PRELIMINARY Draft Users Manual

The MMIFstat Statistical Analysis Package

Version 1.0

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1 INTRODUCTION

EPA, in cooperation with the Federal Land Management Agencies have developed a meteorological preprocessor for the CALPUFF long range transport dispersion modeling system. The processor, entitled Mesoscale Meteorological Input Formatter (MMIF), reads MM5 and WRF generated gridded fields and reformats and derives data necessary for successful CALPUFF execution. This preprocessor differs from CALMET in that it's primary purpose is to pass through three dimensional meteorological fields.

The MMIFstat program performs statistical analysis on the MMIF output files files and enables the MMIF user to assess the fidelity of the meteorological files and the suitability of the use of the files for subsequent air quality modeling. As time more MM5/WRF simulations become available the user will have the ability to use choose the best performing meteorological model simulation on an application specific basis.

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2 FORMULATION

The MMIFstat package and this documentation was developed in part from ENVIRON International Corporation (ENVIRON) METSTAT program. Key features of this package are:

- Ability to quickly and efficiently evaluate surface meteorological parameters;
- Ability to use readily available surface observation files;
- Ability to select a subset of observations for analysis;
- Applicability on either Linux/Unix or Windows platforms;
- A simple text-based user interface "control" file structured like the MMIF file;
- Ability to produce statistical file easily displayed in common CSV format;
- Dynamic memory allocation to remove grid limits from application;

While certain code and features are common between MMIFstat and METSTAT, aside from the obvious difference that METSTAT reads MM5/WRF files and MMIFstat reads MMIF files, several key differences exist. Namely:

- MMIFstat uses FORTRAN 90 dynamic memory allocation;
- MMIFstat directly ingests DS472.0 surface observations;
- METSTAT analyzes mixing ratio as the water vapor variable, MMIFstat analyzes relative humidity;
- MMIFstat does not adjust model estimates to measurement heights since certain key parameters are not available in MMIF output files

2.1 Statistical Metrics

The MMIFstat package performs statistics for air temperature, relative humidity and winds. The metrics computed are those that have been commonly reported for mesoscale model evaluation for air quality modeling. Namely:

Mean Observation (M_o): calculated from all sites with valid data within a given analysis region and for a given time period (hourly or daily):

$$M_o = \frac{1}{IJ}\sum_{j=1}^{J}\sum_{i=1}^{I} O_j^i$$

where O^i_j is the individual observed quantity at site *i* and time *j*, and the summations are over all sites (*I*) and over time periods (*J*).

Mean Prediction (M_p): calculated from simulation results that are interpolated to each observation used to calculate the mean observation (hourly or daily):

$$M_p = \frac{1}{IJ}\sum_{j=1}^{J}\sum_{i=1}^{I} P_j^i$$

where P^i_j is the individual predicted quantity at site *i* and time *j*. Note that mean observed and predicted winds are vector-averaged (for east-west component *u* and north-south component *v*), from which the mean wind speed and mean resultant direction are derived.

Least Square Regression: performed to fit the prediction set to a linear model that describes the observation set for all sites with valid data within a given analysis region and for a given time period (daily or episode). The y-intercept *a* and slope *b* of the resulting straight line fit are calculated to describe the regressed prediction for each observation:

$$\hat{P}^i_j = a + bO^i_j$$

The goal is for a 1:1 slope and a "0" y-intercept (no net bias over the entire range of observations), and a regression coefficient of 1 (a perfect regression). The slope and intercept facilitate the calculation of several error and skill statistics described below.

Bias Error (B): calculated as the mean difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$B = \frac{1}{IJ}\sum_{j=1}^{J}\sum_{i=1}^{I}\left(P^i_j - O^i_j\right)$$

Gross Error (E): calculated as the mean *absolute* difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly

$$E = \frac{1}{IJ}\sum_{j=1}^{J}\sum_{i=1}^{I}\left|P^i_j - O^i_j\right|$$

or daily):

Note that the bias and gross error for winds are calculated from the predicted-observed residuals in speed and direction (not from vector components *u* and *v*). The direction error for a given prediction-observation pairing is limited to range from 0 to ±180°.

Root Mean Square Error (RMSE): calculated as the square root of the mean squared difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$RMSE = \left[\frac{1}{IJ}\sum_{j=1}^{J}\sum_{i=1}^{I}\left(P^i_j - O^i_j\right)^2\right]^{1/2}$$

The RMSE, as with the gross error, is a good overall measure of model performance. However, since large errors are weighted heavily (due to squaring), large errors in a small subregion may produce a large RMSE even though the errors may be small and quite acceptable elsewhere.

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Systematic Root Mean Square Error ($RMSE_S$): calculated as the square root of the mean squared difference in *regressed* prediction-observation pairings within a given analysis region and for a given time period (hourly or daily):

$$RMSE_S = \left[\frac{1}{IJ} \sum_{j=1}^{J} \sum_{i=1}^{I} \left(\hat{P}_j^i - O_j^i \right)^2 \right]^{1/2}$$

where the regressed prediction is estimated for each observation from the least square fit described above. The $RMSE_S$ estimates the model's linear (or systematic) error; hence, the better the regression between predictions and observations, the smaller the systematic error.

Unsystematic Root Mean Square Error ($RMSE_U$): calculated as the square root of the mean squared difference in prediction-regressed prediction pairings within a given analysis region and for a given time period (hourly or daily):

$$RMSE_U = \left[\frac{1}{IJ} \sum_{j=1}^{J} \sum_{i=1}^{I} \left(P_j^i - \hat{P}_j^i \right)^2 \right]^{1/2}$$

The unsystematic difference is a measure of how much of the discrepancy between estimates and observations is due to random processes or influences outside the legitimate range of the model.

A "good" model will provide low values of the RMSE, explaining most of the variation in the observations. The systematic error should approach zero and the unsystematic error should approach RMSE since:

$$RMSE^2 = RMSE_S^2 + RMSE_U^2$$

It is important that RMSE, $RMSE_S$, and $RMSE_U$ are all analyzed. For example, if only RMSE is estimated (and it appears acceptable) it could consist largely of the systematic component. This error might be removed through improvements in the model inputs or use of more appropriate options, thereby reducing the error transferred to the photochemical model. On the other hand, if the RMSE consists largely of the unsystematic component, this indicates that further error reduction may require model refinement (new algorithms, higher resolution grids, etc.), or that the phenomena to be replicated cannot be fully addressed by the model. It also provides error bars that may be used with the inputs in subsequent sensitivity analyses.

Index of Agreement (IOA): calculated following the approach of Willmont (1981). This metric condenses all the differences between model estimates and observations within a given analysis region and for a given time period (hourly and daily) into one statistical quantity. It is the ratio of the total RMSE to the sum of two differences – between each prediction and the observed mean, and each observation and the observed mean:

$$IOA = 1 - \left[\frac{IJ \cdot RMSE^2}{\sum_{j=1}^{J} \sum_{i=1}^{I} \left| P_j^i - M_o \right| + \left| O_j^i - M_o \right|} \right]$$

Viewed from another perspective, the index of agreement is a measure of the match between the departure of each prediction from the observed mean and the departure of each observation from the observed mean. Thus, the correspondence between predicted and observed values across the domain at a given time may be quantified in a single metric and displayed as a time series. The index of agreement has a theoretical range of 0 to 1, the latter score suggesting perfect agreement.

2.2 Statistical Benchmarks

In 2001, the Texas Natural Resource Conservation Commission (TNRCC) sponsored an MM5 modeling project in which we derived and proposed a set of daily performance "benchmarks" for typical meteorological model performance (Emery et al., 2001). These standards were based upon the evaluation of a variety of about 30 MM5 and RAMS air quality applications conducted up to that point, as reported by Tesche et al. (2001). The purpose of these benchmarks was not necessarily to give a passing or failing grade to any one particular meteorological model application, but rather to put its results into the proper context. For example, expectations for modeling of complex terrain might not be as high as flat homogeneous terrain. The key to the benchmarks is to understand how poor or good the results are relative to the universe of other model applications run throughout various areas of the U.S. Certainly, an important criticism of past EPA guidance statistics for acceptable photochemical performance is that they were relied upon much too heavily to establish an acceptable model simulation of a given area and episode. Often lost in the statistical evaluation is the need to critically evaluate all aspects of the model via diagnostic and process-oriented approaches. The same must stressed for the meteorological performance evaluation.

Emery et al. (2001) carefully considered the appropriateness and adequacy of the proposed benchmarks based upon the results of MM5 simulations performed and reported in that study. Based upon these considerations, the final daily proposed benchmarks are given below:

Wind Speed	RMSE:	≤ 2 m/s
	Bias:	≤ ±0.5 m/s
	IOA:	≥ 0.6
Wind Direction	Gross Error:	≤ 30 deg
	Bias:	≤ ±10 deg

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Temperature	Gross Error:	$\leq$ 2 K
	Bias:	$\leq$ ±0.5 K
	IOA	≥ 0.8

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3 CODE STRUCTURE AND COMPILATION

MMIFstat is written in Fortran 90 and consists of a main calling routine and several subroutines and Fortran 90 modules. The code is quite modular and commented and should be quite easy to maintain and extend to other tasks. All of the program data structures are dynamically allocated to eliminate the need to recompile the code for different grid structures.

The program code is arranged into the following file structure:

MMIFstat.f	Main driving routine
averag_0.f	Utility code to compute average of input array, accounting for missing data in an alternative array.
average,f	Utility code to compute average of input array
biaserr.f	Utility code to compute bias and error of scalar values
biaserrw.f	Utility code to compute bias and error of wind data
getioa.f	Utility code to compute index of agreement
getrmse.f	Utility code to compute root mean squared error
grid_calmet.f	Code to read MIFF header and set grid parameters
interp.f	Interpolate gridded fields
isearch15.f	Utility code to search character array for a specific value
istrln.f	Utility code to return the length of a string
juldate.f	Utility code to convert Gregorian to Julian date
lcpgeo.f	Utility code to convert from lambert conformal to geographic coordinates, and vice versa.
met_fields.f	Module containing meteorological fields
polgeo.f	Utility code to convert from polar stereograph to geographic coordinates, and vice versa
readasc.f	Code to read RALPHv2 file and fill data arrays
readcalhdr.f	Code to read MIFF header
readcalmet.f	Code to read MMIF file and fill data arrays
read_statlib.f	Code to read and process the DS472 Station Library file
read_tdl.f	Code to read a DS472 data file
regress.f	Utility code to perform a linear regression
site_fields.f	Module containing station location fields
stat_fields.f	Module containing statistical fields
stats.f	Utility code containing statistical processing
uv2spdr.f	Utility code to convert wind components to speed/direction
wrtfils.f	Code to write all output files

3.1 Compiling MMIFstat on Windows

The code includes a batch file named "compile.bat" which can be used to compile the program on Windows using the Intel FORTRAN (ifort) compiler. MMIF has been tested

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with ifort version 11.1 on Windows VISTA. The MMISstat executable has been tested on Windows VISTA and Windows 7.

MMIFstat is compiled by either double-clicking compile.bat in Windows explorer, or by opening a Command Prompt (DOS box), changing to the appropriate directory, and typing "compile.bat" at the prompt.

3.2 Compiling MMIFstat on Linux/Unix

The code includes a "makefile" for compilation on Linux/Unix systems. The code was developed and tested using the Portland Group Fortran 90 compiler (pgf90) under Fedora Core 8.

MMIF is compiled by issuing the "make" at a command prompt within the source directory. It will generate an executable program called "MMIFstat" in the source directory. If changing compilers, it is best to remove all .o and .mod files before recompiling.

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4 Running MMIFStat

Application of MMIFstat is quite straight forward. Once the MMIF program has been executed to generate the CALPUFF ready meteorological file, the MMIFstat program is run to evaluate how closely the fields are able to replicate the observed parameters in the area.

4.1 Observation Formats

The MMIFstat program is able to read two different surface observation formats. Both of these formats have long history of use in the Mesoscale air quality community and are quite familiar to my potential uses for this tool. One format is the Technique Development Lab (TDL) U.S. and Canada Surface Hourly Observations, DS472.0 data. The other is the RAMS RALPH v2 format.

4.1.1 TDL DS472.0 Observations

The DS472.0 dataset provides hourly observations for about 1,000 stations across the United States and Canada. The dataset currently extends from 1976 through 2008, with annual updates. The data are available from the National Center for Atmospheric Research (NCAR) at http://dss.ucar.edu/datasets/ds472.0. First time users to the NCAR archives are required to complete a no cost registration and to appropriately reference the use of the data in any published works that make use of the data.

The DS472.0 archive format changed starting in 1997 MMIFstat only processes the "post 1996" format.

In addition to the DS472.0 datasets for the period of interest, the user is required to also download the most recent station library available at
http://dss.ucar.edu/datasets/ds472.0/station_libraries/

NCAR requests the following acknowledgement in all documents that make use of this dataset: "The data for this study are from the Research Data Archive (RDA) which is maintained by the Computational and Information Systems Laboratory (CISL) at the National Center for Atmospheric Research (NCAR). NCAR is sponsored by the National Science Foundation (NSF). The original data are available from the RDA (http://dss.ucar.edu) in dataset number ds472.0."

4.1.2 RALPH v2 Observation

The RALPH v2 format was chosen for a couple of reasons. First, this format has been widely used in model evaluation of both MM5 and WRF through its use in the ENVIRON METSTAT program. Additionally the format is quite easy to understand and is relatively self documenting. . The data are space-delimited to allow for Fortran free-format list-directed read. The data records are ordered first by site, then by time. A sample file and description follow:

```
999999 2
4
WINDSPEED  m/s
WIND_DIRECTION  deg
TEMPERATURE  K
MIX_RATIO  g/kg
1999 09 13  0000 WRCC3811       35.590  -88.910   0.    1.54 000  270. 000  302.6 000  9.66 000
1999 09 13  0000 WRCC3866        32.550  -88.560   0. -999.00 000 -999. 000  300.4 000 17.00 000
1999 09 13  0000 WRCC3904        30.580  -96.360   0.    0.00 000    3. 000  307.0 000 12.01 000
1999 09 13  0000 WRCC3927        32.890  -97.040   0.    3.09 000  110. 000  308.2 000 11.69 000
1999 09 13  0000 RAOB72240       30.120  -93.220   0.    0.00 000    5. 000  302.6 000 15.19 000
1999 09 13  0000 WRCC3940        32.310  -90.070   0.    2.06 000  100. 000  302.6 000 14.32 000
1999 09 13  0000 WRCC12912       28.860  -96.920   0.    5.66 000  130. 000  302.6 000 15.28 000
1999 09 13  0000 WRCC12916       29.990  -90.250   0.    2.06 000   70. 000  300.9 000 20.04 000
```

Record 1: A marker (999999) denoting the beginning of a new file or new section of a file, and RALPH version number (2)

Record 2: Number of variables on file for each observation

Record 3+: Specific variable names and units; allowed names/units are (note that these are case-sensitive):

WINDSPEED, m/s, knots, mph, km/hr
WIND_DIRECTION, deg
TEMPERATURE, C, F, K
MIX_RATIO, g/g, kg/kg, g/kg
DEWPOINT, C, F, K
REL_HUMIDITY, %, fraction
STN_PRES, Pa, mb, in

Each Observation Record:

4-digit year
2-digit month
2-digit date
4-digit UTC data time
8-character station ID
real station latitude
real station longitude
real station elevation (not used by METSTAT)
real/integer pairs of data values and quality flags (METSTAT ignores the quality flags, missing values are -999.0)

There must be as many value/flag pairs as specified in the header. Values are in the order specified in the header and are of the specified units. Wind direction is Earth-relative, not rotated to the meteorological model projection. While the RALPH format provides the flexibility for many data types, the MMIFstat package only uses the WINDSPEED, WIND_DIRECTION, TEMPERATURE, and REL_HUMIDITY variables.

4.2 MMIF/CALMET Model Formats

The MMIFstat program was designed to be compatible with the MMIF program. However, MMIFstat may be used with CALMET generated files providing that a version 5.8 or later CALMET was run with a Lambert Conic Conformal (LCC) projection.

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4.3 MMIFstat Execution

When executing, the MMIFstat program will by default open and read a control file name "MMIFstat.inp" that must exist in the current directory. If a filename is given on the command line, that file is read as the control file. The control file contains all the user configuration, flags, and filenames to the observation files and the MMIF output file.

Some examples from the DOS prompt are:

C:\MMIFstat\MMIF
C:\MMIFstat\MMIF control.inp

4.3.1 Control File Format

The MMIFstat control file has the following syntax:

The first 20 characters of each record are reserved for a record description, with the exception of the MMIF input file list (the last lines). These first 20 characters are ignored by the program. Input data are supplied starting on column 21 in free format. The following describes each line of the control file.

Run Description	Run description string that gets written into output files.
Hourly Output File:	Name of hourly summary output file.
Daily Output File:	Name of daily summary output file.
Daily Station File:	Station specific daily output file.
Obs/Model Out File:	File containing obs/model pairs for all stations (None if not required)
Observation Format:	Either RALPH or DS472

If the observation format is DS472:

Station List File:	Name of Station library file downloaded from NCAR (Sec. 4.1.1)
Number of Obs Files:	Number of DS472 files to process
Obs File Name:	Filename for DS472 Observation files (record repeats for each file)

If the observation format is RALPH

Station RALPH File:	Name of the RALPH file

Start Time y m d h	Start time for statistics processing (yyyy mm dd hh) format
End Time y m d h	Ending time for statistics processing (yyyy mm dd hh) format
Time Zone	Number of hours to add to time to convert the OBS into local time The DS472 data are in GMT so this value is -8 for PST, -7 for MST, -6 for CST, -5 for EST.
# Sites to Process	Number of sites to process

If the # of sites is greater than 0

Site Name	Name of station to process (record repeats for each station)

If the # of sites is less than 0

X coordinate Range	Westerly and Easterly range (km) to process
Y coordinate Rage	Southerly and Northerly range (km) to process

If the # of sites is equal to 0 no record is required

This is followed by the names of the MMIF output files listed one file per line. Any time-stamps found in the MMIF files that are before the Start time are skipped.

4.4 MMIFStat Evaluation Products

The MMIFstat program generate four different output files. The output files all have a Comma Separated Value (CSV) format, are self documenting, and are easily imported into common desktop productivity software (i.e. Microsoft Excel) for subsequent formatting and analysis. The output formats are described in-turn in the following sections. The Hourly Output and Daily Output files can be used in Excel macro included in the distribution to easily prepare summary graphics.

4.4.1 Hourly Output File

The Hourly Output file contains hourly statistical summaries and has the same format as the METSTAT Hourly Output file. The files differ however in that the METSTAT output moisture variable is expressed as water vapor mixing ratio and the MMIFstat output moisture variable is relative humidity.

The first record is a comment line that displays the MMIFstat run description (the first line of the MMIFstat.inp file) along with the MMIFstat version number (i.e. 1.0) and release level (i.e. 20100221). The second record contains a description of all the variables in the file. A textual description is shown in Table 4-1. Each subsequent record contains the data for a single hour.

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Table 4-1: Variables and Description in Hourly Output File.

Identifier	Description/Units
mo/dy	Month/Day
hr	Hour (00 through 23)
ObsWndSpd	Mean wind speed observations at monitor sites (m/s)
PrdWndSpd	Mean model predicted wind speed at monitor sites reporting valid data (m/s)
BiasWndSpd	Wind speed bias (m/s)
RMSEWndSpd	Wind speed total RMSE (m/s)
RMSESWndSpd	Wind speed systematic RMSE (m/s)
RMSEUWndSpd	Wind speed unsystematic RMSE (m/s)
IOAWndSpd	Wind speed index of agreement
ObsWndDir	Mean wind direction observations at monitor sites (degree)
PrdWndDir	Mean model predicted wind direction at monitor sites reporting valid data (degree)
BiasWndDir	Wind direction bias (deg)
ObsTemp	Mean air temperature observation at monitor sites (K)
PrdTemp	Mean model predicted air temperature at monitor sites reporting valid data (K)
BiasTemp	Air temperature bias (K)
RMSETemp	Air temperature total RMSE (K)
RMSESTemp	Air temperature systematic RMSE (K)
RMSEUTemp	Air temperature unsystematic RMSE (K)
IOATemp	Air temperature index of agreement
ObsHum	Mean relative humidity observation at monitor sites (%)
PrdHum	Mean model predicted relative humidity at monitor sites reporting valid data (%)
BiasHum	Relative humidity Bias (%)
RMSEHum	Relative humidity total RMSE (%)
RMSESHum	Relative humidity systematic RMSE (%)
RMSEUHum	Relative humidity unsystematic RMSE (%)
IOAHum	Relative humidity index of agreement

4.4.2 Daily Output File

The Daily Output file contains daily statistical summaries has the same format as the METSTAT Daily Output file. The files differ however in that the METSTAT output moisture variable is expressed as water vapor mixing ratio and the MMIFstat output moisture variable is relative humidity.

The first record is a comment line that displays the MMIFstat run description (the first line of the MMIFstat.inp file), along with the MMIFstat version number (i.e. 1.0) and release level (i.e.

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20100221). The second record contains a header record, including the date for each day. The subsequent records contain the variable, metric, unit, and value for that variable/metric for each day, and averaged over the whole analysis period.

4.4.3 Daily Station File

The Daily Station file contains daily statistical summaries at each station in the domain, along with the latitude/longitude of the stations. This file is designed to provide summary data for further analysis and graphing in external software.

The first record is a comment line that displays the MMIFstat run description (the first line of the MMIFstat.inp file), along with the MMIFstat version number (i.e. 1.0) and the release level (i.e. 20100221). The second record contains the number of days of data in the file, and the number of sites in the file. The third record contains a description of each field in the subsequent data record. The remaining data records in the file contain the date, station name, longitude (degree), latitude (degree), variable name, metric, unit and value.

4.4.4 Hourly Obs/Model File

The hourly obs/model file contains the observed and model predicted values for all periods used in the evaluation. This file is included to allow the use of supplemental analysis tools, and as a QA tool to check the model predicted and observed data in the event that a statistical metric does not look reasonable. This output file can be quite large. If this file will not be examined, MMIFstat will by-pass creating this file if the filename is given as “None” in the MMIFstat.inp file.

The first record is a comment line that displays the MMIFstat run description (the first line of the MMIFstat.inp file), along with the MMIFstat version number (i.e. 1.0) and the release level (i.e. 200100221). The second record contains a description of each field in the subsequent data records. Each data record contains the date, the hour, the location of the station in fractional grid coordinates, and the observed and predicted wind components, temperatures and relative humidity. Note that the observed wind components may not agree with the observation files since these wind observations have been rotated into the MMIF Lambert Conformal Conic projection.

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