Calpuff Analysis of Current PSD Class I Increment Consumption in North Dakota and Eastern Montana Using Actual Annual Average SO_2 Emission Rates

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Draft

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North Dakota Department of Health
Division of Air Quality
1200 Missouri Avenue
Bismarck, ND 58506

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1. **Introduction**

The North Dakota Department of Health (NDDH) has conducted an air quality modeling analysis to determine the current status of Prevention of Significant Deterioration (PSD) Class I increment consumption for SO_2 in North Dakota and eastern Montana. The purpose of this analysis was to determine the current level of PSD Class I increment consumption, including the use of actual emission rates. Completion of this analysis satisfies a commitment made to EPA on March 13, 2001[1].

PSD Class I areas in North Dakota and eastern Montana are depicted in Figure 1-1. These include the Theodore Roosevelt National Park (TRNP) and Lostwood Wilderness Area in North Dakota, and the Medicine Lake Wilderness Area and Fort Peck Indian Reservation in Montana. The TRNP is divided into three geographically separated units: North Unit, South Unit, and Elkhorn Ranch Unit. All of these Class I areas were addressed in the NDDH modeling analysis.

Consistent with current Interagency Workgroup for Air Quality Modeling (IWAQM) guidance[2], the Calpuff long-range modeling system[3,4] was used for the NDDH analysis. EPA has proposed inclusion of Calpuff in the Guideline on Air Quality Models[5] as a refined modeling technique for general use in evaluating long-range transport of pollutants. The Calpuff modeling system has been

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[1]NDDH, 2001. March 13 letter from Francis Schwindt, North Dakota Department of Health to Richard Long, EPA Region VIII.

[2]EPA, 1998. IWAQM Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts. Publication No. EPA-454/R-98-019, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711.

[3]Earth Tech, Inc., 2000. A User's Guide for the Calmet Meteorological Model (Version 5). Earth Tech, Inc., Concord, MA 01742.

[4]Earth Tech, Inc., 2000. A User's Guide for the Calpuff Dispersion Model (Version 5). Earth Tech, Inc., Concord, MA 01742.

[5]CFR, 1999. EPA Guideline on Air Quality Models. 40 CFR (Code of Federal Regulations) Part 51, Appendix W.

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widely applied by States, EPA, and the National Park Service (NPS) to evaluate PSD increments and Air Quality Related Values (AQRV's) in PSD Class I areas.

The NDDH emission inventory for PSD Class I increment analysis included generally the actual SO_2 emissions associated with all major SO_2 sources located within 250 km, and all minor SO_2 sources located within 50 km of subject Class I areas. Source locations are also shown in Figure 1-1. To more accurately determine the current status of Class I increment consumption, the NDDH emission inventory was derived from hourly CEM (continuous emission monitor) data, when available.

The NDDH implementation of the Calpuff model followed IWAQM guidance, including the use of five years of conventional meteorological data. The NDDH used a non-traditional approach in the interpretation of model output to determine Class I increment compliance. Complete emission inventories for the baseline period and for the current period (2000-2001) were developed. Increment consumption was then determined as a function of the difference in model output for these two inventories. The NDDH approach also incorporated the use of receptor averaging to provide a uniform prediction for each Class I area. This interpretation of model output is described fully in Section 4.0.

Implementation of the Calpuff modeling system by NDDH included use of the Calmet meteorological model (Version 5.2), the Calpuff dispersion model (Version 5.4), and the Calpost postprocessing program (Version 5.2). Earth Tech (Earth Tech, Inc., Concord, MA), the primary model developer, also provides several utility programs to accommodate pre-processing of meteorological and geophysical data for Calmet. To the extent possible, the NDDH used the utilities provided by Earth Tech. But several additional software programs, developed by NDDH, were necessary to accommodate format conversions and substitutions for missing data. None of the programs developed by NDDH affected the integrity of the original data.

As part of the Class I area increment analysis, the NDDH conducted a model performance evaluation (described in Appendix B) to

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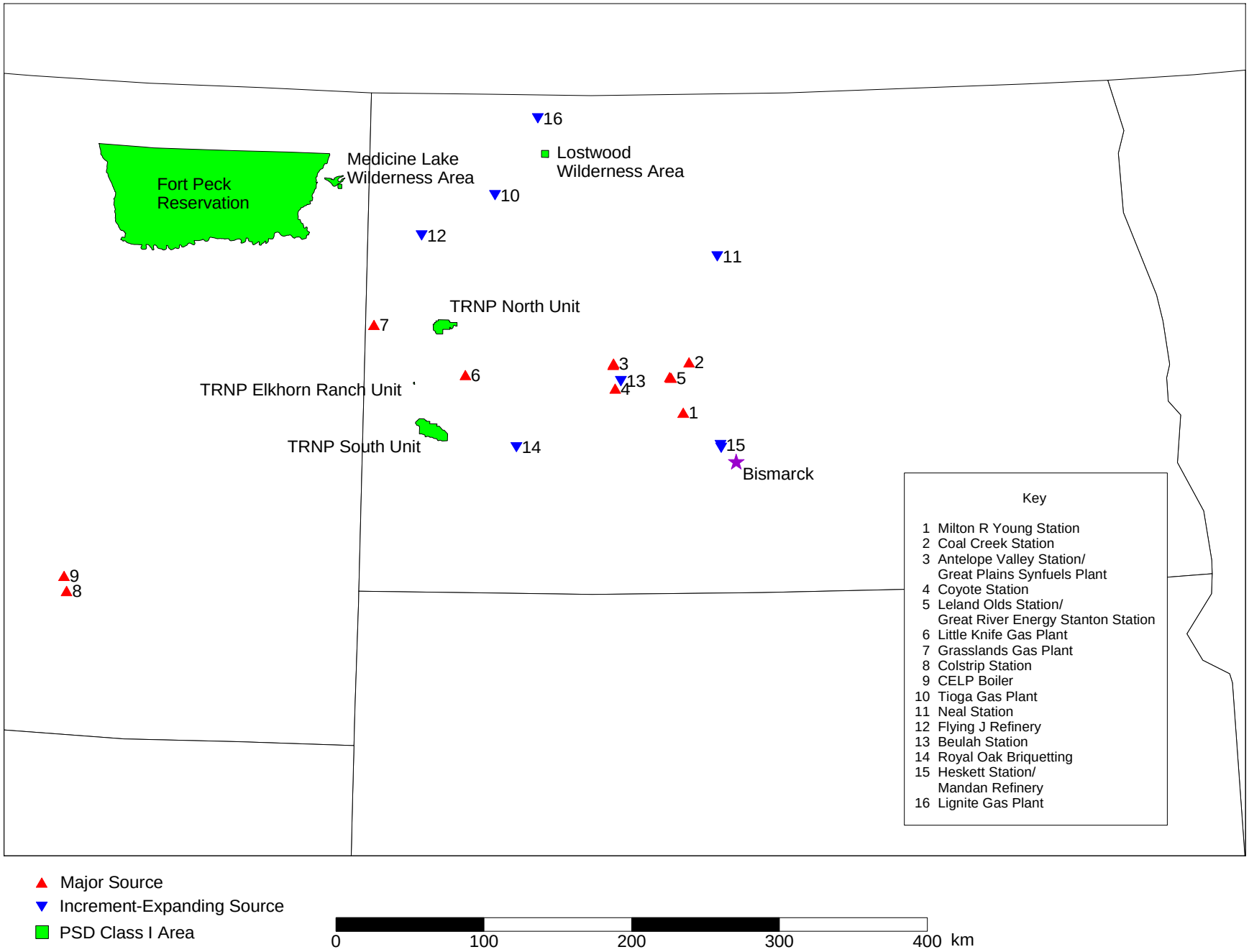
Figure 1-1: Class I Areas and Increment-Affecting Source Locations



determine the effectiveness of Calpuff in reproducing SO_2 concentrations observed at monitoring sites in North Dakota. The performance evaluation also served as the basis to "tune" model input (control file) settings to provide optimal agreement between predictions and observations. As a result of the evaluation and tuning process, some of the input settings utilized by NDDH differ from those recommended by IWAQM.

The NDDH analysis of Class I increment consumption of SO_2 reflects a work in progress because the baseline emission inventory for oil and gas related facilities has not yet been fully developed. Results of the current iteration, however, demonstrate compliance with PSD Class I increments for SO_2.

This report is organized into three additional sections and four appendices. Section 2 describes the preparation and processing of meteorological data using Calmet and supporting software. Section 3 describes the preparation of input data for Calpuff. Application of Calpuff, and model results are discussed in Section 4. Appendix A documents NDDH code changes to Calmet. The NDDH report on Calpuff performance evaluation is included as Appendix B. The complete list of IWAQM-recommended settings for Calmet input control file is provided in Appendix C, and the complete list of IWAQM-recommended settings for Calpuff control file is provided in Appendix D.

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2. **Meteorological Data Processing - Calmet**

Execution of the Calmet meteorological model requires establishment of the modeling domain (meteorological grid), preprocessing and quality assuring meteorological and geophysical input data, and determination of appropriate control file settings. Meteorological input data include surface, upper-air, and precipitation data. Geophysical input data include terrain and land-use data. Meteorological data were obtained from the National Climatic Data Center (NCDC), and geophysical data were acquired from the United States Geological Survey (USGS).

The NDDH processed five years of conventional meteorological data to use with Calpuff.

2.1 Modeling Domain

The NDDH meteorological grid was designed to provide a modeling domain which would encompass all SO_2 sources located up to 250 km away from any North Dakota Class I area. The dimensions of the grid are 640 km east-west by 460 km north-south. The extent of NDDH Calmet grid, with respect to PSD Class I areas, is illustrated in Figure 2-1.

Selection of grid cell size reflects a compromise between the desire to define meteorological and geophysical variations on a very small scale, and the computer time and resources necessary to do so. The NDDH elected to set grid cell size to 10 km, which has precedent in other PSD Class I analyses (involving long range transport) conducted nationally. Given the gently rolling nature of North Dakota terrain, relatively uniform land-use characteristics, and the general lack of terrain features or water bodies large enough to cause persistent, strong local-scale flows, the NDDH believes the 10 km resolution is reasonable. Grid cell size is also depicted in Figure 2-1.

In the vertical, the NDDH meteorological grid is defined by eight vertical layers. Cell face heights are set at 22, 50, 100, 250, 500, 1000, 2000, and 4000 meters above-ground level (AGL). Again, the use of eight layers is consistent with guidance provided for the modeling system, and with other PSD Class I analyses conducted nationally.

Because the NDDH Calmet domain is large, the grid system, meteorological data, and geophysical data were fit to Lambert conformal mapping to account for the earth’s curvature.

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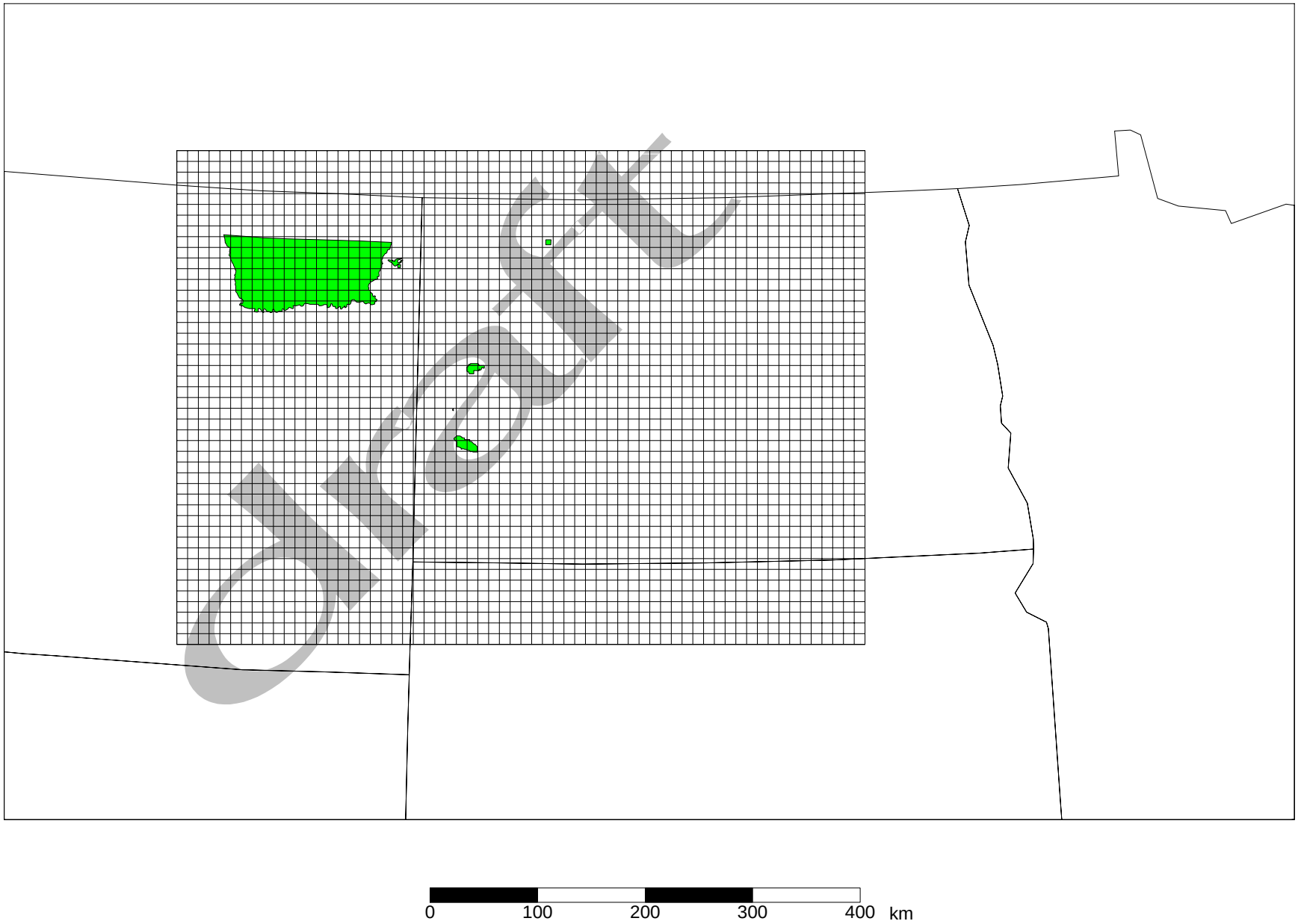
Figure 2-1: Location of Meteorological Grid and Class I Areas



2.2. Meteorological Data

2.2.1 Surface Meteorological Data

Surface meteorological data for the five-year period 1990-1994 were obtained in TD-1440 format from the National Climatic Data Center (NCDC). Data were obtained for 25 stations (National Weather Service, Federal Aviation Administration, U.S. Military, Environment Canada) located within or near the NDDH Calmet grid. Location of these stations is shown in Figure 2-2.

Some adjustments to the surface data files were required before Earth Tech programs METSCAN and SMERGE could be applied. Stations other than first-order National Weather Service (NWS) were missing opaque cloud cover for the entire five-year period. Based on a comparison of total and opaque cloud cover in the first-order NWS data sets, the NDDH developed an objective scheme to extrapolate opaque from total cloud cover. This scheme was coded into a computer program (TOT2OPQ) and applied to all surface data sets with missing opaque cloud cover.

EPA recommendations were followed to substitute for other missing data[6,7] (i.e., ceiling height, wind, pressure, temperature, relative humidity). The EPA substitution scheme was coded into a computer program (SUB144) and applied to all surface data sets. Substitutions were made if data elements were missing for one or two consecutive hours. Except for opaque cloud cover, substitutions were not made for longer missing periods (Calmet ignores stations with missing data). This is not an issue, because Calmet accommodates missing hourly surface data. Stations with missing data are simply ignored in the Calmet gridding of surface data elements for that hour.

Earth Tech program METSCAN was next applied to scan each data set for missing or unreasonable values. A few very minor changes were resultantly applied. Lastly, Earth Tech program SMERGE was applied to merge individual station data sets into a single input file (SURF.DAT) compatible with Calmet.

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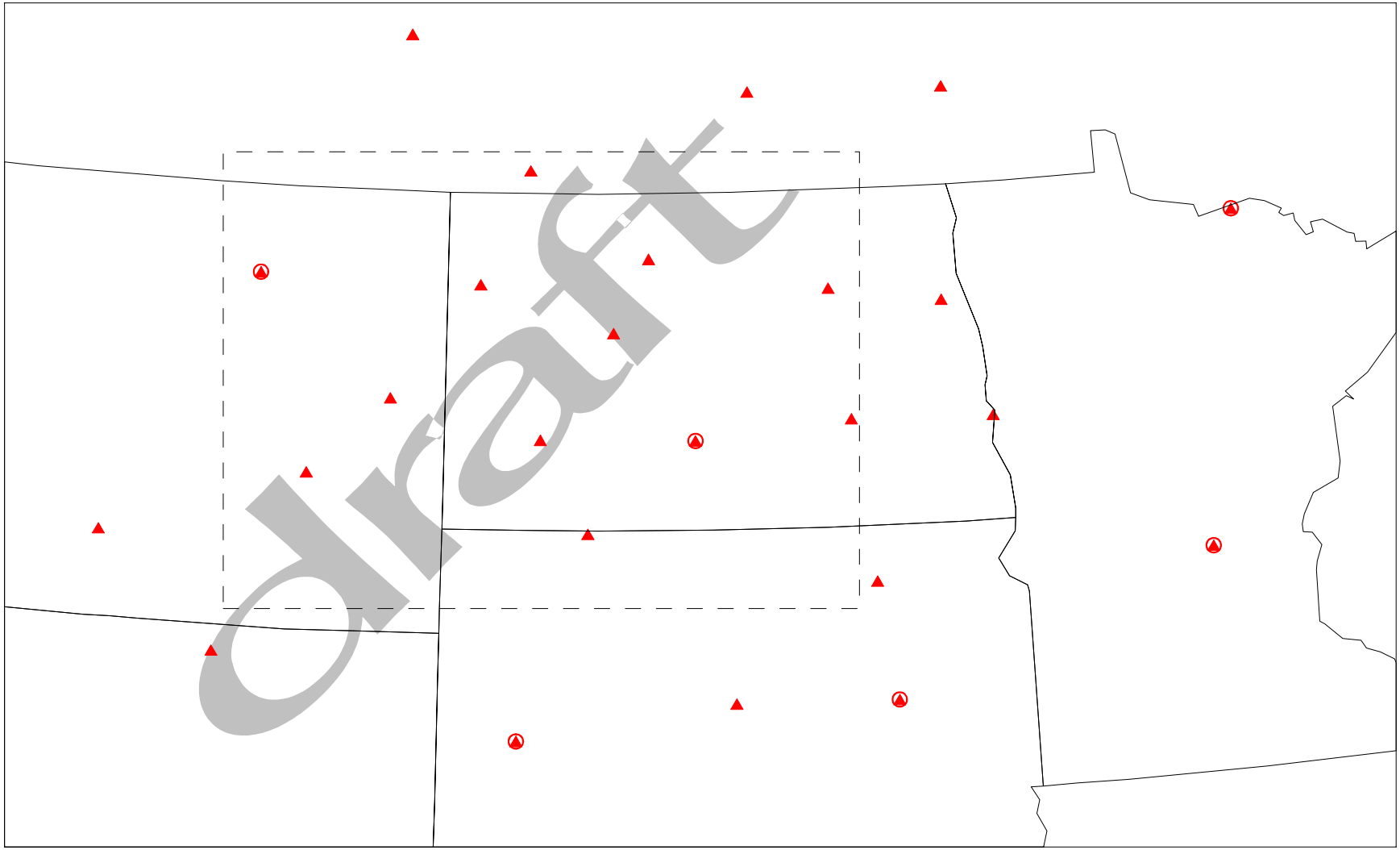
[6]Atkinson, Dennis and Russell F. Lee, 1992. Procedures for Substituting Values for Missing MWS meteorological Data for Use in Regulatory Air Quality Models.

[7]EPA, 1987. On-Site Meteorological Program Guidance for Regulatory Modeling Application. Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711.

Figure 2-2: Surface / Upper-air Meteorological Stations



Surface Station

Surface + Upper-air Station

The NDDH procedure for preparation of surface meteorological data is depicted schematically in Figure 2-3.

The occurrence of missing data elements in the TD-1440 data sets was generally very limited, and within the tolerances suggested by EPA. Note that none of the missing data substitution procedures applied by NDDH affected the integrity of the original, raw data.

2.2.2 Upper-Air Meteorological Data

Upper-air meteorological data for 1990 through 1994 were obtained in TD-6201 format from NCDC. Data were obtained for six upper-air stations located within or near the NDDH Calmet grid. The locations of these stations are shown in Figure 2-2.

Because of Calmet's fairly strict requirements on the completeness of upper-air data records and the frequency of missing upper-air data, it was desirable to automate the upper-air data processing with computer programs as much as possible. Since Earth Tech's program READ62 did not correct errors or fill in for missing data, much of the upper-air data processing was accomplished by running programs written by NDDH staff, along with a fair amount of manual file editing. The procedure consisted of preparing the TD-6201 data file for Earth Tech's program READ62, execution of a modified version of READ62, execution of two NDDH programs to fill in some missing data, and some manual editing to handle more complicated problems or fill in extended missing periods.

The first NDDH upper-air data program (DEL62) input the TD-6201 sounding data for one station for one year, made the hours of observation consistent at 00Z and 12Z (hours GMT or UTC), and output only the first line of data (lowest 79 sounding levels) for each sounding. Then, program READ62 was executed to convert upper-air data to the format Calmet requires and output only the desired variables pressure, height above mean sea level (MSL), temperature, and wind at sounding levels up to the top level desired, 500 mb in this case. Calmet requires sounding data at levels up to the calculated mixing height for all hours processed. It was necessary to extract data up to 500 mb to accommodate mixing heights up to approximately 4000 meters AGL at stations as high as Rapid City, South Dakota (elevation 966 m MSL).

Since program READ62 only flags missing soundings but does not fill in any missing data, the rest of the data preparation and missing data substitution is left up to the user. In addition, READ62 (version available in 1996-97) created some problems that were

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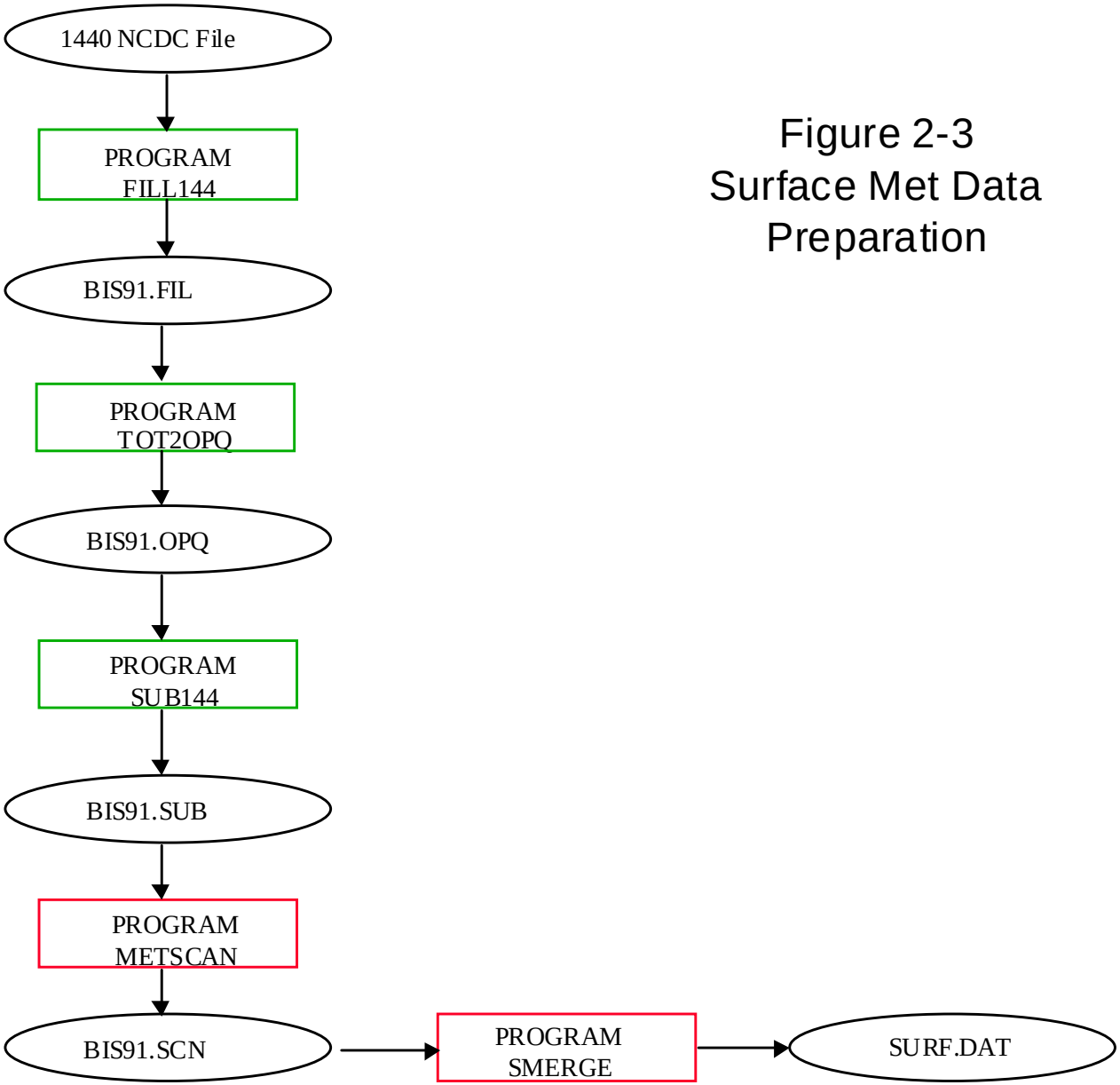

Figure 2-3
Surface Met Data
Preparation

corrected in later NDDH programs or by modifying READ62. READ62 rejected some surface data records because they were coded as having been substituted for missing data by NCDC. Since surface data must be complete (in upper-air data files) and the NCDC substitutions looked reasonable, READ62 was modified to accept this type of data. Also, READ62 overlooked some occurrences of two consecutive missing soundings and did not code missing temperatures correctly for Calmet input, which were remedied in a later NDDH program. Most of these READ62 problems were corrected by Earth Tech in a more recent version, but these NDDH modifications were necessary because preprocessing of raw data was performed in 1997.

Two NDDH programs (FIXR62 and FILLSHRT) performed much of the remaining upper-air data preprocessing. The first program copied soundings at the beginning and end of the year, when necessary, to ensure that upper-air data bracketed the entire calendar year of surface data, as required by Calmet. Since Calmet requires the surface level and top level to be present and complete for all soundings, the program either filled in the missing data or output informative messages indicating where manual substitution was required. Following EPA guidance[6,7], missing data at the top or surface level were interpolated in time from the same station's data for one or two consecutive missing observations and were substituted from a nearby station's data at the same time for three or more consecutive missing observations.

Unlike the requirements for surface meteorological data, Calmet requires soundings to be present for every standard 12-hour observation time. Since no soundings may be left missing, periods with completely missing soundings were filled in either by execution of the NDDH program FILLSHRT or manual substitution. For periods with one or two consecutive missing soundings, the program filled in the missing soundings from adjacent soundings in time for the same station. The substitutions were designed to retain appropriate representative diurnal variations in the substituted soundings. For periods with three or more consecutive missing soundings, the missing soundings were substituted by copying soundings from a representative nearby station for the same times using a text editor. Some editing of the substituted soundings was required to adjust the new soundings to the new station and its different elevation. Program FIXR62 also found missing temperatures, which were converted incorrectly in READ62, and replaced them with the correct code (in the correct units). The result was a file for each upper-air station and year containing sounding data in Calmet-ready format for every 12-hour observation.

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The NDDH procedure for preparation of upper-air meteorological data is depicted schematically in Figure 2-4.

2.2.3 Precipitation Data

Hourly precipitation data for the five-year period 1990-1994 were obtained from Earth Info, Incorporated (Boulder, CO). Data were included for 96 stations located in North Dakota, eastern Montana, northern South Dakota, and western Minnesota. Location of these stations is shown in Figure 2-5.

Software provided with the Earth Info distribution allowed extraction of hourly precipitation data in TD-3240 variable record length format. The Earth Tech program for processing precipitation data (PXTRACT) requires data in TD-3240 fixed record length format. Therefore, the NDDH prepared a program (CONV3240) to convert precipitation files from variable to fixed record length format.

Earth Tech program PXTRACT was executed to extract individual station precipitation data from the TD-3240 files, and PMERGE was executed to consolidate individual station data into the single file required by Calmet (PRECIP.DAT). No substitutions were made for missing data (i.e., Calmet substitutes internally from nearest available station).

2.3 Geophysical Data

Most of the terrain elevation and land use data required by Calmet were downloaded from the United States Geological Survey (USGS) internet web site. Grid cell terrain elevations were derived from 1:250,000-Scale Digital Elevation Models (DEM) and land use data were derived from 1:250,000-Scale Land Use and Land Cover (LULC) files. The LULC coding of land use categories is equivalent to that required by Calmet.

The NDDH Calmet grid extends into Canada, which is not covered by USGS DEM’s or LULC files. Terrain elevations for Canada were obtained from DEM’s included with the EPA CD distribution “Calmet, Calpuff, and Calpost Modeling System Version 1.0". Because of the relative homogeneity of land use in northeastern Montana and northern North Dakota, land use categories for grid cells located in Canada were simply extrapolated from adjoining Montana and North Dakota grid cells.

Current Earth Tech programs for processing terrain elevation and land use data, and creating the GEO.DAT file required by Calmet were

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Figure 2-4
Upper-Air Met Data Preparation

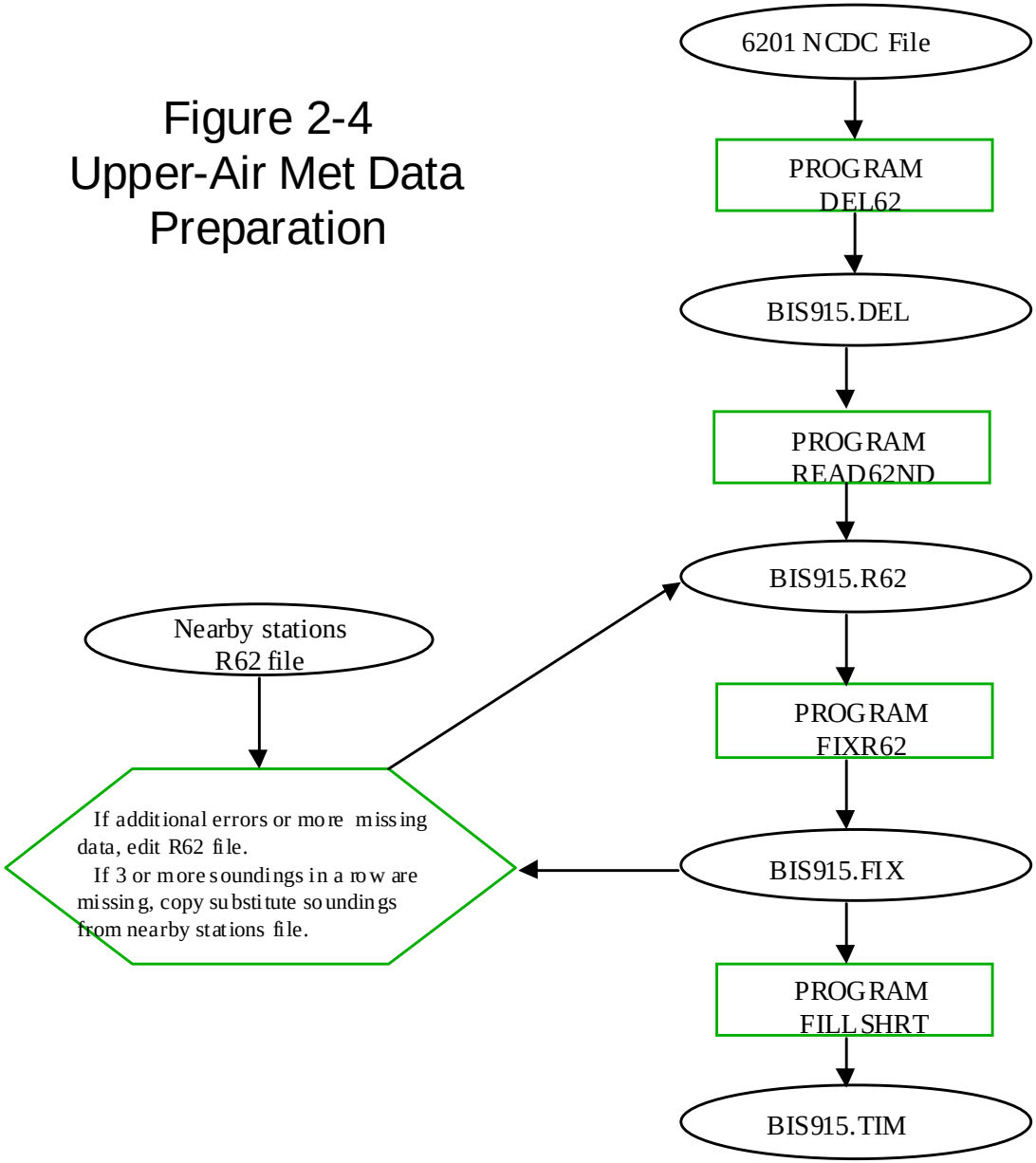
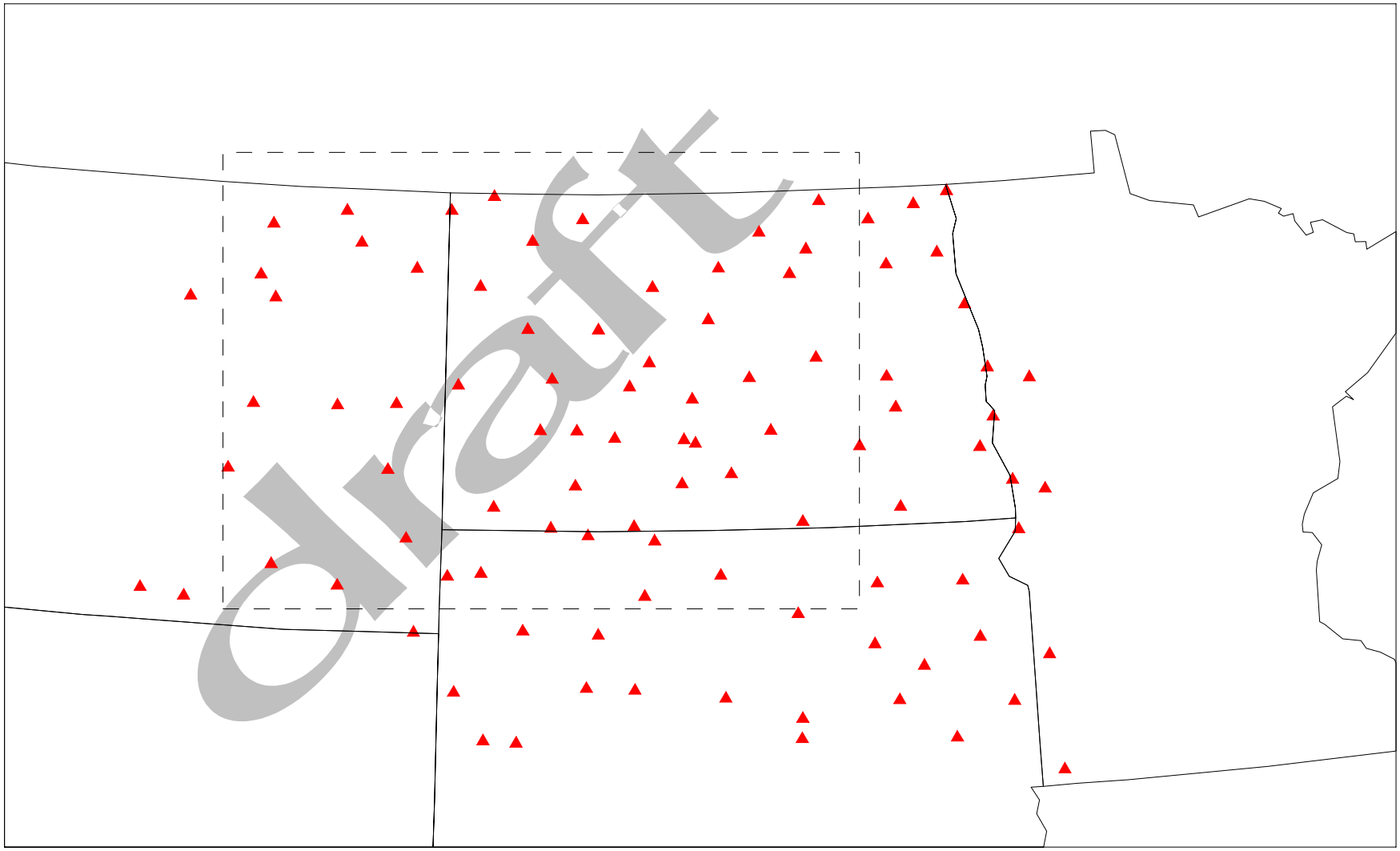


Figure 2-5: Precipitation Stations



not available at the time the NDDH developed geophysical data. For terrain elevation processing, the NDDH developed software to allocate DEM data values to appropriate Calmet grid cells (TERSUM), and then average over all allocated values to determine the composite elevation for each cell (TERAVG).

Land use processing commenced with allocating LULC data values to corresponding Calmet grid cells (via NDDH program TERSUM). For each grid cell, a composite land use type was assigned based on the most frequently allocated value. Other land-use-related parameters required for the GEO.DAT file include surface roughness length (Z_o), albedo, Bowen ratio, soil heat flux, and leaf area index. Values for these parameters are related to land use type as shown in the Calmet User's Guide. The distribution of land use types within each grid cell was used to establish composite values for these parameters. For example, if half of the LULC land use data values allocated to a grid cell were type 10 (Bowen ratio = 1.5) and the other half type 20 (Bowen ratio = 1.0), the composite Bowen ratio for the cell was set to 1.25. In the case of Z_o, the composite value reflects the log-weighted average. NDDH coded the above procedure into program LANDAVG. Coding is consistent with the current Earth Tech program, MAKEGEO.

The resultant fields of terrain elevation, land use type, Z_o, albedo, Bowen ratio, soil heat flux, and leaf area index were edited into the GEO.DAT file for processing with Calmet.

2.4 Calmet Code Revision

Based on a thorough examination of plotted wind fields generated from Calmet processing of 1990-1994 meteorological data sets, the NDDH noted a chronic discontinuity between surface and upper wind levels. To mitigate this problem, the Calmet option to extrapolate surface wind observations to upper layers was deployed, using similarity theory (Option 4) and layer-dependent bias settings. Calmet Version 5.x extrapolates surface winds both for setting the initial guess field, and for introducing observations in the Step 2 wind field procedure. Unfortunately, the model utilizes the bias factors for the initial guess field, only. The Step 2 vertical extrapolation has equal effect through all upper layers. The NDDH considered this unrealistic because resultant upper-layer wind fields reflected localized surface-layer (low-level) perturbations consistently, upward through all upper levels, even in the top layer (4000 m). It was believed that such low-level features should dampen with height and not extend up into the middle troposphere. In other words, the Step 2 vertical extrapolation essentially undid

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the effective Step 1 (dampened) vertical extrapolation of the wind fields.

To address this problem, the NDDH modified the Calmet code to simply eliminate the vertical extrapolation in the Step 2 wind field procedure, resulting in a more realistic transition from surface to upper layers. This modification was made with concurrence from Joe Scire (Earth Tech) and John Vimont (National Park Service). NDDH changes to Calmet code are documented in Appendix A. The modified Calmet version was used to process 1990-1994 data.

2.5 Calmet Control File Settings

Calmet control file settings utilized in the processing of 1990-1994 data were generally consistent with guidance from the Interagency Workgroup on Air Quality Modeling (IWAQM)[2]. However, extensive testing of Calmet output, with visual feedback (plotted 2-D fields), suggested that adjustment to a limited number of IWAQM settings was required to achieve reasonable representations of wind and mixing height fields. Further, the adjustment of a limited number of additional settings was found to provide better agreement with monitored observations based on a Calmet/Calpuff performance evaluation conducted by NDDH (Appendix B) and such changes were judged to be scientifically consistent.

IWAQM recommendations for Calmet control file settings fall into two categories. Group A (NDDH terminology) includes those variables for which IWAQM provides a default value as a general recommendation for all analyses. Group B includes those variables where IWAQM recognizes the value will need to be tailored for a given application, and default values are therefore not provided.

The Group B settings utilized by NDDH for Calmet processing of 1990-1994 data are summarized in Table 2-1. Most of these settings involve straightforward variables, related to the Calmet/Calpuff meteorological grid, which have been previously discussed. The remaining Group B variables (RMAX1, RMAX2, RMAX3, TERRAD, R1, R2) control the influence of station observations and terrain features in development of the final wind field. Initial values for these latter variables were based on guidance from the National Park Service. The NDDH then tuned the initial values to optimum settings using iterative testing with visual feedback.

NDDH settings for Group A variables were based both on the iterative testing process described above, and on a model performance evaluation. Initial iterative testing ensured that Calmet settings

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provided a reasonable appearance of wind and mixing height fields. Then a model performance evaluation was conducted by NDDH to establish optimum and final Calmet/Calpuff control file settings. The performance evaluation was based on a comparison of observations and model predications at two monitoring sites, one located at the TRNP South Unit. The evaluation proceeded in an iterative manner to determine the effect of adjustments to settings in the Calmet and Calpuff input control files on model skill. The NDDH performance evaluation is described in Appendix B.

As a result of the iterative testing process and performance evaluation, the NDDH elected to modify IWAQM values for a limited number of Calmet Group A control file settings. Non-IWAQM settings utilized by the NDDH for the Calmet control file, and which provided optimum agreement with monitored observations, are listed in Table 2-2. These non-IWAQM Group A settings are discussed below.

IKINE - The inclusion of kinematic effects provided significantly better agreement of Calpuff results with monitored observations. From a scientific standpoint, it appears there is no consensus on use of kinematic effects.

BIAS(NZ) - NDDH bias settings were developed through iterative testing with visual feedback. The IWAQM recommendation provides neutral bias (between surface and upper-air data) for all vertical layers. In light of its testing, the NDDH does not believe it is reasonable to assume equal weighting of upper-air wind data with surface data at the lowest level, and to assume equal weighting of surface data with upper-air at top levels.

LVARY - Given the size of the meteorological grid, the NDDH felt it necessary to deploy this option (varying radius of influence) to ensure that at least one station would be available for wind field interpolation.

ZUPWIND(2) - The NDDH was concerned that IWAQM was recommending a value of 1000 m while the model (Earth Tech) default is 2500 m, thus prompting the NDDH compromise value of 2000 m. But regardless of the selected value for this initial guess wind field input, subsequent wind field development should converge to the same result.

MNMDAV/ILEVZI - The NDDH found that IWAQM default values for these parameters, relating to spatial averaging of mixing heights, produced entirely unacceptable results for the mixing

height field. Severe gradients (bull's eyes) in mixing height were observed in the immediate vicinity of meteorological stations, and a significant increase in the value of these input parameters was required to mitigate the anomaly. The NDDH notes that because MNMDAV is a function of grid cell size, IWAQM should not specify an absolute default value for this parameter.

ZIMAX/ZIMAXW - Because the NDDH Calmet/Calpuff grid extends into the western part of the upper Great Plains, maximum mixing height was increased to 4000 m to be consistent with maximum mixing heights reported for this region (Holzworth, 1972)[8].

The complete list of IWAQM-recommended settings for the Calmet control file is included as Appendix C.

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[8]Holzworth, 1972. Mixing Heights, Wind Speeds, and Potential throughout the Contiguous United States. EPA Publication No. AP-101, Office of Air Programs.

Table 2-1

Calmet Control File Settings - Group B

Variable	Description	Value
NSSTA	No. of surface stations	24
NUSTA	No. of upper-air stations	6
NPSTA	No. of precipitation stations	96
NX	No. of east-west grid cells	64
NY	No. of north-south grid cells	46
DGRIDKM	Grid spacing (km)	10
XORIGKM	Southwest grid cell X coordinate	-380
YORIGKM	Southwest grid cell Y coordinate	140
LLCONF	Lambert conformal coordinates	T
XLAT1	Latitude of 1st standard parallel	46.0
XLAT2	Latitude of 2nd standard parallel	48.5
RLON0	Reference longitude	102
RLAT0	Origin latitude	44
NZ	No. vertical layers	8
RMAX1	Max surface over-land extrapolation radius (km)	300
RMAX2	Max aloft over-land extrapolation radius (km)	1200
RMAX3	Max over-water extrapolation radius (km)	500
TERRAD	Radius of influence of terrain features (km)	100
R1	Relative weight at surface of Step 1 field & observation	125
R2	Relative weight aloft of Step 1 field & observation	100
ISURFT	Surface station to use for surface temperature	1*
IUPT	Station for lapse rates	1*

* Represents Bismarck NWS

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Table 2-2

Non-IWAQM Group A Settings Used by NDDH in Calmet Control File

Variable	IWAQM	NDDH
IKINE	0	1
BIAS(NZ)	0,0,0,0, 0,0,0,0,	-1.0, -0.9, -0.7, 0.0, 0.5, 1.0, 1.0, 1.0
LVARY	F	T
ZUPWIND(2)	1000 m	2000 m
MNMDAV	1	8
ILEVZI	1	4
ZIMAX	3000 m	4000 m
ZIMAXW	3000 m	4000 m

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3. **Calpuff Input Data**

Along with the Calmet-processed meteorological data, Calpuff requires the user to provide an emissions inventory, receptor locations, input control file settings, and (optionally) hourly ozone data before the model can be executed.

3.1 Emission Inventory

To address Class I increment consumption, the NDDH developed a source inventory for current (Year 2000/2001) SO_2 emissions, and another source inventory for baseline SO_2 emissions. Net increment consumption was determined as a function of the difference in model results for these two inventories (i.e., current inventory minus baseline inventory). The baseline inventory included sources which no longer existed in Year 2000, or which had reduced emissions by Year 2000, and therefore had the effect of expanding increment. Sources whose emissions remained essentially unchanged from the baseline to Year 2000 were not included in the analysis.

SO_2 increment-affecting sources located in the vicinity of the six subject Class I areas were shown in Figure 1-1. These sources include primarily electrical generating stations, natural gas processing plants, and well-site facilities (not shown in the figure) related to oil and gas production. With the exception of well-site oil and gas facilities, all sources located within 250 km of subject Class I areas were included in the emission inventories (current and baseline). Because well-site oil and gas facilities are numerous and generally have very small SO_2 emissions, their inclusion was limited to a distance of 50 km from Class I areas. These distance limits are consistent with previous NDDH PSD Class I modeling analyses.

Even though numerous oil and gas production facilities are found in the vicinity of Medicine Lake and Fort Peck Class I areas, emission/stack data were not obtainable for such facilities located in Montana. Therefore, the local well-site oil and gas facility contribution was not accounted for in Calpuff modeling for Montana Class I areas, and model predictions for these areas may accordingly be misrepresented.

Annual average SO_2 emission rates, expressed as the total actual annual emission divided by the annual hours of operation, were utilized in the NDDH baseline and current emission inventories. Use

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of the annual average is based on the state's legal review of the Air Pollution Control Rules.[9]

3.1.1 Current Inventory

Annual-average SO_2 emission rates and dynamic stack operating parameters (exit velocity and temperature) for the current inventory were derived from Continuous Emission Monitoring (CEM) hourly data for years 2000 and 2001, where available. The annual average was calculated as the average for all non-zero hours. CEM hourly data for emission rates and flow rates (exit velocity) for electrical generating stations (larger than 25 megawatts) were available and downloaded from the EPA Acid Rain Web Site on the internet. Year 2001 data were available for the first three quarters, only. All CEM hourly data for other sources (Year 2000 only), as well as the hourly stack exit temperature for electrical generating stations, were obtained directly from the plant operators. Values for fixed stack parameters (stack height and diameter) were obtained from NDDH records/permits. Basically, CEM hourly data were available for all electrical generating stations, and for most natural gas processing plants.

For sources with no hourly data, total annual emissions and operating hours were obtained from Annual Emission Inventory Reports for Year 2000. Stack exit velocity and temperature were obtained from recent stack test data. Stack height and diameter were obtained from NDDH records/permits.

Year 2000 actual emission rates reflecting annual average operation for oil and gas production sources (treaters and flares) were derived from the ND State Industrial Commission's (SIC) Oil and Gas data base. The data base includes information on gas production (flared and lease-use), and the H_2S content of the gas, such that SO_2 emission rates for well-site flares and treaters can be calculated. Dynamic stack operating parameters for oil and gas production sources were derived from the calculated heat of combustion using procedures described in the "Williston Basin

[9]NDDH, 2002. Summary of legal Issues Relating to Administration of the Prevention of Significant Deterioration (PSD) Provisions of North Dakota's State Implementation Plan (SIP). North Dakota Department of Health, Bismarck, North Dakota 58506.

Regional Air Quality Study"[10], and modified using SCREEN3[11] (EPA screening model) adjustments for effective flare plume height and radiational heat loss. Flare and treater stack height were obtained directly from the SIC data base.

In summary, the current emissions inventory was grouped into non oil and gas sources with annual averages derived from CEMs hourly stack data, non oil and gas sources with annual averages derived from Annual Emission Inventory Reports, and oil and gas sources with annual averages derived from the SIC Oil and Gas data base. In all cases, the annual average SO_2 represents total actual annual emissions divided by hours (or days) of operation. The emission characterization for each current inventory source is provided in Table 3-1.

It should be noted that the Great Plains Synfuels Plant and the Little Knife Gas Processing Plant, which have been included in previous NDDH analyses of Class I increment consumption, were not included in the current emissions inventory for the present analysis. Based on the state's legal review, it was concluded that all emissions from these facilities are exempt from increment consumption, because Class I variances were granted for major modifications at both facilities.

The complete current emissions inventory for non oil and gas sources, including all information required by Calpuff, is provided as Table 3-2. Current inventory information for the numerous oil and gas sources can be provided on computer media if requested. Source locations in Table 3-2, provided in Lambert coordinates, were obtained from NDDH permits. Stack base elevations were derived from USGS digital elevation models (DEM).

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[10]NDDH, 1990. Williston Basin Regional Air Quality Study. North Dakota Department of Health, Bismarck, ND 58506.

[11]EPA, 1995. SCREEN3 Model User's Guide. Publication No. EPA-454/B-95-004, Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina, 27711.

Table 3-1
Current Source Inventory

Source	Emission Characterization	Status		Figure 1-1 Loc. Key
		PSD/ Baseline	Inc. Consuming/ Expanding	
Antelope Valley Station	Average - Hrs Operation	PSD	Consuming	3
Coal Creek Station	Average - Hrs Operation	PSD	Consuming	2
Coyote Station	Average - Hrs Operation	PSD	Consuming	4
Grasslands Gas Plant	Average - Hrs Operation	PSD	Consuming	7
Colstrip Station (3&4)	Average - Hrs Operation	PSD	Consuming	8
CELP Boiler	Average - Hrs Operation	PSD	Consuming	9
Leland Olds Station	Average - Hrs Operation	Baseline	Consuming	5
Stanton Station	Average - Hrs Operation	Baseline	Consuming	5
Milton R. Young Station	Average - Hrs Operation	Baseline	Consuming	1
Heskett Station	Average - Hrs Operation	Baseline	Expanding	15
Mandan Refinery	Average - Hrs Operation	Baseline	Expanding	15
Lignite Gas Plant	Average - Hrs Operation	Baseline	Expanding	16
Tioga Gas Plant	Average - Hrs Operation	Baseline	Expanding	10
Oil & Gas Related*	Average - Days Operation	Both	Both	-

* All facilities located within 50 km of Class I areas.

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Table 3-2
Calpuff Input Data for Current Source Inventory

```
Source        X          Y      Stack    Base     Stack    Exit  Exit    Bldg.  Emission
 No.     Coordinate Coordinate Height Elevation Diameter  Vel.  Temp.   Dwash   Rate
            (km)       (km)      (m)     (m)      (m)    (m/s) (deg. K)          (g/s)
------   ---------- ---------- ------  ------   -------- ----- -------- ----- --------

  1 ! SRCNAM = Antelope Valley Station 1 !
  1 ! X =    12.459,  374.908,   182.9,  588.3,     7.0,   19.0,  358.2,   0.,   199.9,  ! !END!
  2 ! SRCNAM = Antelope Valley Station 2 !
  2 ! X =    12.459,  374.908,   182.9,  588.3,     7.0,   19.1,  356.7,   0.,   187.3,  ! !END!
  3 ! SRCNAM = Coal Creek Station 1 !
  3 ! X =    63.487,  375.784,   201.0,  602.0,     6.7,   25.9,  358.5,   0.,   430.2,  ! !END!
  4 ! SRCNAM = Coal Creek Station 2 !
  4 ! X =    63.487,  375.784,   201.0,  602.0,     6.7,   24.9,  354.5,   0.,   376.5,  ! !END!
  5 ! SRCNAM = Coyote Station !
  5 ! X =    13.513,  357.842,   152.0,  556.9,     6.4,   25.4,  370.7,   0.,   487.7,  ! !END!
  6 ! SRCNAM = Grasslands Gas Plant !
  6 ! X =  -149.696,  401.234,    65.0,  615.9,    0.86,   15.1,  571.9,   0.,    14.3,  ! !END!
  7 ! SRCNAM = Colstrip Station 3 !
  7 ! X =  -357.648,  220.211,   210.9,  988.7,     7.3,   26.9,  361.3,   0.,    93.6,  ! !END!
  8 ! SRCNAM = Colstrip Station 4 !
  8 ! X =  -357.648,  220.211,   210.9,  988.7,     7.3,   27.6,  362.7,   0.,    90.6,  ! !END!
  9 ! SRCNAM = CELP Boiler !
  9 ! X =  -359.424,  230.411,    61.0,  945.1,     2.5,   22.6,  433.2,   0.,    52.9,  ! !END!
 10 ! SRCNAM = Leland Olds Station 1 !
 10 ! X =    51.326,  365.208,   106.7,  518.3,     5.3,   19.7,  450.0,   0.,   525.4,  ! !END!
 11 ! SRCNAM = Leland Olds Station 2 !
 11 ! X =    51.326,  365.208,   152.4,  518.3,     6.7,   25.0,  448.6,   0.,  1060.5,  ! !END!
 12 ! SRCNAM = Stanton Station !
 12 ! X =    50.407,  365.773,    77.7,  518.3,     4.6,   19.9,  411.1,   0.,   305.8,  ! !END!
 13 ! SRCNAM = Milton R Young Station 1 !
 13 ! X =    59.519,  341.409,    91.4,  597.4,     5.8,   18.5,  449.1,   0.,   644.6,  ! !END!
 14 ! SRCNAM = Milton R Young Station 2 !
 14 ! X =    59.519,  341.409,   167.6,  597.4,     7.6,   19.2,  361.8,   0.,   573.1,  ! !END!
 15 ! SRCNAM = Heskett Station 1 !
 15 ! X =    84.794,  319.565,   91.44,  514.8,     2.2,  20.67,  461.7,   0.,    31.1,  ! !END!
 16 ! SRCNAM = Heskett Station 2 !
 16 ! X =    84.794,  319.565,   91.44,  514.8,    3.65,  17.37,  419.7,   0.,    74.5,  ! !END!
 17 ! SRCNAM = Mandan Refinery - Boilers !
 17 ! X =    85.215,  317.679,    31.8,  518.3,     1.7,   12.5,  424.7,   0.,    17.8,  ! !END!
 18 ! SRCNAM = MR - FCU/CO !
 18 ! X =    85.215,  317.679,    60.7,  518.3,     3.4,    9.9,  547.0,   0.,   133.2,  ! !END!
 19 ! SRCNAM = MR - Alky Furnace !
 19 ! X =    85.215,  317.679,    53.0,  518.3,     2.0,    6.1,  447.0,   0.,     0.9,  ! !END!
 20 ! SRCNAM = MR - Ultra Furnace !
 20 ! X =    85.215,  317.679,    29.1,  518.3,     1.3,    5.9,  530.8,   0.,     1.9,  ! !END!
 21 ! SRCNAM = MR - SRU !
 21 ! X =    85.215,  317.679,    60.8,  518.3,     0.6,    5.7,  589.0,   0.,     5.3,  ! !END!
 22 ! SRCNAM = Lignite Gas Plant !
 22 ! X =   -38.885,  541.932,    38.1,  598.0,     0.4,   19.9,  893.0,   0.,    13.2,  ! !END!
 23 ! SRCNAM = Tioga Gas Plant !
 23 ! X =   -67.762,  489.627,    50.3,  686.0,    0.91,    7.7,  782.0,   0.,    37.3,  ! !END!
```

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3.1.2 Baseline Inventory

SO_2 emission rates for baseline sources were computed as total actual emissions for the baseline period, divided by actual hours of operation for the period. The baseline period reflects the two-year period prior to the western North Dakota minor-source baseline date (December 19, 1977), or a different period representative of "normal" operation, as determined by the NDDH.

For electrical generating stations, total emissions for the baseline period were calculated as a function of mine-average sulfur content and actual coal usage. For natural gas processing plants, total emissions for the baseline period were taken from Annual Emission Inventory Reports, or calculated from raw gas volume and H_2S content. Actual hours of baseline period operation for both electrical generating stations and natural gas processing plants were obtained from Annual Emission Inventory Reports.

Baseline period emissions for well-site oil and gas production sources (treaters and flares) were derived from the SIC Oil and Gas data base information on gas production and H_2S content. Because the SIC had reservations about the quality and quantity of gas production data contained in the data base for the baseline period (1976-1977), the NDDH elected to extrapolate (in time) production data from the period of the "Williston Basin Regional Air Quality Study" (i.e., the period 1987-1988). According to SIC, this latter period represents the approximate earliest point in the chronology of the data base that consistent confidence can be placed in the completeness and reliability of the gas production data. Days of production were also extrapolated from this period.

A complete description of the NDDH methodology for determining baseline emission rates is contained in "Prevention of Significant Deterioration Sulfur Dioxide Baseline Emission Rates (Draft)."[12] The extrapolation of oil and gas data from the Williston Basin Study is also discussed.

For electrical generating stations and natural gas processing plants, dynamic stack operating parameters for the baseline inventory were derived from stack test reports. Stack height and diameter were taken from NDDH records/permits. For oil and gas sources, dynamic stack parameters (as well as stack diameter) were

[12]NDDH, 2002. Prevention of Significant Deterioration Sulfur Dioxide Baseline Emission Rates. North Dakota Department of Health, Bismarck, ND 58506

derived from calculated heat of combustion, as described in Section 3.1.1. Flare and treater stack height were obtained directly from the SIC data base.

The status of each baseline inventory source is summarized in Table 3-3. The complete baseline emission inventory for non oil and gas sources, including all data required by Calpuff, is provided as Table 3-4. Baseline inventory information for oil and gas sources can be provided on computer media if requested. Source locations in Table 3-4, based on Lambert coordinates, were obtained from NDDH permits. Stack base elevations were derived from USGS digital elevation models (DEM).

It should be noted that the referenced baseline inventory for oil and gas related sources reflects a "first cut", as incorporated in this analysis, because a number of issues related to its development have not been (and may not be) resolved. These issues include:

- It may not be possible to determine exactly which wells were tied into gas gathering systems as of the minor-source baseline date (December 19, 1977).

- How to define "normal operation" for oil and gas wells.

- Whether the baseline emission rate (representing two years prior to the baseline date) should be calculated as the average over the actual hours of operation, or as a true annual average (average over all hours in a year), given the intermittent operation of many of the wells.

- If an oil and gas well should be given full credit for its baseline emissions, when it appears (from modeling) that those emissions may have caused an exceedance of National Ambient Air Quality Standards (NAAQS).

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Table 3-3
Baseline Source Inventory

Source	Inc. Consuming/Expanding	Figure 1-1 Loc. Key
Leland Olds Station	Consuming	5
Stanton Station	Consuming	5
Milton R. Young Station	Consuming	1
Heskett Station	Expanding	15
Mandan Refinery	Expanding	15
Lignite Gas Plant	Expanding	16
Tioga Gas Plant	Expanding	10
Beulah Station (shut down)	Expanding	13
Neal Station (shut down)	Expanding	11
Flying J Refinery (shut down)	Expanding	12
Royal Oak Briquetting (shut down)	Expanding	14
Oil & Gas Related *	Both	-

* All facilities located within 50 km of Class I areas.

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Table 3-4
Calpuff Input Data for Baseline Source Inventory

```
Source       X          Y      Stack    Base     Stack    Exit  Exit    Bldg.  Emission
 No.     Coordinate Coordinate Height Elevation Diameter  Vel.  Temp.   Dwash   Rate
            (km)       (km)      (m)     (m)      (m)    (m/s) (deg. K)          (g/s)
------   ---------- ---------- ------  ------   -------- ----- -------- ----- --------

 1 ! SRCNAM = Leland Olds Station 1 !
 1 ! X =    51.326,  365.208,   106.7,  518.3,     5.3,   19.7,  450.0,   0.,   407.6,  ! !END!
 2 ! SRCNAM = Leland Olds Station 2 !
 2 ! X =    51.326,  365.208,   152.4,  518.3,     6.7,   25.0,  448.6,   0.,   766.0,  ! !END!
 3 ! SRCNAM = Stanton Station !
 3 ! X =    50.407,  365.773,    77.7,  518.3,     4.6,   19.9,  411.1,   0.,   268.6,  ! !END!
 4 ! SRCNAM = Milton R Young Station 1 !
 4 ! X =    59.519,  341.409,    91.4,  597.4,     5.8,   18.5,  449.1,   0.,   585.9,  ! !END!
 5 ! SRCNAM = Milton R Young Station 2 !
 5 ! X =    59.519,  341.409,   167.6,  597.4,     7.6,   19.2,  361.8,   0.,   618.1,  ! !END!
 6 ! SRCNAM = Heskett Station 1 !
 6 ! X =    84.794,  319.565,   91.44,  514.8,     2.2,  20.67,  461.7,   0.,    65.2,  ! !END!
 7 ! SRCNAM = Heskett Station 2 !
 7 ! X =    84.794,  319.565,   91.44,  514.8,    3.65,  17.37,  419.7,   0.,   152.2,  ! !END!
 8 ! SRCNAM = Mandan Refinery - Boilers !
 8 ! X =    85.215,  317.679,    31.8,  518.3,     1.7,   12.5,  424.7,   0.,    78.4,  ! !END!
 9 ! SRCNAM = MR - FCU/CO !
 9 ! X =    85.215,  317.679,    60.7,  518.3,     3.4,    9.9,  547.0,   0.,   212.4,  ! !END!
10 ! SRCNAM = MR - Alky Furnace !
10 ! X =    85.215,  317.679,    53.0,  518.3,     2.0,    6.1,  447.0,   0.,    20.2,  ! !END!
11 ! SRCNAM = MR - Ultra Furnace !
11 ! X =    85.215,  317.679,    29.1,  518.3,     1.3,    5.9,  530.8,   0.,     1.9,  ! !END!
12 ! SRCNAM = Lignite Gas Plant !
12 ! X =   -38.885,  541.932,    38.1,  598.0,     0.4,   19.9,  893.0,   0.,    36.0,  ! !END!
13 ! SRCNAM = Tioga Gas Plant !
13 ! X =   -67.762,  489.627,    30.5,  686.0,     1.7,    7.7,  782.0,   0.,   135.3,  ! !END!
14 ! SRCNAM = Beulah Station 1+2 !
14 ! X =    17.404,  362.995,    23.0,  567.0,     1.7,   7.6,   477.0,   0.,   17.27,  ! !END!
15 ! SRCNAM = Beulah Station 3-5 !
15 ! X =    17.404,  362.995,    30.5,  567.0,     2.1,  14.6,   527.0,   0.,   28.29,  ! !END!
16 ! SRCNAM = Neal Station 1+2 !
16 ! X =    82.646,  447.977,    42.4,  488.0,     1.8,  25.0,   470.0,   0.,    44.7,  ! !END!
17 ! SRCNAM = Flying J Refin - Heaters + Boiler 2 !
17 ! X =  -117.411,  462.238,    17.3,  575.0,     0.9,   3.2,   700.0,   0.,    3.19,  ! !END!
18 ! SRCNAM = Flying J Refin - Boiler 1 !
18 ! X =  -117.411,  462.238,    30.2,  575.0,     1.2,   3.4,   464.0,   0.,    1.32,  ! !END!
19 ! SRCNAM = Flying J Refin - Boiler 3 !
19 ! X =  -117.411,  462.238,     9.1,  575.0,     0.8,   6.3,   464.0,   0.,    1.89,  ! !END!
20 ! SRCNAM = Royal Oak - Boilers 1-3 !
20 ! X =   -53.232,  318.050,    19.2,  751.0,     1.4,   9.8,   520.0,   0.,    21.7,  ! !END!
21 ! SRCNAM = Royal Oak - ACC !
21 ! X =   -53.232,  318.050,    26.2,  751.0,    3.35,  9.35,  1172.0,   0.,   200.5,  ! !END!
```

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- Whether the inventory should be limited to wells within 50 km of Class I areas (also an issue for current (Year 2000) oil and gas inventory).

In addition, the NDDH has determined that reliable production data are available for a limited number of oil and gas wells in the SIC data base for the baseline period. The NDDH is currently in the process of replacing SO_2 values estimated from the Williston Basin Study with the actual baseline values.

3.2 Ozone Data

Calpuff requires background ozone values. The NDDH elected to utilize the option of providing an input file of hourly ozone values, rather than assume the constant default value in Calpuff. Hourly ozone data were obtained from a NDDH monitoring site located about 140 km east of TRNP Elkhorn Ranch Unit. This places the site within the corridor of primary plume transport between major generating stations and Theodore Roosevelt National Park. Ozone data were concurrent with Calmet meteorological data (i.e., 1990-1994).

3.3 Receptor Locations

Receptor locations for the Class I Calpuff analysis are shown in Figures 3-1 and 3-2. Figure 3-1 identifies receptor locations for North Dakota Class I areas and Figure 3-2 depicts receptor locations for Montana Class I areas. Numbers in the figures correspond to the receptor numbering convention employed in Calpuff input/output files. Receptor coverage includes 22 receptors (Nos. 1-22) at TRNP South Unit, 16 receptors (Nos. 23-38) at TRNP North Unit, 1 receptor (No. 39) at TRNP Elkhorn Ranch Unit, 5 receptors (Nos. 40-44) at Lostwood Wilderness Area, 1 receptor (No. 45) at Medicine Lake Wilderness Area, and 4 receptors (Nos. 46-49) at Fort Peck Reservation.

Maximum receptor spacing in North Dakota Class I areas is on the order of 4-5 kilometers. Given the distance of the largest-contributing sources from Class I areas (150-200 km), concentration gradients in the vicinity of Class I areas were not expected to be significant. Based on subsequent model execution which confirmed this expectation, receptor coverage was deemed sufficient.

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Figure 3-1: Receptor Locations - North Dakota Class I Areas

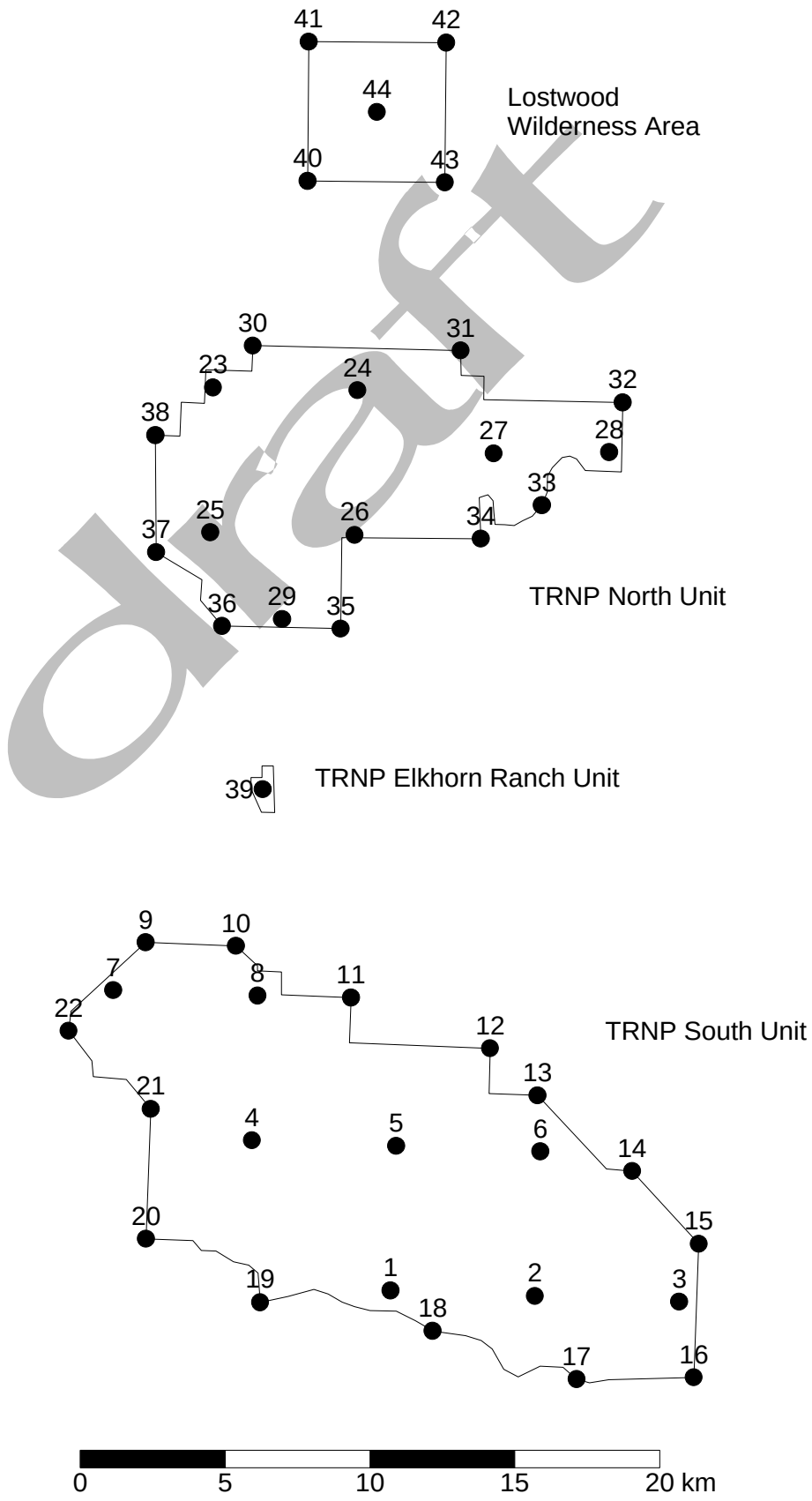

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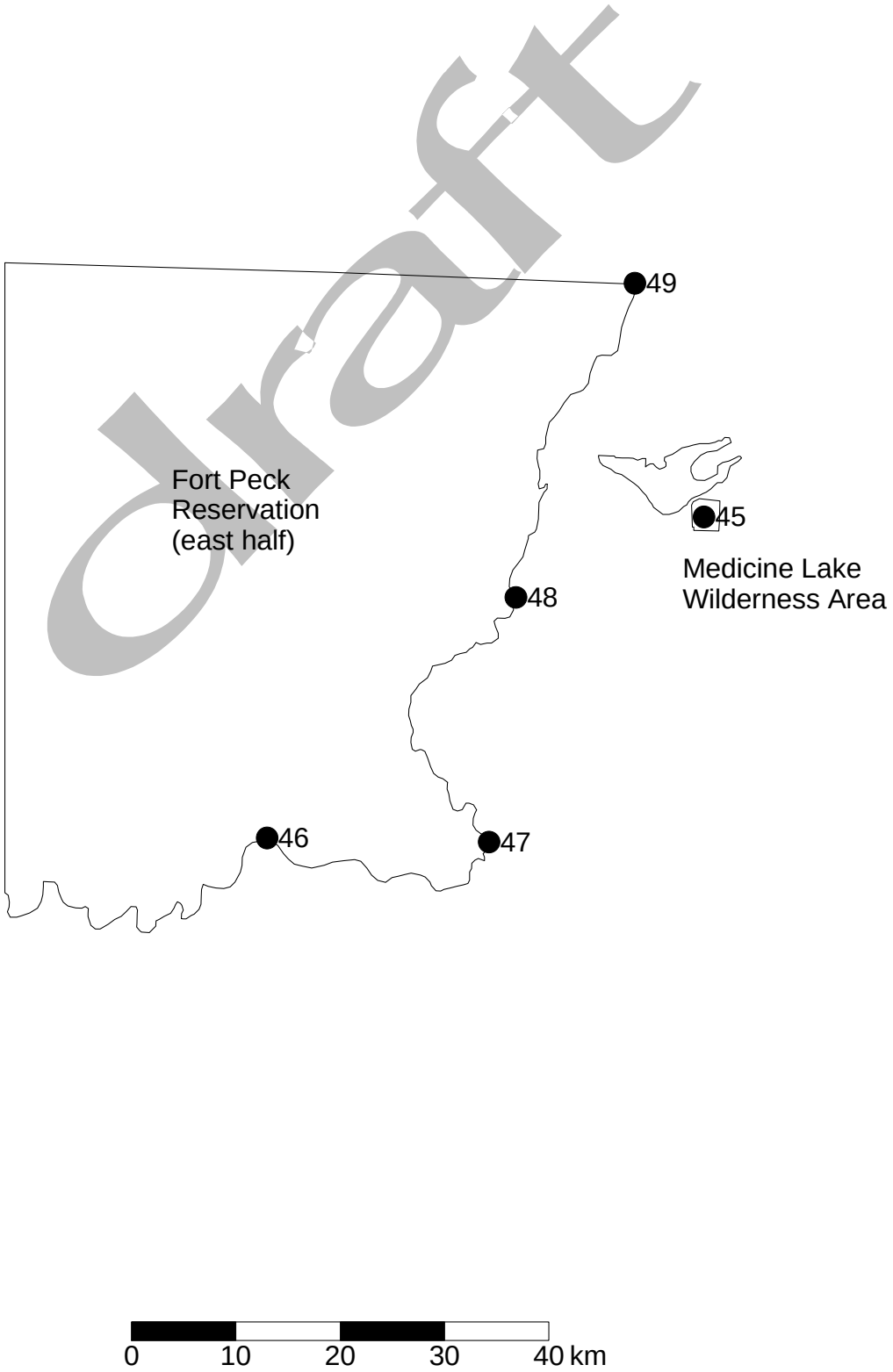
Figure 3-2: Receptor Locations - Montana Class I Areas



Receptor coverage for Medicine Lake and Fort Peck Class I areas was limited because they are located even farther from largest-contributing sources, and (as indicated in Section 3.1) the local minor-source contribution could not be accounted for. Most of Fort Peck is located more than 300 km from major North Dakota sources. Also, some compromise in receptor resolution was necessary to achieve practical Calpuff execution times.

The receptor network depicted in Figures 3-1 and 3-2 was utilized for both the present and previous NDDH Calpuff analyses. As part of the hearing process the NDDH is seeking input regarding the adequacy of the receptor grid.

3.4 Calpuff Control File Settings

Calpuff control file settings for the NDDH Class I increment analysis were generally consistent with IWAQM guidance. However, the adjustment of a limited number of settings was found to provide better agreement with monitored observations based on a Calmet/Calpuff performance evaluation conducted by NDDH (Appendix B), and such changes were judged to be scientifically viable.

IWAQM recommendations for Calpuff control file settings fall into two categories. Group A (NDDH terminology) includes those variables where IWAQM provides a default value as a general recommendation for all analyses. Group B includes those variables where IWAQM recognizes the value will need to be tailored for a given application, and default values are therefore not provided.

The Group B settings utilized by NDDH are summarized in Table 3-5. These settings are straightforward, involving variables related to defining the meteorological and computational grids, and the use of default values for dry and wet deposition parameterization. Note that the computational grid utilized by Calpuff can be designated a subset of the meteorological grid produced by Calmet. But as shown in Table 3-5, NDDH set the computational grid equivalent to the full meteorological grid.

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Table 3-5
Calpuff Control File Settings - Group B

Variable	Description	Value
CSPEC	Names of species modeled (MESOPUFF II = SO_2, SO_4, NO_x, HNO_3, NO_3)	MESOPUFF II
NX	No. of east-west grids in met. data	64
NY	No. of north-south grids in met. data	46
NZ	No. of vertical layers in met. data	8
DGRIDKM	Grid spacing (km)	10
XORIGKM	Southwest corner of met. data grid (X)	-380
YORIGKM	Southwest corner of met. data grid (Y)	140
XLAT	Latitude of center of met. domain	47
XLONG	Longitude of center of met. domain	102
XTZ	Base time zone of meteorology	7
IBCOMP	Southwest X-index of computational domain	1
JBCOMP	Northwest Y-index of computational domain	1
IECOMP	Northeast X-index of computational domain	64
JECOMP	Northeast Y-index of computational domain	46
Dry Gas Dep	Chemical parameters of gaseous deposition species	Model defaults
Dry Part Dep	Chemical parameters of particulate deposition species	Model defaults
Wet Dep	Wet deposition parameters	Model defaults
IRESPLIT	Hours when puff is eligible for split (1-24)	18-23
NREC	Number of discrete receptors	49

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NDDH settings for Calpuff Group A variables were largely consistent with IWAQM recommendations, but included adjustments to a limited number of variables based on the model performance evaluation. As discussed in Section 2.5, the performance evaluation was based on a comparison of observations and predictions at two monitoring sites, and proceeded in an iterative manner to determine the effect of adjustments to control file settings on model skill. The NDDH performance evaluation is described in Appendix B.

As a result of the performance evaluation, the NDDH chose to modify a limited number of IWAQM Group A control file settings. Non-IWAQM settings utilized by the NDDH for the Calpuff control file, and which provided optimum agreement with monitored observations, are shown in Table 3-6. These non-IWAQM Group A settings are discussed below.

MSPLIT - The option for puff splitting was recommended by John Irwin (EPA) when modeling source-receptor distances of 200 km or more, because of the tendency for Calpuff to otherwise overpredict at these distances. Deployment of this option also provided better agreement with observations.

MDISP - Use of dispersion coefficient option 2 provided significantly better agreement with observations. The NDDH also believes this selection is more consistent with the “state-of-the-art” in air quality modeling.

BCKO3 - Though the NDDH utilized the hourly file option for ozone background, the BCKO3 value is substituted by Calpuff when hourly data are missing. Based on local monitoring data, NDDH judged the IWAQM value of 80 ppb to be much higher than typical for North Dakota, and therefore reset the value to 30 ppb.

BCKNH3 - The NDDH value of 2 ppb reflects the annual average of local, unbiased monitoring data.

XSAMLEN - The NDDH set this value lower than the IWAQM recommendation, but notes that the only consequence for doing so would be extra computer time due to more puffs on the grid. The goal was to improve model resolution by increasing the number of puffs and decreasing mass per puff. Again, because

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Table 3-6
Non-IWAQM Group A Settings Used by NDDH
in Calpuff Control File

Variable	IWAQM	NDDH
MSPLIT*	0	1
MDISP	3	2
BCKO3	80 ppb	30 ppb
BCKNH3	10 ppb	2 ppb
XSAMLEN	1.0	0.5
XMAXZI	3000 m	4000 m

* Puff splitting was not deployed in Calpuff control file for oil and gas sources. This concession to model execution time is reasonable, because puffs would not grow vary large given the maximum 50 km source-receptor distance.

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this parameter is a function of grid cell size, the NDDH believes IWAQM should not have provided a default value.

XMAXZI - Value was increased to 4000 m for consistency with ZIMAX/ZIMAXW setting in Calmet.

The complete list of IWAQM-recommended settings for the Calpuff control file is included as Appendix D.

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4. Calpuff Application and Results

4.1 Calpuff Application

Calpuff was executed using meteorological data processed as described in Section 2, and the emission inventories and other input data discussed in Section 3. The model was applied to the current (Year 2000/2001) source inventory (Table 3-2), and then to the baseline source inventory (Table 3-4).

To determine increment consumption in the traditional manner, the Calpuff (hourly) results for the baseline source inventory would be subtracted from the results for the current source inventory, and the difference (summarized with Calpost) would be compared to allowable Class I increments (i.e., 25 $\mu g/m^3$ for 3-hour and 5 $\mu g/m^3$ for 24-hr average). As a result of the state's legal review, the NDDH elected to employ an alternative interpretation of increment consumption. This approach involves determining a fixed modeled baseline concentration, adding the allowable increment (i.e., 25 $\mu g/m^3$ for 3-hour, 5 $\mu g/m^3$ for 24-hour) to the baseline concentration to establish a MAAL (Maximum Allowable Ambient Level), and then comparing the modeled results for the current source inventory against the MAAL. The NDDH approach was implemented as follows:

1) Calpuff was applied for the current (Year 2000/2001) source inventory (Table 3-2), and then for the baseline source inventory (Table 3-4). Calpuff was applied separately for each year of meteorological data (1990-1994).

2) Receptor averaging was performed to derive uniform predictions over each Class I area. To implement receptor averaging, the NDDH developed the Calavg software program. Calavg was applied to the Calpuff (hourly) output for baseline inventory sources, and then to the Calpuff output for current inventory sources. All receptors identified in Figures 3-1 and 3-2 were included in the averaging procedure. Execution of Calavg resulted in revised Calpuff-compatible files (for baseline and current source inventories) which included one central receptor for each Class I area.

3) Calpost (Earth Tech) was applied to the averaged baseline file and then to the averaged current file to provide summary results for 3-hour and 24-hour averages. Calpost provided the high and the second-high prediction (3-hour and 24-hour) for each Class I area.

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4) Using results from Step 3, the second-high baseline prediction was used to determine the MAAL for each averaging period for each Class I area. That is, the MAAL equals the second-high prediction plus conventional allowable increment (25 $\mu g/m^3$ for 3-hour averages and 5 $\mu g/m^3$ for 24-hour averages). MAAL's were determined independently for each year of modeled meteorological data and for each Class I area.

5) Finally, the second-high prediction for the current source inventory (Step 3) was used to determine compliance with the MAAL for each averaging period for each Class I area. Compliance was assumed if the second-high prediction was lower than the MAAL. Compliance was determined independently for each year of modeled meteorological data and for each Class I area.

The NDDH variable-increment approach is illustrated in Figures 4-1 and 4-2. This illustration demonstrates the application of the procedure to the Theodore Roosevelt National Park (TRNP) South Unit for 24-hour averages for 1990 meteorological data.

Determination of the MAAL is illustrated in Figure 4-1. Block 24-hour baseline predictions (averaged over receptors) are plotted as a function of time for 1990 meteorological data. The second-high prediction of 8.9 $\mu g/m^3$ is represented by the lower dashed line in the Figure. Upon adding the conventional allowable 24-hour increment of 5 $\mu g/m^3$ to the second-high prediction, one obtains the MAAL of 13.9 $\mu g/m^3$, which is represented by the upper dashed line in the Figure.

Compliance with the MAAL is illustrated in Figure 4-2. Block 24-hour current-inventory predictions (averaged over receptors) are plotted as a function of time for 1990 meteorological data. The previously determined MAAL (13.9 $\mu g/m^3$) is also represented in Figure 4-2. The second-high prediction of 13.7 $\mu g/m^3$, represented by the lower dashed line, is less than the MAAL and, therefore, demonstrates compliance under this approach.

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Figure 4-1: Illustration of MAAL Determination for TRNP South Unit

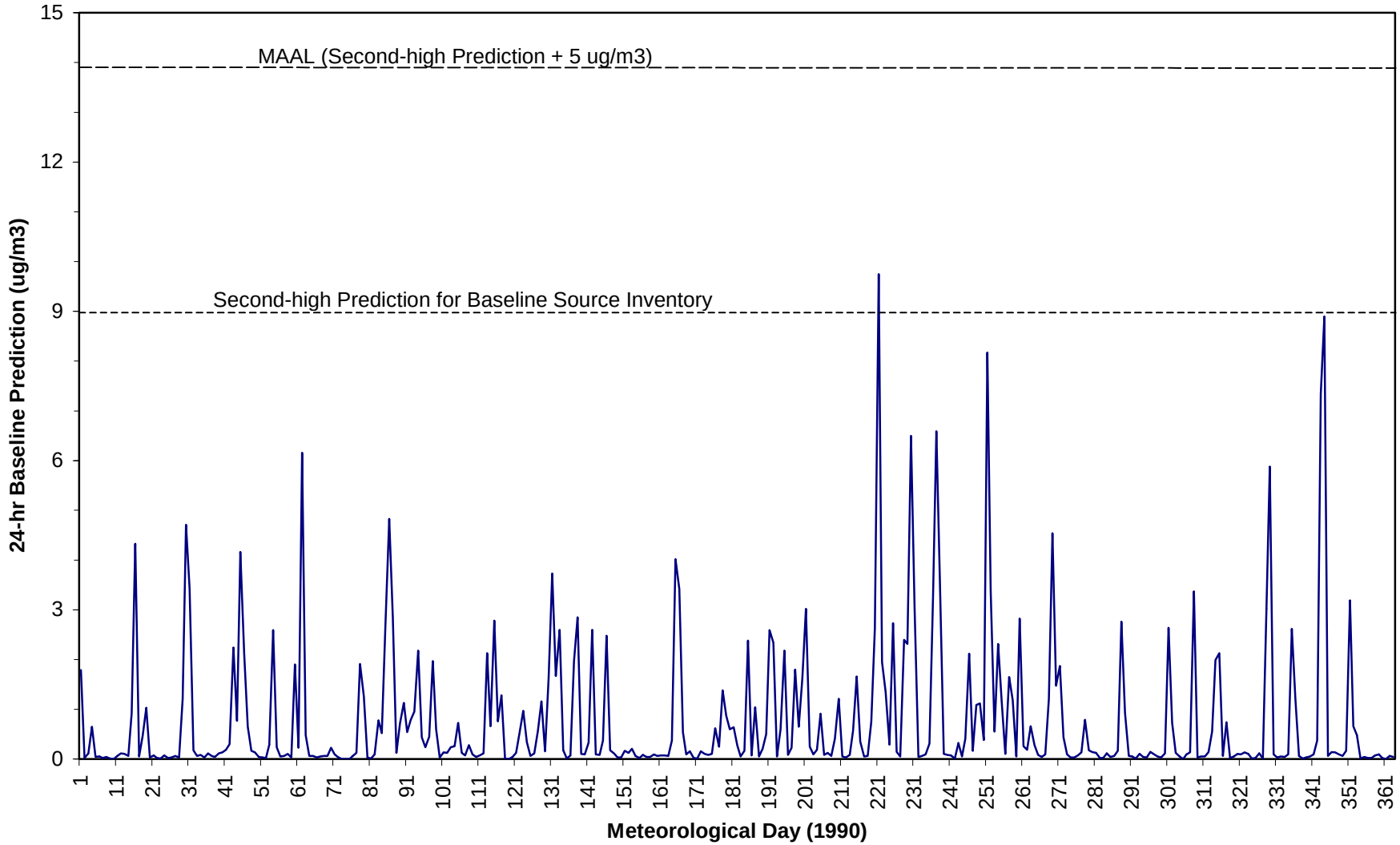
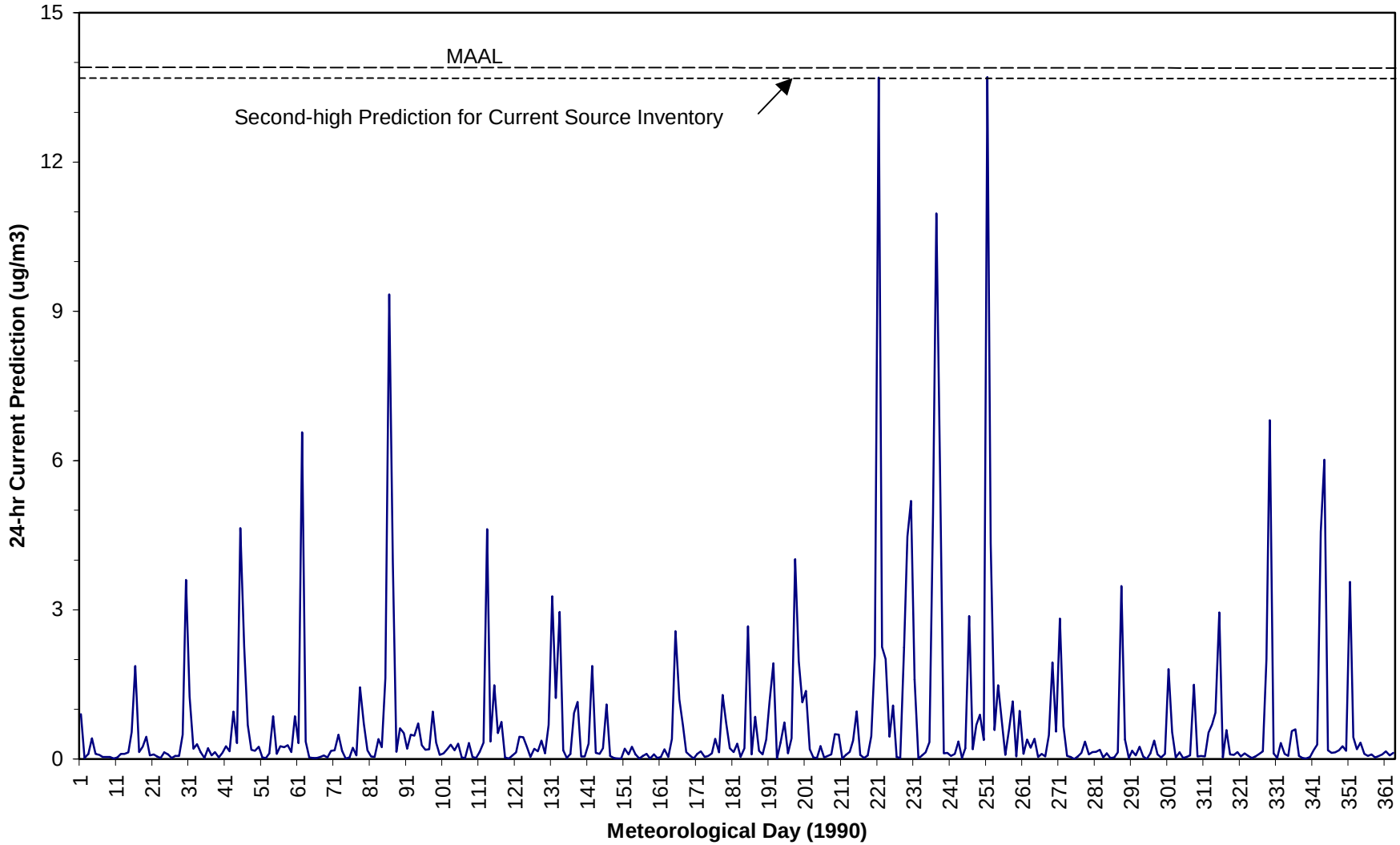


Figure 4-2: Illustration of MAAL Compliance for TRNP South Unit



4.2 Results

Results of the Calpuff SO_2 modeling analysis for current Class I increment consumption in North Dakota and eastern Montana Class I areas are summarized in Tables 4-1 through 4-6. A separate table is provided for each Class I area. The tables provide the MAAL and the second-highest model prediction (for the current source inventory) for 3-hour and 24-hour averages for each year of meteorological data. Also included is the number of predicted exceedances of the MAAL (using the current source inventory). MAAL's and second-high predictions are provided in units of micrograms per cubic meter ($\mu g/m^3$).

As shown in Tables 4-1 through 4-6, the modeling analysis demonstrates compliance with increments at all Class I areas. Though single exceedances of the MAAL were found for some meteorological years at some Class I areas, one exceedance per year is allowed under the rules, thus, these single exceedances do not constitute violations.

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Table 4-1
Calpuff Class I Increment Results for SO_2
TRNP South Unit
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Average					
MAAL	45.3	46.2	44.7	45.9	43.8
2nd High Current Prediction	34.4	31.2	24.8	28.9	21.7
No. of Exceedances of MAAL	0	0	0	0	0
24-hr Average					
MAAL	13.9	14.5	12.1	12.0	13.2
2nd High Current Prediction	13.7	12.0	6.4	7.8	9.7
No. of Exceedances of MAAL	0	1	0	0	0

Table 4-2
Calpuff Class I Increment Results for SO_2
TRNP North Unit
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Average					
MAAL	73.7	80.5	72.7	81.6	85.8
2nd High Current Prediction	25.7	33.6	26.5	23.0	23.5
No. of Exceedances of MAAL	0	0	0	0	0
24-hr Average					
MAAL	26.5	25.5	22.2	23.2	26.2
2nd High Current Prediction	10.6	12.6	7.6	9.0	9.2
No. of Exceedances of MAAL	0	0	0	0	0

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Table 4-3
Calpuff Class I Increment Results for SO_2
TRNP Elkhorn Ranch Unit
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Average					
MAAL	94.0	79.5	65.1	80.1	75.7
2nd High Current Prediction	20.7	26.1	21.6	25.6	20.6
No. of Exceedances of MAAL	0	0	0	0	0
24-hr Average					
MAAL	23.8	25.3	23.1	26.5	22.5
2nd High Current Prediction	9.7	11.7	7.1	9.0	13.4
No. of Exceedances of MAAL	0	0	0	0	0

Table 4-4
Calpuff Class I Increment Results for SO_2
Lostwood Wilderness Area
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Average					
MAAL	46.0	47.8	45.7	47.3	49.5
2nd High Current Prediction	26.3	28.5	28.7	27.8	26.7
No. of Exceedances of MAAL	0	0	0	0	0
24-hr Average					
MAAL	14.0	14.7	13.5	14.2	11.4
2nd High Current Prediction	12.0	10.9	9.9	8.1	8.4
No. of Exceedances of MAAL	0	1	0	0	0

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Table 4-5
Calpuff Class I Increment Results for SO_2
Medicine Lake Wilderness Area
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Average					
MAAL	43.9	38.2	38.5	38.7	36.2
2nd High Current Prediction	27.5	16.7	19.8	20.9	18.3
No. of Exceedances of MAAL	0	0	0	0	0
24-hr Average					
MAAL	11.4	8.7	10.5	11.2	10.5
2nd High Current Prediction	7.6	4.7	8.0	9.0	8.7
No. of Exceedances of MAAL	0	0	1	0	0

Table 4-6
Calpuff Class I Increment Results for SO_2
Fort Peck Reservation
($\mu g/m^3$)

	1990	1991	1992	1993	1994
3-hr Average					
MAAL	39.9	34.7	35.7	36.8	35.1
2nd High Current Prediction	22.5	12.9	15.7	17.6	13.8
No. of Exceedances of MAAL	0	0	0	0	0
24-hr Average					
MAAL	9.3	8.8	9.5	9.3	9.2
2nd High Current Prediction	5.5	5.2	7.7	6.1	5.8
No. of Exceedances of MAAL	1	0	0	0	0

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5. Summary

The Calpuff modeling system has been applied to determine the current status of PSD Class I increment consumption for SO_2 in North Dakota and eastern Montana. Based on the state's legal review, a non-conventional approach was applied to the interpretation of model results. This approach included the use of receptor averaging, and the establishment of a modeled baseline concentration for the 3-hour and 24-hour averaging periods. Results of the increment analysis revealed compliance at all Class I areas.

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Appendix A
Calmet Code Changes

To defeat vertical extrapolation in Step 2 wind field development (while leaving in for initial guess), the following section of Calmet (Version 5.0, Level 970825) Subroutine DIAGNO was changed from:

```
        52 IF(ICALC.LT.0)  GO TO 850
C
C     EXTRAPOLATE SURFACE WINDS
C     EXTRAPOLATION OPTIONS:
C       1) IF IABS(IEXTRP)=1, THEN DO NOT EXTRAPOLATE FROM SURFACE DATA
C       2) IF IABS(IEXTRP)=2, THEN USE POWER LAW
C       3) IF IABS(IEXTRP)=3, THEN USE FEXTRP MULTIPLIER
C       4) IF       IEXTRP=4, THEN USE SIMILARITY THEORY
C       5) IF IEXTRP<=0, THEN DO NOT USE LEVEL 1 DATA FROM UA WINDS
C
      IF(IABS(IEXTRP).EQ.1) GO TO 91
```

to:

```
        52 IF(ICALC.LT.0)  GO TO 850
C
C     EXTRAPOLATE SURFACE WINDS
C     EXTRAPOLATION OPTIONS:
C       1) IF IABS(IEXTRP)=1, THEN DO NOT EXTRAPOLATE FROM SURFACE DATA
C       2) IF IABS(IEXTRP)=2, THEN USE POWER LAW
C       3) IF IABS(IEXTRP)=3, THEN USE FEXTRP MULTIPLIER
C       4) IF       IEXTRP=4, THEN USE SIMILARITY THEORY
C       5) IF IEXTRP<=0, THEN DO NOT USE LEVEL 1 DATA FROM UA WINDS
C
      go to 91
```

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Appendix B
Calpuff Performance Evaluation

Evaluation of

Calpuff Model Performance

Using Year 2000 Data

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November 2001

North Dakota Department of Health
1200 Missouri Avenue
Bismarck, ND 58506

Introduction

Performance of the Calpuff model (Version 5.4, Level 000602_1), as implemented by the North Dakota Department of Health (NDDH) for Year 2000 data, was evaluated using SO_2 observations from the NDDH Dunn Center and Theodore Roosevelt National Park (TRNP) South Unit monitoring sites. Meteorological input data for Calpuff were developed using the Calmet meteorological model (Version 5.2, Level 000602a). Source emission rates were based on CEM's hourly data (where available) or annual average emission for Year 2000.

The performance evaluation proceeded in an iterative manner to determine the effect of adjustments to settings in the Calmet and Calpuff input control files on model skill. The majority of these settings were left equivalent to recommendations in "IWAQM Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts," 1998. But changes to a limited number of settings were judged to be scientifically advantageous for the region of model application, and resulted in improved model agreement with observations. A single Calpuff receptor was included for each monitoring site.

The iterative procedure resulted in a final set of Calmet/Calpuff input conditions which yielded very good agreement with observations. All of the predicted/observed ratios fell within the factor-of-two criteria suggested by EPA.

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Source Inventory

The evaluation analysis accounted for all SO_2 sources located within a reasonable distance of the two monitoring sites, and which operated during Year 2000. The inventory included all significant SO_2 sources within 250 km of the sites. Oil and gas production sources (i.e., treaters and flares) were also included. But because of their greater number and smaller size, the modeled inventory of oil and gas sources was limited to those located within 50 km of each monitoring site.

SO_2 sources included in the evaluation analysis are identified in Table 1. Source locations with respect to monitoring sites are depicted in Figure 1 (oil and gas source locations not shown).

SO_2 emission rates and stack operating parameters (i.e., exit velocity and temperature) were based on CEM's hourly data for Year 2000 where available. For significant sources with no CEM's data, constant emission rates and operating parameters reflecting annual average

operation for Year 2000 were utilized. Annual average stack data for oil and gas production sources were derived from monthly production data for Year 2000. The emission characterization for each source is indicated in Table 1. As shown in Table 1, hourly emissions data were available for a majority of significant sources, and for most of the largest sources.

Emission rates for oil and gas production sources were derived from the ND State Industrial Commission's Oil and Gas data base. The oil and gas sources were screened to eliminate those with zero or minimal emissions. Stack operating parameters for oil and gas production sources were derived using procedures described in the "Williston Basin Regional Air Quality Study" (1990), and modified using SCREEN3 (EPA screening model) adjustments for effective flare plume height and radiational heat loss.

Calmet Input Data

The location of the 10 km computational grid utilized by the NDDH for the Year 2000 analysis is represented in Figure 1. The grid is defined by eight vertical layers. Meteorological input data for Calmet was based on 32 surface stations, 5 upper-air stations, and 89 precipitation stations located in or near the computational grid. GOES ASOS satellite data were used to supplement surface observations for ceiling height and sky cover. All meteorological data were obtained from the National Climatic Data Center (surface and precipitation data), or Forecast Systems Laboratory (upper-air data). Geophysical data were developed using the USGS GTOPO30 data set for terrain elevations and the USGS Global data set for land use.

Processing of meteorological data relied on Earth Tech software, as well as supplemental software developed by NDDH for format conversions and missing data substitution. Methodology for meteorological data preparation is generally consistent with that described in "Calpuff Class I Area Analysis for Milton R. Young Generating Station" (Draft), 1999. That methodology was modified for the Year 2000 analysis largely because of the inclusion of GOES ASOS satellite data. Methodology specific to the Year 2000 analysis has been informally described, and will be formally documented in a future report. Note that the possibility/effect of alternative approaches to meteorological data preparation was not considered in the performance evaluation.

Processing of terrain and land use data was strictly objective, and relied exclusively on Earth Tech software. Note that the seasonal scheme for land use related parameters, which has been informally

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documented, is not incorporated in the final iteration of the performance evaluation, which provided the best agreement with observations. Rather, Calmet default parameters were assumed for the entire year.

Calmet/Calpuff Control File Settings

For the most part, Calmet and Calpuff input control file settings, as implemented by the NDDH, were consistent with IWAQM recommendations. However, extensive testing of Calmet output, with visual feedback (plotted data), suggested that adjustment to a limited number of IWQAM settings was required to achieve reasonable results for wind and mixing height fields. Further, the adjustment of a limited number of additional settings was found to provide better agreement with observations in the performance evaluation, and such changes were judged to be scientifically consistent.

Non-IWAQM settings utilized by the NDDH for Calmet and Calpuff control files, and which provided optimum agreement with monitored observations, are listed in Table 2. These Non-IWAQM settings are discussed below.

Calmet

IKINE - The inclusion of kinematic effects provided significantly better agreement of Calpuff results with monitored observations. From a scientific standpoint, it seems inconsistent for IWAQM to recommend wind adjustment using Froude number effects (IFRADJ), and not kinematic effects.

BIAS(NZ) - NDDH bias settings were developed through significant testing with visual feedback. The IWAQM recommendation provides neutral bias (between surface and upper-air data) for all vertical layers. In light of its testing, the NDDH does not believe it is reasonable to assume equal weighting of upper-air wind data with surface data at the lowest level, and to assume equal weighting of surface data with upper-air data at top levels.

LVARY - The NDDH felt it necessary to deploy this option to ensure that at least one station would always be available.

ZUPWND(2) - The NDDH was concerned that IWAQM was recommending a value of 1000 m while the model (Earth Tech) default is 2500 m, thus prompting the NDDH compromise value of 2000 m. But regardless of the selected value for this initial guess wind field

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input, subsequent wind field development should converge to the same result.

MNMDAV/ILEVZI - The NDDH found that IWAQM default values for these parameters, relating to spatial averaging of mixing heights, produced entirely unacceptable results for the mixing height field. Severe gradients (bull's eyes) in mixing height were observed in the immediate vicinity of meteorological stations, and a significant increase in the value of these input parameters was required to mitigate the anomaly. The NDDH notes that because MNMDAV is a function of grid cell size, IWAQM should specify "User Defines" for this parameter.

ZIMAX/ZIMAXW - Because the NDDH Calmet/Calpuff grid extends into the western part of the upper Great Plains, maximum mixing height was increased to 4000 m to be consistent with maximum mixing heights reported for this region (Holzworth, 1972).

<u>Calpuff</u>

MSPLIT - The option for puff splitting was recommended by John Irwin (EPA) when modeling source-receptor distances of 200 km or more, because of the tendency for Calpuff to otherwise overpredict at these distances. Deployment of this option also provided better agreement with observations.

MDISP - Use of dispersion coefficient option 2 provided significantly better agreement with observations. The NDDH also believes this selection is more consistent with the "state-of-the-art" in air quality modeling.

BCKO3 - Though the NDDH is utilizing the hourly file option for ozone background, the BCKO3 value is substituted by Calpuff when hourly data are missing. Based on local monitoring data, NDDH judged the IWQAM value of 80 ppb to be much higher than typical for North Dakota, and therefore reset the value to 30 ppb.

BCKNH3 - The NDDH value of 2 ppb reflects the annual average of local, unbiased monitoring data.

XSAMLEN - The NDDH set this value lower than the IWAQM recommendation, but notes that the only consequence for doing so would be extra computer time due to more puffs on the grid. The goal was to improve model resolution by increasing the number of puffs and decreasing mass per puff. Again, because this parameter

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is a function of grid cell size, the NDDH believes the recommended XSAMLEN value should be “User Defined”.

XMAXZI - Value was increased to 4000 m for consistency with ZIMAX/ZIMAXW setting in Calmet.

Some other deviations from IWAQM guidance, which had no consequence for model predictions, were also involved in the NDDH implementation. These related to printed output options and parameters for the Lambert conformal map projection used by the NDDH.

Results

Results of the performance evaluation are summarized in Figure 2 for the Dunn Center monitoring site, and in Figure 3 for the TRNP South monitoring site. The Figures include quantile-quantile plots of the highest 50 predictions and observations for 3-hour and 24-hour averaging times. The plots include “factor-of-two” curves for assessing performance. Note that these results represent the final iteration of the performance evaluation process, as reflected by the control file settings in Table 2.

Inspection of the quantile-quantile plots in Figures 2 and 3 reveals that the capability of the NDDH Calpuff modeling system to reproduce observed SO_2 concentrations is very good. All predicted-to-observed ratios fall within the factor-of-two criteria suggested by EPA, and in most cases are much better. Though some of the 50 highest 24-hour averages at both monitoring sites were underpredicted, it appears the modeling system produces no systematic bias toward underprediction on overprediction when considering the ensemble results.

One caveat regarding these results in that TRNP South Unit monitoring data for Year 2000 included extensive missing periods (about 700 hours total). Therefore, maximum observations may be under-represented in the comparative analysis, moving the bias more toward underprediction, particularly for 24-hour averages.

Conclusions

The evaluation of Calpuff performance for Year 2000 data at Dunn Center and TRNP South Unit monitoring sites indicates the modeling system performs well, when implemented using IWAQM control file settings as modified by NDDH (Table 2). Predicted-to-observed ratios for the fifty highest predicted/observed concentrations fell within the factor-of-two criteria suggested by EPA, and did not exhibit systematic bias toward

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underprediction or overprediction. Therefore, the NDDH implementation of the Calpuff modeling system, using currently processed meteorological/geophysical data and IWAQM control file settings as modified by NDDH, should be acceptable for regulatory Class I area modeling in North Dakota.

The NDDH recognizes that minor improvement in model performance is still possible. But the implication of these performance evaluation results is that caution must attend any suggested changes to input or methodology. Changing all control file settings to IWAQM-recommended values, for example, would likely move some predicted-to-observed ratios outside of the factor-of-two window.

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Table 1
Source Inventory (SO_2)

Source	Emission Characterization	Figure 1 Loc. Key
Coal Creek Station	Actual Hourly	1
Antelope Valley Station	Actual Hourly	2
Coyote Station	Actual Hourly	3
Leland Olds Station	Actual Hourly	4
Milton R. Young Station	Actual Hourly	5
Heskett Station	Actual Hourly	6
Stanton Station	Actual Hourly	4
Great Plains Synfuels Plant	Actual Hourly*	2
Little Knife Gas Plant	Actual Hourly	7
Grasslands Gas Plant	Actual Hourly	8
Tioga Gas Plant	Annual Average	9
Lignite Gas Plant	Annual Average	10
Mandan Refinery	Annual Average	6
Boundary Dam Station	Annual Average	11
Shand Station	Annual Average	12
Colstrip Station	Actual Hourly	13
CELP Boiler	Annual Average	14
Sidney Station	Annual Average	15
Oil & Gas Related**	Annual Average	—

* Hourly CEM's data were available for GPSP main stack only. Annual average emission assumed for other three units.

** All facilities located within 50 km of monitoring sites.

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Table 2
Non-IWAQM Settings Used by NDDH
in Calmet/Calpuff Control Files

Parameter	IWAQM	NDDH
Calmet		
IKINE	0	1
BIAS(NZ)	0,0,0,0, 0,0,0,0	-1.0, -0.9, -0.7, 0.0, 0.5, 1.0, 1.0, 1.0
LVARY	F	T
ZUPWND(2)	1000 m	2000 m
MNMDAV	1	8
ILEVZI	1	4
ZIMAX	3000 m	4000 m
ZIMAXW	3000 m	4000 m
Calpuff		
MSPLIT*	0	1
MDISP	3	2
BCKO3	80 ppb	30 ppb
BCKNH3	10 ppb	2 ppb
XSAMLEN	1.0	0.5
XMAXZI	3000 m	4000 m

* Puff splitting was not deployed in Calpuff control file for oil and gas sources. This concession to model execution time is reasonable, because puffs would not grow very large given the maximum 50 km source-receptor distance.

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Figure 1: Monitor and Source Locations

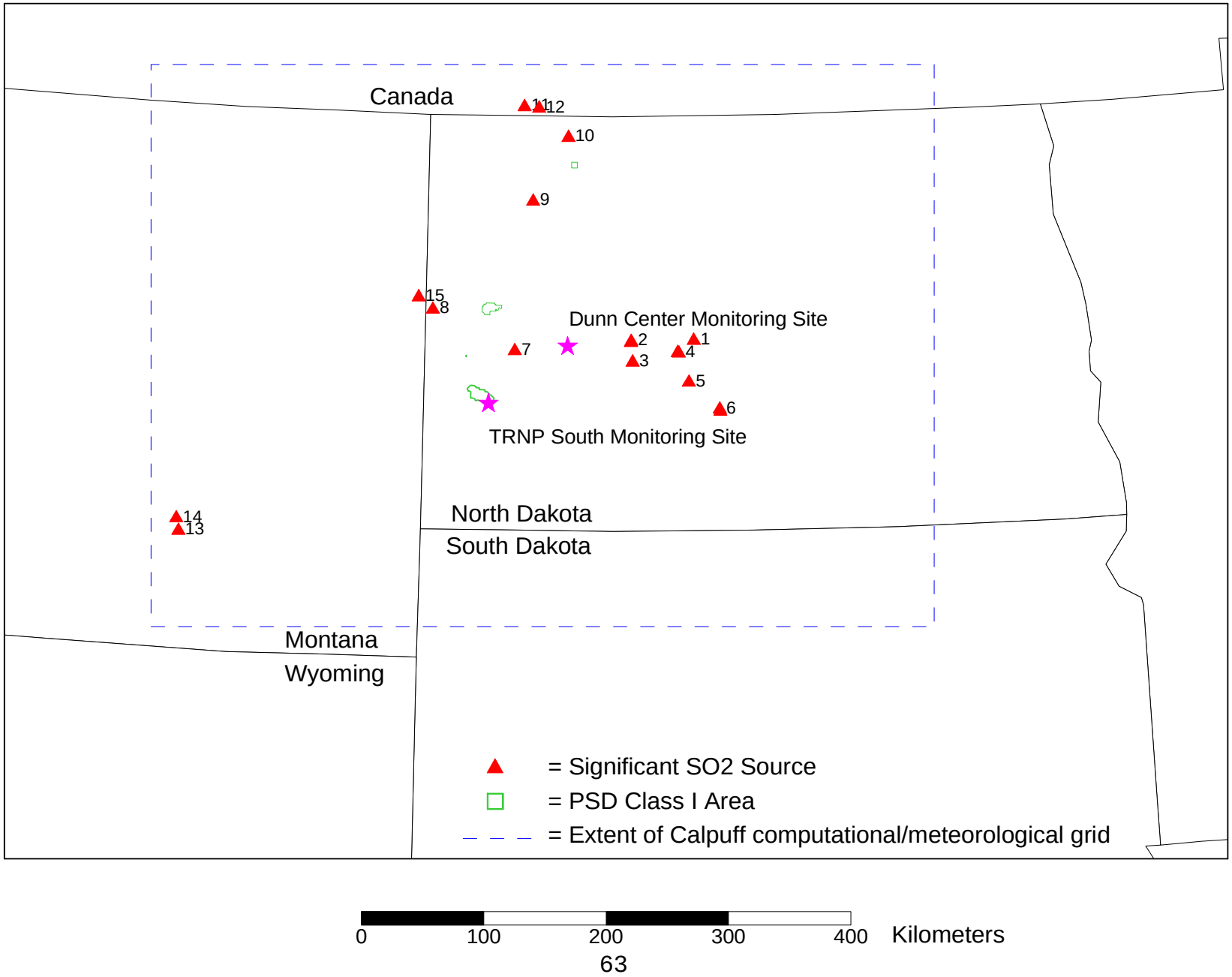
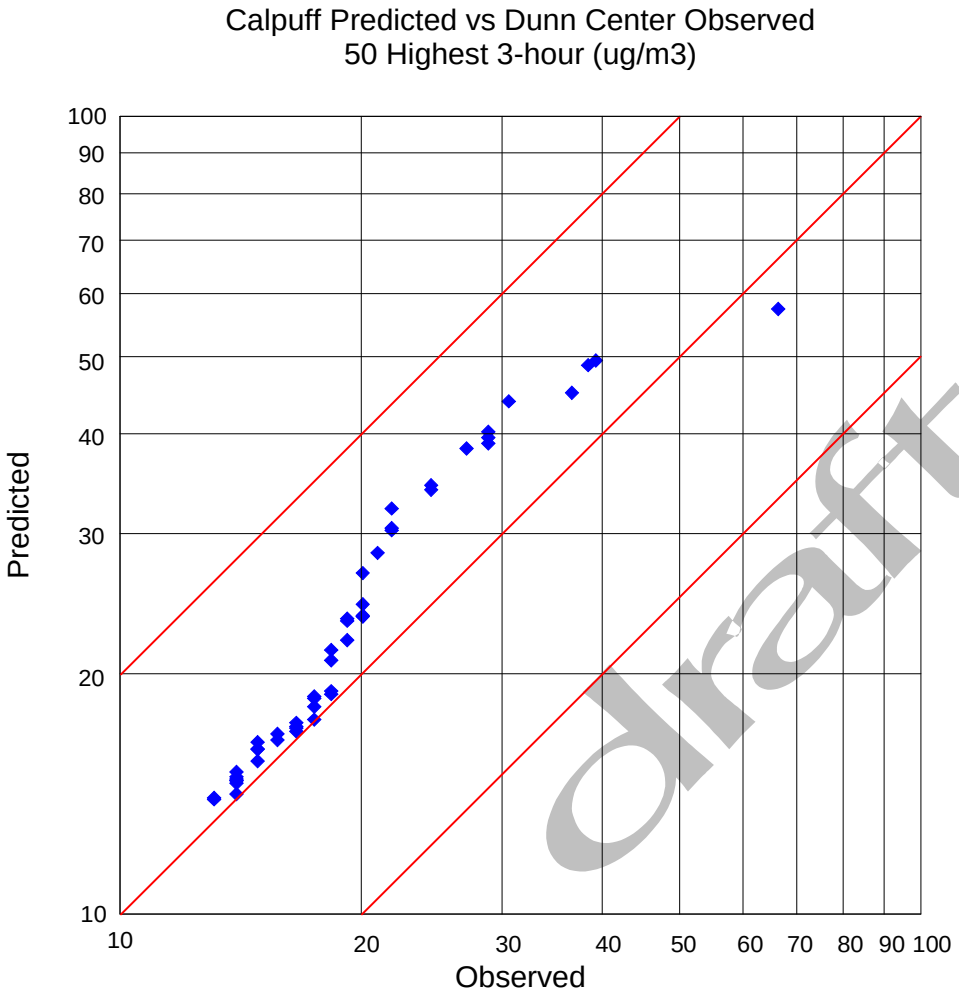


Figure 2



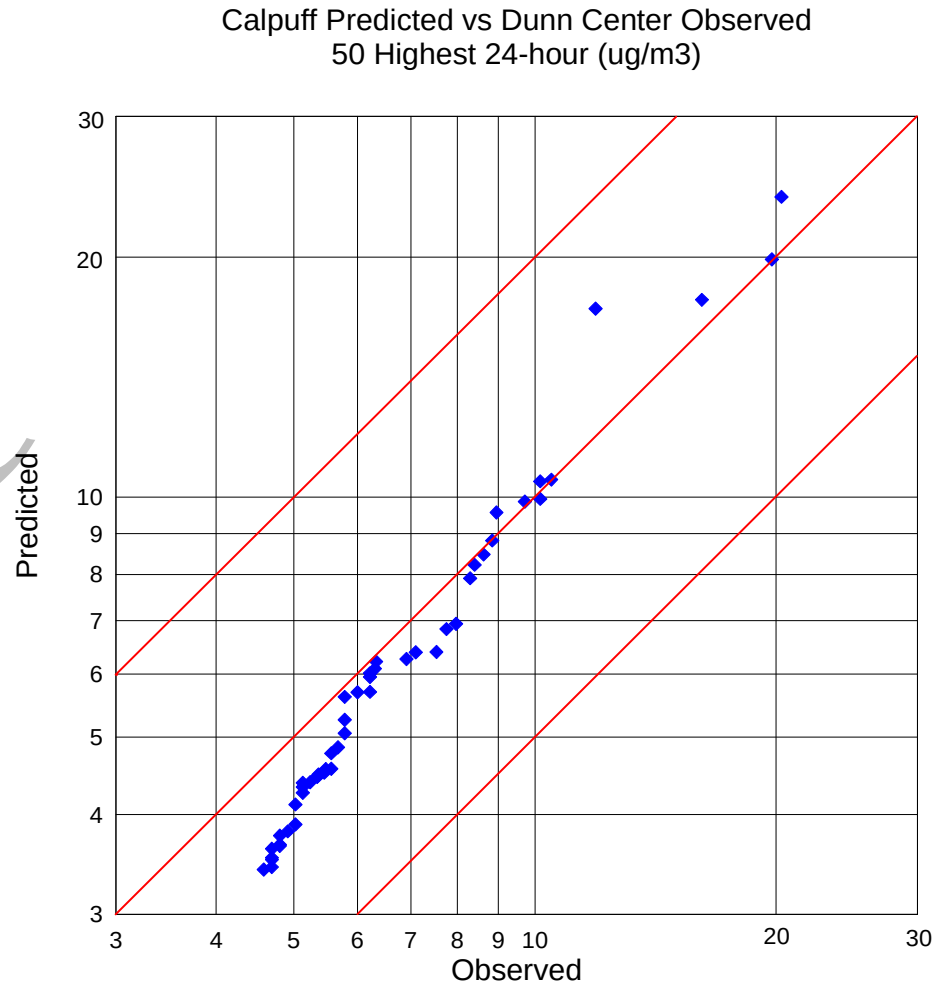


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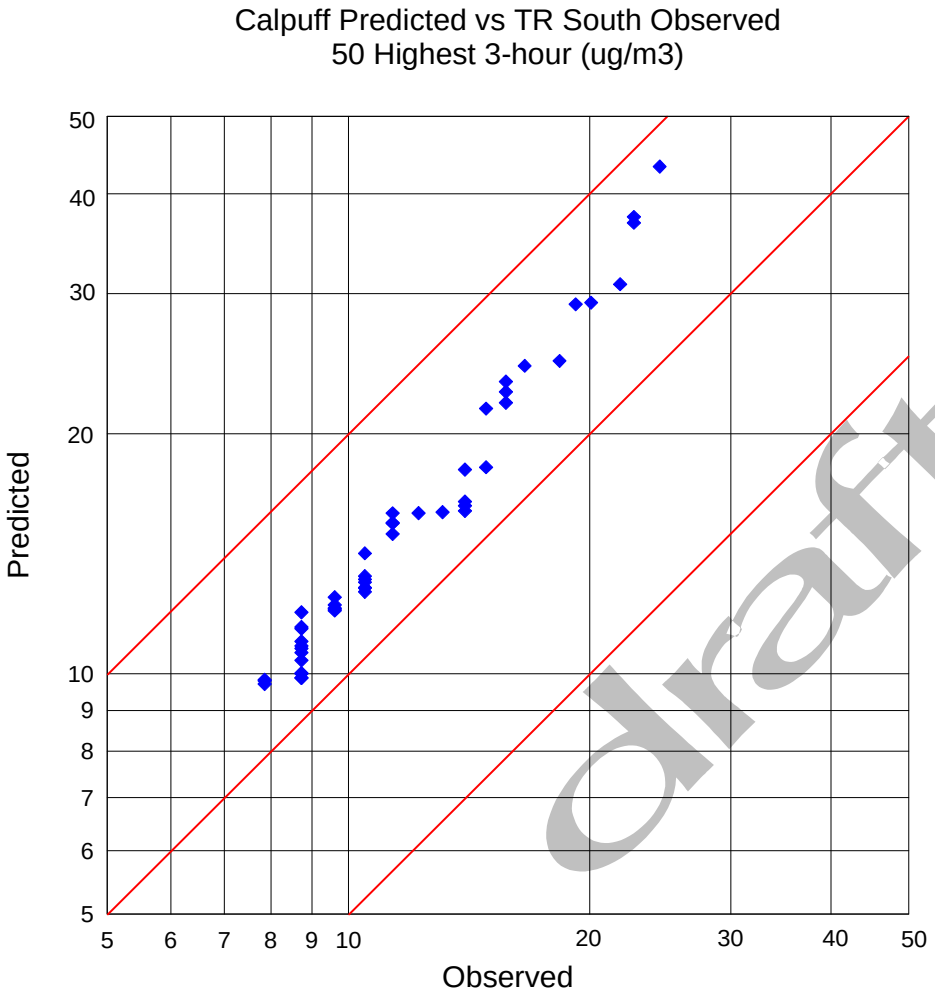
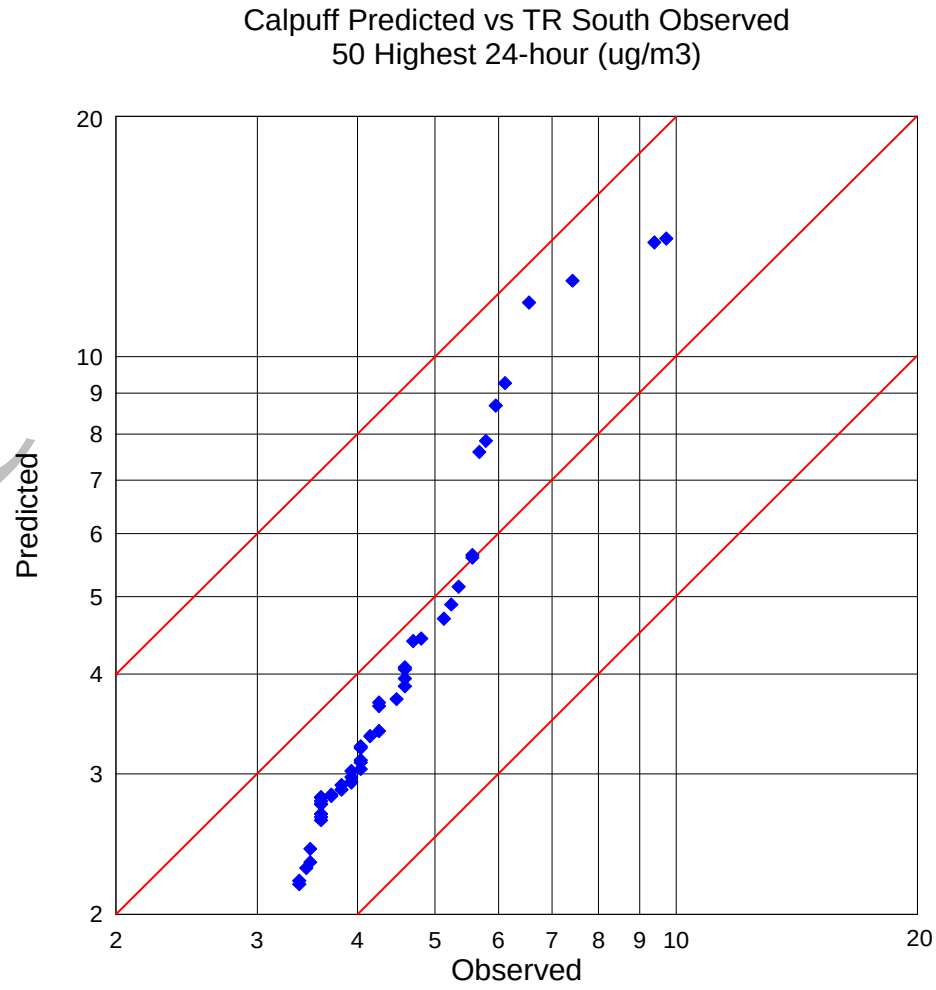
Figure 3





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Appendix C

IWAQM Recommendations

for Calmet Control File

Variable	Description	Value
GEO.DAT	Name of Geophysical data file	GEO.DAT
SURF.DAT	Name of Surface data file	SURF.DAT
PRECIP.DAT	Name of Precipitation data file	PRECIP.DAT
NUSTA	Number of upper air data sites	User Defined
UPn.DAT	Names of NUSTA upper air data files	UPn.DAT
IBYR	Beginning year	User Defines
IBMO	Beginning month	User Defines
IBDY	Beginning day	User Defines
IBHR	Beginning hour	User Defines
IBTZ	Base time zone	User Defines
IRLG	Number of hours to simulate	User Defines
IRTYPE	Output file type to create (must be 1 for CALPUFF)	1
LCALGRD	Are w-components and temperature needed?	T
NX	Number of east-west grid cells	**User Defines**
NY	Number of north-south grid cells	**User Defines**
DGRIDKM	Grid spacing	**User Defines**
XORIGKM	Southwest grid cell X coordinate	User Defines
YORIGKM	Southwest grid cell Y coordinate	User Defines
XLAT0	Southwest grid cell latitude	User Defines
YLON0	Southwest grid cell longitude	User Defines
IUTMZN	UTM Zone	User Defines
LLCONF	When using Lambert Conformal map coordinates, rotate winds from true north to map north?	F
XLAT1	Latitude of 1st standard parallel	**30**
XLAT2	Latitude of 2nd standard parallel	**60**

Variable	Description	Value
RLON0	Longitude used if LLCONF = T	**90**
RLAT0	Latitude used if LLCONF = T	**40**
NZ	Number of vertical layers	**User Defines**
ZFACE	Vertical cell face heights (NZ+1 values)	**User Defines**
LSAVE	Save met. data fields in an unformatted file?	T
IFORMO	Format of unformatted file (1 for CALPUFF)	1
NSSTA	Number of stations in SURF.DAT file	User Defines
NPSTA	Number of stations in PRECIP.DAT	User Defines
ICLOUD	Is cloud data to be input as gridded fields? (0 = No)	0
IFORMS	Format of surface data (2 = formatted)	2
IFORMP	Format of precipitation data (2 = formatted)	2
IFORMC	Format of cloud data (2 = formatted)	2
IWFCOD	Generate winds by diagnostic wind module? (1 = Yes)	1
IFRADJ	Adjust winds using Froude number effects? (1 = Yes)	1
IKINE	Adjust winds using kinematic effects? (1 = Yes)	0
IOBR	Use O'Brien procedure for vertical winds? (0 = No)	0
ISLOPE	Compute slope flows? (1 = Yes)	1
IEXTRP	Extrapolate surface winds to upper layers? (-4 = use similarity theory and ignore layer 1 of upper air station data)	-4
ICALM	Extrapolate surface calms to upper layers? (0 = No)	0
BIAS	Surface/upper-air weighting factors (NZ values)	NZ*0

Variable	Description	Value
IPROG	Using prognostic or MM-FDDA data? (0 = No)	0
LVARY	Use varying radius to develop surface winds?	**F**
RMAX1	Max surface over-land extrapolation radius (km)	**User Defines**
RMAX2	Max aloft over-land extrapolation radius (km)	**User Defines**
RMAX3	Maximum over-water extrapolation radius (km)	**User Defines**
RMIN	Minimum extrapolation radius (km)	0.1
RMIN2	Distance (km) around an upper air site where vertical extrapolation is excluded (Set to -1 if IEXTRP = ±4)	4
TERRAD	Radius of influence of terrain features (km)	**User Defined**
R1	Relative weight at surface of Step 1 field and obs	**User Defines**
R2	Relative weight aloft of Step 1 field and obs	**User Defines**
DIVLIM	Maximum acceptable divergence	5.E-6
NITER	Max number of passes in divergence minimization	50
NSMTH	Number of passes in smoothing (NZ values)	2, 4*(NZ-1)
NINTR2	Max number of stations for interpolations (NA values)	**99**
CRITFN	Critical Froude number	1
ALPHA	Empirical factor triggering kinematic effects	0.1
IDIOPT1	Compute temperatures from observations (0 = True)	0
ISURFT	Surface station to use for surface temperature (between 1 and NSSTA)	**User Defines**
IDIOPT2	Compute domain-average lapse rates? (0 = True)	0
IUPT	Station for lapse rates (between 1 and NUSTA)	**User Defines**
ZUPT	Depth of domain-average lapse rate (m)	200

Variable	Description	Value
IDIOPT3	Compute internally inital guess winds? (0 = True)	0
IUPWND	Upper air station for domain winds (-1 = 1/r**2 interpolation of all stations)	-1
ZUPWND	Bottom and top of layer for 1st guess winds (m)	1, 1000
IDIOPT4	Read surface winds from SURF.DAT? (0 = True)	0
IDIOPT5	Read aloft winds from UPn.DAT? (0 = True)	0
CONSTB	Neutral mixing height B constant	1.41
CONSTE	Convective mixing height E constant	0.15
CONSTN	Stable mixing height N constant	2400
CONSTW	Over-water mixing height W constant	0.16
FCORIOL	Absolute value of Coriolis parameter	1.E-4
IAVEXZI	Spatial averaging of mixing heights? (1 = True)	1
MNMDAV	Max averaging radius (number of grid cells)	1
HAFANG	Half-angle for looking upwind (degrees)	30
ILEVZI	Layer to use in upwind averaging (between 1 and NZ)	1
DPTMIN	Minimum capping potential temperature lapse rate	0.001
DZZI	Depth for computing capping lapse rate (m)	200
ZIMIN	Minimum over-land mixing height (m)	50
ZIMAX	Maximum over-land mixing height (m)	3000
ZIMINW	Minimum over-water mixing height (m)	50
ZIMAXW	Maximum over-water mixing heigh (m)	3000
IRAD	Form of temperature interpolation (1 = 1/r)	1
TRADKM	Radius of temperature interpolation (km)	500

Variable	Description	Value
NUMTS	Max number of stations in temperature interpolations	5
IAVET	Conduct spatial averaging of temperature? (1 = True)	1
TGDEFB	Default over-water mixed layer lapse rate (K/m)	-0.0098
TGDEFA	Default over-water capping lapse rate (K/m)	-0.0045
JWAT1	Beginning landuse type defining water	999
JWAT2	Ending landuse type defining water	999
NFLAGP	Method for precipitation interpolation (2 = 1/r**2)	2
SIGMAP	Precip radius for interpolations (km)	100
CUTP	Minimum cut off precip rate (mm/hr)	0.01
SSn	NSSTA input records for surface stations	User Defines
USn	NUSTA input records for upper-air stations	User Defines
PSn	NPSTA input records for precipitation stations	User Defines

draft

Appendix D

IWAQM Recommendations for Calpuff Control File

Variable	Description	Value
METDAT	CALMET input data filename	CALMET.DAT
PUFLST	Filename for general output from CALPUFF	CALPUFF.LST
CONDAT	Filename for output concentration data	CONC.DAT
DFDAT	Filename for output dry deposition fluxes	DFLX.DAT
WFDAT	Filename for output wet deposition fluxes	WFLX.DAT
VISDAT	Filename for output relative humidities (for visibility)	VISB.DAT
METRUN	Do we run all periods (1) or a subset (0)?	0
IBYR	Beginning year	User Defined
IBMO	Beginning month	User Defined
IBDY	Beginning day	User Defined
IBHR	Beginning hour	User Defined
IRLG	Length of run (hours)	User Defined
NSPEC	Number of species modeled (for MESOPUFF II chemistry)	5
NSE	Number of species emitted	3
MRESTART	Restart options (0 = no restart), allows splitting runs into smaller segments	**0**
METFM	Format of input meteorology (1 = CALMET)	1
AVET	Averaging time lateral dispersion parameters (minutes)	60
MGAUSS	Near-field vertical distribution (1 = Gaussian)	1
MCTADJ	Terrain adjustments to plume path (3 = Plume path)	**3**
MCTSG	Do we have subgrid hills? (0 = No), allows CTDM-like treatment for subgrid scale hills	**0**
MSLUG	Near-field puff treatment (0 = No slugs)	0

Variable	Description	Value
MTRANS	Model transitional plume rise? (1 = Yes)	1
MTIP	Treat stack tip downwash? (1 = Yes)	1
MSHEAR	Treat vertical wind shear? (0 = No)	0
MSPLIT	Allow puffs to split? (0 = No)	**0**
MCHEM	MESOPUFF-II Chemistry? (1 = Yes)	1
MWET	Model wet deposition? (1 = Yes)	1
MDRY	Model dry deposition? (1 = Yes)	1
MDISP	Method for dispersion coefficients (3 = PG & MP)	3
MTURBVW	Turbulence characterization? (Only if MDISP = 1 or 5)	3
MDISP2	Backup coefficients (Only if MDISP = 1 or 5)	3
MROUGH	Adjust PG for surface roughness? (0 = No)	0
MPARTL	Model partial plume penetration? (0 = No)	1
MTINV	Elevated inversion strength (0 = compute from data)	0
MPDF	Use PDF for convective dispersion? (0 = No)	0
MSGTIBL	Use TIBL module? (0 = No) allows treatment of subgrid scale coastal areas	0
MREG	Regulatory default checks? (1 = Yes)	1
CSPECn	Names of species modeled (for MESOPUFF II, must be SO2, SO4, NOX, HNO3, NO3)	**User Defined**
Specie Names	Manner species will be modeled	**User Defined**
Specie Groups	Grouping of species, if any.	**User Defined**
NX	Number of east-west grids of input meteorology	User Defined
NY	Number of north-south grids of input meteorology	User Defined
NZ	Number of vertical layers of input meteorology	User Defined

Variable	Description	Value
DGRIDKM	Meteorology grid spacing (km)	User Defined
ZFACE	Vertical cell face heights of input meteorology	User Defined
XORIGKM	Southwest corner (east-west) of input meteorology	User Defined
YORIGIM	Southwest corner (north-south) of input meteorology	User Defined
IUTMZN	UTM zone	User Defined
XLAT	Latitude of center of meteorology domain	User Defined
XLONG	Longitude of center of meteorology domain	User Defined
XTZ	Base time zone of input meteorology	User Defined
IBCOMP	Southwest X-index of computational domain	**User Defined**
JBCOMP	Southwest Y-index of computational domain	**User Defined**
IECOMP	Northeast X-index of computational domain	**User Defined**
JECOMP	Northeast Y-index of computational domain	**User Defined**
LSAMP	Use gridded receptors? (T = Yes)	F
IBSAMP	Southwest X-index of receptor grid	User Defined
JBSAMP	Southwest Y-index of receptor grid	User Defined
IESAMP	Northeast X-index of receptor grid	User Defined
JESAMP	Northeast Y-index of receptor grid	User Defined
MESHDN	Gridded recpetor spacing = DGRIDKM/MESHDN	1
ICON	Output concentrations? (1 = Yes)	1
IDRY	Output dry deposition flux? (1 = Yes)	1
IWET	Output west deposition flux? (1 = Yes)	1
IVIS	Output RH for visibility calculations (1 = Yes)	1
LCOMPRS	Use compression option in output? (T = Yes)	T

Variable	Description	Value
ICPRT	Print concentrations? (0 = No)	0
IDPRT	Print dry deposition fluxes (0 = No)	0
IWPRT	Print wet deposition fluxes (0 = No)	0
ICFRQ	Concentration print interval (1 = hourly)	1
IDFRQ	Dry deposition flux print interval (1 = hourly)	1
IWFRQ	West deposition flux print interval (1 = hourly)	1
IPRTU	Print output units (1 = g/m**3; g/m**2/s)	1
IMESG	Status messages to screen? (1 = Yes)	1
Output Species	Where to output various species	**User Defined**
LDEBUG	Turn on debug tracking? (F = No)	F
Dry Gas Dep	Chemical parameters of gaseous deposition species	**User Defined**
Dry Part. Dep	Chemical parameters of particulate deposition species	**User Defined**
RCUTR	Reference cuticle resistance (s/cm)	30.
RGR	Reference ground resistance (s/cm)	10.
REACTR	Reference reactivity	8
NINT	Number of particle-size intervals	9
IVEG	Vegetative state (1 = active and unstressed)	1
Wet Dep	Wet deposition parameters	**User Defined**
MOZ	Ozone background? (1 = read from ozone.dat)	1
BCKO3	Ozone default (ppb) (Use only for missing data)	**80**
BCKNH3	Ammonia background (ppb)	**10**
RNITE1	Nighttime SO2 loss rate (%/hr)	0.2
RNITE2	Nighttime NOx loss rate (%/hr)	2
RNITE3	Nighttime HNO3 loss rate (%/hr)	2

Variable	Description	Value
SYTDEP	Horizontal size (m) to switch to time dependence	550.
MHFTSE	Use Heffter for vertical dispersion? (0 = No)	0
JSUP	PG Stability class above mixed layer	5
CONK1	Stable dispersion constant (Eq 2.7-3)	0.01
CONK2	Neutral dispersion constant (Eq 2.7-4)	0.1
TBD	Transition for downwash algorithms (0.5 = ISC)	0.5
IURB1	Beginning urban landuse type	10
IURB2	Ending urban landuse type	19
Use Following Only For Single-Point Meteorological Input (CALPUFF Screen)		
ILANDUIN	Land use type (20 = Unirrigated agricultural land)	20
ZOIN	Roughness length (m)	0.25
XLAIIN	Leaf area index	3
ELEVIN	Met. Station elevation (m above MSL)	0
XLATIN	Met. Station North latitude (degrees)	**User Defined**
XLONIN	Met. Station West longitude (degrees)	**User Defined**
ANEMHT	Anemometer height of ISC meteorological data (m)	10.0
ISIGMAV	Lateral turbulence (Not used with ISC meteorology)	1
IMIXCTDM	Mixing heights (Not used with ISC meteorology)	0
End of Single Point Meteorology Input Variables		
XMXLEN	Maximum slug length in units of DGRIDKM	1
XSAMLEN	Maximum puff travel distance per sampling step (units of DGRIDKM)	1

Variable	Description	Value
MXNEW	Maximum number of puffs per hour	99
MXSAM	Maximum sampling steps per hour	99
SL2PF	Maximum Sy/puff length	10
PLX0	Wind speed power-law exponents	0.07,0.07,0.10,0.15,0.35,0.55
WSCAT	Upper bounds 1st 5 wind speed classes (m/s)	1.54,3.09,5.14,8.23.10.8
PGGO	Potential temperature gradients PG E and F (deg/km)	0.020, 0.035
SYMIN	Minimum lateral dispersion of new puff (m)	1.0
SZMIN	Minimum vertical dispersion of new puff (m)	1.0
SVMIN	Array of minimum lateral turbulence (m/s)	6*0.50
SWMIN	Array of minimum vertical turbulence (m/s)	0.20, 0.12, 0.08, 0.06, 0.03, 0.016
CDIV	Divergence criterion for dw/dz (1/s)	0.01
WSCALM	Minimum non-calm wind speed (m/s)	0.5
XMAXZI	Maximum mixing height (m)	3000
XMINZI	Minimum mixing height (m)	50
PPC	Plume path coefficients (only if MCTADJ = 3)	0.5,0.5,0.5,0.5,0.35,0.35
NSPLIT	Number of puffs when puffs split	3
IRESPLIT	Hours when puff are eligible to split	**User Defined**
ZISPLIT	Previous hour's mixing height (minimum), (m)	100
ROLDMAX	Previous Max mixing height/current mixing height ratio, must be less then this value to allow puff split	0.25

Variable	Description	Value
EPSSLUG	Convergence criterion for slug sampling integration	1.0E-04
PESAREA	Convergence criterion for area source integration	1.0E-06
NPT1	Number of point sources	User Defined
IPTU	Units of emission rates (1 = g/s)	1
NSPT1	Number of point source-species combinations	0
NPT2	Number of point sources with fully variable emission rates	0
Point Sources	Point sources characteristics	User Defined
Area Sources	Area sources characteristics	User Defined
Line Sources	Buoyant lines source characteristics	User Defined
Volume Sources	Volume sources characteristics	User Defined
NREC	Number of user defined receptors	User Defined
Receptor Data	Location and elevation (MSL) of receptors	User Defined