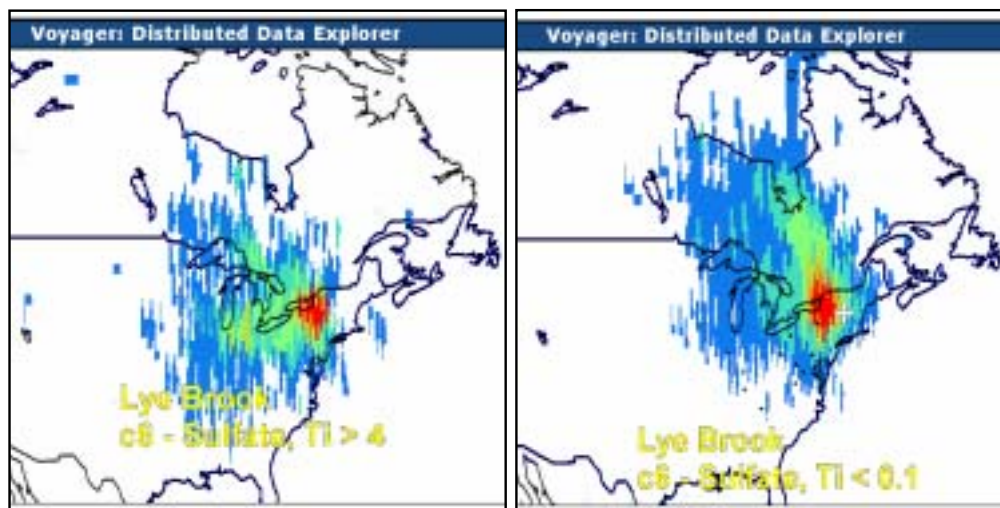


MANE-VU Mid-Atlantic/Northeast Visibility Union

Combined Aerosol & Trajectory Database Analysis Tool Development: Final Interim Report



Final Interim Report

Prepared by
Center for Air Pollution Impact and Trend Analysis (CAPITA)
Washington University in St. Louis

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for the
Mid-Atlantic/Northeast Visibility Union
and
Midwest Regional Planning Organization

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About MANE-VU

The Mid-Atlantic/Northeast Visibility Union (MANE-VU) was formed by the Mid-Atlantic and Northeastern states, tribes, and federal agencies to coordinate regional haze planning activities for the region. MANE-VU members include Connecticut, Delaware, the District of Columbia, Maine, Maryland, Massachusetts, New Hampshire, New Jersey, New York, Pennsylvania, the Penobscot Indian Nation, Rhode Island, the St. Regis Mohawk Tribe, and Vermont. Also participating as non-voting members of MANE-VU are the U.S. Environmental Protection Agency (EPA), the National Park Service, the U.S. Fish and Wildlife Service, and the U.S. Forest Service.

MANE-VU was formed to encourage a coordinated approach to meeting the requirements of EPA's regional haze rules and reducing visibility impairment in major national parks and wilderness areas in the Northeast and Mid-Atlantic region. MANE-VU provides technical assessments and assistance to its members, evaluates linkages to other regional air pollution issues, provides a forum for discussion, and encourages coordinated actions. MANE-VU also facilitates coordination with other regions.

The Ozone Transport Commission Executive Staff Office provides management and administration for MANE-VU. The Mid-Atlantic Regional Air Management Association and the Northeast States for Coordinated Air Use Management conduct MANE-VU's technical projects.

COMBINED AEROSOL & TRAJECTORY DATABASE ANALYSIS TOOL DEVELOPMENT

Preparation of this report was made possible by grants from the U.S. Environmental Protection Agency (EPA) to the Mid-Atlantic/Northeast Visibility Union (MANE-VU) and the Midwest Regional Planning Organization (Midwest RPO).

MANE-VU is coordinating efforts to reduce regional haze in the Mid-Atlantic and Northeast region and is collaborating in that effort with the Mid-Atlantic Regional Air Management Association (MARAMA) and the Northeast States for Coordinated Air Use Management (NESCAUM).

Midwest RPO is coordinating efforts to reduce regional haze in the midwestern states.

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DISCLAIMERS

This report was sponsored in part by the Mid-Atlantic/Northeast Visibility Union (MANE-VU) and the Midwest Regional Planning Organization (Midwest RPO). It was prepared by the Center for Air Pollution Impact and Trend Analysis (CAPITA) at Washington University in St. Louis., under contract to the Mid-Atlantic Regional Air Management Association (MARAMA). The opinions, findings, conclusions, and recommendations are those of the authors and do not necessarily represent the views of MANE-VU, the Midwest RPO, or MARAMA. MANE-VU, the Midwest RPO, and MARAMA, their officers, employees, contractors, and subcontractors make no warranty, expressed or implied, and assume no legal liability for the information in this report. MANE-VU, the Midwest RPO, and MARAMA have not approved or disapproved this report, nor have they passed upon the accuracy or adequacy of the information contained herein.

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ACRONYMS

ATAD	Atmospheric Transport and Diffusion
CAPITA	Center of Air Pollution Impact and Trend Analysis
CASTNET	Clean Air Status and Trends Network
CATT	Combined Aerosol and Trajectory Tool
CIRA	Cooperative Institute for Research in the Atmosphere
dVoy	Distributed Voyager
GIS	Geographic Information System
IMPROVE	Interagency Monitoring of Protected Visual Environments
MARAMA	Mid-Atlantic Regional Air Management Association
MVC	Model-View-Controller
PMF	Positive Matrix Factorization, a source apportionment software tool developed by Pentti Paatero
RPO	Regional Planning Organization
SQL	Structured Query Language
UNMIX	A source apportionment software tool developed by Ronald Henry
VIEWS	Visibility Information Exchange Web System

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INTERIM FINAL REPORT ON COMBINED AEROSOL & TRAJECTORY DATABASE ANALYSIS TOOL DEVELOPMENT

PROJECT BACKGROUND

The source-receptor relationship of particulate matter can be estimated by a number of alternative techniques. Some techniques are based explicitly on meteorological transport, others on chemical fingerprinting, and some combine the transport and chemical approaches using either statistical or physical chemical inverse modeling methods.

The simplest source identification is through the use of “back trajectories.” By this method, the air mass is traced backwards from the receptor. A somewhat refined version is the residence time analysis, where one takes into account the speed at which air masses are transported. Air mass history analysis, particularly when combined with statistical filtering of high and low concentrations, can quickly reveal the general source regions of the measured pollutants (Poirot et al., 2001). Such analysis can be repeated for any of the measured chemical species. However, since many of the chemical elements are contributed by a variety of source types, this technique only yields rough, directional source attribution of specific species, not source types.

Chemical source apportionment is based on the assumption that each aerosol source type has a unique chemical signature or “fingerprint.” The fingerprint itself may be derived either from detailed source characterization or extracted from the ambient data using clustering algorithms. Existing apportionment algorithms include PMF (Paatero, 1998) and UNMIX (Henry, 2000). The result of source apportionment calculations is the re-mapping of the individual species concentrations into groups by aerosol source types. However, by themselves, the chemical fingerprinting algorithms do not elucidate the source location. Combining the back-trajectory and chemical tracer methods can yield considerable new information about the aerosol source types.

A particularly attractive source-attribution technique, *Paired Aerosol / Trajectory Analysis*, developed by Poirot and Wishinski combines the chemical and transport techniques by establishing the major aerosol types at a specific receptor location and time (PMF and UNMIX) and estimating the geographic transport regions for each aerosol type (Residence Time Analysis). An example paired aerosol / trajectory analysis for the Lye Brook, NH is shown in Figure 1. The analysis indicates that high (illustrated as yellow-red in Figure 1) secondary coal contribution at Lye Brook originates from the Upper Ohio River region while low (illustrated as green-blue in Figure 1) secondary coal values occur during transport from Quebec. High biomass smoke is transported from the N-NW direction while low biomass Smoke occurs during transport from Quebec and the Ohio RV Region. High residual oil aerosol types are transported from the East Coast Megalopolis as compared to low residual oil that occurs during transport from Quebec.

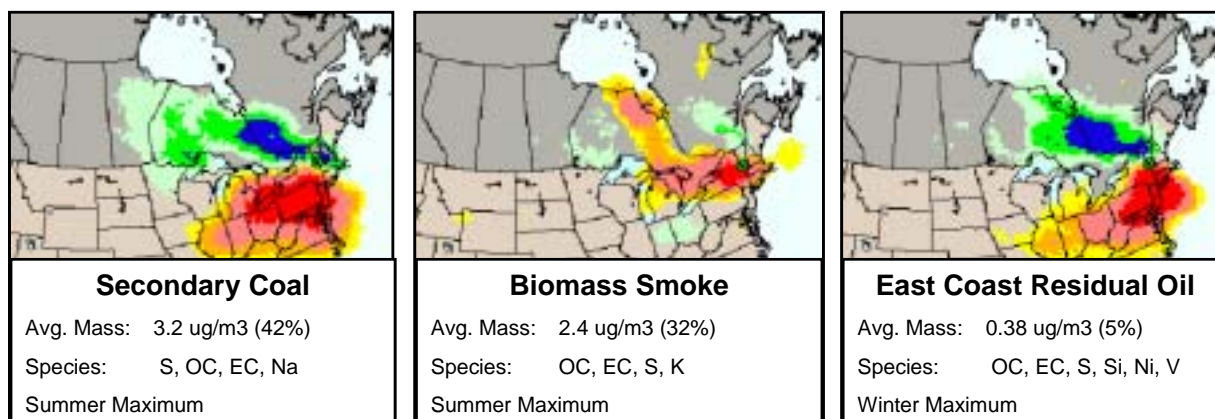


Figure 1. Illustration of Paired Chemical and Trajectory Analysis for Lye Brook, NH adapted from Wishinski and Poirot (2002) and based on Positive Matrix Factorization (PMF) results from B. Coutant and ATAD trajectories from K. Gebhart.

The effectiveness of the paired aerosol / trajectory analysis approach in source apportionment and transport encourages us to develop a tool to make facilitate this type of analysis to a broader audience. This project will develop an interactive data query and analysis tool for paired chemical and trajectory analysis.

PROJECT OBJECTIVES

The objective of this project is to design and implement a combined aerosol and trajectory tool (CATT) with capabilities for database access, filtering, and aggregation in exploring the aerosol source features based on chemical and transport characteristics. Specifically, this project will:

- Develop a relational database that incorporates both aerosol chemistry and gridded trajectory data.
- Design a relational schema of the combined data sets to allow specific queries for extracting pertinent subsets from the data, as well as perform aggregations on the combined data sets.
- Develop graphical user interfaces accessible through the web for accessing and browsing the data sets.

The resulting database will be transferable and expandable to accommodate additional dates, sites, and trajectory data.

DATA USED IN PROJECT

MANE-VU and the Midwest RPO supported a recent study to perform source attribution (PMF and UNMIX) for 16 receptor sites extending from Illinois through Tennessee to New England (Battelle and Sonoma Technology, 2002) (Figure 2). The aerosol receptor modeling data were derived from IMPROVE and CASTNET monitoring data, covering the period since 1988. The receptor modeling data have been assembled into a consistent data set and will be used in this project.

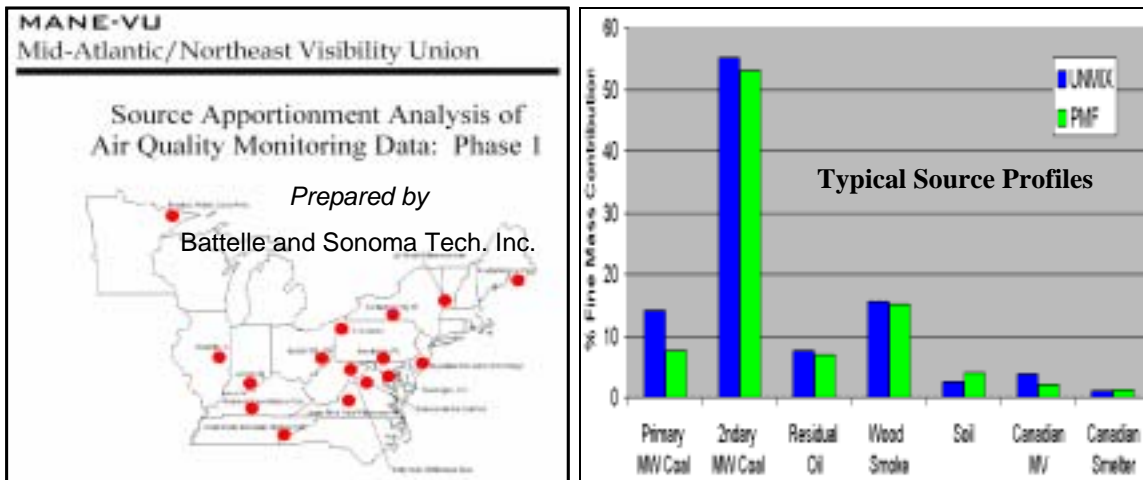


Figure 2. PMF/UNMIX Source Profiles for 16 receptor sites. The results of the Battelle/Sonoma PMF and UNMIX modeling are source profile time series for each location

Gridded back-trajectory data for the 16 sites and about 1000 sample days were also provided for this study. The trajectory calculations were conducted by Paul Wishinski at Vermont DEC and are given as residence time, calculated as “hours per grid cell” for the 80 x 80 km stereographic grid covering North America and the surrounding oceans. The residence time calculations are based on daily ATAD trajectories provided Kristi Gebhart at CIRA.

Portions of the VIEWS databases are also available for this project. IMPROVE speciated PM data are accessible through a CAPITA-VIEWS ‘wrapper’ that can send CAPITA SQL queries to the VIEWS relational database. Other related data such as GIS base map layers and meteorological data are available to the combined aerosol and trajectory tool.

PROJECT DELIVERABLES

The outputs of this project will provide MANE-VU and the Midwest RPO with:

1. A relational database that incorporates both PMF/UNMIX results and gridded trajectory data.
2. SQL filtering and aggregation queries for
 - a. aggregated trajectory data based on chemical specifications
 - b. aggregated chemical data based on geographic specifications
3. A graphic interface for user input (query) and for data output as rendered images or as exportable numeric data.
4. The transfer of the resulting database to a designated SQL server and instructions for augmenting the database with additional chemical and trajectory data.

The current status and plan for each of these deliverables is summarized below.

Deliverable 1: Relational Database

Status: The creation of a SQL relational database containing the speciated chemical data and residence time data has been completed.

The PMF and UNMIX data were provided in Excel spreadsheet format and the associated metadata describing their format and structure were obtained verbally from Rich Poirot. The spreadsheet data were reformatted and imported in the SQL server as two tables; a table containing the chemical data and a table containing the location coordinate information for each monitoring stations.

The residence time data were provided by Paul Wishinski on CD-ROM including full metadata documentation. The data were imported in the SQL server as two SQL tables; a table containing the residence time data and a table containing the latitude/longitude information for each location at which residence times were calculated.

The combined aerosol and trajectory database schema is shown in Figure 3. The core database consists of two “fact tables,” one for the aerosol chemistry/model data (dSourceApp) and another for trajectory residence time (dTrajResTime). The key fields in the dSourceApp table will be the site_code, representing the 16 locations, and Date for the sampling date. The dSourceApp table is linked to the monitoring location table (dsourceApp_Loc) that contains the location code, name, latitude, longitude, and other site descriptors.

The dTrajResTime table contains the trajectory data (hours) for each receptor location and receptor date. The dTrajResTime table shares the site_code and date keys with the dSourceApp table. The dTrajResTime table has an additional key field representing the grid points in the 80x80 North American grid. The values in the table consist of the “hours of residence”.

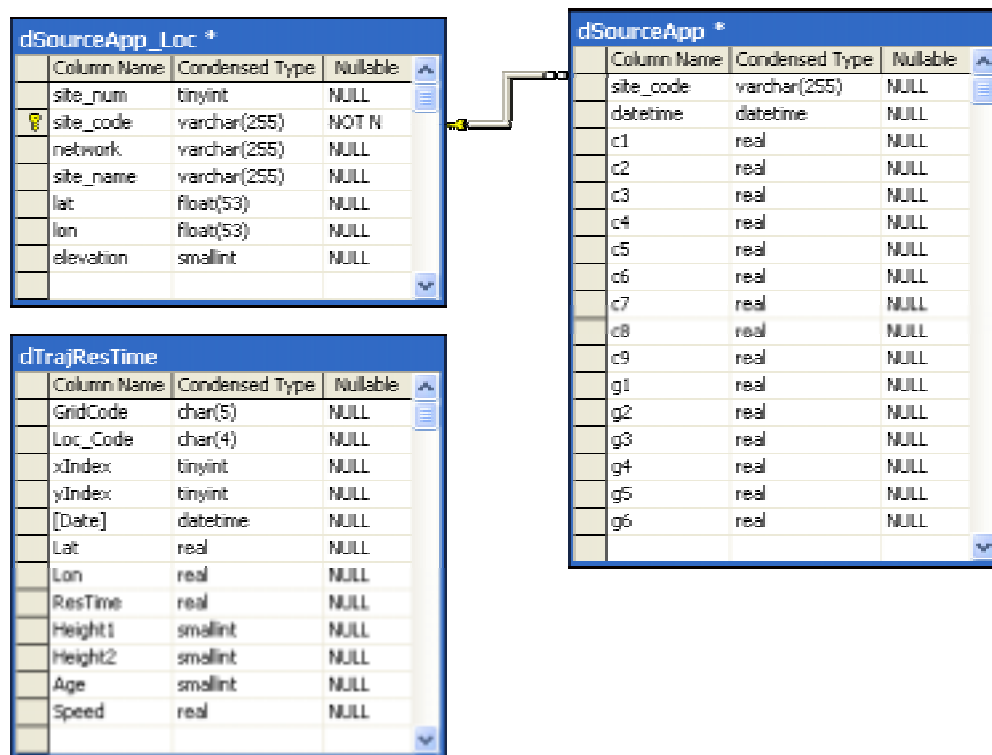


Figure 3. Schema of the combined aerosol-trajectory data sets

Deliverable 2: SQL filtering and aggregation queries

Status: Dataset filtering and aggregation queries have been developed but require refining and user testing.

The design of the relational database schema allows powerful user queries of the chemical and residence time data. The execution of queries that join the two tables can be conducted because the two fact tables share the common keys of loc_code and date/time. The symmetry of this relational schema allows the filtering and aggregation operations to be performed either on the dSourceApp or dTrajResTime tables. Thus, it is possible to perform filter operations on the dSourceApp table (e.g., by specific parameter) and at the same time perform aggregations over the joined dTrajResTime table. Conversely, filter operations can be performed on the dTrajResTime table and the desired aggregations then executed on the dSourceApp table. Figure 4 contains template SQL code for these two types of queries on the dTrajResTime and dSourceApp tables. Templates (settings that are unique to a specific query) are designated by double brackets, "[[____]]". A filter for any parameter for any query can be added by implementing a [[sql_filter_clause]].

```
SELECT Lat as lat,
       Lon as lon,
       Loc_Code as loc_code,
       SUM(ResTime) AS [VALUE]
FROM   dTrajResTime
WHERE  ([Date] IN
       (SELECT datetime
        FROM dSourceApp
        WHERE (Loc_Code = '[[loc_code]]') [[sql_filter_clause]]))
GROUP BY GridCode, Lat, Lon, Loc_Code
ORDER BY Lon ASC

SELECT SUM(ResTime) AS VALUE,
       Lat,
       Lon,
       Loc_Code
FROM   dTrajResTime
WHERE  (Loc_Code = '[[param_abbr]]')
       AND (DATEDIFF(dd, '[[datetime]]', [Date]) < [[datetime_period]])
       AND (DATEDIFF(dd, '[[datetime]]', [Date]) >= 0)
GROUP BY GridCode, Lat, Lon, Loc_Code
```

Figure 4. Template SQL queries for datatables dTrajResTime and dSourceApp.

Additional queries will be implemented through “stored procedures” in the CAPITA SQL server. The purpose of these procedures is to allow specific parameters in a given query to be selected by the user. In figure 5, the variables prefixed with ‘@’ can be supplied dynamically by the user through an appropriate user interface. Stored procedures facilitate optimization by the SQL server engine. The specific user selectable input parameters will be exposed through a user interface for the above simple query; the user interface selections include location, parameter, and minimum and maximum date.

```

CREATE proc sp_fetch_grid
    @parameter    char(10),
    @datetime_min datetime,
    @datetime_max datetime,
    @loc_code     char(10)
AS
SELECT  Restime_Fact.grid_id, SUM(Restime_Fact.grid_hr)
FROM    Obs_Fact INNER JOIN Restime_Fact
        ON Obs_Fact.loc_code = Restime_Fact.loc_code
        AND Obs_Fact.datetime = Restime_Fact.datetime
WHERE   Obs_Fact.parameter = @parameter
        AND Obs_Fact.datetime BETWEEN @datetime_min AND @datetime_max
        AND Obs_Fact.loc_code = @loc_code
GROUP BY Restime_Fact.grid_id
ORDER BY Restime_Fact.grid_id

```

Figure 5. Generalized stored procedure for specific user input.

Deliverable 3: User Interface

Status: A prototype user interface to conduct queries and display results has been developed but requires refinement based on user testing.

Both the inputs and outputs to the data viewing program will be through graphic interfaces accessible through web browsers. The user interface is based on the spatial-temporal environmental data system, distributed Voyager (dVoy), being developed at CAPITA. The browser has three major components: data access, navigation and display which interact following the model-view-controller (MVC) paradigm. The data access (model) layer offers a homogeneous, read-only access mechanism to a changing collection of heterogeneous, autonomous and distributed information sources. The Voyager data access uses a global multidimensional schema consisting of spatial, temporal, parameter and other dimensions common to environmental data. The dVoy interface is particularly well suited to handle the combined aerosol trajectory tool (CATT). For this project, the basic dVoy architecture was used and customized to accommodate the unique characteristics of CATT. Details of dVoy can be found at <http://capita.wustl.edu/voyager>.

Figure 6 displays the graphical browser interface for point and gridded data. The interface currently consists of three components, a map view, a time view, and a control panel. The components are linked so that a change in one component updates the settings in the others. For example, the time view can be updated by clicking on a particular location in the map view. Likewise, the map view can be updated by clicking on a particular time in the time view. Each click in a view or change of setting in the control panel initiates a query to the SQL database.

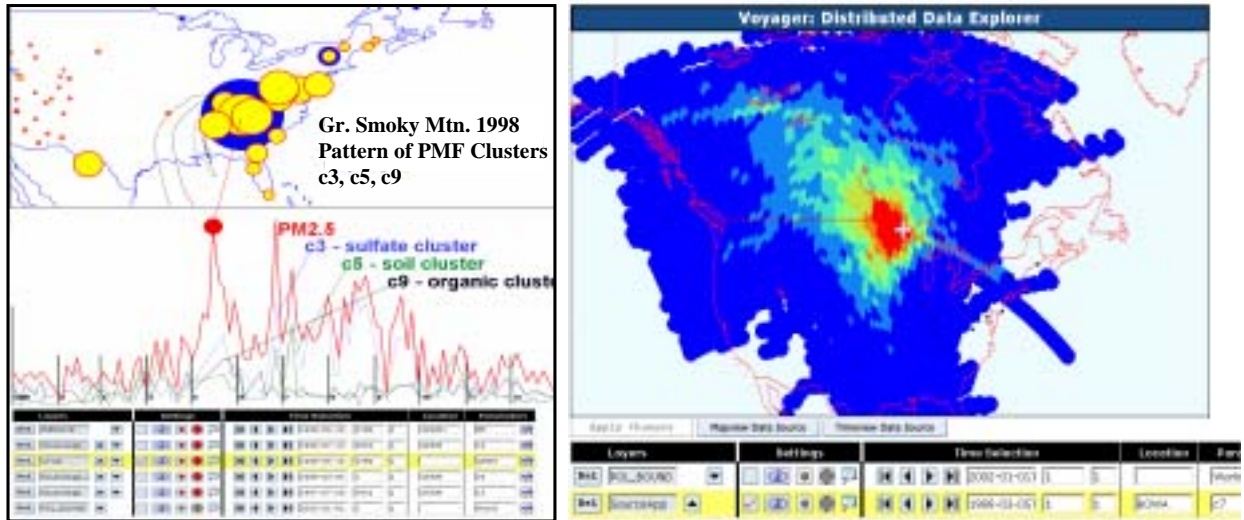


Figure 6. User interface for point data and gridded data. a) the spatial and temporal pattern of point data for PMF c3, c5, and c9 at Great Smoky Mountain. b) The aggregated residence time gridded data for Boundary Waters.

The capability to conduct aggregation queries over time has been developed. Figure 7 display aggregated residence time grids for winter months (Dec. Jan. and Feb.) and summer months (Jun., Jul, and Aug.) for Lye Brook. The aggregated maps indicate that air tends to be transported from the north during the winter and from the west-southwest during the summer.

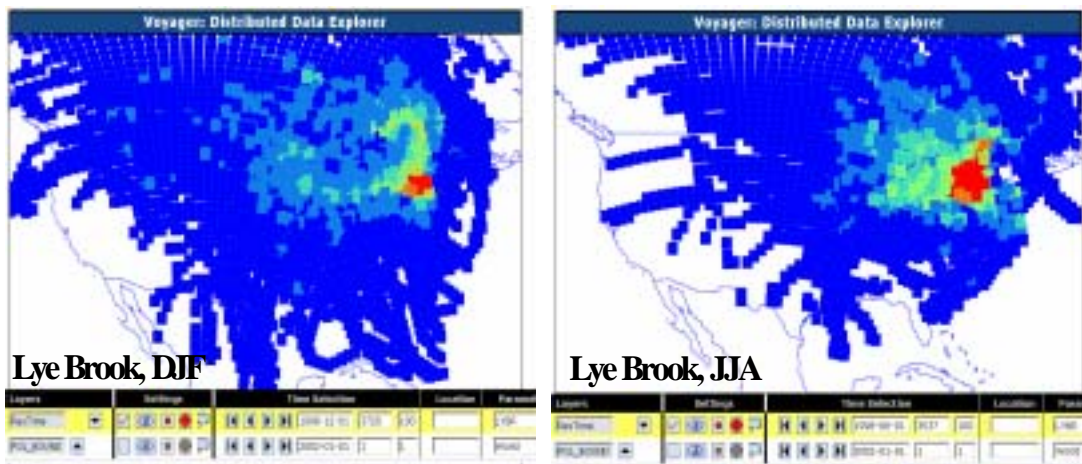


Figure 7. Seasonal residence time, e.g. sum of the residence time over 3 months, for Lye Brook during the winter and summer.

The consistency of the ATAD trajectory and gridded residence time data sets was verified by superimposing the two data sets for various dates and times. As shown in Figure 8 in the verification for the Great Smoky Mountains, the two data sets are aligned. Other sites and times were equally consistent and we were therefore satisfied that the input of the data from their original formats into the SQL database was accurate.

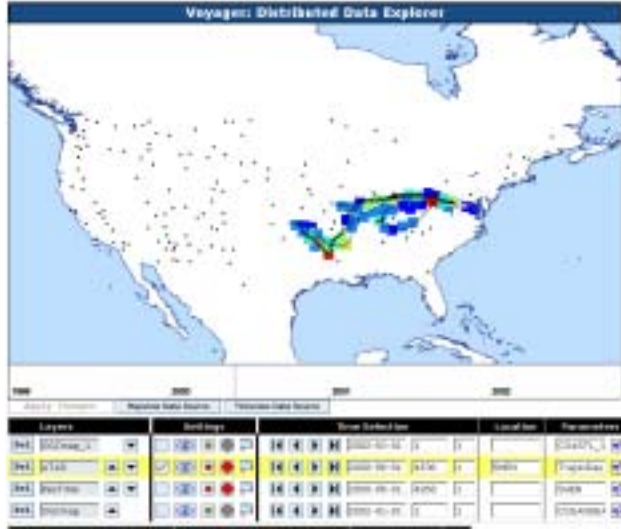


Figure 8. Residence time and ATAD trajectory data superimposed for June 1, 2000. The alignment of the two data sets verifies that the conversion of the data from their original formats into the SQL database was accurate.

The prototype user interface for defining a paired data query from the SQL server is shown in Figure 9. The input form allows the user to specify which parameter to return (display) and a parameter on which to impose the filter. If a paired query had been previously submitted on the dataset, those settings are displayed on the user input form. The form also allows the user to clear the current filter.

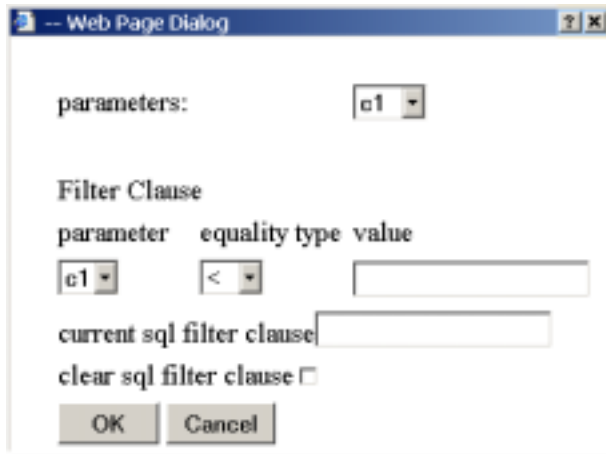


Figure 9. Prototype user interface for defining paired aerosol and trajectory queries.

The results of queries for residence time based on concentrations of the parameter c6 (sulfate and titanium) are shown in Figure 10. The first map displays the residence time when c6 is high while the second map shows residence times filtered for low c6 concentrations. The SQL query code for high c6 concentrations is provided in Figure 11.

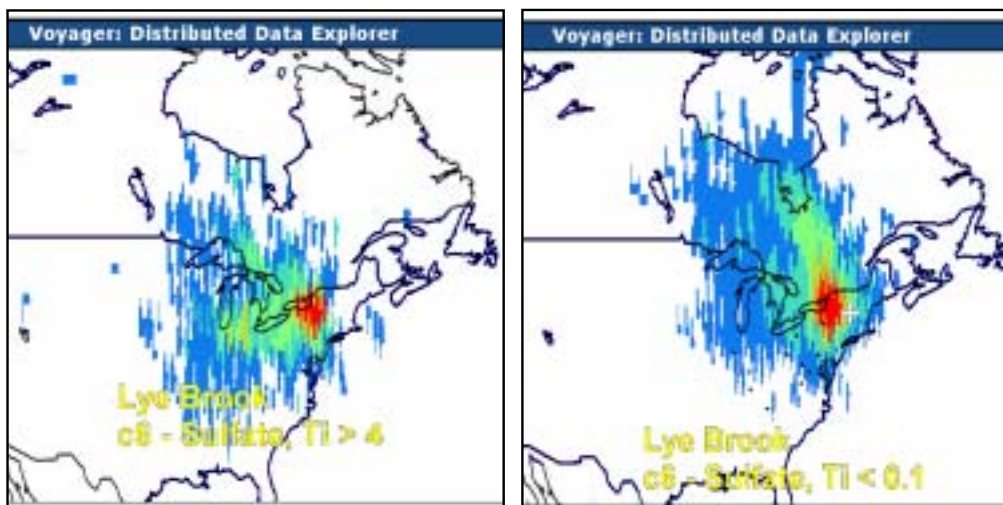


Figure 10. Paired query results for chemical 'source'/ResTime Data and PMF source C6 (Sulfate, Titanium) for Lye Brook.

```

SELECT Lat as lat,
       Lon as lon,
       Loc_Code as loc_code,
       SUM(ResTime) AS LYBR
FROM   dTrajResTime
WHERE  ([Date] IN
        (SELECT datetime
         FROM dSourceApp
          WHERE (Loc_Code = 'LYBR')and c6 > 4)
GROUP BY GridCode, Lat, Lon, Loc_Code
ORDER BY Lon ASC

```

Figure 11. SQL code for executing the paired query of PMF and trajectory databases.

Deliverable 4: Transfer the resulting database to a designated SQL server

Status: Not completed

The task of transferring the relational database from the CAPITA SQL server to another designated by the sponsoring organizations will be conducted after the queries and user interface components of the CATT are in final delivery form and have undergone adequate user testing.

We anticipate the transfer to be a straightforward task. The data and location tables and any stored queries in the aerosol and trajectory database can be directly copied into another relational SQL database. The new database 'address' would need to be recorded in a data catalog from which it would be accessed by the combined aerosol and trajectory tool.

PROJECT STATUS SUMMARY

A summary of the project status is provided in Table 1.

Table 1. Project Status Summary

Task	Deliverable	Status
Develop relational database of PMF/UNMIX and trajectory data	Relational Database of PMF/UNMIX and trajectory data	<i>Complete</i>
Develop specific SQL filtering and aggregation queries	Chemical filtering/aggregation query	<i>Developed, needs testing and feedback</i>
	Trajectory filtering/aggregation query	<i>Developed, needs testing and feedback</i>
	Paired Chemical/Trajectory data query	<i>Partially developed, needs user input, testing, feedback</i>
Develop graphical user interface to database	Graphic interface for user input (query) and for data output through web browsers	<i>Partially developed, needs user input, testing, feedback</i>
Transfer the resulting database to a designated SQL server		<i>Will be addressed after the combined aerosol and trajectory tool is completed.</i>

FUTURE MILESTONES AND DELIVERABLES

A substantial amount of the CATT development has been completed. The second half of the project will focus on user testing, component refinement and implementation.

Project Milestones for January through June 2003

1. February 1, 2003: Complete initial queries, user interface and displays
2. April 1, 2003: Finalize design/implementation of queries, user interface and displays
3. April-June 2003: 'Public' testing and user feedback
4. July 2003: Final combined aerosol / trajectory database tool delivery

Final Deliverable: Combined Aerosol and Trajectory Tool (CATT)

The final combined aerosol and trajectory data analysis tool will provide a user friendly graphical interface to multidimensional data including the UNMIX/PMF and residence time data

as well as complementary data from VIEWS and other meteorology and GIS databases. Figure 13 illustrates the data flow for the CATT system. Users interact with CATT browser that provides a user-specified integrated interface of multiple views to the input data. The views represent a particular ‘slice’ (i.e. space, time, chemical species) of the multiple dimensional database. The data cube is comprised of distributed data sources including the aerosol and trajectory data from either the CAPITA SQL database or a secondary SQL database to which it will be transferred. When the data resides on the CAPITA server it can be directly fed to the data cube and CATT browser. Data on non-CAPITA servers can be included in the CATT system using ‘wrappers’, middleware which encapsulates the data sources and removes data heterogeneity.

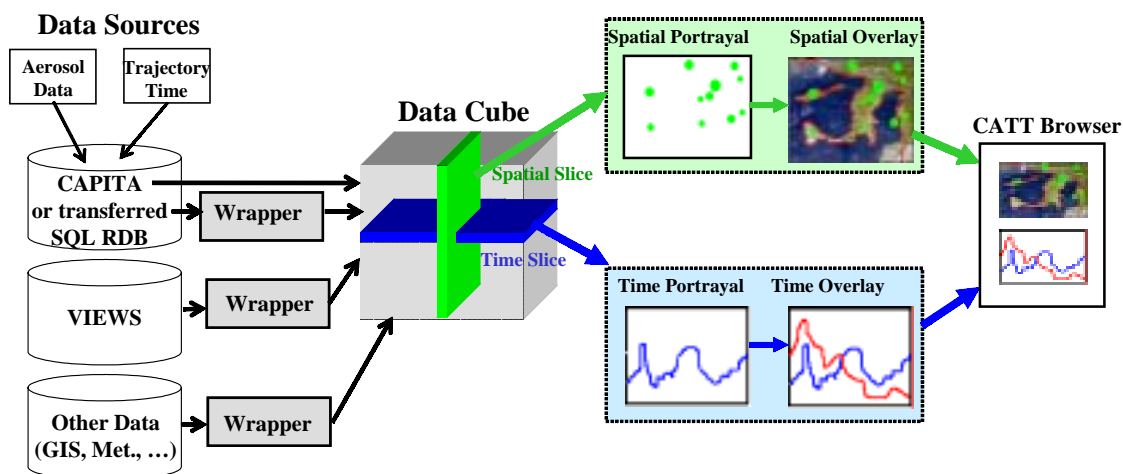


Figure 13. Data flow, processing, and rendering in the Combined Aerosol and Trajectory Tool (CATT).

It should be noted that while the CATT system is based on and shares a number of architectural components with the distributed Voyager system developed at CAPITA, CATT will be a stand-alone system with specialized features for aerosol and trajectory data access and analysis. At the conclusion of this project, the CATT system will attain ‘code freeze’ and will be no longer subject to updates in underlying architectural components allowing reliable use after this project has ended.

An online documentation, tutorial and help facility will be provided to aid users in learning the features of CATT and in browsing and exploring the aerosol and trajectory databases.

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