

A Study of the Multiple Year Variation of Air Quality Impacts Predicted By the CALPUFF Dispersion Model

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ABSTRACT

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The annual variation of air quality impacts has been evaluated by running the CALPUFF dispersion model for a five year period and examining the variation in the predicted impacts from year to year. The CALMET model was run for the years 1990 through 1994 to produce the meteorological fields necessary to run CALPUFF. CALMET was run using the National Weather Service radiosonde data, surface data, and precipitation data. The runs were performed for an array of source locations with impacts predicted at one receptor located in southern Vermont. For each source location the variation in impacts over the five year period is represented by the ratio of highest to lowest predicted values, where predicted values occur for each year. This multiple year variation is calculated for long and short term regulatory standards. The analysis is performed for sulfate concentrations and air quality related values including sulfate dry deposition and visibility.

For the year 1992 a similar analysis is performed in comparing variation in predicted impacts for CALPUFF runs using meteorological fields produced with National Weather Service data and meteorological fields produced using prognostic mesoscale data (MM5 data), input into CALMET.

The multiple year variation is represented by annual variation indicator values. These indicator values may be used as multipliers to apply to air quality impacts when the impact analysis does not rely on 5 years of meteorology to better define an inherent variability range because of the temporal limitation of the meteorological data set.

INTRODUCTION

In the Federal Register Guideline on Air Quality Models section 9.3.1 is devoted to the required length of record of meteorological data for air quality dispersion modeling in permit reviews. The recommended contiguous time period of meteorological data for dispersion modeling is 5 years. This multiple year time frame is required because of the variation in any one year of average transport events and other meteorological variables that affect modeled pollutant impacts. The decision to require 5 years of data is in fact a compromise based on the practical feasibility of performing air quality impact evaluations and the original full recommendations on this issue which were for up to 10 years of meteorology.

In current permit review regulatory analysis for Prevention of Significant Deterioration (PSD)

increment consumption and Air Quality Related Values at Federal Class I areas, air quality impact analysis are commonly based on one year of meteorology. This relaxation of recommendations from those required in the Federal Register described above has occurred primarily because the modeling relies on windfields produced from prognostic models, such as the mesoscale meteorological model (MM5). These windfields are usually utilized in the CALPUFF modeling system by being input into the CALPUFF meteorological processor CALMET.

It is generally agreed that utilization of the prognostic windfields for these regulatory purposes, which usually involve long range transport, will result in production of best windfields. However, at this point in time, performing a regulatory analysis based on the MM5 windfields is limited in the sense that only one year of meteorology is available. The EPA subjects all models that are candidates for inclusion into the federal register to a performance evaluation which includes model uncertainty (EPA Publication, 1981). There is a significant component of model uncertainty that is not evaluated when only one year of meteorology is used. This uncertainty is the multiple year variation which section 9.3.1 in the Guideline on Air Quality Models above addresses. The primary intent of this study is to quantify the extent of this multiple year variation in order that error ranges may be assigned to one year analyses.

APPROACH

To evaluate the potential for multiple year variation in this study a five year data set of meteorology has been compiled and runs performed for an array of source locations oriented around a common receptor. This approach, with a common receptor and multiple source locations, has been used because the receptor location is a Federal Class I area routinely subject to PSD permit reviews.

For this analysis the CALPUFF modeling system has been utilized. The meteorological fields have been produced using the measured National Weather Service (NWS), data sets as inputs, as opposed to the alternative approach, using the prognostic model input from the MM5 model. This is because for this study at least five years of meteorology are needed and this contiguous time frame is not available for prognostic data sets, such as the MM5 model output. For the CALMET runs using NWS inputs a technical study, (Riley, VTAPCD), was relied upon to choose the best CALMET parameter settings to produce accurate windfields for the domain. Essentially, this study has compared windfields produced with the MM5 data to many different alternative windfields produced with the NWS data and based final choice of CALMET parameter settings on the NWS run most similar to the MM5 run at 1000 meters elevation in the atmosphere.

The source locations are oriented with respect to the common receptor location at all directions of the compass and over a range of distances between 5 and 500 km. At each source location CALPUFF runs have occurred for each of the five years of meteorology. A ratio of the highest to lowest predicted values over the five year period has been calculated for sulfate compounds. This ratio will be termed the annual variation indicator. The ratios have been calculated for predicted concentrations, dry deposition, and visibility impacts.

A similar analysis has also been performed for the year 1992 where the high to low ratio has been computed at each source location for two runs in which one utilizes the MM5 windfields and the other utilizes NWS data only. The MM5 windfields for this analysis were produced by the United States Park Service. These fields are at an 80 kilometer resolution. In this analysis the run with the MM5 windfields has utilized *measured surface observations* and precipitation data because of concerns regarding possible bias in surface predictions of important parameters by the MM5 model. Therefore, the primary difference in the meteorological fields produced by the two runs is in the upper air windfields. The intent of this analysis is to examine consistency between results obtained with either method of windfield production.

ANALYSIS

Meteorological Data

In this study, the CALMET Model was run on a large regional domain extending westward to 84 degrees longitude and southward to 37 degrees latitude and north and eastward to encompass the entire state of Maine in which the windfield is resolved at a 40 kilometer resolution in the horizontal grid. See Table 1. For a summary of CALMET parameter settings for runs utilizing radiosonde data.

Table 1. Summary of CALMET Wind Field Options Used for 1990 - 1994.

| Option | Option Setting |
|--|----------------------------|
| Model selection variable (IWFCOD) | 1 = Diagnostic wind module |
| Compute Froude number adjustment effects (IFRADJ) | 1 (Yes) |
| Compute kinematic effects (IKINE) | 0 (No) |
| Use O'Brien procedure for adjustment of the vertical velocity (IOBR) | 0 (No) |
| Maximum radius of influence over land in the surface layer (RMAX1) | 300 KM. |
| Maximum radius of influence over land aloft (RMAX2) | 900 KM. |
| Maximum radius of influence over water (RMAX3) | 500 KM. |
| Radius of influence of terrain features (TERRAD) | 100 KM. |

In the vertical, 8 levels are specified to discern meteorological differences in surface level, transition level, and free atmospheric conditions. This domain is represented in a Lambert - Conformal projection because of its large size. The large dimensions of this domain are necessary for any multiple source analysis required in a Prevention of Significant Deterioration (PSD), permit review. The domain was established at the 40 kilometer resolution to allow reasonable computational times when running the CALMET and CALPUFF model for long time periods. Usage of the windfields computed for this domain are most accurate for transport scenarios which occur above the surface layers, or, as defined by the EPA, long range transport of greater than 50 kilometers. For the CALMET runs the geographical processing to produce terrain heights and land use represented in the model was done using the programs available as recommended by EPA.

For the CALMET runs terrain effects have been calculated from an initial guess windfield to produce a first guess windfield, whose values have then been interpolated with surface observations. National Weather Service (NWS), data has been used as recommended in the IWAQM guidance which consists of upper air radiosonde data, surface observations, and precipitation measurements (EPA Publication, 1998). For the CALMET domain, meteorological data consists of 48 surface stations, 11 radiosonde stations, and 474 precipitation sites. This data has been processed for the years 1990 to 1994. For the precipitation data, preprocessing was necessary to recode the flag indicating data validity before the data could be read by CALMET. For the meteorological data, data format conversion and data filling was necessary. The data filling and correcting for the radiosonde data was necessary for all missing soundings as well as soundings which, for various reasons, were insufficient to run CALMET. The technical report (Riley, VTAPCD), provides more detail regarding the radiosonde substitution routines.

CALPUFF Runs

After the CALMET data was compiled for the five year period 1990 through 1994, 280 CALPUFF runs, and the associated CALPOST runs occurred over the 5 years of meteorology for the 56 source locations described above. For these runs all input parameters in data files utilized were constant except the year of meteorology. Stack parameters were taken from a facility which emits more than 500 tons of air pollutants annually and has stack characteristics of most combustion emission points. For the CALPUFF runs, emissions of SO₂, SO₄, Nox, and PM₁₀ were represented in realistic proportions and to allow visibility calculations. Table 2. Summarizes pollutant representation in the CALPUFF model

Table 2. Pollutant Emissions Represented in the CALPUFF Runs.

| SPECIES | MODELED (1 - yes, 0 - no) | EMITTED (1=yes, 0-no) | DEPOSITED |
|---------|------------------------------|--------------------------|---------------------|
| | | | 1=COMPUTED-GAS |
| | | | 2=COMPUTED-PARTICLE |
| | | | 3=USER-SPECIFIED) |
| SO2 = | 1 | 1 | 1 |
| SO4 = | 1 | 1 | 2 |
| NOX = | 1 | 1 | 0 |
| HNO3 = | 1 | 0 | 0 |
| NO3 = | 1 | 0 | 0 |
| PM10 = | 1 | 1 | 2 |

For visibility calculations CALPOST was utilized in the recommended manner to account for visibility degradation from clean background conditions in the Northeastern U.S. Default (Mesopuff2), chemistry was utilized. All other CALPUFF settings were chosen so that the model performed in an acceptable manner for long range transport impacts at Class I areas. See Table 3. For a summary of the CALPUFF settings utilized.

Table 3. CALPUFF Technical Options From Input Group Two Used in the Runs.

| Option | Option Setting |
|--|--|
| Vertical distribution used in the near field | Gaussian |
| Terrain adjustment method | partial plume path adjustment |
| Subgrid-scale complex terrain | not modeled |
| Near-field puffs modeled as elongated | no |
| Transitional plume rise modeled ? | yes (i.e., transitional rise computed) |

| | |
|---|--|
| Stack tip downwash? | yes (i.e., use stack tip downwash) |
| Vertical wind shear modeled above stack top? | no (i.e., vertical wind shear not modeled) |
| Puff splitting allowed? | no (i.e., puffs not split) |
| Chemical mechanism flag | transformation rates computed internally (MESOPUFF II scheme) |
| Wet removal modeled ? | Yes |
| Dry deposition modeled ? | Yes |
| Method used to compute dispersion coefficients | PG dispersion coefficients for RURAL areas (computed using the ISCST multi-segment approximation) and MP coefficients in urban areas |
| Sigma-v/sigma-theta, sigma-w measurements used? | use both sigma-(v/theta) and sigma-w from PROFILE.DAT to compute sigma-y and sigma-z |
| Back-up method used to compute dispersion when measured turbulence data are missing | PG dispersion coefficients for RURAL areas (computed using the ISCST multi-segment approximation) and MP coefficients in urban areas |
| PG sigma-y,z adj. for roughness? | no |
| Partial plume penetration of elevated inversion? | Yes |
| Strength of temperature inversion provided in PROFILE.DAT extended records? | no (computed from measured/default gradients) |
| PDF used for dispersion under convective conditions? | No |
| Sub-Grid TIBL module used for shore line? | no |
| Boundary conditions (concentration) modeled? | no |

For each air quality related value (AQRV), a short term and a long term (annual), temporal standard were evaluated for the annual variation indicator. For SO₄ concentrations and SO₄ dry deposition the short term standard was the maximum 3 hour impacts and for visibility a maximum 24 hour impact.

RESULTS

The Annual Variation Indicator.

Figures 2 through 7 depict the annual variation indicator (AVI), values as calculated over the 5 years of meteorology. Note that the annual variation indicator represents the ratio of highest / lowest values over the 5 years of meteorology. Therefore a value of 1 for the AVI would indicate that there is no annual variation. In each of these figures, the AVI value is depicted for plotted source locations where the impacts have been computed at Lye Brook, Vermont, located at the confluence of all the source locations. Figure 1. Depicts the color legend of the annual variation indicators at source locations.

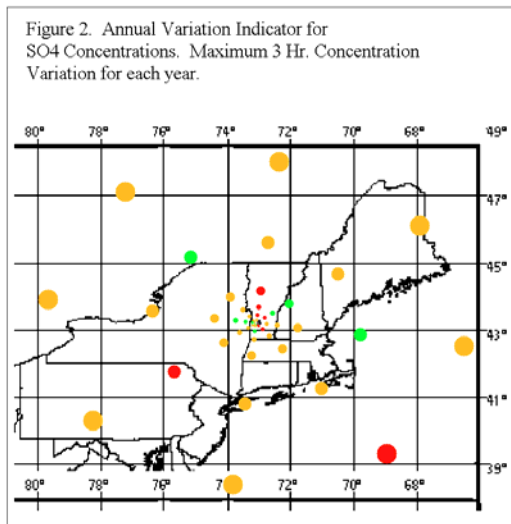
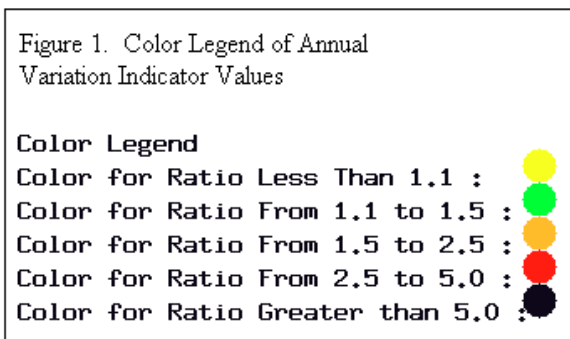


Figure 3. Annual Variation Indicator for SO₄ Concentrations. Annual Average Concentration Variation for Each Year.

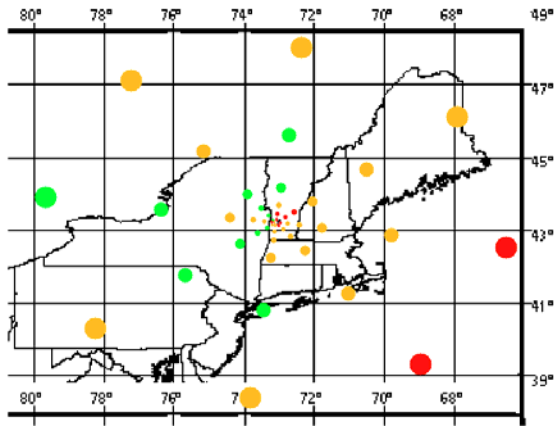


Figure 4. Annual Variation Indicator for SO₄ Dry Deposition. Maximum 3 Hr. Variation for Each Year.

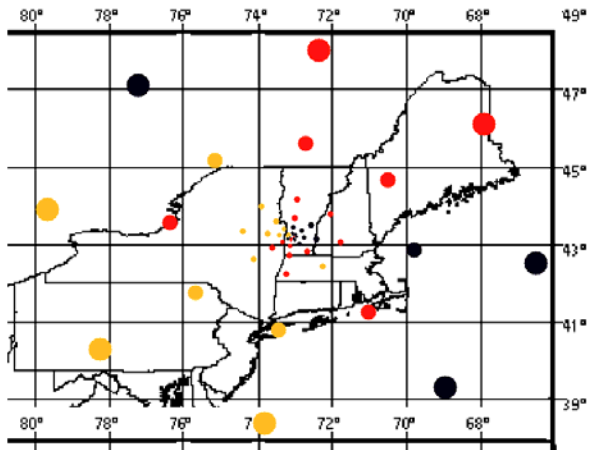


Figure 5. Annual Variation Indicator for SO4 Dry Deposition. Annual Average concentration variation for each year.

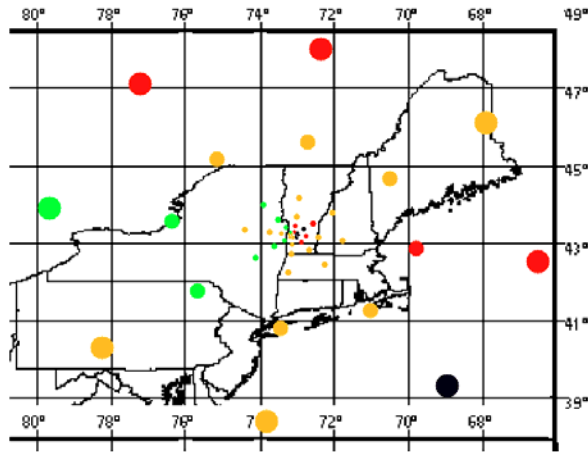
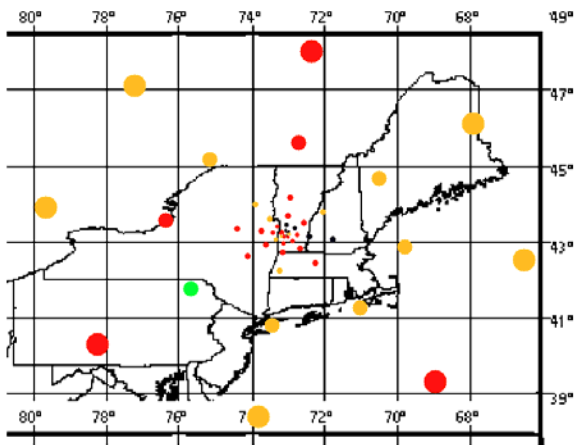
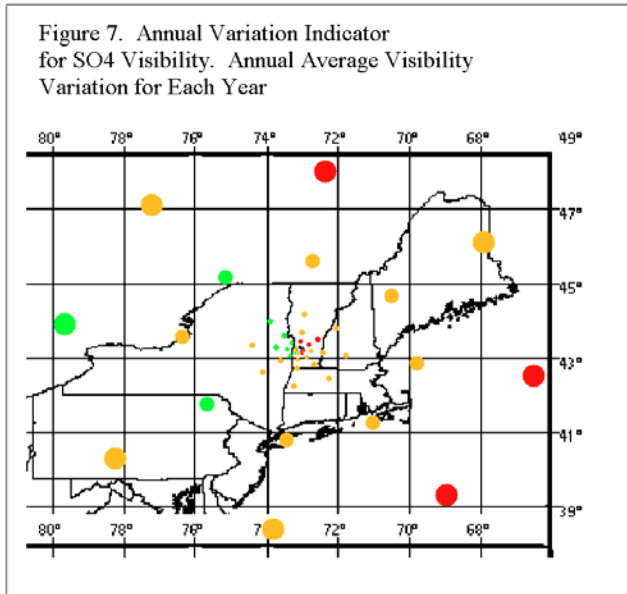


Figure 6. Annual Variation Indicator for SO4 Visibility. Maximum 24 HR Visibility Variation for Each Year





Tables 4. And 5. Below provide a tabulated numeric summary of the results plotted in figures 2 through 7.

Table 4. Average Annual Indicator Values by Distance

| .Pollutant /Standard | 10 km | 25 km | 50 km | 100 km | 250 km | 500 km | Average |
|-----------------------------------|-------|-------|-------|--------|--------|--------|---------|
| 3 hr SO ₄ Conc | 3.2 | 2.5 | 2.0 | 2.1 | 2.0 | 2.2 | 2.35 |
| Annual SO ₄ Conc | 3.3 | 2.3 | 2.0 | 1.7 | 1.7 | 2.4 | 2.21 |
| 3 hr SO ₄ Dry Dep. | 4.9 | 4.6 | 3.9 | 2.9 | 3.4 | 4.0 | 3.95 |
| Annual SO ₄ Dry Dep. | 3.7 | 3.0 | 2.0 | 1.8 | 2.0 | 3.1 | 2.63 |
| 24 hr SO ₄ Visibility | 3.9 | 4.2 | 3.8 | 3.4 | 2.4 | 2.7 | 3.40 |
| Annual SO ₄ Visibility | 3.4 | 2.2 | 2.0 | 1.9 | 1.8 | 2.6 | 2.32 |

Table 5. Average Annual Indicator Values by Direction.

| Pollutant / Standard | North east | East | South east | South | South west | West | North west | North |
|--|------------|------|------------|-------|------------|------|------------|-------|
| 3 hr SO4 Conc. | 2.8 | 2.6 | 2.9 | 1.9 | 2.3 | 1.7 | 1.9 | 2.9 |
| Annual SO4 Conc. | 3.3 | 2.6 | 2.6 | 1.9 | 1.5 | 2.1 | 1.5 | 2.2 |
| 3 hr SO4 Dry Dep. | 5.0 | 5.8 | 4.7 | 3.2 | 3.3 | 2.3 | 2.7 | 4.6 |
| Annual SO4 Dry Dep. | 3.7 | 3.6 | 3.7 | 2 | 1.5 | 1.8 | 1.8 | 2.9 |
| 24 Hr. Visibility | 3.7 | 3.7 | 3.5 | 2.9 | 2.8 | 3.5 | 2.6 | 4.6 |
| Annual Visibility | 3.3 | 2.6 | 2.6 | 2 | 1.7 | 1.7 | 1.5 | 3.3 |
| Average of All Pollutants / Standards by Direction | 3.6 | 3.5 | 3.3 | 2.3 | 2.2 | 2.2 | 2.0 | 3.4 |

From Tables 4 and 5. And the plotted results some observations may be made. The range of AVI values for all pollutant measures and standards ranges from 1.7 to 4.9. In general, the AVI values are larger for the short - term averages and smaller for the annual averages. The annual average AVI values are somewhat indicative of the overall climatological variation in average transport vectors for any given year. As a group, the annual average AVI values are significantly lower for sources west of the receptor for which impacts occur during prevailing westerly flow. For sources east, or prevailingly downwind of the receptor, there are fewer events over the course of a year which register impacts at the source. Therefore the variation in impacts between years is likely to be greater for these source locations.

The short term AVI values are indicative of the variation in transport events resulting in maximum impacts. There is no obvious directional bias in the values for the short term values. Table seven averages the AVI values for distances greater than and less than 50 kilometers. Noter that values are smaller for all standards and pollutant measures greater than 50 kilometers.

For the visibility impacts one reason for the larger AVI values is because of the relative humidity functional value that varies greatly at high humidities. No explanation is given why the SO4 dry deposition impacts have such high indicator values except to note the complexity of this calculation in comparison to SO4 concentration impacts.

Comparison of Results Obtained With The MM5 Windfield and The National Weather Service Observations Only

Figures 8 through 13 depict the MM5 - Radiosonde (MM5-RAD) windfield comparison indicator values where these values represent the ratio of impacts at each source location for two one year runs for the year 1992 where one run utilized the MM5 windfields in an unadjusted manner and the other run relied on CALMET windfields produced from the radiosonde and surface NWS measurements only. Therefore a value of one for the MM5-RAD indicator means there is no difference in the impacts predicted with either windfield. In each of these figures, the MM5-RAD indicator is depicted for plotted source locations where the impacts have been computed at Lye Brook, Vermont, located at the confluence of all the source locations. Figure 1. Depicts the color legend of the annual variation indicators at source locations.

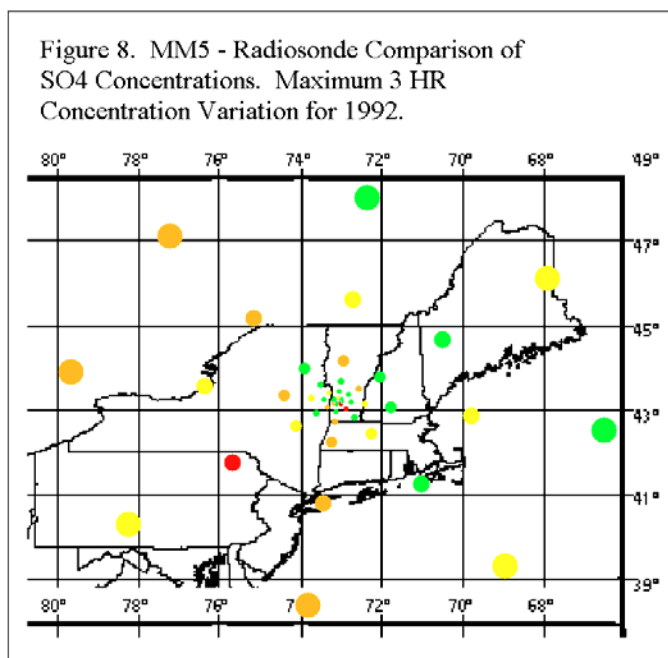


Figure 9. MM5 - Radiosonde Comparison of SO4 Concentrations. Annual Average Concentration Variation for 1992.

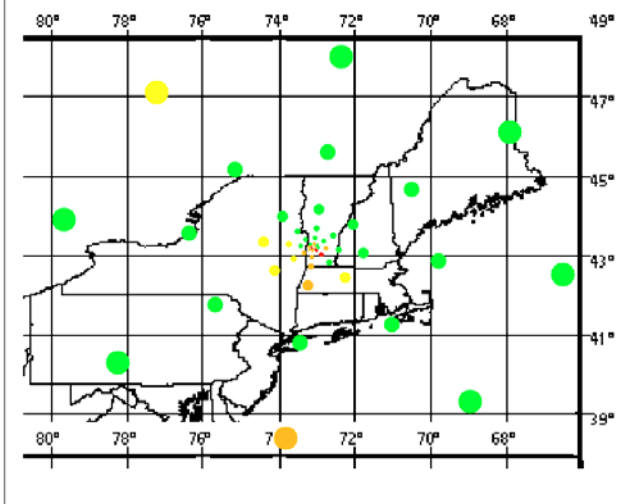


Figure 10. MM5 - Radiosonde Comparison of SO4 Concentrations. Maximum 3 HR Variation for 1992.

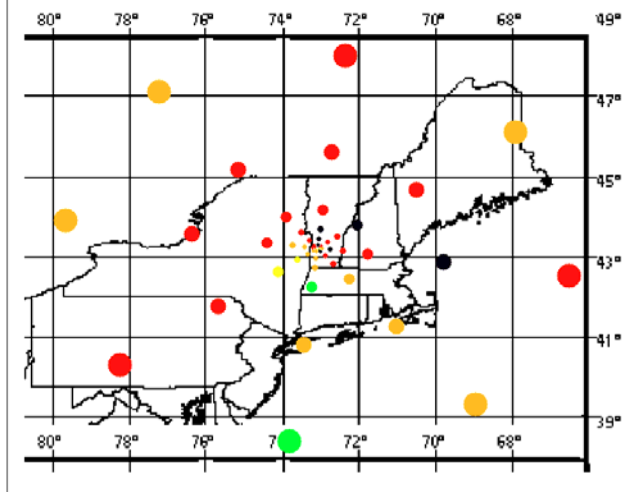


Figure 11. MM5 - Radiosonde Comparison of SO4 Dry Deposition. Annual Average Variation for 1992.

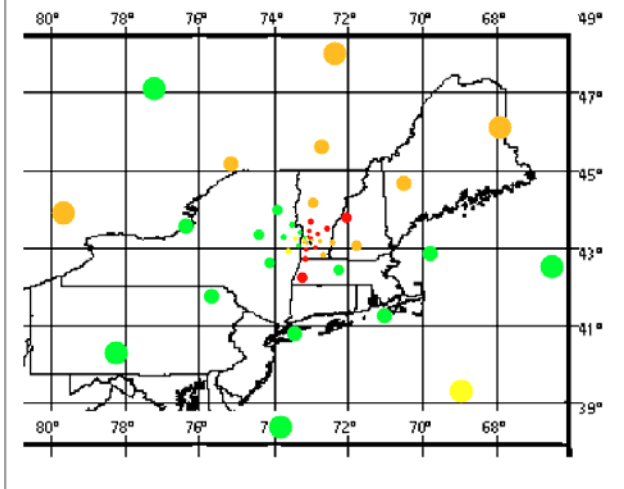
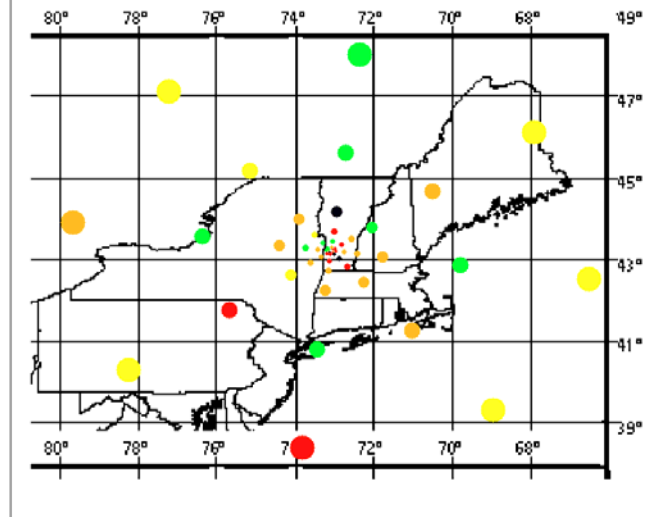
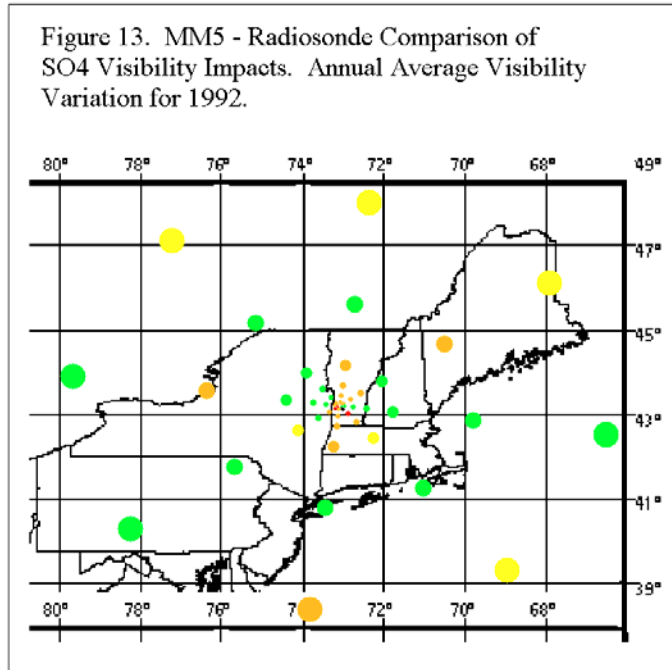


Figure 12. MM5 - Radiosonde Comparison of SO4 Visibility Impacts. Maximum 24 HR Visibility Variation for 1992.





Tables 6. And 7. Below provide a tabulated numeric summary of the results plotted in figures 8 through 13.

Table 6. MM5- Radiosonde Indicator Values by Distance

| Pollutant /Standard | 10 km | 25 km | 50 km | 100 km | 250 km | 500 km | Average |
|----------------------|-------|-------|-------|--------|--------|--------|---------|
| 3 hr SO4 Conc | 1.7 | 1.7 | 1.4 | 1.5 | 1.7 | 1.5 | 1.6 |
| Annual SO4 Conc | 2.0 | 1.9 | 1.3 | 1.3 | 1.3 | 1.4 | 1.5 |
| 3 hr SO4 Dry Dep. | 3.7 | 3.7 | 3.3 | 3.2 | 3.6 | 2.6 | 3.4 |
| Annual SO4 Dry Dep. | 2.8 | 2.6 | 2.4 | 2.1 | 1.6 | 1.5 | 2.1 |
| 24 hr SO4 Visibility | 3.3 | 2.8 | 2.2 | 2.3 | 1.8 | 1.5 | 2.3 |
| Annual | 2.7 | 2.0 | 1.7 | 1.4 | 1.5 | 1.3 | 1.7 |

| | | | | | | | | |
|-------------------|--|--|--|--|--|--|--|--|
| SO4 Visibility | | | | | | | | |
|-------------------|--|--|--|--|--|--|--|--|

Table 7. MM5- Radiosonde Indicator Values by Direction

| Pollutant / Standard | Northeast | East | Southeast | South | Southwest | West | Northwest | North |
|----------------------|-----------|------|-----------|-------|-----------|------|-----------|-------|
| 3 hr SO4 Conc. | 1.4 | 1.2 | 2.0 | 1.8 | 1.9 | 1.5 | 1.5 | 1.3 |
| Annual SO4 Conc. | 1.3 | 1.4 | 2.1 | 1.9 | 1.5 | 1.3 | 1.3 | 1.4 |
| 3 hr SO4 Dry Dep. | 3.9 | 4.3 | 3.3 | 1.8 | 2.3 | 2.9 | 3.5 | 5.0 |
| Annual SO4 Dry Dep. | 3.2 | 1.8 | 2.6 | 2.6 | 1.4 | 1.3 | 1.4 | 2.9 |
| 24 Hr. Visibility | 2.3 | 2.0 | 3.6 | 2.8 | 2.3 | 1.7 | 1.3 | 2.7 |
| Annual Visibility | 1.7 | 1.3 | 2.6 | 1.9 | 1.8 | 1.5 | 1.4 | 1.7 |

From figures 8 through 13 and Tables 6 and 7. some observations may be made. The MM5-RAD Indicator values range between 1.3 and 3.7 for all standards and pollutant measures. For all standards and pollutant measures except the 3 HR SO4 Dry Deposition the MM5-RAD Indicator values are, for most source locations and on average, values less than 2.0. These values are significantly lower than the corresponding AVI values for source locations. There is less evidence of a consistent directional variation in the MM5-RAD indicator values such as there is for the annual variation indicator values. Similarly to the AVI results the MM5-RAD Indicator values are less for the annually averaged impacts. No explanation is given why the SO4 dry deposition impacts have such high indicator values except to note the complexity of this calculation in comparison to SO4 concentration impacts.

Although there is certainly some variation in the impacts predicted resulting from the two meteorological fields, the magnitude of variation, typically less than on order of two for concentration and visibility impacts, lends some credibility to the meteorological fields generated from the N.W.S. data for these applications.

Table 8. Overall Average Annual Variation Indicator Values and MM5- Radiosonde Indicator Values for distances less than or greater than 50 km.

| Pollutant / Standard | Less than 50 km Annual Var. Indicator | Less than 50 km MM5-Rad. Indicator | Greater than 50 km Annual Var. Indicator | Greater than 50 km MM5-Rad Indicator |
|----------------------|---------------------------------------|------------------------------------|--|--------------------------------------|
| 3 hr SO4 Conc. | 2.6 | 1.6 | 2.1 | 1.6 |
| Annual SO4 Conc. | 2.5 | 1.7 | 1.9 | 1.3 |
| 3 hr SO4 Dry Dep. | 4.5 | 3.6 | 3.4 | 3.1 |
| Annual SO4 Dry Dep. | 2.9 | 2.6 | 2.3 | 1.7 |
| 24 Hr. Visibility | 4.0 | 2.8 | 2.8 | 1.9 |
| Annual Visibility | 2.5 | 2.1 | 2.1 | 1.4 |

CONCLUSIONS

In Table 8. The average annual variation indicator values can serve as factors to adjust pollutant impacts predictions obtained using only one year of meteorology. These factors account for the range in variation of impacts likely for five or more years of meteorology. These values are only valid for a receptor location at Lye Brook, Vermont. However, similar values may occur for other receptor locations in the Northeastern United States.

Indicator values have also been computed by comparing pollutant impacts predictions from CALPUFF runs utilizing meteorological data sets produced with and without the MM5 prognostic windfields with the intent of examining consistency between results obtained with either method of windfield production. In table 8. These values provide a guide to this aspect of model uncertainty for the combinations of pollutant measures and standards examined at this receptor location. For predictions of highest 3 HR SO4 concentrations, annual average SO4 concentrations, highest 24 HR visibility impacts and annual average visibility impacts at distances greater than 50 kilometers from the receptor location this factor of model uncertainty is less than two.

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3. Riley, D.C. Vermont Air Pollution Division Technical Summary CALPUFF Modeling Protocol CALMET Meteorological Windfields for 1995, Dec. 2002.