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A case study of sulfur dioxide concentrations in Muscatine, Iowa and the ability for AERMOD to predict NAAQS violations

Charlene Marie Becka
University of Iowa

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A CASE STUDY OF SULFUR DIOXIDE CONCENTRATIONS IN MUSCATINE, IOWA AND THE ABILITY FOR AERMOD TO PREDICT NAAQS VIOLATIONS

by

Charlene Marie Becka

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Thesis Supervisor: Professor Patrick O’Shaughnessy

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Iowa City, Iowa

CERTIFICATE OF APPROVAL

MASTER'S THESIS

This is to certify that the Master's thesis of

Charlene Marie Becka

has been approved by the Examining Committee for the thesis requirement for the Master of Science degree in Civil and Environmental Engineering at the December 2014 graduation.

Thesis Committee: Patrick O'Shaughnessy, Thesis Supervisor

David Cwiertny

Scott Spak

ABSTRACT

Sulfur dioxide is a primary pollutant and a known respiratory irritant. While there is a small level of background SO_2, elevated concentrations are caused by industrial emissions. Muscatine, IA was designated as an area of nonattainment due to the persistent elevated levels of SO_2 in the area. There are currently no available methods for predicting potential SO_2 violations in Muscatine, and very little research was found investigating predictive modeling efforts.

This thesis examines atmospheric conditions in Muscatine caused by SO_2 emissions from facilities near the city. The main goals were to examine the plume dispersion model AERMOD for its ability to accurately map pollution levels, and to determine whether AERMOD could be used to predict SO_2 concentrations when using meteorological forecast models as weather inputs. An historical analysis was performed using meteorological records from 2007 and AERMOD. The maximum emission limit was used in AERMOD. The resulting predicted concentrations were compared with concentrations reported at a monitoring site within the city. A forecasting analysis was also completed using two weather model forecasts (WRF and NAM) from March 2012 as meteorological input for AERMOD. Accurate daily SO_2 emissions were obtained from each facility, and the corresponding rates were used in AERMOD. The resulting predicted concentrations were compared with monitored concentrations during the same time period.

Overall, the historical analysis showed AERMOD’s tendency to overestimate SO_2 concentrations, particularly on days that also resulted in high monitored levels. The forecasting analysis resulted in favorable results with respect to the WRF weather forecast, but the NAM forecast created concentrations in AERMOD that were poorly correlated with monitored values. AERMOD still was likely to overestimate concentrations, but these overestimations were lessened due to more accurate emission information. Further research will be needed to further advance the prediction of pollution levels.

PUBLIC ABSTRACT

Sulfur dioxide is a pollutant and a known respiratory irritant. While there is a small level of background SO2, elevated concentrations are caused by industrial emissions, and Muscatine, IA has experienced persistently elevated levels of SO2. There are currently no available methods for predicting potential SO2 violations in Muscatine, and very little research was found investigating predictive modeling efforts.

This thesis examines atmospheric conditions in Muscatine and elevated SO2 concentrations. The main goals were to examine the plume dispersion model AERMOD for its ability to accurately map pollution levels, and to determine whether AERMOD could be used to predict SO2 concentrations when using meteorological forecast models as weather inputs. An historical analysis was performed using meteorological records from 2007, AERMOD, and the maximum emission limits. The resulting predicted concentrations were compared with concentrations reported at a monitoring site in Muscatine. A forecasting analysis was also completed using two weather model forecasts from March 2012 as meteorological input for AERMOD. Daily SO2 emissions were obtained from each facility, and the corresponding rates were used in AERMOD. The resulting predicted concentrations were compared with monitored concentrations.

The historical analysis showed AERMOD’s tendency to overestimate SO2 concentrations, particularly on days that resulted in high monitored levels. The forecasting analysis resulted in one of the weather forecast models accurately predicting days with violations. AERMOD still was likely to overestimate concentrations, but these overestimations were lessened due to more accurate emission information. Further research will be needed to further advance the prediction of pollution levels.

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1 INTRODUCTION

1.1 Muscatine, IA

The city of Muscatine is a rural community located along the Mississippi River in southeastern Iowa surrounded by industrial facilities. In July, 2013 the Environmental Protection Agency (EPA) designated Muscatine as an area of nonattainment for sulfur dioxide (SO_2) meaning the area persistently exceeded the National Ambient Air Quality Standards (NAAQS) for SO_2 (EPA 2013). Prior to 2010 the EPA had established a 24-hour primary standard of 140 ppb and an annual average of 30 ppb. As SO_2 is a known respiratory irritant and can worsen asthma symptoms (Chen 2007), these primary standards were revoked in 2010 and replaced with a one-hour standard of 75 ppb in order to reduce impact on public health (EPA 2013). Muscatine was in violation of the one-hour standard 37 times in 2011 and 36 times in 2012. There were also 40 violations reported in 2013 through June 24 (Iowa DNR 2013). An area is determined to be in nonattainment when the annual 99th percentile of daily maximum 1-hour average concentrations averaged over three years exceeds 75 ppb.

Industrial facilities are required to obtain a Title V permit from the EPA detailing all air pollution emission sources and their corresponding emission rates. There are ten companies possessing Title V permits for SO_2 emissions and three SO_2 monitoring sites in Muscatine. The monitoring sites include Musser Park, Garfield School, and Greenwood Cemetery. For this study four facilities with Title V permits were considered (Grain Processing Corporation, MidAmerican Energy, Monsanto, and Muscatine Power and Water), and monitored values observed at Musser Park were used. The Iowa Department of Natural Resources (IDNR) analysis of the SO_2 concentrations paired with the hourly wind direction in 2010 showed that the highest SO_2 concentrations in excess of 120 ppb were produced by winds from the south of this monitoring site. Concentrations coinciding with all other wind directions reached less than 10 ppb. With this information, the SO_2 sources located to the south of Muscatine are the focus of this evaluation.

Muscatine is an ideal location for a meteorological and air pollution case study as it has been the focus of many air dispersion models conducted by the IDNR. Because Muscatine is situated in a rural region of the state, the high concentrations of SO_2 recorded can be attributed to industrial facilities within the county. Muscatine's proximity to the National Weather Service office in Davenport, IA (DVN) is also advantageous as that is where ground-level and upper air soundings are observed and official records are well kept for the Muscatine region. These observations are used in modeling software and, as DVN is approximately 30 miles east of Muscatine, they can be trusted as a representative sampling of conditions in the modeled area.

1.2 Atmospheric Conditions

The dispersion of a pollutant plume depends on the meteorological conditions at the emission location and the area immediately surrounding it over the depth of the planetary boundary layer (PBL). The PBL is the lowest level of the atmosphere which comes in contact with the ground, and the characteristics of this layer are directly impacted by the heating and cooling of the planetary surface. One of the most notable weather features found in the PBL that influences air pollution concentrations is an inversion. An inversion is a stable layer of air in which temperature increases or remains constant as height increases. This layer prevents air from rising past the height of the inversion. Inversions are known to limit the dispersion of pollutants and can cause NAAQS violations if they are strong or persistent.

Inversions can be classified into three basic categories: subsidence, frontal, or radiation. Subsidence inversions occur when air is sinking. This causes the air to warm and the relative humidity to decrease substantially at the base of the inversion. A frontal inversion occurs in the presence of a front. This front may be small (mesoscale) or large (synoptic scale). The frontal inversion is identified by an increase in temperature with height paralleled by an increase in the dew points over the same height. Radiation inversions occur very close to the surface and are typically very shallow in depth, though they can encompass a large increase in temperature. These inversions are caused by radiational cooling that occurs overnight, particularly when the wind is light, therefore they are almost exclusively found on morning weather soundings (12 Z, or 6 AM CST).

The strength of an inversion is a combination of the depth over which it spans, the quantitative change in temperature, and the meteorological conditions occurring at that point. For example a radiation inversion can show a large increase in temperature, but, due to its shallow nature, the occurrence of moderate wind speeds are able to mix the cold air near the surface with the warm air aloft. This is known as “mixing out” the inversion which can either decrease the inversion’s strength or eliminate it entirely. It is difficult to overcome these inversions in calm conditions, especially with low solar input. Conversely, an inversion that shows either small increase or no change in temperature with height but spans a large depth of the atmosphere can show great strength due to the considerable amount of mixing and surface heating it will take to eliminate it completely. In the case of air pollution, the lower the inversion is to the ground, the more likely it is to trap pollutants near the surface.

Surface wind speeds can also impact pollution levels for a given location by providing mixing and turbulence, or a lack thereof. High winds can result in a horizontal plume and cause considerable turbulence. The turbulence can cause the formation of eddies capable of forcing large concentrations of pollutants down to the ground level, though this is typically less of an issue with high stacks. Conversely, high winds can also provide mixing between the plume and fresh air which helps dilute pollutant concentrations. In the event of calm conditions there is limited dilution of the pollutants in the plume, and the constituents are allowed to settle over a relatively short range. This can also cause high concentrations of pollutants at the ground especially when an inversion is also present.

1.3 Modeling

Due to the complex nature of the PBL and the meteorological conditions found within it, computer models are often used to analyze plume dispersion. The American Meteorological Society-Environmental Protection Agency Regulatory Model (AERMOD) is the standard model used by the EPA and the IDNR when evaluating pollutant dispersion from an industrial source. AERMOD is a steady-state dispersion model which is partly based on the Gaussian plume model (Cimorelli 2005). AERMOD uses meteorological conditions to approximate the structure of the PBL based on terrain and heat flux algorithms (Cimorelli 2005). AERMOD is meant for modeling pollutant dispersion from stationary industrial sources over a short range (less than 50 km) and has been shown to perform well over flat terrain with high stacks producing buoyant plumes (Perry 2005). This scenario is similar to that found in Muscatine.

Since AERMOD strictly models the dispersion of a pollutant, any chemical changes that create or sequester SO_2 are not considered. Unlike NO_2 and fine particulate matter ($PM_{2.5}$), which can form in the atmosphere regardless of emissions, SO_2 is less reactive. Because of this, emitted SO_2 can be assumed to remain unchanged in the atmosphere until deposition by way of precipitation or until atmospheric conditions have diluted the ambient concentrations to negligible levels. SO_2 does decay in the atmosphere, though the rates of deposition are typically greater than the rate of decay (Eliassen 1975). AERMOD allows for SO_2 decay if selected, but this is not used except for urban environments. Because Muscatine is considered rural, SO_2 decay was not used in this analysis. Since SO_2 is relatively nonreactive in the short term, its dispersion is based entirely on the meteorological conditions to which it is subject, making AERMOD an appropriate model to utilize for analysis.

Typically, AERMOD is operated using weather data supplied by government agencies, in this case the IDNR. Upper air and surface weather information are compiled by the IDNR and formatted for AERMOD use. The meteorological data is compiled for each hour within a five year span which is completed every five years. This allows AERMOD to be used in retrospective analyses which examine statistical probabilities of exceedances for regulation purposes. In this way, AERMOD can identify high pollution impact areas (Seangkiatiyuth 2011).

There are many changes associated with dispersion modeling accuracy. These include, but are not limited to, resolving boundary layer characteristics (Hamdi 2007), resolving complex terrain (Venkatram 2001), applying appropriate meteorological scales (Palau 2005), accounting for anthropogenic feedbacks of pollutants (Mena-Carrasco 2014), correctly mapping emissions (Baklanov 2006), and accounting for chemical processes (Grell 2011). When predicting pollution levels is the objective, there is added difficulty in accurately resolving meteorological variables such as temperature and wind speed (Perez 2006). AERMOD has been previously paired with a regional Weather Research and Forecast model (WRF) to evaluate particulate matter dispersion in India (Kesarkar 2007). In that particular study the WRF was used to interpolate surface conditions in a rural area lacking meteorological data, and the results indicated that AERMOD showed promising results recreating particulate levels but underestimated the concentrations at the receptor sites (Kesarkar 2007). A separate study used AERMOD and a non-steady-state puff model (CALPUFF) to predict ambient SO_2 concentrations in Pennsylvania and New Jersey using actual emission rates from factories in the studied area (Dresser 2011). The results showed that AERMOD performed well but under predicted concentrations when compared to real time data collected (Dresser 2011).

In terms of SO_2 prediction, plume dispersion models other than AERMOD have been used to provide missing monitored concentrations due to equipment failure or calibration (Sahin 2011). Other studies have examined pollutant forecasting using meteorological data. This included investigations into ozone (Shrestha 2009), NO_2 (Buns 2012), and $PM_{2.5}$ (Zhou 2014) though AERMOD was not used in any of these cases. Some studies have considered seasonal variations, including case studies for both winter and summer events (Finardi 2008). Prediction time varied from nowcasting using high resolution, local mesoscale models (Schroeder 2006) to prediction values one day in advance (Perez 2006, Zhou 2014). New methods are being developed, including the use of statistics and climatology, to improve on air quality forecasting (Zhang 2012). Overall there are relatively few studies involving pollutant forecasting, and even fewer specifically investigating SO_2. Of the pollutant forecasting studies, very few used AERMOD to model the plume dispersion.

1.4 Study Objectives

The main goal of this study was to evaluate AERMOD as a potential model for predicting days on which SO_2 NAAQS violations may occur in Muscatine. The hypothesis was that predictable, repeatable meteorological patterns contribute to high concentrations of permitted pollutants. The research was pursued in three specific aims. The first aim was to model Muscatine, IA using AERMOD software for one year and obtain dates that produced high 24-hour averaged SO_2 concentrations within the model. It was hypothesized that the highest concentrations produced by AERMOD would occur on days with similar meteorological conditions. The second aim was to evaluate the meteorological data for the ten days with the highest 24-hour averages produced by AERMOD as well as the ten days of the year with the highest 24-hour averages that were observed at the Musser Park monitoring station. It was hypothesized that features such as inversions and wind profiles would be similar in both data sets. The third aim was to evaluate the meteorological conditions within AERMOD during the hours at which the top three modeled concentrations occurred. It was hypothesized that these conditions would be similar to those found in aims one and two. The fourth aim was to evaluate AERMOD’s ability to predict future SO_2 concentrations using weather forecast models as the meteorological input conditions. It was hypothesized that AERMOD would be able to produce high SO_2 concentrations on days when the problematic meteorological conditions are forecasted to occur.

2 METHODS AND MATERIALS

2.1 Historical Analysis

Monitored SO_2 data collected in 2007 from the Thermo Scientific 43i Pulsed Fluorescence SO_2 Analyzer located in Musser Park, IA was obtained from the IDNR. This data contained hourly SO_2 concentrations throughout the year, with the exception of a span of time between August 23 and August 30 when the data were not collected. The timeframe of missing data was excluded from all analysis.

To model the emissions in Muscatine, AERMOD software was used (Lakes Environmental Software, Waterloo, Ontario). The IDNR had previously used AERMOD to analyze SO_2 levels in Muscatine. The AERMOD configuration produced included pertinent sources with the highest emission rates detailed in the Title V permits for each source. This method of modeling creates a worst-case-scenario with all sources emitting at the maximum capacity and follows EPA guidelines for regulatory purposes. The files created by the IDNR to configure the Muscatine sources in AERMOD were obtained from the IDNR in order to accurately model SO_2 emissions in accordance with EPA standards of operations. The IDNR model used elevated, rural terrain. It also used regulatory default settings which did not include SO_2 decay or deposition during wet or dry conditions, but building downwash was accounted for.

Though there are ten companies with Title V permits in Muscatine, only four were modeled by the IDNR in this particular file due to their location relative to the city: Grain Processing Corp, Monsanto, MidAmerican Energy, and Muscatine Power and Water. Each company has multiple emission points for SO_2, creating a total of 149 emission sources within the model. Of these emission points, 148 were point sources and one was a volume source. A list of emission points and their emission rates can be found in Appendix A.

The four companies included in the model are all located south of Musser Park. The proximity of Grain Processing Corp and Muscatine Power and Water to Musser Park can be seen in Figure 1 with the crosshatch in Musser Park at the top of the figure representing the receptor site and circled crosshatches representing modeled emission points. Sources from Monsanto and MidAmerican Energy are not pictured in Figure 1 but are approximately two and five miles to the south, respectively. The highest emission rate originated from Grain Processing Corp at 4,086.7 lb/hr, and the lowest rate originated from Monsanto at 159.6 lb/hr.

Meteorological data from 2007 processed for input into AERMOD was obtained from the IDNR and included upper air profiles and surface analysis for DVN. This meteorological data was used within AERMOD to replicate weather conditions for each hour over the course of one year. AERMOD was then run for January 1 through December 31 of 2007 and hourly concentrations of SO_2 were produced. Given the AERMOD output, 24-hour moving averages were computed with the use of a spreadsheet over the course of the year with the exception of January 1 when not enough data were present from the previous day to complete the averages. The 24-hour average at any given hour was calculated from the hourly concentration at that hour and the 23 hours prior. For example, the 24-hour average for January 2 at 11:00 PM includes the hourly data from midnight beginning January 2 through 11:00 PM on the same day. The 24-hour average for January 3 at midnight includes the hourly data from January 2 at 1:00 AM through January 3 at midnight. This was completed for both the modeled and monitored data.

Based on the 24-hour averages, the ten 24-hour periods with the highest concentrations were determined for both the modeled and observed data. Upper air soundings and surface observations (METARs) were collected for the corresponding days. Because the 24-hour moving averages can incorporate meteorological data over the span of two calendar days, soundings and METARs were also collected for the days preceding those producing a 24-hour average with elevated concentrations. This information was processed and the results can be found in the following section.

The top three modeled hourly concentrations were also determined. The processed AERMOD meteorological data used to determine the dispersion at those hours was collected and the stability class for each of the hours was determined using the Turner method which is based on wind speed and solar radiation (Cooper 2011). The classes are rated A through F where F is the most stable. The class A designation means the air is unstable and strongly supports vertical mixing, and it corresponds with light winds and moderate to strong solar radiation. The class F designation means vertical mixing is extremely limited and is given on clear nights with very light winds.

2.2 Weather Forecast Model Analysis

Monitored SO_2 data was obtained from the IDNR for Musser Park in Muscatine, IA for February 28 through March 31, 2012. This data contained hourly SO_2 concentrations during that time period.

Emission inventories and continuous emissions monitor (CEM) reports from March 2012 were obtained from the IDNR for Grain Processing Corp, Monsanto, MidAmerican Energy, and Muscatine Power and Water. The emission inventories contain operating rates and schedules for all emission points at each facility. CEM reports contain measured daily, and sometimes hourly, emissions from each facility. During March of 2012, GPC and MidAmerican Energy had very high SO_2 emission rates compared to Muscatine Power and Water and Monsanto. There was also considerable variability in the emissions on a daily basis for GPC and MidAmerican Energy which covered a range of 3000 lb/d between the highest and lowest daily emission rates. Muscatine Power and Water also had a variable daily emission rate, but the range was only spanned approximately 200 lb/d. Due to the lack of specific emission information, Monsanto was assumed to have a constant emission rate for the month. The variability in daily emissions can be seen in Figure 2.

The emission inventories and CEM reports were obtained to provide accurate emission information for AERMOD. The AERMOD configuration used in the previous part of this study was altered to reflect the daily emissions detailed in the CEM reports. In the emission inventories for Grain Processing Corp, Monsanto, and MidAmerican Energy facilities, one main emission point was noted to emit more than 99% of all emissions from each facility. Because the CEM reports did not detail actual daily emissions at each point, rather a summation of all points, all of the pollutants were considered to be emitted from the primary emission point in the AERMOD configuration. The Muscatine Power and Water facility had two primary emission points, and the CEM report documented daily emissions at each point so both were included in the AERMOD configuration. It is important to note that while many emission points are listed for each facility, as can be seen in Appendix A, some points did not have documented SO_2 emissions for 2012 and could therefore be ignored in AERMOD. The resulting five emission points were EP001.0, MON195, LGSEP1, MPW70, and MPW80. Hourly emission files were created in AERMOD for the facilities from February 28 through March 31, 2012.

The first analysis in this study used historical meteorological data from 2007 provided by the IDNR, but an alternative source of meteorological data was needed to predict concentrations. In this case, weather forecast models were used as meteorological inputs for AERMOD. As AERMOD is unable to utilize raw weather model data, the Mesoscale Model Interface program (MMIF) was obtained from the EPA. This is a beta program developed by the EPA to convert WRF model data into surface and upper air files useable by AERMOD.

Previously run WRF model simulations were obtained from the University of Iowa for February 28 through March 30, 2012. This is a nested grid model with the highest resolution of 0.4 km occurring over Iowa City and decreasing resolution to 12 km over the Midwest. Over Muscatine the resolution was 4 km. This WRF was run as a retrospective simulation in which the model was partially constrained by providing observational nudging both at the surface and above the planetary boundary layer in order to keep the model's solutions close to the actual conditions experienced in 2012. Most notably, the wind vectors and temperatures within the PBL were nudged. More details regarding the WRF settings and parameters can be found in Appendix B. The model was run in contiguous eight day cycles over the course of several months including those which are of interest in this study. The initial 24 hours of each run were considered a spin-up period, and only the simulation for the remaining six days was analyzed. For the purposes of this analysis, one simulation was selected starting at 12 Z for every day between February 28 and March 30, 2012 containing 72 hours of simulated weather conditions. The WRF files were processed through MMIF to obtain surface and upper air files suitable for AERMOD. It is important to note that, though WRF files contained 72 hours of weather data, this analysis only considered hours 18 through 41 in each file. These hours coincide with a day two forecast. A day three forecast was not included for the WRF data due to the characteristics of the WRF model used. Because the WRF model was nudged, the day two forecast for any given day would be identical to the day three forecast from the day prior thus creating redundant data.

North American Mesoscale Forecast System (NAM) model forecasts were obtained from February 28 through March 30, 2012 at the grid cell which contains Muscatine, IA. This is a 12 km resolution daily model run by the National Weather Service (NWS) four times daily at 00 Z, 6 Z, 12 Z, and 18 Z (6 PM CST, midnight CST, 6 AM CST, and noon CST respectively). The NAM is also a WRF model, though specific settings have been assigned. Most notably is the 12-hour spin-up period, the lower resolution over Muscatine, and different microphysics methods though other differences were also noted (Rogers 2014). A more detailed account of the NAM setup can be found in Appendix B. For this analysis, the 12 Z model runs were chosen using 72 hours of forecasted weather conditions. The NAM was initialized off of current meteorological conditions at the time the model begins running. Since it is predicting into the future it is unbound, meaning the forecast can be inaccurate especially the farther past initialization the model proceeds.

It is important to note that while the NAM is a version of the WRF, the NAM file structure is different from that of the WRF. Additionally, the file types differ between the two models used in this analysis. Because MMIF can only process WRF data files, the NAM forecasts were manipulated into a WRF format using WRF processing software (WPS). The NAM files were obtained in grib2 format, which is a compressed file format. WPS was used to unpack the NAM files and translate them into WRF format. The finished files were processed through MMIF to produce surface and upper air files.

The surface and upper air files produced by MMIF were run through AERMOD. Separate SO_2 concentrations were obtained using the WRF and NAM forecast information.

2.3 Computer Code

The processing and commands used to manipulate the WRF and NAM files and run MMIF were executed in a Linux environment. The binary processes included were netCDF 3.6.3, nco-4.4.5 built against the net CDF libraries, MMIF v3.0_2013-10-17, WRFV3.6 built against netCDF, and WPSV3.6 built against netCDF and WRF. More recent versions of netCDF were tried, though there were problems with compatibility.

Processing WRF through MMIF was fairly straightforward and only involved compiling the individual hourly forecasts into 72-hour files. These were then run through MMIF using a batch script similar to that found in Appendix C. The result was surface and upper air files suitable for AERMOD. MMIF allows the user to choose how many levels above the surface are used in analysis up to 3500 m. In this analysis, the levels chosen were 2 m, 10 m, 30 m, 60 m, and 120 m. This was in an attempt to capture low level inversions produced by the model.

Because MMIF does not recognize non-WRF files, modifications were made to the NAM files in order to make them readable through MMIF. The NAM files downloaded were in three hour increments and in grib2 format as hourly forecasts were not available. The command ungrib.exe was executed in WPS which unpacked the NAM data into its full size. MMIF also requires the files be in netCDF format, so metgrid.exe was executed on the unpacked NAM data. These were done sequentially for each model run using a single script which can be found in Appendix C**.** The three hour NAM files were then catenated into 72-hour forecasts using the script found in Appendix C.

Next, global attributes were applied to the catenated NAM files. This provides the location of Muscatine so the weather forecast specific to that location can be examined. The script can be found in Appendix C. Because the variables in the NAM file have different parameters than those recognized by MMIF, WRF parameters were applied to the NAM files. This involved three steps: creating a WRF donor file, setting up an environment to modify the variables, and using a script written in R computer code to modify the variables. The WRF donor file was adjusted from 96 hours to 72 hours using the script in Appendix C. A separate file was used to create an environment to manipulate the variables by ensuring only a single 72-hour NAM forecast was manipulated to the donor file. The final script in this process involved executing the R script which strips the WRF file of its variables and replaces them with the NAM data. This allows the variables to be in the correct order and format for processing through MMIF. Essentially it is a WRF file filled with NAM data. The scripts for these processes can be found in Appendix C.

The final step was to process the properly formatted NAM data through MMIF using the script in Appendix C. The result was surface and upper air data suitable for use in AERMOD. The same level settings for the upper air files that were applied to the WRF forecasts were also applied to the NAM forecast files.

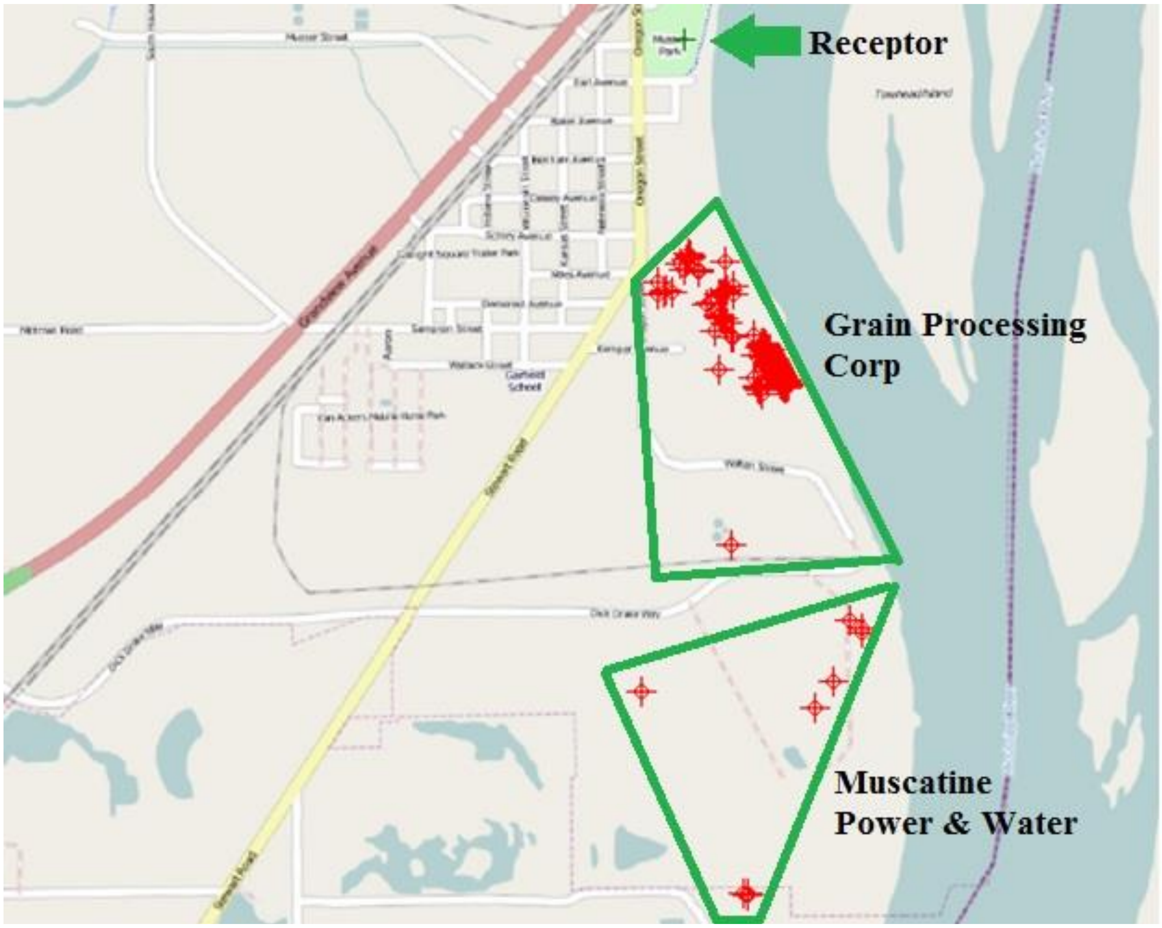

Figure 1: A map of sources and receptor in Muscatine, IA. The receptor is in Musser Park at top near the arrow, and the emission points are within the boxes in the middle and bottom of the figure.

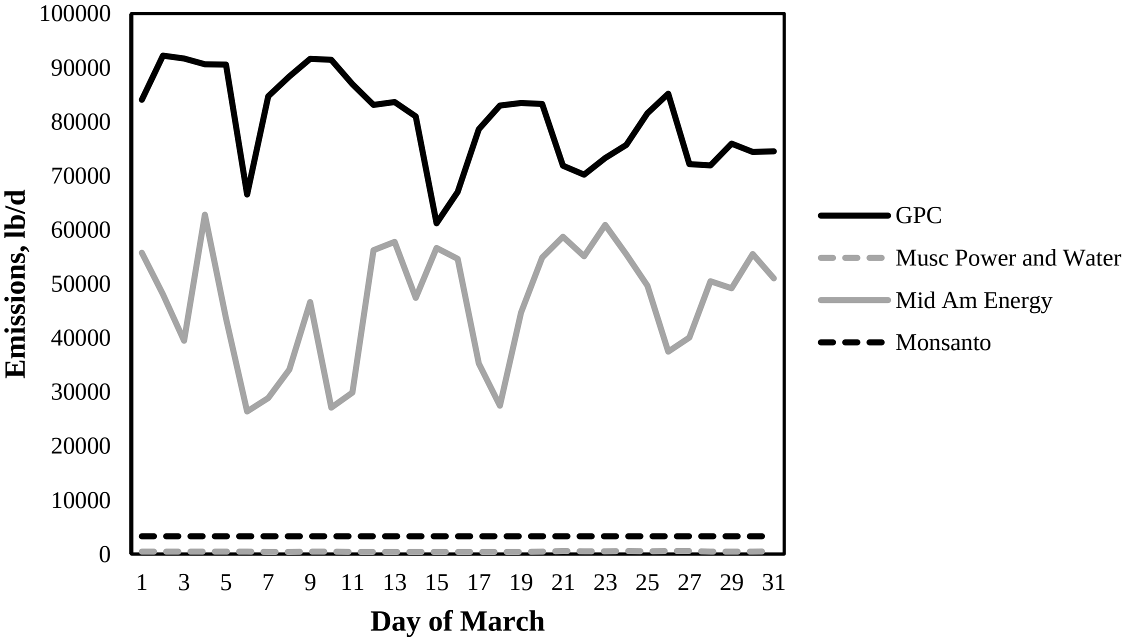

Figure 2: Daily SO_2 emissions in March 2012

3 RESULTS

3.1 Historical Analysis Concentrations

The modeled hourly concentrations were compared to the corresponding monitored hourly concentrations throughout 2007. As shown in Figure 3, the model predicted much higher concentrations than those actually observed. There were also significantly more days with spikes in concentrations in the model output compared to those in the actual data. This can be partially explained by the fact that, per EPA modelling requirements, AERMOD models are to be developed for a worst-case scenario where all sources are emitting the maximum emission rate for the duration of the modeled period whereas the actual plants would not typically be operating at such high capacity throughout the year. However, spikes in the monitored data coincide with spikes in modeled data meaning the model was able to predict the days of elevated concentrations when the plants were likely in operation.

The hourly modeled concentrations were plotted on a log scale against the corresponding hourly monitored concentrations from 2007 in Figure 4. The results are very noisy with little correlation between the modeled and monitored points and with some modeled values being a factor of ten above the monitored values. A quantile-quantile (Q-Q) plot was also created, as is shown in Figure 4, where the modeled concentrations were ordered from largest to smallest and plotted against the ordered monitored concentrations. In this Q-Q plot, good model performance will result in points along the 1-1 line (Perry 2004). While the resulting line in Figure 5 is relatively linear, its slope is below the 1-1 line which reinforces the aforementioned statement concerning AERMOD’s over-estimation of SO_2 concentrations. It should be noted that for concentrations less than 200 ppb, the points fall very close to the 1-1 line, but then diverge with higher concentrations. This means that, while the model over-predicts concentrations, the difference between the concentrations increases as the measured concentrations increases.

The 24-hour moving averages are plotted by date in Figure 3. In the majority of cases, the model over-predicted the averages as was expected due to the high hourly concentrations from

AERMOD. However, there were several days on which highest monitored concentration averages surpassed the model's predicted average concentrations. This included the four days with the highest monitored average concentrations. Overall, spikes in the monitored data coincide with spikes in modeled concentrations, though the model produced a larger number of pronounced spikes than what actually occurred. A summary of the findings from the analysis of the moving 24-hour averages from Figure 3 can be seen in Table 1. There were 27 days where AERMOD produced a 24-hour average concentration higher than 50 ppm in which the monitored data was lower than 50 ppm. 24-hour average concentrations above 50 ppb were observed in both the monitored and modeled data on 13 days. There were five days where only the monitored 24-hour average concentrations exceeded 50 ppb.

The modeled 24-hour averages were plotted against the corresponding monitored 24-hour averages in Figure 4. Due to the extremely noisy hourly results from Figure 4, the 24-hour averaged values were used for the remainder of the analysis as they have a lower degree of noise. There is still a considerable amount of noise, but there is some degree of correlation. This means that the 24-hour averaged modeled values are more representative of actual conditions, though they still frequently exceed monitored values. A Q-Q plot was also constructed which plotted the modeled concentrations against those monitored, as can be seen in Figure 5. The resulting line produced a slope very close to the 1-1 line. In this case at low concentrations the model over-predicts, but at high concentrations the model under-predicts the 24-hour averages. According to Figure 5, the modeled 24-hour averages are a more accurate approximation of the actual concentrations than the hourly data.

Based on the data in Figure 3, the ten days with the highest modeled 24-hour averages and the ten days with the highest monitored 24-hour averages were determined. This resulted in the identification of 18 calendar days over the course of 2007 because peak events occurred on April 22 and May 30 in both the monitored and model analyses.

3.2 Meteorological Phenomena

For the 18 days previously determined and the day prior to each, meteorological sounding data were compiled and can be found in Appendix D. Since upper air soundings are taken twice per day, there are four soundings for each peak concentration occurrence. In all of the 18 days of high SO_2 concentrations at least one inversion was observed below 700 mb on the day of the peak as well as the day prior with the majority of the lowest inversions starting below 850 mb. While the exact depth of the PBL changes daily at any given location, 850 mb (approximately 1500 m) is a critical point as this can generally be considered the top of the PBL in the Midwest since no mountains are present. Table 2 summarizes the lowest inversions found in the modeled and monitored data by classifying them into four categories where an unknown classification means there were strong characteristics of multiple types or the inversion was so small that not enough data was present to classify it otherwise. It is also noted the number of surface-based and elevated inversions.

In the dates observed, all but seven soundings showed inversions below 700 mb. In both the monitored and modeled peaks, the radiation inversion is found most often. Subsidence inversions are also found frequently in both cases. Frontal inversions were reported frequently in the monitored data, but there were significantly fewer occurrences in the modeled data. In both data sets the majority of the inversions are surface based, meaning the increase in temperature began at ground level. As mentioned previously, the lower inversions have a greater potential to trap pollutants near the ground, and our results support that statement. While the occurrence of a low-level inversion presents the possibility of air quality deterioration, not every inversion will cause dangerously high levels of a pollutant. Other meteorological variables must be considered, particularly those at the ground level.

The collected METARs were compiled and processed into a wind rose, as shown in Figure 6. This is a collection of wind data during the two days noted for each peak concentration occurrence. The dominant wind direction during times when high concentrations were recorded or predicted was from the south, representing 41% of the total observed hours. Winds from the south-southeast, south, and south-southwest represent approximately 65% of the observed hours. A closer examination of the METARs revealed that the winds from other directions occurred at the beginning of the day prior to a high-level event or at the end of the day in which the peak occurred. This means the wind was turning to a southerly direction early before the high occurrence, or the winds were shifting from the south to a different direction after the high concentrations had occurred. These wind shifts coincide with lower hourly concentrations. It is clear that a southerly wind is crucial in developing elevated concentrations over the Musser Park monitoring station. This is expected as all of the stations modeled are located south of the receptor site, and winds with a predominantly southerly component would allow the plume to disperse over the city. The occurrence of a southerly wind is also similar to results found by the IDNR (EPA 2013). Not every southerly wind causes a problematic increase in pollutant levels for Muscatine, as there is a high probability of southerly winds in the spring and summer, but the combination of a south wind and a low level inversion was observed in all of the 18 high-concentration events. The identification of these two meteorological phenomena occurring simultaneously on any given day is essential in predicting high SO_2 concentrations in Muscatine.

The three highest hourly concentrations produced by AERMOD are shown in Table 3 along with the pertinent meteorological features corresponding to each event. In two of the cases the high modeled concentration occurred in the late evening when the ground would have been starting to cool but the air above it would have remained warm. In the third case the high modeled concentration occurred early in the morning shortly around sunrise. At this point in time the ground would have been the coolest during the day while the air above it would have remained relatively warm. Once the sun rose, the ground would have heated and caused a reduction in stability. In all three cases the surface winds were very light and the sky was clear.

Because of these factors, all three classes were categorized in the F stability class, meaning the model created very stable conditions and vertical mixing was limited.

In addition to the stable conditions, the wind direction was also noted in Table 3. As was noted previously, a southerly wind was observed as the predominant wind on days with high modeled and observed SO_2 concentrations. In all three cases noted the wind direction was from the south-southeast. The stable conditions prevented vertical mixing and allowed the emitted SO_2 to remain in the lowest level of the PBL. The very light wind allowed minimal horizontal dispersion northward across Muscatine meaning the emissions stayed within a very short distance from the emission site, leading to a spike in SO_2 concentrations over Musser Park.

3.3 Meteorological Model Prediction

The hourly concentrations forecasted by WRF and AERMOD (A-WRF) for each day of March 2012 were plotted with the actual hourly concentrations. Figure 7 displays the data on a daily basis with concentrations being in $\mu g/m^3$ on a logarithmic scale. The horizontal line at 200 $\mu g/m^3$ displays the approximate level of a NAAQS violation (approximately equivalent to 75 ppb). The conversion between $\mu g/m^3$ and ppb is dependent on temperature and pressure, so the conversion factor varies from one hour to the next. It was beyond the scope of this research to extract these variables from the weather forecast model and factor them into the conversion. This was also neglected when analyzing the NAM concentrations.

Overall, the WRF model processed through AERMOD produced results that correlated reasonably well with those obtained from the monitoring station. A-WRF predicted fifteen violations, though the actual number reported that month was nine. Eight of the monitored violations were correctly identified by the A-WRF configuration with only one unreported violation. This leaves a total seven false positives. A-WRF also correctly predicted 15 days on which violations did not occur out of a possible 22 days. These results are displayed in Table 4.

The percent differences between the monitored concentrations were also calculated and displayed in Table 4. Equation 1 was used to solve for the percent difference in the number of total violations. Equation 2 shows the percent of correct violations forecasted by the model. Similarly, Equation 3 was used to solve for the percent of false positives compared to nonviolation days. Equation 4 displays the method for solving the percent of unreported violations in relation to total monitored violations. Finally, Equation 5 shows the percent of correct nonviolation days forecasted.

$$Percent\ difference = \frac{Total\ Model\ Violations - Total\ Monitored\ Violations}{Total\ Monitored\ Violations} \tag{Equation 1}$$

$$Percent = \frac{Correct\ Model\ Violations}{Total\ Monitored\ Violations} \tag{Equation 2}$$

$$Percent = \frac{Correct\ Model\ Violations}{Total\ Monitored\ Violations} \tag{Equation 3}$$

$$Percent = \frac{Unreported\ Model\ Violations}{Total\ Monitored\ Violations} \tag{Equation 4}$$

$$Percent = \frac{Correct\ Model\ Nonviolation\ Days}{Total\ Monitored\ Nonviolation\ Days} \tag{Equation 5}$$

The highest A-WRF and monitored concentrations for each day of the month were plotted on a on a logarithmic scale and can be seen in Figure 8. For nearly all days, A-WRF overestimated the peak concentration which is similar to the results previously found using AERMOD and the compiled meteorological data from the IDNR. In general, the A-WRF data followed a similar trend to the monitored level. The median A-WRF and monitored concentrations for each day of the month were also plotted as seen in Figure 9. The A-WRF concentrations follow the general trend of the monitored concentrations, though the magnitude of the A-WRF concentrations is lower those monitored. This results indicates that the A-WRF forecasted concentrations are frequently lower than the monitored concentrations, but, when examined in conjunction with the results from Figure 8, it also shows that the A-WRF forecast produces higher concentration spikes.

The forecasted concentrations produced by NAM and AERMOD (A-NAM) were plotted on a logarithmic scale with the monitored hourly concentrations and can be seen in Figure 10. The 200 µg/m^3 line was also included as a reference for violations. Two sets of forecasted concentrations were examined; day two and day three. Day two forecast concentrations occurred during hours 18 through 41 of the model run. Day three concentrations occurred during hours 42 through 67 of the model run. In other words, the model was initialized at 12 Z which is 6 AM CST and considered to be hour zero. This study did not consider concentrations during the calendar day on which the initialization occurred, but rather examined the concentrations for the two days following the model initialization. It is important to note that the NAM forecasts are in six hour blocks, instead of hourly in the case of WRF. This means that only six SO_2 concentrations are resolved for each calendar day instead of 24.

Overall the concentrations predicted by the A-NAM configuration were poorly correlated with the levels obtained from the monitoring station, and the results can be found in Table 4. A-NAM day two forecasts picked up eight violations out of nine observed compared to only six forecast from A-NAM day three data. Only two correct violations were predicted with A-NAM day two forecasts leaving seven unreported violations and six false positives. A-NAM day three forecasts predicted three correct violations, six unreported violations, and three false positives. A-NAM day two data correctly produced sixteen days when violations did not occur compared to nineteen predicted by A-NAM day three forecasts.

The A-NAM day two and A-NAM day three concentrations were also plotted with the corresponding monitored values and can be seen in Figure 11. This method reduces the number of exceedances produced by the monitored concentrations from nine to five, though the A-NAM day two and A-NAM day three forecasts still missed multiple reported violations.

The daily maximum A-NAM day two and A-NAM day three concentrations were plotted with the monitored daily maximum concentrations in Figure 12. Unlike with the A-WRF concentrations, there is less correlation between the modeled and the monitored values. While the model follows the same general trend between days four and fifteen, the model greatly diverges in the latter half of the month. Similarly to the A-WRF forecast, the A-NAM forecast is generally consistently higher than the monitored levels, though the difference between the values is not as pronounced. The frequency that A-NAM day two and A-NAM day three forecasts are higher than the monitored concentrations is also lower than with the A-WRF forecasts.

The A-WRF forecasts correctly predicted the highest number of correct violations compared to A-NAM day two and A-NAM day three forecasts which correctly forecasted less than half of the recorded violations. A-WRF had the lowest percent of unreported violations with only 11% of actual violations going unforecasted compared with more than 75% being unforecasted for A-NAM day two and 67% for A-NAM day three. However, A-WRF had the highest percent of false positives with more than 30% of nonviolation days being forecasted to have violations. Due to the high number of false positives, A-WRF also had the lowest percent of correct nonviolation days with 68% correctly forecasted nonviolation days compared with 73% for A-NAM day two and 86% A-NAM day three.

As was demonstrated previously, wind direction is a large factor in whether a violation was expected to occur. The hours during which the A-WRF model forecasted violations were plotted on a wind rose and can be seen in Figure 13. Similarly, the wind roses representing violations forecasted by A-NAM day two and A-NAM day three forecasts are shown in Figure 14 and Figure 15 respectively. In all cases, the violations were produced under conditions where the wind vector included a southerly component, with most of the violations being forecasted to occur with south and south-southeasterly winds.

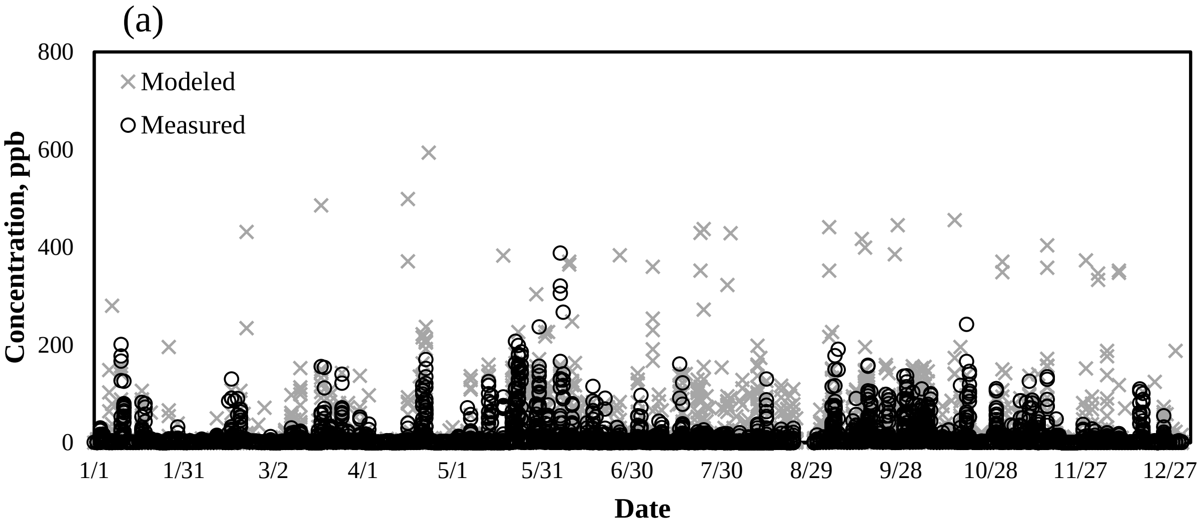

Figure 3: A daily account of modeled and monitored concentrations for 2007 for (a) hourly concentrations and (b) moving 24-hour concentrations.

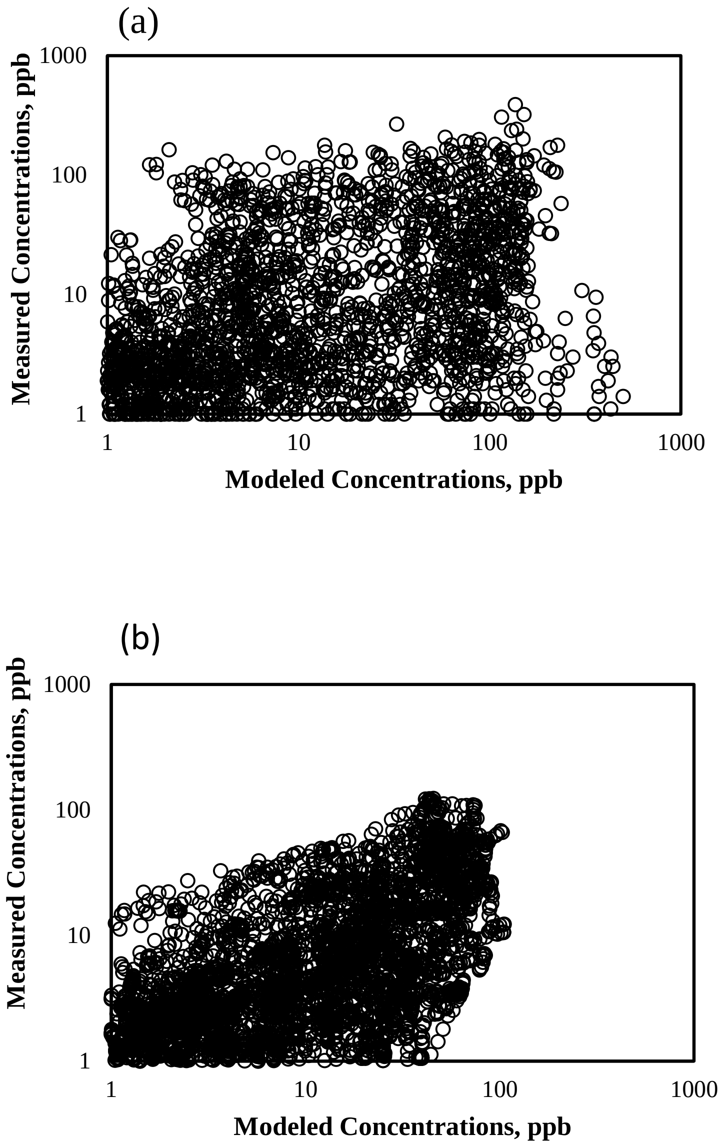

Figure 4: Correlation plot of modeled concentrations vs. monitored concentrations in 2007 for (a) hourly concentrations and (b) moving 24-hour concentrations.

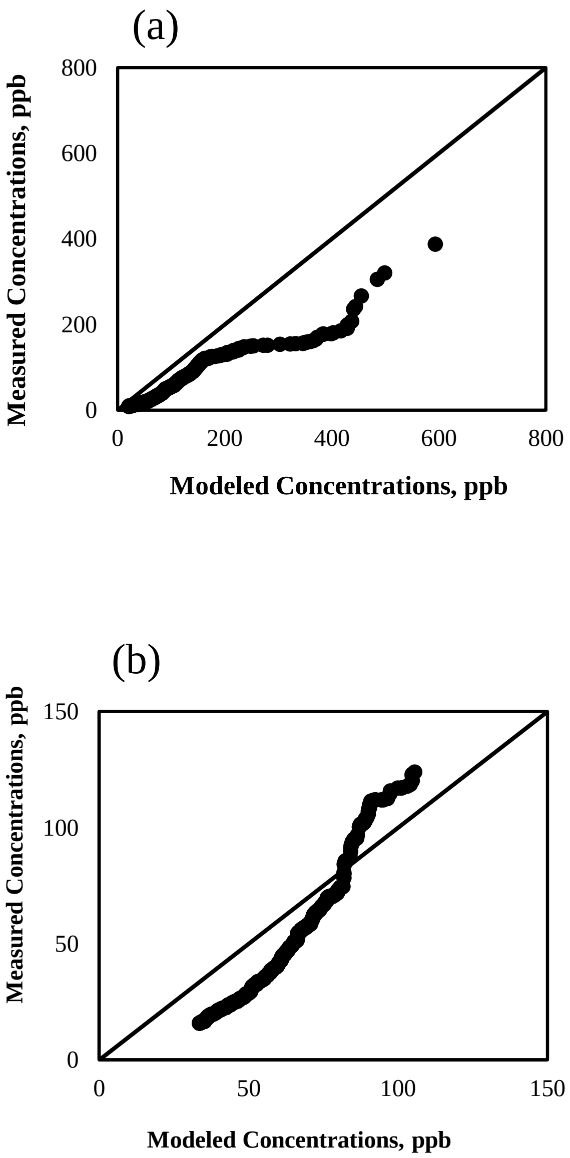

Figure 5: Correlation plot of modeled relative to monitored concentrations in 2007 for (a) hourly concentrations and (b) moving 24-hour concentrations

Table 1: A Comparison of AERMOD Predicted Concentrations Above 50 ppb to Monitored Concentrations Above 50 ppb for 2007

Days AERMOD concentrations exceeded 50 ppb when monitored levels were less than 50 ppb	Days AERMOD concentrations and monitored levels exceeded 50 ppb	Days AERMOD concentrations were under 50 ppb but monitored levels exceeded 50 ppb
27	13	5

Table 2: Inversion Information for the 10 Days with the Highest Monitored Concentrations and the 10 Days with the Highest Modeled Concentrations in 2007

Inversion Type	Monitored Days	Modeled Days
Radiation	11	13
Subsidence	9	10
Frontal	9	4
Unknown	1	1
Surface-Based	17	19
Elevated	13	9

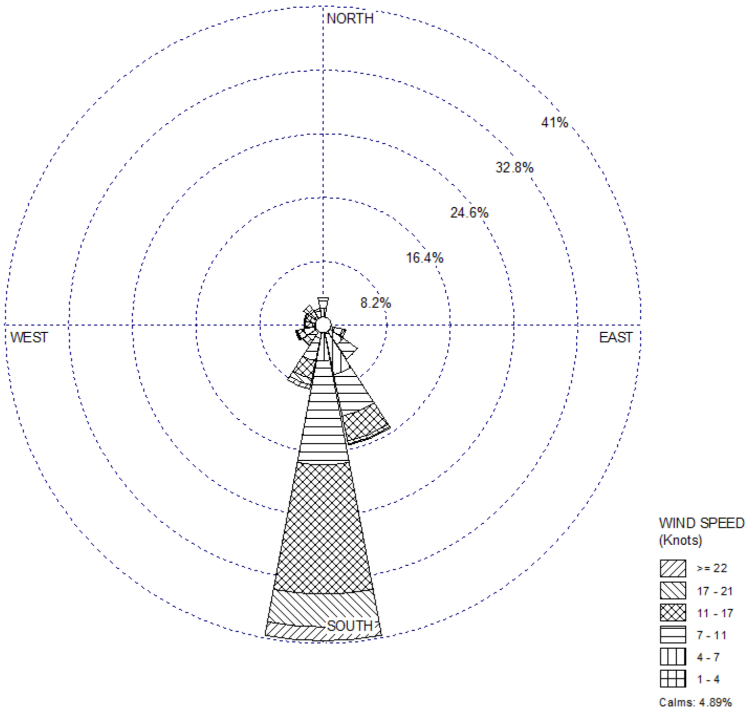

Figure 6: DVN meteorological data from days with high modeled and monitored SO_2 concentrations in 2007 compiled into a wind rose

Table 3: Dates of High Modeled Concentrations and Corresponding Meteorological Data in 2007

Date	Hour	Cloud Cover	Solar Radiation	Wind Speed (m/s)	Stability Class	Wind Direction
23-Apr	20	0	Night	1.33	F	SSE
16-Apr	20	0	Night	1.31	F	SSE
18-Mar	7	0	Night	1.03	F	SSE

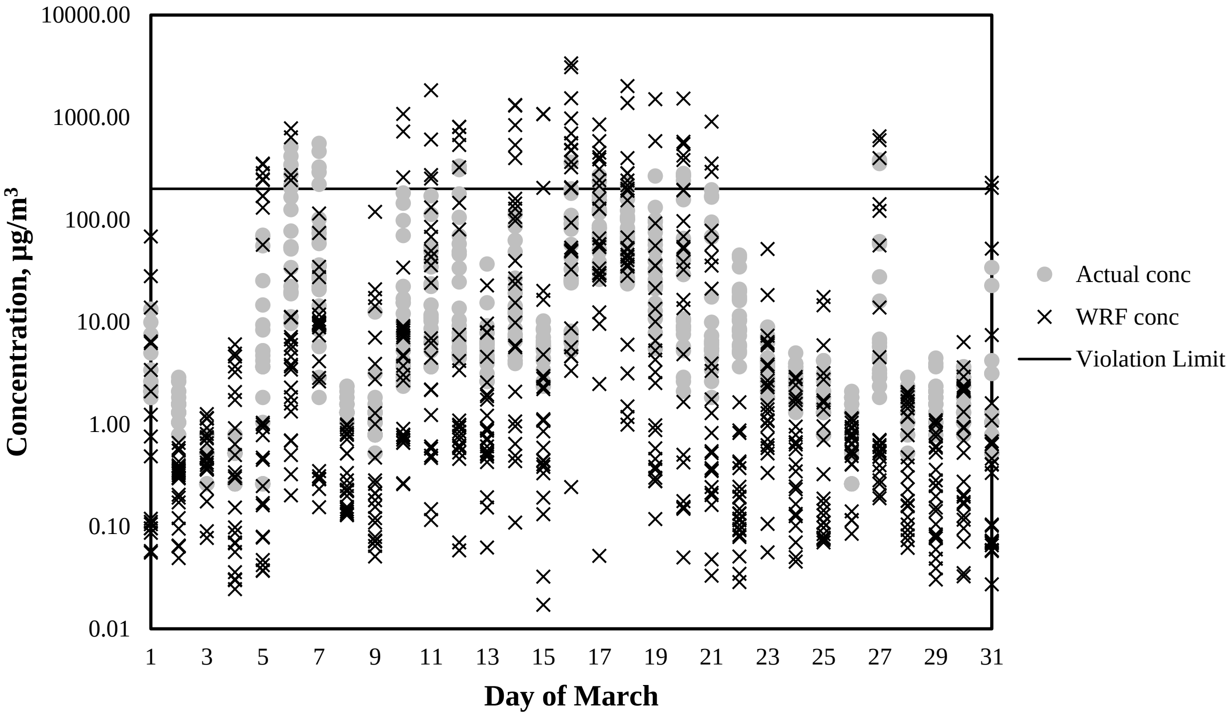

Figure 7: A-WRF forecast hourly concentrations vs. monitored hourly concentrations in March 2012

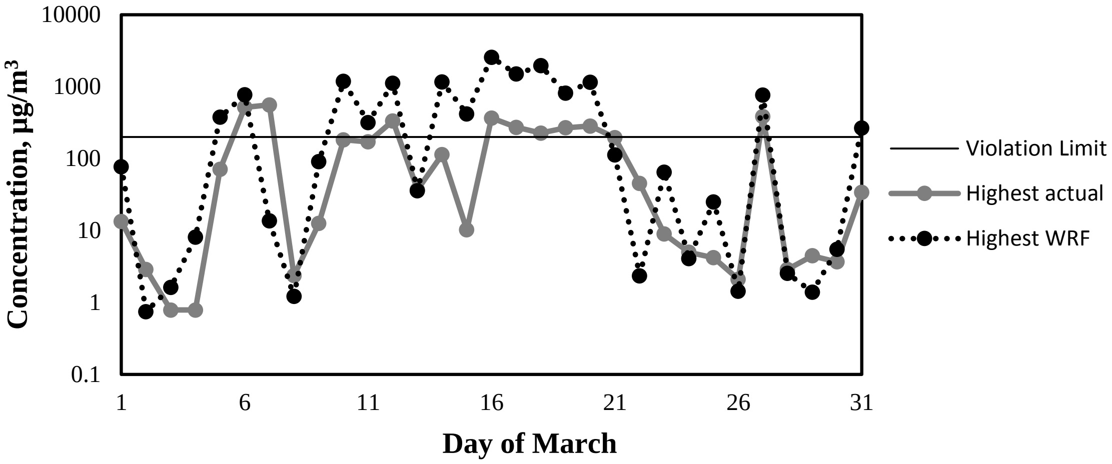

Figure 8: The highest daily A-WRF concentrations and the highest daily monitored concentrations for March 2012

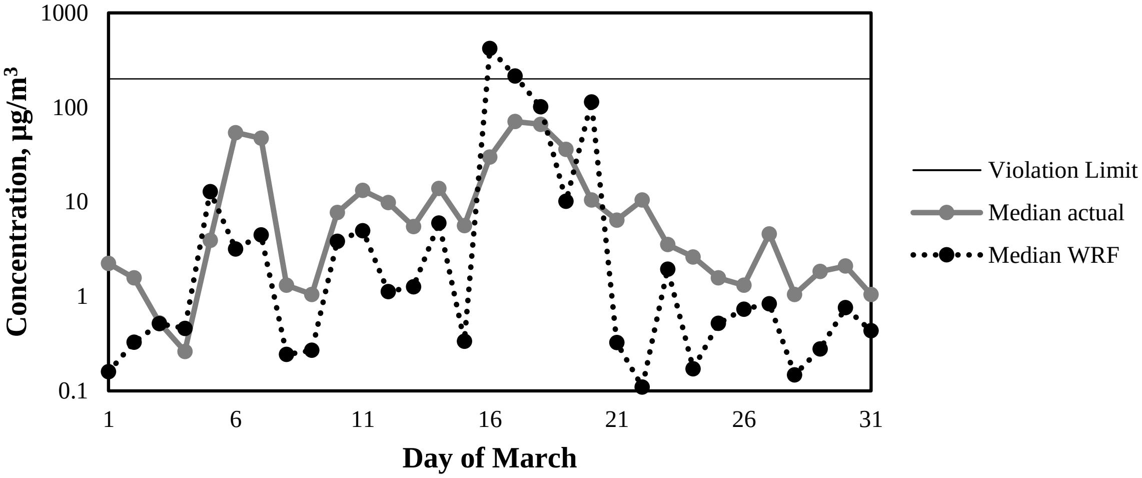

Figure 9: A-WRF daily median forecast concentrations and daily median monitored concentrations for March 2012

Table 4: Comparison of Predicted Violations from A-WRF and A-NAM Forecasts to Actual Monitored Violations in March 2012

	Violations		Correct violations		False positives		Unreported violations		Correct nonviolations	
	Number	Percent Difference	Number	Percent	Number	Percent	Number	Percent	Number	Percent
Monitored	9								22	
A-WRF	15	66.7%	8	88.9%	7	31.8%	1	11.1%	15	68.2%
A-NAM Day 2	8	-11.1%	2	22.2%	6	27.3%	7	77.8%	16	72.7%
A-NAM Day 3	6	-33.3%	3	33.3%	3	13.6%	6	66.7%	19	86.4%

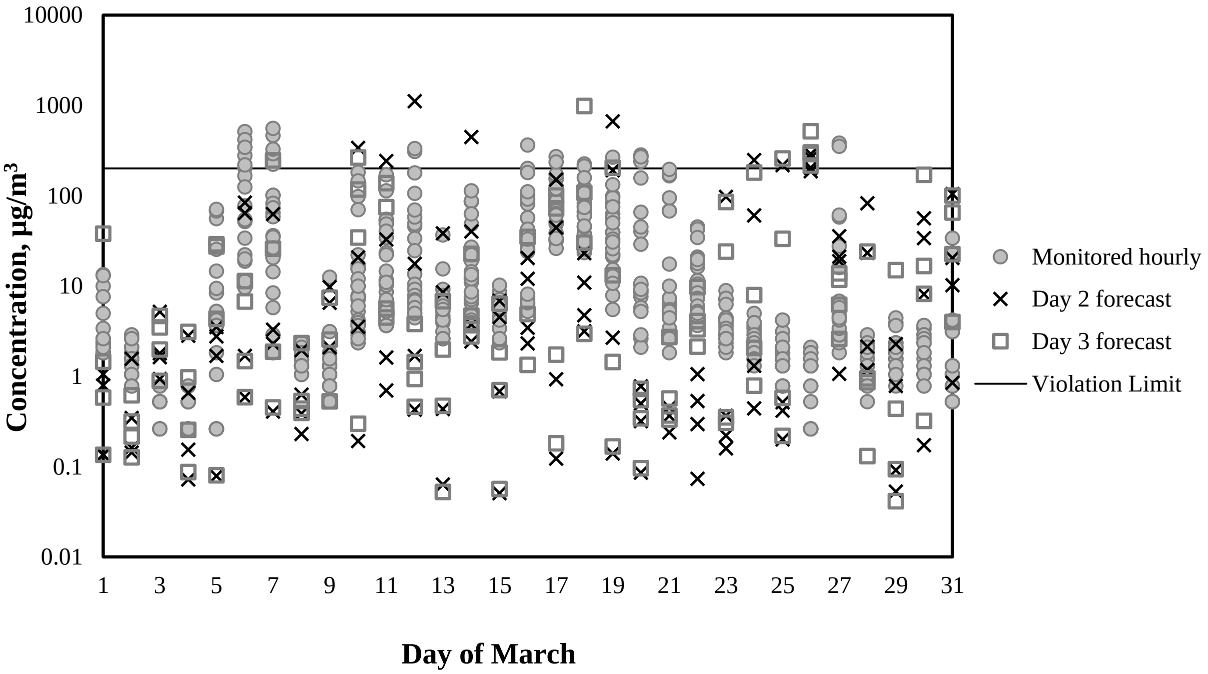

Figure 10: A-NAM day 2 forecast concentrations, A-NAM day 3 forecast concentrations, and monitored hourly concentrations

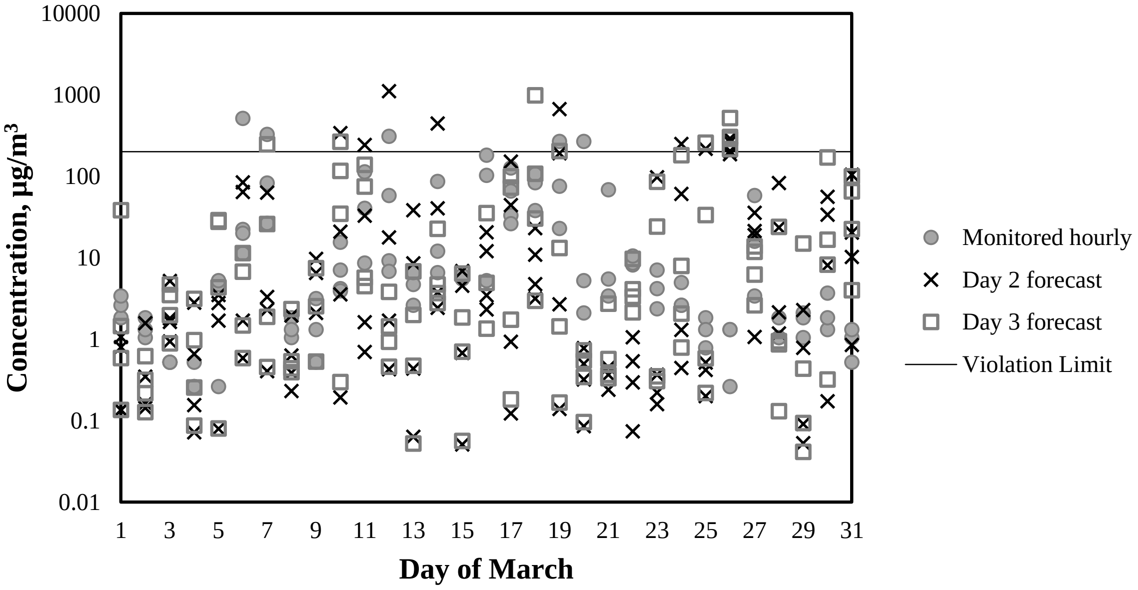

Figure 11: A-NAM day 2 forecast concentrations, A-NAM day 3 forecast concentrations, and corresponding monitored concentrations for March 2012

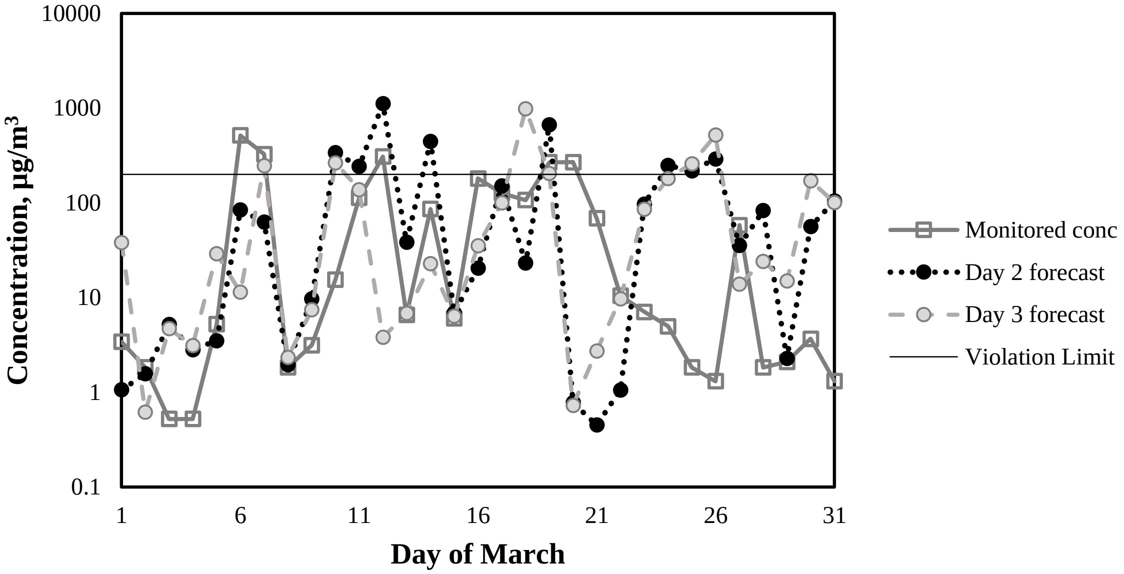

Figure 12: A-NAM highest daily forecast concentrations and monitored highest daily concentrations for March 2012

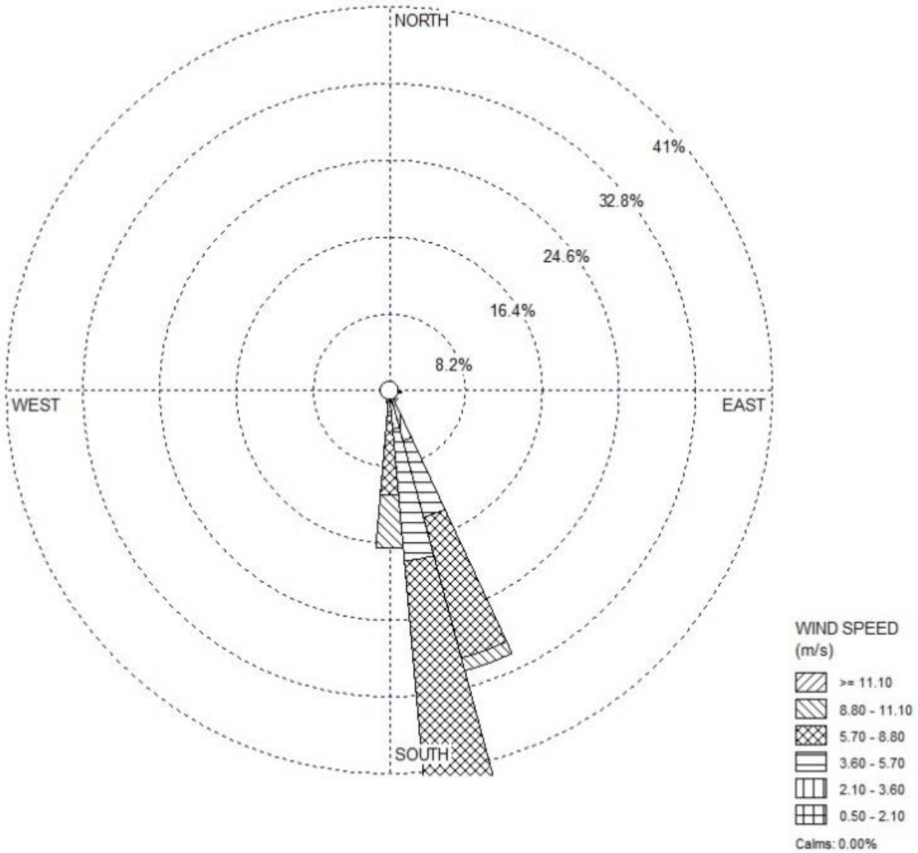

Figure 13: A-WRF forecasted hourly violations in March 2012 compiled into a wind rose

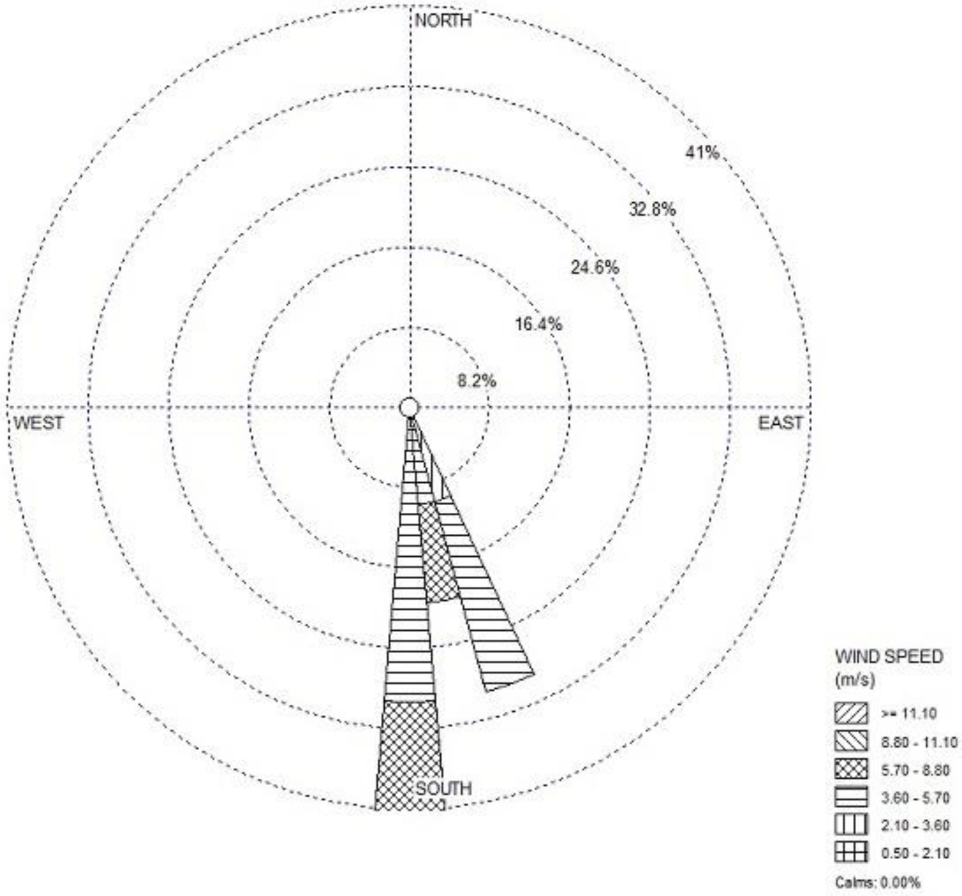

Figure 14: A-NAM day 2 forecasted violations for March 2012 compiled into a wind rose

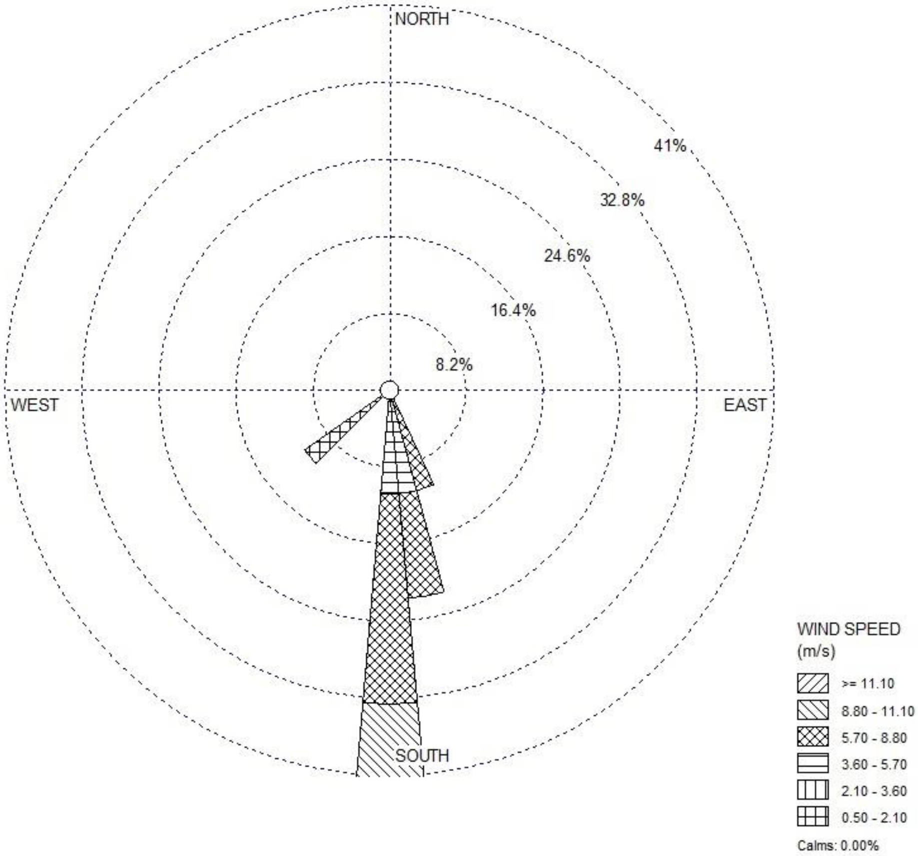

Figure 15: A-NAM day 3 forecasted violations for March 2012 compiled into a wind rose

4 CONCLUSIONS

This case study evaluated AERMOD as a potential model for predicting specific days in which SO_2 NAAQS violations may occur in Muscatine, IA. AERMOD produces high pollutant concentrations when the provided meteorological conditions inhibit plume dispersion, such as the occurrence of low-level inversions. Based on the positioning of the emission sources relative to the receptor, the model is accurate in correlating a southerly wind with a spike in SO_2 concentrations in Musser Park. Based on the 18 days evaluated, due to having the highest modeled and monitored 24-hour averages, AERMOD also identified days when these two meteorological events coincided and thus displayed high levels of SO_2 at the receptor site. When considering the times when the model created high concentrations, surface and upper air stability were well modeled on both a daily and hourly level based on the observation of low-level inversions and the highly stable classification of the top occurrences. The highest modeled values all occurred on clear nights with low wind speeds from the south-southeast.

Using the EPA technique of modeling a worst-case scenario leads to inaccuracies in the predicted pollutant concentrations. In most cases AERMOD greatly overestimated the levels of SO_2 in Musser Park. Without more accurate SO_2 emission rate estimations from the industrial facilities, it is unlikely that AERMOD will produce ground-level concentrations close to those observed in Muscatine. When more accurate emission rates are used in AERMOD and paired with weather forecast models, the inaccuracies produced by AERMOD are reduced. Overestimation of the concentrations is still evident, but the magnitude and frequency was minimized.

The accuracy of predicting violations depends on the weather forecast model used and its characteristics. The hourly, high resolution, retrospective WRF model created weather conditions which correlated to more accurate SO_2 levels in AERMOD and correctly forecasted the majority of the violations with the fewest number of unforecasted violations. However, it also created the highest number of false positives and the lowest number of correct nonviolation days. The concentrations produced in AERMOD using the NAM forecast, which has lower resolution and provided a concentration every six hours, were poorly correlated with the monitored SO_2 violations. Both the A-NAM day two and A-NAM day three forecasts missed the majority of the reported violations and still created multiple false positives. The A-NAM forecasts correctly predicted more nonviolation days compared with the A-WRF, but at the expense of missing other violations.

Overall the A-WRF model produced a superior forecast to that from the A-NAM, which was expected considering the model was nudged by observations meaning it was forced to be more representative of the actual meteorological conditions that occurred. The A-NAM model was inferior in predicting violations, which is also expected due to the lower resolution and the fewer number of predicted concentrations each day. The a-NAM day three forecasts correlated marginally better than the A-NAM day two forecasts, but both missed a substantial number of violations. In both models, the wind direction played a key role in the forecasting of a violation. As expected, both A-WRF and A-NAM only produced violation level concentrations on days with southerly winds.

5 DISCUSSIONS AND FUTURE RESEARCH

5.1 Discussions

Based on the results from this analysis, the current model setup could be used to obtain a monthly or seasonal assessment of violations in the Muscatine area. While the A-WRF configuration correctly predicted the majority of the actual violations, it predicted nearly doubled the total number of violations over the course of a month. The A-NAM configuration was inaccurate in placing the predicted violations on the correct days, though the total number of violations was closely correlated to the number of recorded violations within the month. When considering the accuracy based on monthly counts, the A-NAM setup is superior to the A-WRF. This approach could lead to a more representative regulatory analysis for the IDNR or other regulatory agencies. The archived NAM data files can be readily obtained and processed in a fashion similar to that of this study. The detailed emission information used in this analysis could also be processed into AERMOD, and the product has the potential to be a more representative assessment of the pollution potential of a facility.

While it was demonstrated that the process of predicting daily SO_2 violations is possible, there is considerable room for improvement. Two of the main options for more accurate solutions are improving on the AERMOD configuration and/or improving the weather forecast model.

Adjustments within the AERMOD configuration could include refinements in the terrain to fully account for elevation variations that may impact concentrations. In the case of this research, no elevation files were used in AERMOD as per the IDNR’s setup. For regulatory purposes terrain files are not considered, though terrain settings built into AERMOD are utilized. In the case of Muscatine, the area including all emission points and the receptor is at a nearly constant elevation. There are bluffs to the north of the area of focus, though it was determined that their impact would be minimal due to the distance and positioning relative to the emission points and receptor. An improvement to future research could include additional terrain details.

Emission settings in AERMOD could also impact future results. Reliable emission data can contribute to prediction error (Buns 2012), so more detailed emission information could also lead to more accurate forecasts though these would likely be difficult to obtain. Because the CEMS and emission inventories generally did not cover hourly emissions from each emission point individually, those who wish to continue with this research would likely need to develop a working relationship with the industries in the area of interest. If possible, the facilities could provide a more detailed account of the hourly emission from various points including diurnal variability. Finally, adjustments could be made to the stack information within the model. Because AERMOD uses algorithms to adjust for a meandering plume on low wind days as well as downwash, changes in the stack height within the model would likely lead to changes in the concentrations at the ground level.

It is likely that errors in the meteorological forecasting are greater than errors due to other factors such as emissions (Zhang 2012). Modifying the weather forecast model would also allow for changes in the concentrations. WRF, being a research weather model, allows for customization in many aspects of the model. This research did not have the luxury of running WRF to be specific to this project, so customization was not able to be analyzed. Weather models provide more accurate forecasts with higher resolution (Fay 2006), so using WRF with higher resolution could possibly resolve more of the spatial differences in the terrain as well as important variables such as temperature and wind vectors. Since Muscatine is in a river valley, microclimates can develop that low resolution models may smooth out. With higher resolution, the effects of these microscale weather phenomena could possibly be better resolved.

Additionally, a single weather forecast model will statistically be less accurate over a long period of time when compared to a model ensemble (Durai 2014). Using multiple forecast models with slight modifications made to variables and parameters could lead to better concentration data at the surface. While an individual model may do well on any given day, using an ensemble would help to smooth out the days when an individual model is less accurate which would lead to a more accurate forecast over a long period of time.

An additional detail to be considered from the analysis is the seasonal variability in the accuracy. While the A-WRF was more accurate in producing violations on the days in which they occurred compared to the A-NAM, it is possible that the NAM was not using the most accurate seasonal settings. With regional and global models, equations are switched between a summer and winter set during the transition seasons. In this particular case, Eastern Iowa experienced record heat in March, 2012. If the NAM was still using the winter formulas, this would have significant impact on the results. However, because this study was done only over a small portion of a single season, it is unknown whether either model may have performed better during a different part of the year.

In terms of practicality, this method could be used in two ways. The first involves alerting the public in advance of a possible violation. Similarly to how the EPA forecasts for high levels of pollutants such as ozone, air quality alerts could be issued in advance for other pollutants such as SO_2. This would allow sensitive individuals to take the necessary precautions before the forecasted event instead of first subjecting them to the adverse conditions, as is currently the situation.

The second practical use would be alerting facilities in advance of a potential violation. While it is not clear whether an industrial facility would be receptive to this notice, those that are willing could adjust production and cut emissions temporarily in hope of avoiding the exceedance. This use would likely need community or government involvement in order to fully implement.

This study used accurate daily emission information, though this will not be possible if this method is used in a true forecasting capacity. The exact emissions of a facility will not be known in advance, though it is possible that an estimation may be available. A solution could involve running the forecasted weather information through multiple AERMOD scripts each with variable emission information. In this case, the modeler could advise a facility that there may be an exceedance at a certain level of emissions, but cutting emissions by a percentage determined by AERMOD would likely not lead to a violation. In this way, quantitative cuts to production could be suggested for the facility.

It is important to note that short term hourly weather forecast models (such as the High Resolution Rapid Refresh model, HRRR) were not used in this analysis due to the fact that there would not be adequate time to alert the public or adjust production. Due to the complexity of weather forecast models, runs take several hours to complete. For example, the information from the ECMWF model (a European weather model) initialized at 12 Z (6 AM CST) does not become available until nearly 18 Z. While the short term models have fewer forecasted hours and thus a shorter run time, the first few hours of the run will not be useful no matter how accurate. This is due to the fact that by the time the forecasted weather information is available to process through AERMOD it would already be several hours into the forecast period. For this reason, forecast models that produce information more than 24 hours into the future are needed.

Additionally, once the forecast is available it will need to be processed through MMIF and eventually through AERMOD. Finally the alerts would need to be distributed either to the public or the industrial facilities. In all, a reasonable estimation of time needed from model initiation to air quality alert would be along the lines of eight to ten hours. The most practical application for this would be forecasting for an alert for the day following the model initialization. One of the benefits from using Linux to process the information, is that scripts can be created to automate the process. This means that the process can be run at a specific time every day without human interaction.

5.2 Future Research

This study constitutes a first step in examining the potential of forecasting SO_2 violations, however there is much more research that can be done. A longer term study can be done to improve upon some of the flaws previously discussed.

Ideally, future research would include working with multiple high resolution, unbound WRF models (or other hourly forecast models) with small variations in the parameters and variables. These models would be monitored over the course of one year for accuracy, and adjustments would be made to the parameters if necessary. Notes would also be taken on the seasonal variability in the accuracy of the individual models. These models would be run daily, initialized from current weather information, for one calendar year. The resulting forecast data would then be processed through MMIF, or using the WPS process described in this analysis, to obtain surface and upper air files suitable for use in AERMOD.

At the end of the calendar year, CEMS reports and emission inventories would be collected from necessary facilities that contribute to pollution in the area. Ideally, the researcher would have established communication with the facilities in hopes of obtaining more detailed hourly emissions. This emission data would be entered into AERMOD. Additionally, seasonal cycles for each facility would be established. Staggered variations in emission rates would be calculated in order to produce multiple AERMOD scripts. The previously forecasted weather information would be utilized in these AERMOD scripts to observe the validity of a staggered approach to emissions. In a true forecast, the exact emission rates for each facility would be unknown. Ensembles can also be used with accuracy for emissions (Zhang 2012), so the previously established seasonal variability can be used within an ensemble emissions forecast.

Researchers involved in similar analyses should be very familiar operating in a Linux environment. If models other than WRF are used, the researchers also should have a firm understanding of WPS and the R programming language. This will help to debug any problems that arise in the execution of this process.

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APPENDIX A: EMISSION POINT INFORMATION

ID	Company	Source	Height (ft)	Rate (lb/hr)	Equipment
MPW7890	Muscatine Power and Water	Volume	10	0.0507	
MPW60	Muscatine Power and Water	Point	122.8	0.0172	
MPW70	Muscatine Power and Water	Point	220	293	
MPW80	Muscatine Power and Water	Point	225	652.461	
MPW90	Muscatine Power and Water	Point	300	73	
MPW928A	Muscatine Power and Water	Point	8	0.227	
MPW928B	Muscatine Power and Water	Point	5	0.0812	
MPW928C	Muscatine Power and Water	Point	5	0.581	
MPW7892	Muscatine Power and Water	Point	6.8	0.0162	
MPW168V	Muscatine Power and Water	Point	13.5	0.005	
	TOTAL EMISSION RATE (lb/hr):			**1019.4393**	

ID	Company	Source	Height (ft)	Rate (lb/hr)	Equipment
LGSEP1	MidAmerican Energy	Point	610	2242	LGS Boiler
LGSEP2	MidAmerican Energy	Point	80	11.904	Aux Boiler A
LGSEP3	MidAmerican Energy	Point	80	11.904	Aux Boiler B
LGSEP4	MidAmerican Energy	Point	66	1.993	Emergency Generator A
LGSEP5	MidAmerican Energy	Point	66	1.993	Emergency Generator B
LGSEP32	MidAmerican Energy	Point	24.4	0	Fire Pump
	TOTAL EMISSION RATE (lb/hr):			**2269.794**	

ID	Company	Source	Height (ft)	Rate (lb/hr)	Equipment
MON21	Monsanto	Point	41	0.0429	Boiler 5
MON33	Monsanto	Point	82	0.0429	Boiler 6
MON37	Monsanto	Point	114	0.0094	CAC Ketene Furnace
MON38	Monsanto	Point	76	0.0044	CAC Process Incinerator
MON45	Monsanto	Point	80	0.0726	Boiler 7
MON195	Monsanto	Point	150	159.444	Boiler 8
MON234	Monsanto	Point	160	0.02	CAC Process Flare
	TOTAL EMISSION RATE (lb/hr):			**159.6362**	

ID	Company	Source	Height (ft)	Rate (lb/hr)	Equipment
EP001.0	Grain Processing Corp	Point	219	3870.571	GEP Stack (Blrs 1-4 & 6-7)

EP014.0	Grain Processing Corp	Point	56	0.753	WM, #1Wet Germ Cyclone
EP015.0	Grain Processing Corp	Point	94	11.18	WM, #1 & #2 Germ Dryers
EP032.1	Grain Processing Corp	Point	75	0.663	DH1, #1 Rotary Dryer
EP032.2	Grain Processing Corp	Point	75	0.663	DH1, #2 Rotary Dryer
EP032.3	Grain Processing Corp	Point	91	0.663	DH1, #3 Rotary Dryer
EP032.4	Grain Processing Corp	Point	81	0.663	DH1, #4 Rotary Dryer
EP032.5	Grain Processing Corp	Point	65	0.663	DH1, #5 Rotary Dryer
EP032.6	Grain Processing Corp	Point	65	0.663	DH1, #6 Rotary Dryer
EP040.0	Grain Processing Corp	Point	58	3.93	DH2, Rotary Dryer
EP043.1	Grain Processing Corp	Point	96	8.056	GP1 #1 & #2 Scrub Units
EP046.0	Grain Processing Corp	Point	78	6.74	GP1, #3 Unit Scrubber
EP066.0	Grain Processing Corp	Point	124	0.006	Maltrin, #1 Spray Dryer
EP079.0	Grain Processing Corp	Point	84	2.585	DH3, Primary Dyer (NW)
EP080.0	Grain Processing Corp	Point	84	2.585	DH3, Primary Dryer (SW)
EP081.0	Grain Processing Corp	Point	84	2.585	DH3, Primary Dryer (SE)
EP082.0	Grain Processing Corp	Point	84	2.585	DH3, Primary Dryer (NE)
EP096.0	Grain Processing Corp	Point	53	0.65	WM,#2 Wet Germ Cyclone
EP097.0	Grain Processing Corp	Point	84	22.518	WM, #3 Germ Cyclone
EP108.1	Grain Processing Corp	Point	98	1.447	DH4, #1 Rotary Dryer
EP108.2	Grain Processing Corp	Point	98	1.447	DH4, #2 Rotary Dryer
EP108.3	Grain Processing Corp	Point	98	1.447	DH4, #3 Rotary Dryer
EP125.0	Grain Processing Corp	Point	98	1.096	DH4, #4 Rotary Dryer
EP126.0	Grain Processing Corp	Point	75	11.18	WM, #4 Germ Dryer
EP127.0	Grain Processing Corp	Point	98	1.28	DH4, #5 Rotary Dryer
EP132.2	Grain Processing Corp	Point	126	0.011	
EP135.0	Grain Processing Corp	Point	94	0.014	
EP137.0	Grain Processing Corp	Point	98	1.911	DH4, #6 Rotary Dryer
EP142.0	Grain Processing Corp	Point	70	0.095	PH, Boiler #10
EP153.0	Grain Processing Corp	Point	70	0.095	PH, Boiler #11
EP164.0	Grain Processing Corp	Point	98	2.29	DH4, #7 Rotary Dryer
EP168.0	Grain Processing Corp	Point	152	0.019	
EP173.0	Grain Processing Corp	Point	148	4.51	GP2,#4 Gluten Flash Dryer
EP 174.0	Grain Processing Corp	Point	82	0.37	
EP177.0	Grain Processing Corp	Point	117	0.212	PH, Boiler #12
EP178.0	Grain Processing Corp	Point	65	53.46	WM, #5 Germ Dryer
EP186.0	Grain Processing Corp	Point	137	0.026	Maltrin, #6 Spray Dryer Stk A
EP194.0	Grain Processing Corp	Point	68	2.939	WM,#3 Germ Transfer & Rec
EP195.0	Grain Processing Corp	Point	66.5	0.001	
EP200.0 thru EP261.0	Grain Processing Corp	Point	51.8	22.841	Steep Tanks (62)
EP264.0	Grain Processing Corp	Point	43	1.147	Steep Water Tank
EP265.0	Grain Processing Corp	Point	28	0.002	Distillery Steep Water Tank
EP266.0	Grain Processing Corp	Point	60	0.182	Sulfur Burner

EP268.0	Grain Processing Corp	Point	29	0.172	Gluten Filter Vent Fan #1
EP269.0	Grain Processing Corp	Point	38	0.172	Gluten Filter Vent Fan #2
EP270.0	Grain Processing Corp	Point	29	0.172	Gluten Filter Vent Fan #3
EP271.0	Grain Processing Corp	Point	37	0.172	Gluten Filter Vent Fan #4
EP272.0	Grain Processing Corp	Point	37	0.172	Gluten Filter Vent Fan #5
EP273.0	Grain Processing Corp	Point	29	4.97	Wet Mill Grind Bin #1-2
EP274.0	Grain Processing Corp	Point	38	5.818	Wet Mill Grind Bin #3
EP275.0	Grain Processing Corp	Point	29	4.121	Wet Mill Grind Bin #4
EP276.0	Grain Processing Corp	Point	37	4.791	Wet Mill Grind Bin #5
EP277.0	Grain Processing Corp	Point	37	4.791	Wet Mill Grind Bin #6
EP278.0	Grain Processing Corp	Point	30	0.1	Starch Wall Fan
EP280.0	Grain Processing Corp	Point	69	4.842	N Wet Corn Drag Vent Fan
EP281.0	Grain Processing Corp	Point	69	2.374	S Wet Corn Drag Vent Fan
EP282.0	Grain Processing Corp	Point	59	5.884	Wet Corn Drag Vent
EP283.0	Grain Processing Corp	Point	1	0.032	GP1 VF Pump Discharge
EP284.0	Grain Processing Corp	Point	1	0.032	
EP544.0	Grain Processing Corp	Point	50	0.267	Distilling, CO2 Scrubber
EP546.0	Grain Processing Corp	Point	25	0.0034	#3 Alpha Laval
EP548.0	Grain Processing Corp	Point	35	1	Biogas Flare
EP551.0	Grain Processing Corp	Point	69	0.084	East Tank & C400 Thrus Tank
	TOTAL EMISSION RATE (lb/hr):			**4086.7134**	

APPENDIX B: WEATHER FORECAST MODEL PARAMETERS

WRF Model Parameters

Variable	Configuration
Domains	12 km over Midwest, 4 km over eastern Iowa, 1.3 km over Johnson county and western Cedar county, 0.44 km over Iowa City
Nesting	One way nesting
Vertical Resolution	35 levels First layer depth ~20 m Model top 50 mbar
Spin-up Period	24 h
Run Time Before Initialization (excluding spin-up)	30 days
Land Cover	USGS 24-category Land Use Categories
Treatment of Snow (albedo, influence on surface energy and moisture balance)	ifsnow = 1
Initial and Boundary Conditions	NARR
isfflx	1
icloud	1
Data Assimilation to Improve Initial and Boundary Conditions via Objective Analysis (OBSGRID)	yes – obsgrid
Data Source for Objective Analysis	ds461.0 data files
Objective Analysis Descriptions	OBSGRID run with Cressman analysis with radius influence of 4, 1.33, 0.44
Observation Nudging (obs_nudge_opt)	Yes – used on all domains except the coarsest 12 km domain
Observation Nudging Design and Settings	Winds, temperature, and water vapor are nudged in the 4, 1.3, and 0.4 km domains (but not the 12 km). Coefficients are 6.0E-4 for all three
Grid (Analysis) Nudging via FDDA. Settings Above the Surface Layer (grid_fdda)	Yes – grid nudging for the outer 12 km domain at 3 hr time interval. The winds in the PBL were nudged. u,v: 3.0E-4. Nudged for T, q above the PBL and for winds throughout all layers

Grid (Surface) Nudging in the Surface Layer (grid_sfdda)	No – surface FDDA nudging using grid_sfdda not used
PBL Scheme (bl_pbl_physics)	ACM2
Microphysics Scheme (mp_physics)	Morrison
Radiation Scheme (ra_lw_physics, ra_sw_physics)	RRTMG, SW and LW Timesteps 12, 4 and 1 min depending on domain.
Land Surface Scheme (sf_sfclay_physics and sf_surface_physics)	Pleim-Xiu
Cumulus Scheme (cu_physics)	Kain-Fritsch
Soil Moisture Treatment / Soil Layers	Default: 2 layers.
Timestep	90 sec at 12 km; 30/10/3.3 sec at the finer resolutions
Dynamics Damping (w_damping, damp_opt)	w_damping = 1 damp_opt = 3
WRF Version	Ran WRF 3.4.1
Evaluation Period	08/15/2011-09/15/2012
Summary of Evaluation Method	METSTAT evaluation in each domain

NAM Model Parameters

Variable	Configuration
Model Domain	12 km parent over North America
Nesting	4 km CONUS, 6 km Alaska, 3 km Hawaii/Puerto Rico, 1.33 km “fire weather” next
Vertical Resolution	60 levels, model top at 2 mb, first layer above ground ~ 20 m
Initial Conditions/Spin-up	12-h spin-up with NAM data assimilation system
Objective Analysis	NCEP Gridpoint Statistical Interpolation analysis
Land-Cover	20 MODIS-IGBP land-use categories
Boundary Conditions	Parent domain: 6-h old GFS forecast, boundary tendencies updated every 3-h. Nest domains: one-way timestep from parent domain
PBL Scheme	Mellor-Yamada-Janic Level 2.5
Land Surface	NOAH-LSM, 4 soil layers
Convection	Betts-Miller-Janic, convection with reduced triggering in the NAM nests
Microphysics	Ferrier
Radiation	GFDL
Timestep	12 km parent domain 26.67 seconds, physics is called every 6 timesteps, radiation called every hour

APPENDIX C: LINUX CODE SCRIPTS

WPS Ungrib and Metgrid Script

```
#!/bin/bash

## Process Files using WPS

##Set up For Loops

##Create Folder with Date names

##Setup Grib Data Links

RUNFOLDER=/home/eng/build/WPS/WPS
DATAFOLDER=/data
ORIGINALGRIBDATA=$DATAFOLDER/external/raw-data/nam-2012
GRIBDATAFILENAMEHEADER="nam_218_"
GRIBDATAFOLDER=$DATAFOLDER/grib-data
METGRIDDATAFOLDER=$DATAFOLDER/external/metgrid-WPS-NAM
DATELIST=$DATAFOLDER/NAM-DateList.txt
PROCESSLOGFILE=$RUNFOLDER/Process.log
NAMELISTWORKINGFILE=$RUNFOLDER/namelist.wps
NAMELISTPREFILE=$RUNFOLDER/namelist.wps_pre
NAMELISTPOSTFILE=$RUNFOLDER/namelist.wps_post

##Colors
NORMAL="\e[0m"
RED="\e[0;31m"
GREEN="\e[0;32m"
PURPLE="\e[0;35m"

##PreCleanUp:
cd $RUNFOLDER
rm -v $PROCESSLOGFILE $NAMELISTWORKINGFILE  >> $PROCESSLOGFILE
touch $PROCESSLOGFILE

## RunTime Break Settings
#set -e

for dateVar in $(cat $DATELIST)
do
	# Delete grib Links in GRIBDATA
	#set +e
	echo -e "\n "$RED"Beginning data dump for $dateVar...$NORMAL\n	clearing grib-data,"
	# Delete nam_ files and PFILE's
	rm -v ./GRIBFILE.* >> $PROCESSLOGFILE
	rm -v $GRIBDATAFOLDER/*.grb2 >> $PROCESSLOGFILE
```

```
        rm -v nam_* PFILE* >> $PROCESSLOGFILE
        #set -e
        echo -e "        loading grib data for $dateVar,"
        ln -s $ORIGINALGRIBDATA/$GRIBDATAFILENAMEHEADER$dateVar*
$GRIBDATAFOLDER/
        echo -e "        linking grib files in WPS Working Folder,"
        cd $RUNFOLDER
        ./link_grib.csh $GRIBDATAFOLDER/
        echo -e "        Updating namelist.wps file for $dateVar..."
        cp $NAMELISTPREFILE $NAMELISTWORKINGFILE
        STARTDATE=$(date -d $dateVar +%Y-%m-%d)
         ENDDATE=$(date -d "$dateVar+3 days" "+%Y-%m-%d")
        echo -e " start_date =  '"$STARTDATE"_12:00:00','"$STARTDATE"_12:00:00'," >>
$NAMELISTWORKINGFILE
        echo -e " end_date =  '"$ENDDATE"_12:00:00','"$ENDDATE"_12:00:00'," >>
$NAMELISTWORKINGFILE
        cat $NAMELISTPOSTFILE >> $NAMELISTWORKINGFILE
        echo -e "opt_output_from_metgrid_path = '$METGRIDDATAFOLDER/$dateVar/'" >>
$NAMELISTWORKINGFILE
        echo -e "\n/" >> $NAMELISTWORKINGFILE
        echo -e "        Done Updating NameList.wps file."
        echo -e "$GREEN        Now Ready to unGrib.$NORMAL\n\n"
        sleep 2
        echo -e "\n\nUnGRIBing..."
        touch ungrib_$dateVar.log
        # Actual Ungrub command...
        ./ungrib.exe &> ungrib_$dateVar.log

        echo -e "$PURPLE\n\n\nFinished UnGRIBing\n$RED\nBeginning MetGrid
Processing.$NORMAL"
        echo -ne "        Preparing Folder:  "
        mkdir -pv $METGRIDDATAFOLDER/$dateVar
        echo ""
        echo -e "        Ready to MetGrid.\n\n"
        sleep 2
        echo -e "$GREEN Beginning MetGrid...$NORMAL"
        touch metgrid_$dateVar.log
        ./metgrid.exe $METGRIDDATAFOLDER/$dateVar/ &> metgrid_$dateVar.log
        echo -e "$PURPLE\n\n\nFinished with MetGrid. $NORMAL Moving onto next DataSet...\n"
        sleep 2
        #read
done

echo -e "$RED\n\nFor Routine Finished!!!!\n$NORMAL"
```

NAM Catenation Script

```
#!/bin/bash

## RyanN 8-23-2014

## Vars

clear # Clear Screen
#DEBUG MODE
DEBUG="no"

#RUN Folder Stuff
RUNFOLDER=/data/bin/ncrcat-bin
PROCESSLOGFILE=$RUNFOLDER/cat_NAM_Process.log

#DATAFILE
DATAFOLDER=/data/external/metgrid-WPS-NAM
DATAFILE_HEADER="met_em.d02.2012"
DATAFILE_FOOTER=":00:00.nc"

#DATEFILE
DATELIST=/data/NAM-DateList.txt

#OUTPUT
OUTPUT_FOLDER=/data/external/metgrid-72hrs
OUTPUT_HEADER=met-NAM_d02_72_
OUTPUT_FOOTER="-12z.nc"

##Colors
NORMAL="\e[0m"
RED="\e[0;31m"
GREEN="\e[0;32m"
PURPLE="\e[0;35m"
GREY="\e[0;90m"

TAB="\t\t"
NTAB="\n$TAB"

##PreCleanUp:
cd $RUNFOLDER
clear #Clear Terminal Screen
echo -e "\n\nSpinning-Up Catenation Processing Script for RAW NAM Data...$NORMAL"
#rm -v $PROCESSLOGFILE >> $PROCESSLOGFILE
echo "Begin Log - $(date -I)..." > $PROCESSLOGFILE

sleep 2
```

```
for dateVar in $(cat $DATELIST)
do
	clear #Clear Screen

	echo -e "\n"$PURPLE"***\tStarting ncrCAT for $GREEN$(date -I -d "$dateVar")
$PURPLE\n***\n***\tCatenating 72 hours...\n$NORMAL"
FILE1_12=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar" "+%m-
%d_12")$DATAFILE_FOOTER
FILE1_18=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar" "+%m-
%d_18")$DATAFILE_FOOTER
FILE2_00=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+1 days" "+%m-
%d_00")$DATAFILE_FOOTER
FILE2_06=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+1 days" "+%m-
%d_06")$DATAFILE_FOOTER
FILE2_12=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+1 days" "+%m-
%d_12")$DATAFILE_FOOTER
FILE2_18=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+1 days" "+%m-
%d_18")$DATAFILE_FOOTER
FILE3_00=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+2 days" "+%m-
%d_00")$DATAFILE_FOOTER
FILE3_06=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+2 days" "+%m-
%d_06")$DATAFILE_FOOTER
FILE3_12=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+2 days" "+%m-
%d_12")$DATAFILE_FOOTER
FILE3_18=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+2 days" "+%m-
%d_18")$DATAFILE_FOOTER
FILE4_00=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+3 days" "+%m-
%d_00")$DATAFILE_FOOTER
FILE4_06=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+3 days" "+%m-
%d_06")$DATAFILE_FOOTER
FILE4_12=$DATAFOLDER/$dateVar/$DATAFILE_HEADER-$(date -d "$dateVar+3 days" "+%m-
%d_12")$DATAFILE_FOOTER
OUTFILE=$OUTPUT_FOLDER/$OUTPUT_HEADER$(date -d "$dateVar" "+%Y-%m-
%d")$OUTPUT_FOOTER
	echo -e $PURPLE"\tUsing Files from $(date -I -d
"$dateVar"):$GREY$NTAB'$FILE1_12'$NTAB'$FILE1_18'" #>> $PROCESSLOGFILE
	echo -e $PURPLE"\tUsing Files from $(date -I -d "$dateVar+1
days"):$GREY$NTAB'$FILE2_00'$NTAB'$FILE2_06'$NTAB'$FILE2_12'$NTAB'$FILE2_18'" #>>
$PROCESSLOGFILE
	echo -e $PURPLE"\tUsing Files from $(date -I -d "$dateVar+2
days"):$GREY$NTAB'$FILE3_00'$NTAB'$FILE3_06'$NTAB'$FILE3_12'$NTAB'$FILE3_18'" #>>
$PROCESSLOGFILE
	echo -e $PURPLE"\tUsing Files from $(date -I -d "$dateVar+3
days"):$GREY$NTAB'$FILE4_00'$NTAB'$FILE4_06'$NTAB'$FILE4_12'" #>> $PROCESSLOGFILE
	echo -e "\n\t"$PURPLE"Outputting to file: $RED'$OUTFILE'.$NORMAL" #>>
$PROCESSLOGFILE

	echo -e "\n"$PURPLE"***\tRunning ncrCat for $GREEN$(date -I -d
"$dateVar")$PURPLE...\n***$NORMAL" #>> $PROCESSLOGFILE
	set -e
	if [ "$DEBUG" = "no" ]; then
```

```
	ncrcat -3 -F -D 5 \
		$FILE1_12 \
		$FILE1_18 \
		$FILE2_00 \
		$FILE2_06 \
		$FILE2_12 \
		$FILE2_18 \
		$FILE3_00 \
		$FILE3_06 \
		$FILE3_12 \
		$FILE3_18 \
		$FILE4_00 \
		$FILE4_06 \
		$FILE4_12 \
		-o $OUTFILE \
		>> $PROCESSLOGFILE
	else
		echo -e "		Skipping Actual ncrCAT - DEBUG mode...\n"
		echo -e "Skipping Actual ncrCAT - DEBUG mode...\n" >>$PROCESSLOGFILE
	fi
	set +e
	echo -e "\n***Completed running ncrCAT for: $dateVar." >>$PROCESSLOGFILE
	echo -e $PURPLE"\n***\n***\n***\tCompleted running ncrCAT for: $GREEN$(date -I -d
"$dateVar"), 72-hours, 12z.\n"$PURPLE"***\n***\n***$NORMAL"


	if [ "$DEBUG" != "no" ]; then
		echo -e "$RED  Press enter to continue, DEBUG Mode Enabled...$NORMAL"
		read #wait!!
	fi
sleep 2

done

echo -e "$RED\n\nFor Routine Finished!!!!\n$NORMAL"
```

Global Attributes Script

```
#!/bin/bash
## RyanN - 9-18-2014 Run Global Attributes
##
clear # Clear Screen
#DEBUG MODE
DEBUG="no"

#RUN Folder Stuff
RUNFOLDER=/data/bin
PROCESSLOGFILE=$RUNFOLDER/Global_Process.log

#DATAFILE
DATAFOLDER=/data/external/metgrid-72hrs
DATAFILE_HEADER="met-NAM_d02_72_2012"
DATAFILE_FOOTER="-12z.nc"

#DATEFILE
DATELIST=/data/gatt-DateList.txt

cd $DATAFOLDER

for dateVar in $(cat $DATELIST)
do
    FILE=$DATAFOLDER/$DATAFILE_HEADER-$(date -d "$dateVar" "+%m-
%d")$DATAFILE_FOOTER
    echo -e "Applying Global Attributes to file: "$FILE
    if [ "$DEBUG" = "no" ]; then
    #Begin
    ncatted -O -a WEST-EAST_GRID_DIMENSION,global,o,l,88 $FILE
    ncatted -O -a BOTTOM-TOP_GRID_DIMENSION,global,o,l,27 $FILE
    ncatted -O -a WEST-EAST_PATCH_END_UNSTAG,global,o,l,87 $FILE
    ncatted -O -a WEST-EAST_PATCH_END_STAG,global,o,l,88 $FILE
    ncatted -O -a CEN_LAT,global,o,f,42.01135 $FILE
    ncatted -O -a CEN_LON,global,o,f,-91.96472 $FILE
    ncatted -O -a MOAD_CEN_LAT,global,o,f,43.39888 $FILE
    ncatted -O -a corner_lats,global,o,f,"40.41752, 43.73895, 43.56293, 40.24944, 40.41809,
43.73955, 43.56149, 40.24806, 40.39944, 43.75697, 43.5809, 40.23141, 40.40002, 43.75756, 43.57946,
40.23002" $FILE
    ncatted -O -a corner_lons,global,o,f,"-94.12549, -93.98029, -89.7009, -90.05069, -94.14923, -
94.00525, -89.67609, -90.02707, -94.12625, -93.97946, -89.69888, -90.05249, -94.14996, -94.00443, -
89.67407, -90.02887" $FILE
    fi
    if [ "$DEBUG" != "no" ]; then
        echo -e "$RED  Press enter to continue, DEBUG Mode Enabled...$NORMAL"
        read #wait!!
    fi
```

```
done

echo -e "\n\nDone."
##
```

WRF Donor File Script

```bash
#!/bin/bash

## RyanN 2014-9-19

## Vars

##Example "ncks -d Time,12,86,6 ./wrf_d02_96_2012-02-25_00:00:00 ./wrf-NAM_d02_72_2012-02-25-12z"

clear # Clear Screen
#DEBUG MODE
DEBUG="no"

#RUN Folder Stuff
RUNFOLDER=/data/bin/ncks-bin
PROCESSLOGFILE=$RUNFOLDER/Process.log

#DATAFILE
DATAFOLDER=/data/wrf-0z-data/domain02/merged
DATAFILE_HEADER="wrf_d02_96_2012"
DATAFILE_FOOTER="_00:00:00"

#DATEFILE
DATELIST=/data/bin/dateLists/nkcs-Datelist.txt

#OUTPUT
OUTPUT_FOLDER=/data/wrf-0z-data/72hr-donor
OUTPUT_HEADER="donor_d02_72_2012"
OUTPUT_FOOTER="-12z.nc"

NCKS_CMD="ncks -d Time,12,86,6"

##Colors
NORMAL="\e[0m"
RED="\e[0;31m"
GREEN="\e[0;32m"
PURPLE="\e[0;35m"
GREY="\e[0;90m"

TAB="\t\t"
NTAB="\n$TAB"

##PreCleanUp:
cd $RUNFOLDER
clear #Clear Terminal Screen
echo -e "\n\nSpinning-Up ncks Processing Script for Wrf-Donor Data...$NORMAL"
```

```
echo "Begin Log - $(date -I)..." > $PROCESSLOGFILE #btrFS friendly

sleep 2

for dateVar in $(cat $DATELIST)
do
    clear #Clear Screen

INPUTFILE=$DATAFOLDER/$DATAFILE_HEADER-$(date -d "$dateVar" "+%m-
%d")$DATAFILE_FOOTER
OUTFILE=$OUTPUT_FOLDER/$OUTPUT_HEADER$(date -d "$dateVar" "+%Y-%m-
%d")$OUTPUT_FOOTER
    echo -e "\n\t"$PURPLE"Inputting from file: $RED'$INPUTFILE'.$NORMAL" #>>
$PROCESSLOGFILE
    echo -e "\n\t"$PURPLE"Outputting to file: $RED'$OUTFILE'.$NORMAL" #>>
$PROCESSLOGFILE

    echo -e "\n"$PURPLE"***\tRunning ncks for $GREEN$(date -I -d
"$dateVar")$PURPLE...\n***$NORMAL" #>> $PROCESSLOGFILE

    if [ "$DEBUG" = "no" ]; then
        set -e
        $NCKS_CMD $INPUTFILE $OUTFILE >> $PROCESSLOGFILE
        set +e
        echo -e "\n***Completed running ncks for: $dateVar." >>$PROCESSLOGFILE
        echo -e $PURPLE"\n***\n***\n***\tCompleted running nkcs for: $GREEN$(date -I -d
"$dateVar"), 72-hours, 12z.\n"$PURPLE"***\n***\n***$NORMAL"

    else
        echo -e "        DEBUG mode...\n"
        echo -e "Skipping Actual ncks - DEBUG mode...\n" >>$PROCESSLOGFILE

    fi


    if [ "$DEBUG" != "no" ]; then
        echo -e "$RED  Press enter to continue, DEBUG Mode Enabled...$NORMAL"
        read #wait!!
    fi
sleep 2

done

echo -e "$RED\n\nncks Routine Finished!!!!\n$NORMAL"
```

R Environment Set Up Script

```
#!/bin/bash

## Process Files using R-Script, written for us by Scott Spak
## Ryan Nicholson 9-19-2014

clear # Clear Screen
#DEBUG MODE
DEBUG="no"

##Vars...
RUNFOLDER=/data/bin/R-bin
DATAFOLDER=/data
DATELIST=/data/bin/dateLists/R-DateList.txt
PROCESSLOGFILE=$RUNFOLDER/Process.log
#R-Script
RSCRIPTWORKINGFILE="R-ProcessExec.R"
RSCRIPTBASEFILE="R-ProcessFunction.R"
RLOGFILE=$RSCRIPTWORKINGFILE"out"

#Working WRF File to use
DONORPATH=/data/wrf-0z-data/72hr-donor
DONORHEADER="donor_d02_72_2012"
DONORFOOTER="-12z.nc"

#Source
SOURCEPATH=/data/external/metgrid-72hrs
SOURCEHEADER="met-NAM_d02_72_"
SOURCEFOOTER="-12z.nc"

#Destination
DESTPATH=/data/local-NAM-WRF
DESTHEADER=R-NAM-d02_72_
DESTFOOTER=-12z.nc

##Colors
NORMAL="\e[0m"
RED="\e[0;31m"
GREEN="\e[0;32m"
PURPLE="\e[0;35m"

##PreCleanUp:
cd $RUNFOLDER
echo "Begin. Running in "$(pwd)"."  > $PROCESSLOGFILE

# Process Routine
for dateVar in $(cat $DATELIST)
do
```

```
    #Assemble proper R Script with command execution...
    echo -e "       Creating R file for $dateVar..."
    echo -e "       Creating R file for $dateVar..." >> $PROCESSLOGFILE
    #Blank File, maintain inode...Depend on CoWrite...
    echo "" > $RSCRIPTWORKINGFILE
    cat $RSCRIPTBASEFILE >> $RSCRIPTWORKINGFILE
    #String Manip
        STARTDATE=$(date -d $dateVar +%Y-%m-%d)
        DONORFILE=$DONORPATH/$DONORHEADER$STARTDATE$DONORFOOTER

    SOURCEFILE=$SOURCEPATH/$SOURCEHEADER$STARTDATE$SOURCEFOOTER
        DESTFILE=$DESTPATH/$DESTHEADER$STARTDATE$DESTFOOTER
    #Composite to Append
        COMMANDLINE="metem2wrfout(\"$SOURCEFILE\",\"$DESTFILE\");"

    #Compile R-Script for Execution:
        echo -e "\n$COMMANDLINE\n" >> $RSCRIPTWORKINGFILE

    #Actual Work
    if [ "$DEBUG" = "no" ]; then
        # We're using btrFS - allowing inode cloning:
        cp -v --reflink $DONORFILE $DESTFILE >> $PROCESSLOGFILE

        # Execute R Script
        R CMD BATCH $RSCRIPTWORKINGFILE

        # Copy R-LogFile

        cp -v --reflink $RLOGFILE $DESTPATH/$RLOGFILE-$dateVar >>
$PROCESSLOGFILE

    else
        echo "Debug Mode:"
        echo "Donor File: "$DONORFILE
        echo "   $COMMANDLINE"

    fi

    if [ "$DEBUG" != "no" ]; then
        echo -e "$RED  Press enter to continue, DEBUG Mode Enabled...$NORMAL"
        read #wait!!
    fi
done

echo -e "$RED\n\nFor Routine Finished!!!!\n$NORMAL"
```

R Variable Processing Script

```
metem2wrfout<-function(met_em,wrfout){

# example: metem2wrfout(â€œmet_em_d02_201304.nc","wrfout_d02_201304.nc")

# metem2wrfout(met_em="met-NAM_d02_72_2012-02-25-12z.nc",wrfout="wrf-NAM_d02_72_2012-02-25-12z")
# note: this script does not interpolate in time. Make sure that the empty wrf file only contains the same times as the met_em file

library(ncdf)

m<-open.ncdf(met_em)

w<-open.ncdf(wrfout,write=TRUE)

var_m<-c("VV","UU","TT")

var_w<-c("V","U","T")

p<-get.var.ncdf(m,"PRES")

p2<-get.var.ncdf(w,"P")

pb<-get.var.ncdf(w,"PB")

p3<-p2+pb

h<-dim(p)[3]

h2<-dim(p3)[3]
lt<-dim(p3)[4]

nxp<-dim(p)[1]
nyp<-dim(p)[2]

nxp3<-dim(p3)[1]
nyp3<-dim(p3)[2]

for(i in 1:length(var_w) ){

a<-get.var.ncdf(m,var_m[i])

#make empty target grid
b2<-get.var.ncdf(w,var_w[i])
b<-b2 - b2
nx<-dim(b)[1]
ny<-dim(b)[2]
```

```
# pressure interpolation for each variable, for each grid cell, ignoring surface pressure level

for(j in 1:nx){

for(k in 1:ny){

for(t in 1:lt){

# for edge faces (U&V), use
if (j > nxp) j1<- nxp else j1<-j
if (k > nyp) k1<- nyp else k1<-k
if (j > nxp3) j2<- nxp3 else j2<-j
if (k > nyp3) k2<- nyp3 else k2<-k

b[j,k,,t]<-approx(x=p[j1,k1,2:h,t], y=a[j1,k1,2:h,t], xo= p3[j2,k2,,t])$y

}}}

put.var.ncdf(w,varid=var_w[i],vals=b,start=c(1,1,1,1),count=c(-1,-1,-1,-1))
rm(b,b2)

}

# convert RH to water vapor mixing ratio

rh<-get.var.ncdf(m,"RH")

t<-get.var.ncdf(m,"TT")-273.15

es<-6.112*exp(17.67*t/(t+243.5))

ws<-0.6219907*es/(es+p)

wo<-ws*rh

#make empty target grid
b2<-get.var.ncdf(w,"QVAPOR")
b<-b2 - b2
nx<-dim(b)[1]
ny<-dim(b)[2]

# pressure interpolation for water vapor mixing ratio

for(j in 1:nx){

for(k in 1:ny){

for(t in 1:lt){
```

```
if (j > nxp) j1<- nxp else j1<-j
if (k > nyp) k1<- nyp else k1<-k
if (j > nxp3) j2<- nxp3 else j2<-j
if (k > nyp3) k2<- nyp3 else k2<-k

b[j,k,,t]<-approx(x=p[j1,k1,2:h,t], y=wo[j1,k1,2:h,t], xo=p3[j2,k2,,t])$y

}}}

put.var.ncdf(w,varid="QVAPOR",vals=b,start=c(1,1,1,1),count=c(-1,-1,-1,-1))

close.ncdf(m)

close.ncdf(w)

invisible(0)

}
```

MMIF Processing Script

```
#!/bin/bash

## RyanN 8-21-2014 - Updated 9-19-2014

## Vars
clear # Clear Screen
#DEBUG MODE
DEBUG="no"

#MMIF
RUNFOLDER=/home/eng/build/MMIF
MMIFEXEC=$RUNFOLDER/mmif
MMIFINPUTFILE=$RUNFOLDER/mmif.inp
PROCESSLOGFILE=$RUNFOLDER/MMIF-Process.log
echo -e "\n\n\n\nBegin MMIF Processing...\n\n" > $PROCESSLOGFILE

# "AER_layers   0   0"
#MMIF's INPUTFILE
INPUTFILE_SETTINGS="POINT  latlon     42.01135   -91.96472  -5 ! in GMT-9 zone" #AER_layers  1
4\n"
#DATAFILE
DATAFOLDER=/data/local-NAM-WRF
DATAFILE_HEADER="R-NAM-d02_72_2012"
DATAFILE_FOOTER="-12z.nc"

#DATEFILE
Z_TIME=12
DATELIST=/data/bin/dateLists/MMIF-DateList.txt

#OUTPUT
AERMOD_OUTPUT_FOLDER=/data/aermod-ready/wrf_NAM-12z

##Colors
NORMAL="\e[0m"
RED="\e[0;31m"
GREEN="\e[0;32m"
PURPLE="\e[0;35m"

##PreCleanUp:
cd $RUNFOLDER
clear #Clear Terminal Screen
echo -e "\n\n"$RED"Beginning MMIF Processing Script...$NORMAL"
rm -v $RUNFOLDER/PJHJ.* $MMIFINPUTFILE >> $PROCESSLOGFILE

for dateVar in $(cat $DATELIST)
do
```

```
    echo -e "\n"$RED"***MMIF - $dateVar***$NORMAL\n    Setting-up MMIF's input file...\n"
    echo "start   $(date -d "$dateVar" "+%Y %m %d") $Z_TIME;" >  $MMIFINPUTFILE #Erases previous - only one arrow#
    echo "stop   $(date -d "$dateVar+3 days" "+%Y %m %d") $Z_TIME;" >> $MMIFINPUTFILE
    echo -e "\n\n$INPUTFILE_SETTINGS" >> $MMIFINPUTFILE
    echo -e "\n\n#AERMOD Settings" >> $MMIFINPUTFILE
    echo "Output aermod   useful   $AERMOD_OUTPUT_FOLDER/PJHJ-$(date -d "$dateVar" "+%Y-%m-%d")-"$Z_TIME"z.info.txt" >> $MMIFINPUTFILE
    echo "Output aermod   sfc   $AERMOD_OUTPUT_FOLDER/PJHJ-$(date -d "$dateVar" "+%Y-%m-%d")-"$Z_TIME"z.sfc" >> $MMIFINPUTFILE
    echo "Output aermod   PFL   $AERMOD_OUTPUT_FOLDER/PJHJ-$(date -d "$dateVar" "+%Y-%m-%d")-"$Z_TIME"z.pfl" >> $MMIFINPUTFILE
    echo -e "\n\n#INPUT file names\n"  >> $MMIFINPUTFILE
    echo -e "INPUT '$DATAFOLDER/$DATAFILE_HEADER-$(date -d "$dateVar" "+%m-%d")$DATAFILE_FOOTER'"  >> $MMIFINPUTFILE
    echo -e "\n\n#END OF mmif.inp FILE"  >> $MMIFINPUTFILE

    echo -e "\n Running mmif against $dateVar..."

    if [ "$DEBUG" = "no" ]; then
        set -e
#       echo -e "$MMIFINPUTFILE"
        $MMIFEXEC $MMIFINPUTFILE
        set +e
        echo -e "\nCompleted running MMIFagainst $dateVar." >>$PROCESSLOGFILE
        echo -e "\n"$GREEN"Completed running MMIFagainst $dateVar.$NORMAL"
    else
        echo "Debug Mode:"
        echo "   $MMIFINPUTFILE"
    fi

    if [ "$DEBUG" != "no" ]; then
        echo -e "$RED  Press enter to continue, DEBUG Mode Enabled...$NORMAL"
        read #wait!!
    else
        sleep 2

    fi

done

echo -e "$RED\n\nFor Routine Finished!!!!\n$NORMAL"

#EOF
```

APPENDIX D: SUPPLEMENTAL UPPER AIR INFORMATION

Sounding Data from the Days with the 10 Highest Observed 24-Hour Averages

Date	**Time[1]**	**Inversion Below 700 mb**	**Type**	**Base (mb)**	**Surface Based**	**Height Above Surface (mb)**	**Depth (mb)**	**Temp Spread (C)**
10-Jan	12Z	Yes	Radiation	1000	Yes	0	50	5
11-Jan	00Z	Yes	Frontal	940	No	50	90	3
	12Z	Yes	Frontal	950	No	30	100	5
12-Jan	00z	Yes	Frontal	925	No	65	45	1
21-Apr	12Z	Yes	Radiation	995	Yes	0	20	8
22-Apr	00Z	Yes	Subsidence	850	No	130	40	0
	12Z	Yes	Radiation	990	Yes	0	130	3
23-Apr	00Z	Yes	Subsidence	980	Yes	0	15	0
22-May	12Z	Yes	Frontal	980	Yes	0	30	5
23-May	00Z	No						
	12Z	Yes	Radiation	990	Yes	0	60	-1
24-May	00Z	No						
	12Z	Yes	Radiation	960	No	30	35	1
25-May	00Z	Yes	Frontal	960	No	30	40	1
29-May	12Z	Yes	Radiation	1000	Yes	0	40	3
30-May	00Z	Yes	Subsidence	725	No	265	25	0
	12Z	Yes	Radiation	990	Yes	0	30	3
31-May	00Z	No						
	12Z	Yes	Radiation	980	Yes	0	90	-3
1-Jun	00Z	No						
5-Jun	12Z	Yes	Radiation	975	Yes	0	35	2
6-Jun	00Z	Yes	Subsidence	810	No	170	35	1
	12Z	Yes	Frontal	980	Yes	0	50	3
7-Jun	00Z	Yes	Subsidence	825	No	150	35	-1
	12Z	Yes	Subsidence	875	No	95	55	5
8-Jun	00Z	Yes	Frontal	975	Yes	0	15	0
6-Sep	12Z	Yes	Subsidence	910	No	70	30	1
7-Sep	00Z	Yes	Frontal	890	No	90	30	0
	12Z	Yes	Radiation	980	Yes	0	50	0

---

[1] All times are given in UTC. In Iowa, 12Z weather soundings are taken at approximately 6:00 AM on the date shown. 00Z weather soundings are taken at approximately 6:00 PM on the date prior.

7-Sep	00Z	Yes	Subsidence	820	No	160	20	1
20-Oct	12Z	Yes	Radiation	975	Yes	0	25	6
12-Oct	00Z	Yes	Subsidence	980	Yes	0	20	1
	12Z	Yes	Frontal	975	Yes	0	175	5
22-Oct	00Z	Yes	Unknown	980	Yes	0	10	0

Sounding Data from the Days with the 10 Highest Modeled 24-Hour Averages

Date	Time[2]	Inversion Below 700 mb	Type	Base (mb)	Surface Based	Height Above Surface (mb)	Depth (mb)	Temp Spread (C)
21-Apr	12Z	Yes	Radiation	995	Yes	0	20	8
22-Apr	00Z	Yes	Subsidence	850	No	130	40	0
	12Z	Yes	Radiation	990	Yes	0	130	3
23-Apr	00Z	Yes	Subsidence	980	Yes	0	15	0
21-May	12Z	Yes	Radiation	990	Yes	40	40	8
22-May	00Z	Yes	Subsidence	775	No	105	25	1
	12Z	Yes	Frontal	980	Yes	0	30	5
23-May	00Z	No						
28-May	12Z	Yes	Radiation	1000	Yes	0	20	3
29-May	00Z	No						
	12Z	Yes	Radiation	1000	Yes	0	40	3
30-May	00Z	Yes	Subsidence	725	No	265	25	0
	12Z	Yes	Radiation	990	Yes	0	30	3
31-May	00Z	No						
22-Jul	12Z	Yes	Radiation	1000	Yes	0	20	7
23-Jul	00Z	Yes	Subsidence	860	No	140	50	4
	12Z	Yes	Radiation	1000	Yes	0	25	6
24-Jul	00Z	No						
15-Sep	12Z	Yes	Radiation	1000	Yes	0	20	6
16-Sep	00Z	Yes	Subsidence	850	No	140	175	2
	12Z	Yes	Radiation	990	Yes	0	20	1
17-Sep	00Z	Yes	Frontal	850	No	140	70	4
	12Z	Yes	Frontal	950	No	30	10	7
18-Sep	00Z	Yes	Unknown	990	Yes	0	15	2
4-Oct	12Z	Yes	Radiation	990	Yes	0	20	10
5-Oct	00Z	Missing						
	12Z	Yes	Frontal	990	Yes	0	40	4
6-Oct	00Z	Yes	Subsidence	740	No	140	20	0
	12Z	Yes	Radiation	990	Yes	0	40	2
7-Oct	00Z	No						

---

[2] All times are given in UTC. In Iowa, 12Z weather soundings are taken at approximately 6:00 AM on the date shown. 00Z weather soundings are taken at approximately 6:00 PM on the date prior.

15-Nov	12Z	Yes	Subsidence	840	No	150	40	4
16-Nov	00Z	Yes	Subsidence	1000	Yes	0	30	1
	12Z	Yes	Radiation	990	Yes	0	15	5
17-Nov	00Z	Yes	Subsidence	980	Yes	0	10	0