

Model Performance Evaluation Software: Description and Application to Regional Haze Modeling

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MPE Software





Data for PM Model Performance Evaluation

- IMPROVE: 24 hour PM_{2.5} and component* data, one in three days
- CASTNet: 7-day sulfate, nitrate, ammonium, SO₂, and HNO₃ (may be problematic)
- AQS: hourly to daily PM₁₀, PM_{2.5}, PM_{2.5} speciation*, O₃, NO, NO₂, NO_y, VOC (ppb or ppbC), SO₂
- NADP: wet deposition fluxes, concentrations of sulfate, nitrate, ammonium in precipitation
- Other

*PM fraction can be evaluated if both total mass and component mass are available at the same site



How to Consolidate, Store, and Retrieve Ambient Data for MPE?

What we have:

- Many data sources
- Different formats
- Supporting information sometimes separate from data and sometimes difficult to find

MySQL database

- upload data (measurement, site)
- compile other relevant information
- use query to retrieve data in consistent format

What we need:

- Preferably one data source
- Consistent format
- Supporting information
 - site location
 - sample start time including time zone
 - sample duration
 - units



- Read observations
 - perform time zone changes
 - average to longer periods
 - perform unit conversions (may require meteorology)
- Extract modeling data (NetCDF)
 - calculate grid cell corresponding to latitude/longitude
 - extract model data at grid cell(s)
 - sum components of species (look up table)
 - perform unit conversions



Subdomain and Temporal Options

<u>Subdomains</u>

- All sites
- A list (e.g., a city)
- Ranges
 - latitude and longitude
 - cell numbers in x and y
- Performance evaluation zones
- Temporal
- Subperiods
- Aggregation of high frequency measurements (data completeness criterion)





- Model value at grid cell corresponding to site location
- Linear interpolation using 4 closest grid cell
- Average of all cells within a user specified window
- Best estimate with a user specified window
- Distance-weighting method within user specified window

$$V(x, y) = \sum_{i=1}^{n} w_i V_i; where \ w_i = \frac{h_i^{-2}}{\sum_{i=1}^{n} h_i^{-2}} \ and \ h_i = \sqrt{(x - x_i)^2 + (y - y_i)^2}$$





Statistical Options

- Threshold to be selected by user
- Default output metrics
 - accuracy of peak (unpaired in time): paired and unpaired in space
 - mean observed and modeled value
 - Gross and normalized bias and error
 - Coefficient of correlation
 - Normalized root mean square error
- Optional output metrics
 - ratio of means, fractional bias and error, r², index of agreement, site specific root mean square error, normalized mean bias and error, slope and intercept



An MPE Database and Software Designed for Community Use

- Comprehensive Processor
 - data base; binary to NetCDF converter; software
 - output compatible with common graphics software
- Versatility
 - PM, PM components, gases, deposition fluxes
- User-friendly Design
 - Community input for software features
 - Software engineering standard
 - Based on Fortran 90 and MySQL (free!)
- Documentation



Example Results (BRAVO)

