scheme (Skamarock et al 2008). The GCIP NCEP NAM / ETA 3D data and surface analysis data were used for input into the model. The WRF model simulated meteorological conditions over North America for the 2002 year in seven-day simulation steps (with one overlap day which was used for ramp-up) and produced the standard hourly meteorological output. Most of the basic surface variables needed by AERMET / AERMOD were readily available from WRF and were extracted using a standard WRF data extraction program[2]. Relative humidity and cloud

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[1] The AERMOD modeling suite consists of the AERMET meteorological processor, the AERMAP terrain data (USGS) processor, and the AERMOD dispersion model.

[2] The program, read_wrf_nc.f, can be obtained from the WRF download page: http://www.mmm.ucar.edu/wrf/users/download/get_sources.html

cover were not readily available from WRF. Instead, they were derived from temperature, mixing ratio and pressure based on a UCAR algorithm[3]. All of the AERMET-required upper-air variables were readily available from WRF and were extracted for all 27 levels.

The AERMET processor requires NWS surface and upper air observations as well as user estimation of land surface characteristics (albedo (r), Bowen ratio (B_0), and surface roughness length (z_0)) to derive several boundary layer parameters: sensible heat flux (H), surface friction velocity (u*), convective velocity (w*), the vertical potential temperature gradient above the PBL (VPTG), the height of the convectively-generated boundary layer (CBL), the height of the mechanically-generated boundary layer (MBL), and Monin-Obukhov length (L). These boundary layer variables were not standard output from WRF. Therefore, several AERMET conversion routines were modified to take the necessary WRF surface variables and calculate them. Once all surface and upper-air variables were extracted or derived, they were reformatted into AERMET Stage 3 format for ready use into AERMOD.

The WRF-AERMOD tool was used to model 2002 emissions of criteria pollutants with their standard averaging times from the TVA Allen Fossil (ALF) Plant in Memphis, Tennessee. The NWS 2002 Memphis surface and Little Rock NWS upper air data were also processed through AERMET and used in AERMOD to model emissions from ALF. Both approaches were modeled using a four-nested AERMOD domain with the finest receptor grid closest to the source and extending out 20 kilometers (Figure 1).

3. AERMOD ANALYSES

The ALF site was chosen as the modeling source for several reasons: 1) its location in an urban setting (Memphis) close to a NWS station, which allowed for a good comparison between WRF and NWS meteorology, and 2) a SO_2 monitor located at the ALF site, which allowed for comparison between estimated concentrations and observations. In Memphis, there are three large sources of SO_2 emissions, of which ALF is the largest. The closest source of SO_2 emissions to the ALF site is from the Cargill Corn Milling plant located to the northeast. It emits less than 1/6th of the SO_2 emissions at ALF. With prevailing winds from the southwest and west, impacts from this plant to the ALF monitor are most likely minimal. Therefore, AERMOD-estimated maximum 24-hour SO_2 concentrations from both the WRF tool and the NWS approach (independent of receptor location) were compared to 24-hour averaged SO_2 monitor observations. A cumulative frequency distribution (CFD) was performed to present a running total of SO_2 concentrations in order to see how well each approach compared to observations (Figure 2). The CFD showed that the WRF-AERMOD tool estimated the observed SO_2 concentrations much better than the NWS-AERMOD approach. Additional statistical analyses of the mean bias, mean error, and root mean square error (RMSE) showed that independent of receptor location, WRF-estimated 24-hour SO_2 concentrations with a lower bias, error, and RMSE than NWS (Figure 3).

Chi over Q (χ/Q) values were calculated on the AERMOD results to see if any patterns or similarities existed in the concentration averages. They were calculated for 1-hour, 3-hour, 8-hour, 24-hour, and annual averages. The χ/Q values, or dispersion factors, were obtained by dividing the maximum impact concentrations by the emission estimates in units of seconds / cubic meter. The χ/Q values provide a relatively simple means to estimate the magnitude of pollutant impacts from a source; they are better representative of maximum concentration impacts from dispersion modeling when no chemistry is included. The χ/Q results showed that for short-term averages (< 24-hour), the WRF-AERMOD tool predicted higher maximum concentrations than NWS-AERMOD (Figure 4). For the longer-term averages (24-hour and annual), NWS-AERMOD predicted higher maximum concentrations. Furthermore, both the NWS approach and WRF approach predicted the highest 3-hour and 24-hour concentrations in December, with the 24-hour concentrations predicted on the same day. An analysis of the highest 98th percentile of concentrations for all averaging periods revealed that the majority (75%) of highest concentrations estimated with the WRF-AERMOD tool fell in December. The NWS approach tended to spread the highest 98th percentile of concentrations over several months, with December ranking highest (26%) followed by March (21%) (Figure 5).

Finally, spatial plots were constructed to view the distribution of concentrations around the ALF site. For all averaging periods <= 24 hours, the WRF-AERMOD tool tended to spread concentrations much farther downwind from the source than NWS-AERMOD. For the 24-hour average, even though NWS-AERMOD produced a higher maximum, the spatial plots revealed that WRF-AERMOD tended to predict a larger distribution of high concentrations that extended much farther from the source than the NWS approach (Figure 6). For the annual average, NWS-AERMOD predicted both a higher maximum annual concentration and a larger spread of high concentrations away from the source than the WRF-AERMOD tool.

[3] The UCAR algorithm, cloudf.F, is found in the GRAPH program (/mesouser/MM5V3/GRAPH.TAR.gz) which can be obtained from the UCAR ftp site: anonymous@ftp.ucar.edu.

4. METEOROLOGICAL ANALYSES

The results of the CFD and the χ/Q analysis led to further investigation of the AERMET-generated meteorological conditions that were present during the highest estimated concentrations. Surface conditions were primarily investigated since they were most likely to influence results. A review of the meteorological variables present during the maximum averages showed no obvious concurrent, key meteorological drivers present for either approach. For the highest 24-hour average concentrations that occurred on the same day, both approaches had similar values for wind speeds and direction, MBL heights, and CBL heights. Again, there were no obvious variables that stood out as key drivers.

In an attempt to isolate the key meteorological drivers that were producing the maximum concentrations, a linear regression analysis was performed on both meteorological datasets. At first, the analysis revealed inconclusive results as each approach yielded different key predictors. The analysis of the NWS approach estimated w* as the key predictor whereas the WRF approach estimated VPTG as the most significant predictor. A closer look at the AERMET output from both approaches revealed that the NWS data contained approximately 20% calm wind conditions. Calm conditions are essentially treated as missing in AERMOD and the model will not calculate any derived boundary layer parameters or concentrations during calms. Therefore, all hours containing calms were removed from the NWS dataset with corresponding hours removed from the WRF dataset and another regression analyses was performed on the matched data set. The results of this analyses showed that the MBL height was the most significant predictor for both approaches (Table 1). Clearly, calms strongly influenced the statistical analysis and model performance. However, the disparity between the level of importance attributed to MBL in the NWS versus WRF AERMOD (partial r^2 of 0.49 and 0.15, respectively) results was striking.

To further evaluate the performance of both approaches and potentially explain the patterns seen in the concentration averages, several statistical indicators were calculated for the AERMET output variables. For screening purposes, a measure of performance recommended by the USEPA (USEPA 1992) is the fractional bias (FB):

$$FB = \frac{2}{N}\sum_{i=1}^{N}\frac{(Model - Observed)}{(Model + Observed)}.$$

It is often considered a useful statistic since it is symmetrical and bounded with limits from -2.0 (extreme under-prediction) to +2.0 (extreme over-prediction). Bias values equal to +/-0.67 reveal over / under-prediction by a factor of 2, whereas bias values close to 0 (zero) indicate a high level of agreement between predictions. However, FB results must be interpreted carefully because the sign of FB can be opposite of the sign for the computed bias. In other words, one can have an over-prediction of a variable (a positive bias) but have a negative FB. Because of the large number of meteorological surface variables that are output from AERMET (approximately 20), the FB was used as a screening tool to try and isolate those variables that appeared to have the largest disagreement between NWS and WRF approaches (Figure 7). The FB was calculated for both calm and no-calm conditions. Once the key variables were isolated, mean bias, mean error, the root mean square error (RMSE), and monthly averages were calculated to further evaluate performance (Table 2). For the key variables, most of the results of the statistics and averages reflected calm conditions since results from no-calm conditions were very similar.

Based on the results of the FB analysis, the following surface parameters had a disagreement by at least a factor of 2 (+/- 0.67): sensible heat flux (H), Bowen ratio (B_0), surface roughness length (z_0), Monin-Obukhov length (L), and convective velocity scale (w*). The largest disagreement was with L (1/L) as FB results showed almost no agreement. However, L, H, and B_0 ratio can become unbounded with large extremes and vary widely throughout a day. Therefore, further evaluation of these parameters using other statistical measures and monthly patterns was crucial.

The Monin-Obukhov length (L) is a derived convective boundary layer (CBL) parameter that is estimated in AERMET through an iterative procedure with surface friction velocity, u*. It is a stability parameter that represents the height above which convectively driven turbulence dominates over mechanically driven turbulence (USEPA 2000). In AERMET, H and u* are first calculated, and then used to calculate L using similarity theory. The inverse length is more commonly used in evaluations as L can become unbounded and large. The inverse length is more often expressed in relation to surface roughness length, z_0. Large negative values of z_0/L correspond to large instability due to buoyancy; positive values correspond to stable conditions (Golder 1972). For all comparisons involving L, either the inverse or z_0/L was used. Statistical evaluation of a parameter that has widely varying, large extremes can often produce misleading conclusions. To complicate matters, NWS-AERMET only computes L during non-calm conditions whereas the WRF-AERMOD tool calculates it for all wind speeds. Therefore, a Pasquill stability analysis which compared 1/L with z_0 only during non-calm conditions was performed (Figure 8). It revealed that the NWS approach kept a slightly more stable regime than WRF with as much as 5% more E-F stability classes present throughout the 2002 year. A monthly breakdown of the stability classes for each approach using the criteria of 1/L > 0 for stable conditions showed that NWS tended to stay more stable than WRF, especially during the winter months.

Sensible heat (H) is energy transferred between the surface and air when there is a difference in temperature between them (Wallace and Hobbs 2006). It can be negative or positive, with negative values usually indicative of warmer air temperatures than the surface (inversions). It is important in AERMET as it is used to calculate several parameters: u*, w*, CBL, and L. In WRF, it is directly calculated and output. When NWS data is used, AERMET estimates it using the user-defined Bowen ratio and observed net radiation. If net radiation is not available, solar radiation, temperature, and cloud cover are used. The mean bias, mean error, and RMSE evaluations were difficult to interpret given extreme limits on H; they tended to show that on average, the WRF-AERMOD tool had larger positive values of sensible heat than NWS (Table 2). A monthly analysis of day/night heat fluxes between WRF and NWS revealed that WRF kept positive values of sensible heat flux both day and night throughout the year (Figure 9). For the NWS approach, large negative night fluxes dominated the monthly averages from January-March and November-December. Since negative heat fluxes correspond to a more stable boundary layer, NWS-AERMET was estimating strong inversions at night during the winter and thus keeping a more stable regime than WRF. On the flip side, NWS-AERMET estimated larger average fluxes than WRF in the summer, which reflected a more unstable boundary layer. The discovery that the WRF-AERMOD estimated no negative heat flux values was alarming. Sensible heat flux remains positive at night only under certain conditions (i.e., warm air advection). Further investigation revealed that WRF does directly output both positive and negative values. When heat flux values are read into the AERMET subroutine MPPBL.F, the program sets a positive value (limit of 0.1 W/m^2) under convective conditions. However, the AERMET subroutine changed WRF's negative heat flux values to the positive limit even when convective conditions were not present. This important finding reveals that there may be some inconsistency in the AERMET criteria used to derive and limit heat flux values. Once this discovery was known, a second WRF-AERMOD run was made setting the limited H values to negative. Results showed no change in pollutant concentrations.

The Bowen ratio (B_0) is the ratio of energy fluxes by sensible and latent heating and is sensitive to boundary layer surface moisture. The AERMET processor uses B_0 to calculate H, which is further used to calculate additional boundary layer parameters (as previously mentioned). Since WRF directly calculates sensible and latent heat fluxes, B_0 was easily derived. For the NWS approach, B_0 was estimated by use of the AERSURFACE tool or by direct user-calculation via reference tables (USEPA 2000). Either procedure estimates hourly B_0 values that are dependent on time (i.e., annually, seasonally, or monthly) and by land use characteristics that are defined within user-specified wind sectors. The mean bias results showed that NWS-AERMET estimated higher values of B_0 than the WRF-AERMOD tool. Average monthly B_0 values confirmed that the NWS approach estimated higher values for all months except March (Figure 10). From January-February and in December, the NWS-estimated B_0 values were approximately four (4) times higher than WRF-estimated values. The WRF-estimated values typically ranged from 0.2 during the summer to 0.6 in the winter, with NWS values ranging from 0.3 in the summer to 1.6 in the winter. Given typical documented winter B_0 values of 1.0 - 1.6 for urban / grassland categories, it appears as if the WRF-AERMOD tool underestimated values, resulting in extra evaporation from surface wetness in addition to the normal transpiration rates which would keep the boundary layer more moist throughout the year (Paine 1987; AERMET 2000). It was discovered that the Bowen ratio calculated from WRF's sensible and latent heat fluxes can sometimes become extremely large, unlike the NWS-AERMET approach which defines limited B_0 values. Since analyses of H tended to show that WRF had higher values than NWS, larger latent heat flux values must have dominated the energy balance equation to keep B_0 smaller. However, WRF uses H to derive B_0 - unlike the NWS approach which uses B_0 to derive H. Therefore, its effects on derived boundary layer parameters were most likely less significant. Furthermore, studies show that AERMOD concentrations are not highly sensitive to changes in r and B_0 (Karvounis et al. 2007).

The surface roughness length, z_0, was another surface parameter that appeared to show much disagreement between WRF and NWS. The z_0 is the height at which the mean horizontal wind speed is zero. It quantifies the obstacles to wind flow from various surfaces. Typical values range from 0.001 meters over water to 0.2-3.0 meters for an urban area (Stull 1988). In WRF, z_0 is determined from the model's land use reference tables and remains constant for all hours at a particular location. For the NWS approach, z_0 is determined by the AERSURFACE tool or by direct user estimation using the AERMET user's guide land use reference tables. As with B_0, either estimation produces hourly z_0 values which may vary substantially depending on the seasonal frequency and land surface characteristics. The AERSURFACE-estimated values vary by season; they do not remain constant for all hours. For the ALF site, WRF estimated a constant z_0 of 0.2 meters; NWS estimated z_0 that varied from 0.3 meters in the summer to 1.6 meters in the winter (Figure 11). The NWS-AERMET's large variation in z_0 seemed counterintuitive. For a downtown urban site, z_0 would be higher from the close proximity of structures (buildings), but it would vary little by season. Having a seasonal variation would indicate vegetation changes, but z_0 would be higher in the summer than winter. Average bias results confirmed that WRF estimated lower z_0 values than NWS (Table 2). Typically, higher z_0 values correspond to more wind flow obstacles which, in turn, enhance turbulence and ultimately affect mixing height (Wallace and Hobbs 2006). The increased turbulence associated with higher roughness lengths increases the dispersion of the plume away from the centerline height. The AERMOD model is extremely sensitive to changes in surface roughness and wind speeds; small changes in these variables have been shown to affect the distance within which concentration limits are exceeded by several hundred meters (Grosch and Lee 1999; Faulkner et al 2008). Studies have shown that lower z_0 values in AERMOD tend to increase short-term concentrations (1-hour, 3-hour) and lower the long-term maximum averages (24-hour, annual) (Grosch and Lee 1999).

In order to estimate turbulence in the CBL, AERMET calculates a convective velocity scale, w*, which is directly proportional to H and the CBL and inversely proportional to temperature (T) and density (ρ). It indicates the amount of turbulent kinetic energy in thermal updrafts in the CBL, with typical values for deep layers on the order of 1-2 m/s (Stull 1988). It is only calculated during daytime convection. Both the mean bias results and the monthly averages of w* indicated that the WRF-AERMOD tool tended to produce lower values of w* than NWS-AERMET (Figure 12). The WRF-AERMOD tool's lower w* values were most likely due to the consistently lower estimated CBL heights and a more moist boundary layer. Lower values of w* typically indicate a more neutral regime during daytime convection (Wallace and Hobbs 2006; Stull 1988).

Even though the FB results did not indicate large MBL and CBL disagreement, monthly average snapshots of the data combined with additional statistics were computed for the two variables. The MBL was especially examined since the regression analysis seemed to indicate that it was one of the most important predictors of concentrations. According to the mean bias results, the WRF-AERMOD tool generally tended to produce lower MBL heights than NWS-AERMET. A frequency analysis of plume rise in the MBL between both approaches revealed several important findings (Figures 14). First, NWS-AERMET estimated low plume heights - well below the MBL - throughout the year, whereas the WRF-AERMOD tool estimated higher plume heights with some above the MBL (July). Furthermore, the average MBL heights from NWS-AERMET were significantly higher than the WRF-AERMOD tool, especially in the winter. With typical MBL heights ranging a few hundred meters deep (Yu 1977), NWS-AERMET estimated values unrealistically high, with averages reaching 2000 meters in December, January, and February. That deep of a MBL rivaled the CBL, and it caused much more plume dilution for stable plumes which most likely lowered pollutant concentrations and kept plumes closer in to the source.

For the CBL, first glance of the mean bias, error, and RMSE results showed that WRF tended to keep slightly higher CBL heights than the NWS approach (Table 2). However, monthly averages of CBL heights revealed that NWS-AERMET estimated higher CBL heights in the summer (Jun-Sep) and lower CBL heights in the winter when compared to WRF (Figure 13). This is further confirmed by a frequency distribution of CBL heights which showed that the NWS approach estimated a larger percentage of very low and extremely high CBL heights (Table 3). The NWS-AERMET maximum estimated CBL heights were roughly 300m higher than WRF. These extremes were coupled with the discovery that NWS-AERMET estimated fewer convective hours during the day than WRF. Throughout the year, the WRF-AERMOD tool estimated approximately 2-4 more convective daytime hours than NWS-AERMET. So, even though the WRF-AERMOD tool calculated more hours of CBL heights, the NWS approach had more extremes. The CBL results coincide with NWS-AERMET's larger w* and higher H during the summer.

Finally, based on AERMOD's high sensitivity to winds (Steib 2005), the distribution of surface wind fields from both approaches was evaluated. Wind roses were constructed to determine the frequency of wind speed and direction throughout the year (Figure 15). Calm conditions in the NWS dataset (< 1.3 m/s) were excluded since calms did not influence concentrations. The wind analysis showed that NWS-AERMET winds tended to blow either from the SSW/S or the NNE/NE most of the time; these directions comprised almost 50% of the total hourly winds. The WRF-AERMOD tool's wind distribution was more evenly spread; the largest percentage of the distribution (24%) came from the SW/SSW/S directions. A frequency analysis confirmed that WRF tended to have slightly higher wind speeds for all wind speed categories. The higher wind speeds could be a possible explanation for the greater dispersion of pollutants from the WRF-AERMOD tool. With more persistent wind directions, maximum pollutant concentrations are more likely to impact the same grid cells, in turn producing higher long-term averages. The NWS-AERMET's more restrictive wind distribution was another likely explanation for the higher long-term maximum average concentrations.

The wind analyses unexpectedly revealed that there was some discrepancy between the NWS raw wind data and the AERMET-produced wind data. Hourly raw NWS input variables did not always correspond to the AERMET output variables. This discovery led to an investigation of the NWS raw input data and the AERMET-produced data to determine the extent of the differences between datasets. The AERMOD modeling system does use smoothing in derived boundary layer parameters. However, substantial differences between input and output meteorological variables would not be expected. Wind direction (WDIR), wind speed (WS), temperature (T), cloud cover (CC), and surface pressure (PRES) were statistically compared between raw input and AERMET output (Table 4). Substantial differences were seen in winds and cloud cover with smaller differences seen with pressure.

5. CONCLUSIONS

Comparisons between the WRF-AERMOD tool and the current EPA-recommended NWS approach revealed several significant findings about the performance of each option. For the 2002 episode, the WRF-AERMOD tool estimated higher short-term maximum concentrations (< 24 hour) whereas NWS-AERMOD estimated higher long-term maximum concentrations (>= 24 hour). The spatial plots also revealed that even though NWS produced a higher maximum 24-hour average, WRF-AERMOD tool estimated a larger distribution of higher concentrations. These patterns were most likely due to the differences seen in estimated z_0, wind distribution, and MBL heights. Studies have shown that pollutant concentrations tend to be highly sensitive to variations in z_0 and wind speeds in particular (Faulkner et al. 2008). Furthermore, AERMOD studies have revealed that obtaining representative z_0 values is crucial to model accuracy (Karvounis et al. 2007; Grosch and Lee 1999). Changes in z_0 generate changes in mixing heights and alter the profiles of various meteorological parameters; therefore, representative z_0 values are crucial. Both approaches relied on reference tables for z_0 estimation. With typical z_0 values for urban environments documented around 0.2-1.0 meters and having little seasonal variation (USEPA 2004), it appears as if the NWS approach did not represent the ALF site most accurately.

Both the WRF-AERMOD tool and the NWS approach estimated the majority of highest concentrations in December. For both approaches, December had the lowest average CBL heights, w*, and H; and had the highest RH and MBL heights - all indicators of a stable regime. The largest disagreement between approaches appeared to be with the derived boundary layer parameters. Furthermore, all of the derived boundary layer parameters were interdependent, so a variation in one variable greatly influenced the variation of another variable. Analyses of the stability parameters showed that NWS-AERMET remained more unstable in the summer and more stable in the winter than WRF, with unrealistically deep MBL heights. The large MBL heights allowed for substantial plume dilution for the stable plumes which most likely lowered pollutant concentrations. This is a significant discovery, especially since the regression analysis seemed to indicate that MBL heights are a key player in predicting concentrations.

Bowen ratio (B_0) values between both approaches were significantly different. Based on typical documented ranges for B_0 in urban areas, the WRF-AERMOD tool appeared to underestimate values, keeping a more moist boundary layer than NWS. It was discovered that the Bowen ratio calculated from WRF's sensible and latent heat fluxes sometimes became extremely large, unlike the NWS-AERMET approach which set limited B_0 values. It was inconclusive as to the significance WRF's underestimated B_0 values had on estimated concentrations. Unlike the NWS approach which used B_0 to derive H, the WRF-AERMOD tool had H and derived B_0. With the AERMET processor relying on H to derive additional boundary layer parameters, obtaining representative H values would seem to be of greater importance. However, several studies have shown that AERMOD concentrations are not as highly sensitive to changes in H, r, and B_0 as they are to surface roughness length, z_0 (Karvounis et al. 2007). The AERMOD users manual states, "The sensible heat flux, Bowen ratio and albedo are not used by AERMOD, but are passed through by AERMET for information purposes only" (USEPA 2004).

The significant number of calms (20%) in the NWS dataset made direct comparisons with WRF very difficult and compromised some of the accuracy of the analyses since the NWS approach did not calculate boundary layer parameters during calm conditions - unlike WRF which calculated parameters for every hour (with the exception of those calculated only during daytime convection). More importantly, estimated concentrations were not calculated during calm conditions. Removing 20% of the hourly estimations from the dataset undoubtedly affected the resulting concentration averages. The WRF-AERMOD tool's ability to output all hourly variables with the exception of those that are calculated during daytime convection is a major advantage over the NWS-AERMOD approach. Even though the upper air variables were not analyzed, the WRF-AERMOD tool's 27-layer atmospheric profile was another significant improvement over the NWS-AERMOD 1-layer profile. A detailed vertical stratification unquestionably produced a more representative atmospheric profile than the "standard" approach.

The most important finding in the analyses was the result of the CFD which revealed that the WRF-AERMOD tool estimated 24-hour SO_2 concentrations more closely to observed than the NWS approach. The significant number of calms and missing data, the unrealistic MBL heights, the highly variable z_0, and a 1-layer upper air profile most likely impaired the ability of the NWS-AERMOD approach to fully capture boundary layer and pollutant behavior. Furthermore, estimation of surface characteristics via land use tables or user estimation as required by both approaches may not be the best method, especially for z_0 as the parameter has been documented as highly influencing concentration averages (Karvounis et al. 2007). Finally, it is uncertain whether the NWS approach is truly representative of a modeled site when the source lies in a location far removed from an NWS station or other suitable meteorological monitoring site. Locally-influenced meteorological conditions such as radiation, cloud cover, precipitation, and winds may differ widely between an existing or potential source and meteorological data used for dispersion analysis. Some refinements to the WRF-AERMOD tool's approach in estimating B_0 values closer to those documented in literature as well as modification to the AERMET subroutine to keep H values negative and limit B_0 are necessary. Overall, the tool seemed to provide a better representation of boundary layer physics and pollutant behavior at the ALF site than the current EPA-recommended approach. With some studies backing WRF over MM5 in capturing boundary layer processes (Kwun et al. 2009) and with MM5 no longer supported by its developers, the WRF-AERMOD tool may prove to be a valuable meteorological processing tool for AERMOD applications. Final assessment of tool performance would definitely require further analyses using multiple sites and episodes.

6. FIGURES AND TABLES

6.1 Figures

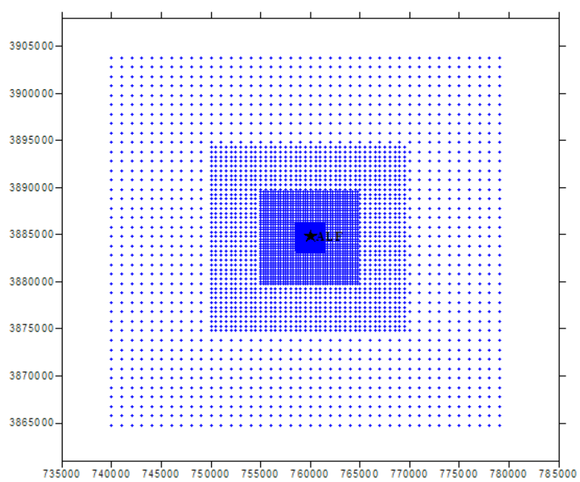


Figure 1: AERMOD domain with ALF location.

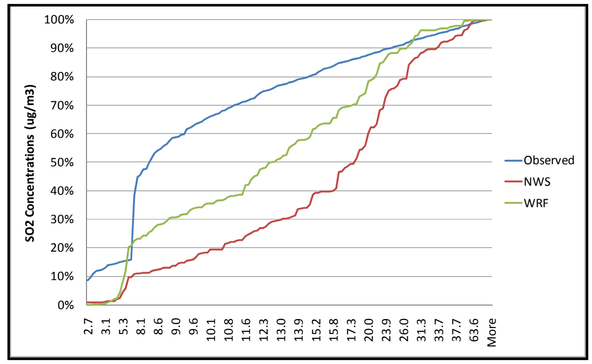


Figure 2: Cumulative Frequency Distributions of 24-hour AERMOD SO_2 Concentrations from NWS-AERMOD and WRF-AERMOD at ALF Monitor (Independent of Receptor Location).

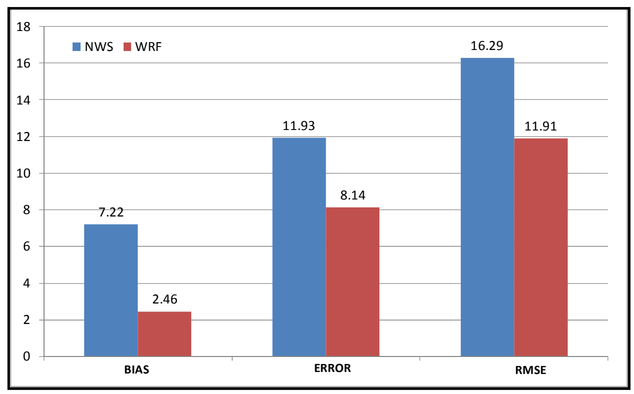


Figure 3: Mean Bias, Mean Error, and Root Mean Square Error (RMSE) Statistics of NWS-AERMOD and WRF-AERMOD estimated 24-hour SO_2 Concentrations at ALF Monitor (Independent of Receptor Location).

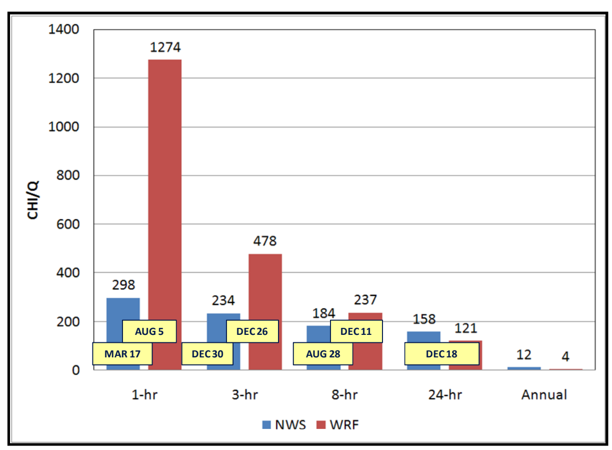


Figure 4: χ/Q estimates of pollutant concentrations for different averaging periods from NWS-AERMOD (blue) and WRF-AERMOD (red). Dates (yellow boxes) indicate days reporting highest concentrations.

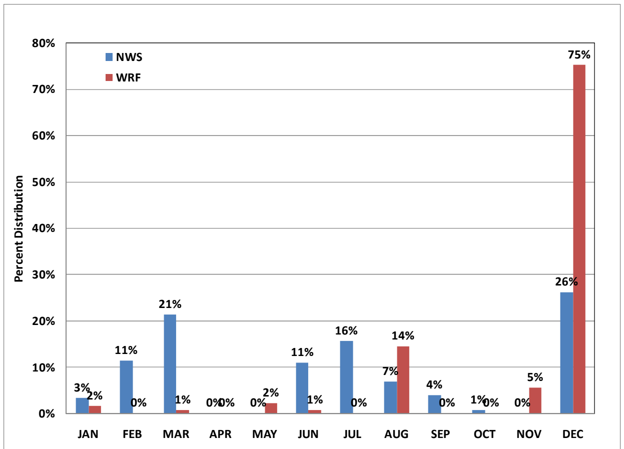


Figure 5: Monthly Distribution (%) of the Highest 98th Percentile of Concentrations from NWS-AERMOD (blue) and WRF-AERMOD (red).

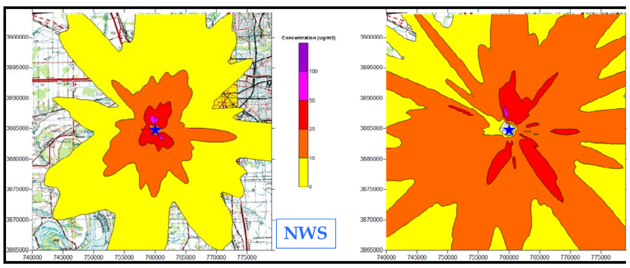


Figure 6: Spatial Plot of 24-hour Average Concentrations from WRF-AERMOD and NWS-AERMOD

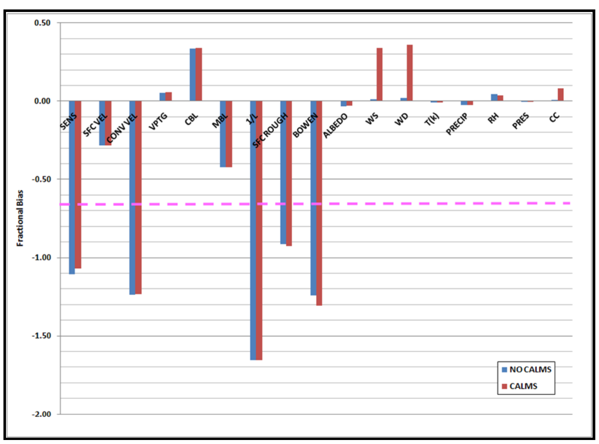
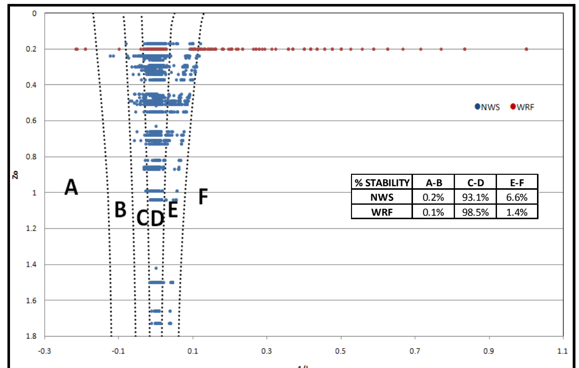


Figure 7: FB Results for Calm Conditions and No Calm Conditions.



% STABILITY	A-B	C-D	E-F
NWS	0.2%	93.1%	6.6%
WRF	0.1%	98.5%	1.4%

1/L > 0	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
NWS	5.8%	4.8%	5.4%	4.6%	3.7%	2.9%	2.6%	3.6%	3.4%	4.6%	5.0%	6.6%
WRF	4.7%	4.1%	4.9%	4.5%	3.2%	2.7%	2.4%	3.5%	3.2%	4.3%	4.5%	5.2%

Figure 8: Pasquill Stability Analysis comparing z_0 with 1/L from NWS-AERMET and the WRF-AERMOD tool.

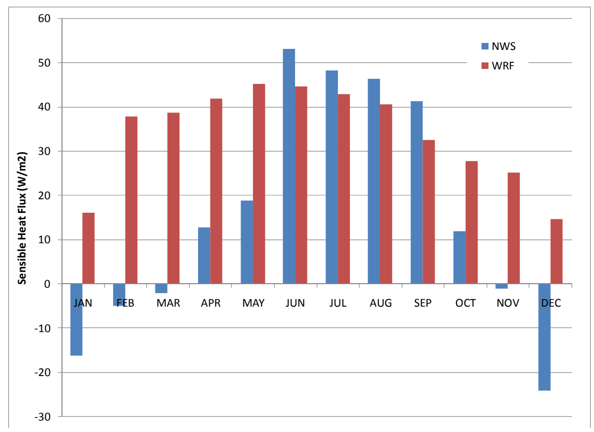


Figure 9: Average monthly sensible heat flux (H) values from NWS-AERMET and the WRF-AERMOD tool.

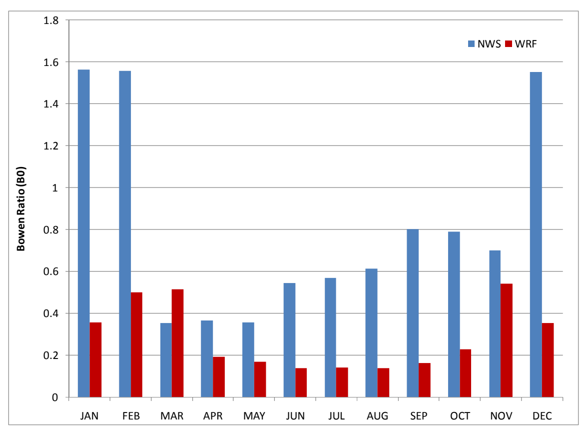


Figure 10: Average Monthly Bowen Ratio (B_0) values from NWS-AERMET and the WRF-AERMOD tool.

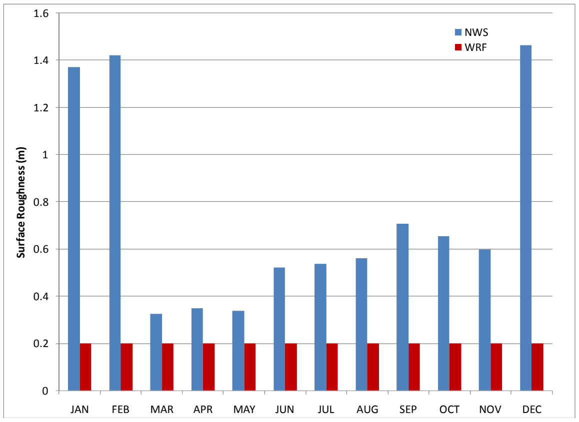


Figure 11: Average Monthly Surface Roughness (z_0) values from NWS-AERMET and the WRF-AERMOD tool.

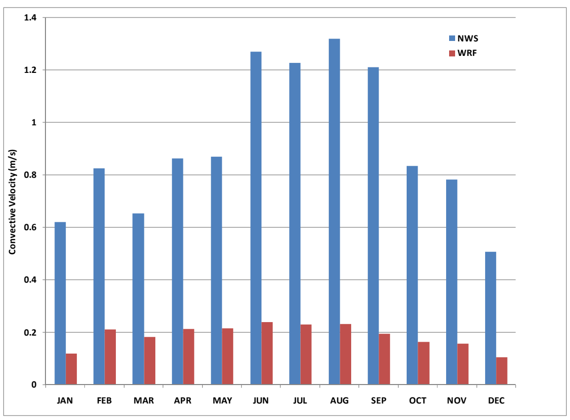


Figure 12: Average Monthly Convective Velocity (w*) values from NWS-AERMET and the WRF-AERMOD tool.

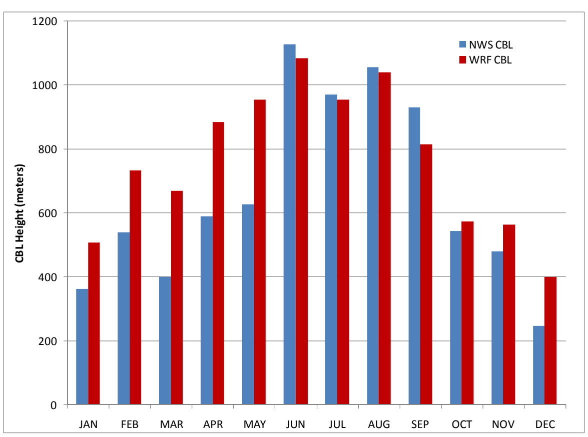
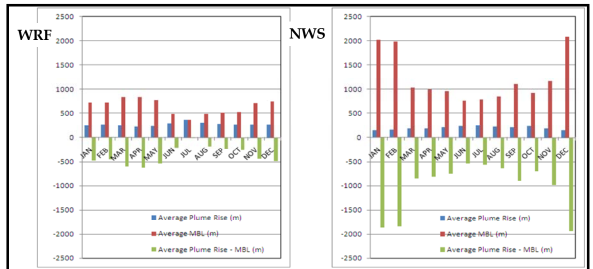
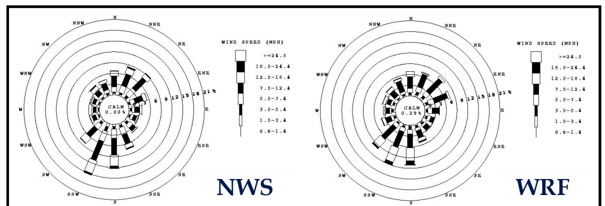


Figure 13: Average Monthly CBL heights (CBL) from NWS-AERMET and the WRF-AERMOD tool.



		JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
WRF	Average Plume Rise (m)	247.3	270.9	241.5	222.4	235.8	288.0	362.8	300.7	278.9	268.0	268.1	263.8
	Average MBL (m)	723.3	718.4	839.3	839.6	776.7	490.1	370.5	485.4	514.8	526.6	704.5	748.0
	Average Plume Rise - MBL (m)	-476.0	-447.5	-597.7	-617.2	-540.9	-202.0	-7.7	-184.7	-235.9	-258.7	-436.5	-484.2
NWS	Average Plume Rise (m)	148.8	152.7	188.4	183.4	211.6	235.8	243.0	218.9	210.4	226.2	185.7	143.9
	Average MBL (m)	2019.0	1987.9	1042.3	1005.3	962.8	767.0	794.8	852.2	1110.6	925.9	1174.2	2085.9
	Average Plume Rise - MBL (m)	-1862.7	-1841.1	-853.9	-821.9	-751.1	-531.1	-556.9	-633.3	-900.2	-699.7	-988.5	-1942.0

Figure 14: Average Monthly Plume Rise and MBL Heights from the WRF-AERMOD tool and NWS-AERMET.



% WS	> 1.3 m/s	> 3 m/s	> 6 m/s	> 8 m/s	> 10 m/s	> 12 m/s
NWS	100	71.85	16.01	4.01	0.48	0.01
WRF	95.06	73.50	16.94	4.37	0.58	0.01

Figure 15: Wind Roses and Wind Speed Distribution from NWS-AERMET and the WRF-AERMOD tool.

6.2 Tables

CALMS INCLUDED

REGRESSION ANALYSIS -- NWS DATA			
STEP	VARIABLE	PARTIAL R-SQ	MODEL R-SQ
1	w*	0.4415	0.4415
2	u*	0.2672	0.7087
3	H	0.0024	0.711
4	T	0.0029	0.7139
5	MBL	0.0026	0.7166
6	z0	0.0014	0.718

REGRESSION ANALYSIS -- WRF DATA			
STEP	VARIABLE	PARTIAL R-SQ	MODEL R-SQ
1	VPTG	0.0409	0.0409
2	MBL	0.0536	0.0945
3	WS	0.0654	0.1599
4	1/L	0.007	0.1669
5	CBL	0.0036	0.1705
6	T	0.0086	0.1791

CALMS REMOVED

REGRESSION ANALYSIS -- NWS DATA			
STEP	VARIABLE	PARTIAL R-SQ	MODEL R-SQ
1	MBL	0.4853	0.4853
2	CBL	0.3494	0.8348
3	1/L	0.0084	0.8431
4	w*	0.0052	0.8484
5	VPTG	0.0429	0.8913
6	u*	0.0061	0.8974

REGRESSION ANALYSIS -- WRF DATA			
STEP	VARIABLE	PARTIAL R-SQ	MODEL R-SQ
1	MBL	0.1520	0.152
2	VPTG	0.0159	0.1679
3	CBL	0.0138	0.1817
4	WS	0.0077	0.1894
5	u*	0.0217	0.211
6	T	0.0035	0.2145

Table 1: Results of the Regression Analysis with Calms Included and Calms Removed.

AERMET VARIABLE	MEAN BIAS	MEAN ERROR	FRACT BIAS	FRACT ERROR	RMSE
H	25.29	42.03	-1.11	3.47	53.75
U*	-0.18	0.26	-0.28	1.00	0.36
W*	-0.73	0.73	-1.23	2.49	0.87
VPTG	0.01	0.01	0.06	0.83	0.03
CBL	150.91	381.13	0.34	1.23	500.69
MBL	-522.18	680.41	-0.42	1.36	973.74
1/L	0.002	0.013	-1.657	3.523	0.053
Z0	-0.54	0.54	-0.91	1.85	0.73
B0	-0.52	0.72	-1.24	2.91	1.77
R	-0.02	0.04	-0.03	0.24	0.09
WS	0.13	1.32	0.01	0.71	1.69
T(K)	-1.82	2.48	-0.01	0.02	3.04
PAMT	-0.11	0.29	-0.03	0.49	1.63
RH	2.11	10.10	0.04	0.32	13.09
PRES	-5.41	5.44	-0.01	0.01	5.73
CCVR	-0.39	2.55	0.01	1.28	3.62

Table 2: Mean Bias, Mean Error, Fractional Bias, Fractional Error, and RMSE (WRF-NWS) for AERMET variables.

CBL HEIGHT DISTRIBUTION					
MET	CBL<100m	CBL>500m	CBL>1000m	CBL>1500m	CBL>2000m
NWS	4.6%	23.0%	11.1%	4.7%	1.1%
WRF	2.1%	31.9%	15.2%	4.9%	0.8%

Table 3: Distribution of CBL heights from NWS-AERMET and the WRF-AERMOD tool.

	Wdir (deg)	Wspd (m/s)	Temp (C)	Tdew (C)	RH (%)	CCVR (0~10)	Psfc (mb)
$\{N\}_{Total}$	6998	8710	8717	n/a	n/a	8563	8754
$\{N\}_{\%}$	79.9%	99.5%	99.6%	n/a	n/a	97.8%	100.0%
$\{Diff\}_{Max}$	180.0	6.7	4.6	n/a	n/a	6.0	0.9
$\{Diff\}_{Min}$	-170.0	-7.7	-3.4	n/a	n/a	-10.0	-13.6
$\{Diff\}_{Aveg}$	-0.5923	0.0063	0.0226	n/a	n/a	0.0252	-0.3140
$\{N\}_{Total}$	- Total number of valid data in comparison						
$\{N\}_{\%}$	- Percentage of total number of valid data in comparison						
$\{Diff\}_{Max}$	- Maximum difference between NWS-raw and NWS-AERMET-ready data						
$\{Diff\}_{Min}$	- Minimum difference between NWS-raw and NWS-AERMET-ready data						
$\{Diff\}_{Aveg}$	- Average difference between NWS-raw and NWS-AERMET-ready data						

Table 4: Comparison of Basic Meteorological Variables from NWS Raw Data and AERMET Output Data.

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