NEWDat Tool for PAMS Data Validation and Analysis

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for
National Ambient Air Monitoring Conference
Atlanta, GA

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## Glossary

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<th>Term</th>
<th>Definition</th>
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<td>ANT</td>
<td>AirNow-Tech</td>
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<tr>
<td>AQS</td>
<td>Air Quality System</td>
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<tr>
<td>Auto-GC</td>
<td>Automated Gas-Chromatograph</td>
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<tr>
<td>EPA</td>
<td>Environmental Protection Agency</td>
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<tr>
<td>NACAA</td>
<td>National Association of Clean Air Agencies</td>
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<tr>
<td>PAMS</td>
<td>Photochemical Assessment Monitoring Stations</td>
</tr>
<tr>
<td>PM$_{2.5}$</td>
<td>Particulate Matter smaller than 2.5 micrometers</td>
</tr>
<tr>
<td>STI</td>
<td>Sonoma Technology, Inc.</td>
</tr>
<tr>
<td>VOC</td>
<td>Volatile Organic Compounds</td>
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Outline

• Overview
• Getting Started
• Live Demonstration
• Next Steps
What Is VOCDat?

• A desktop software program c. 1995
• Used by PAMS community to validate VOC data and prepare data for AQS submission
• Used to analyze carbonyls, air toxics, and speciated PM$_{2.5}$
Motivation to Update VOCDat

- Evolution of desktop operating systems
- New types of auto-GC instruments
- Transition to web-based application
- Extension of existing infrastructure
Benefits of Web Applications

- Reduced hardware requirements
- No downloads or installation
- Centralized updates
- Improved data retention and security
- Collaboration, sharing, and publishing
- AirNow-Tech Integration
- Acquire data from other online systems (AQS, AirNow)
Initial Development Phase
November 2013 – September 2014

Develop the core functionality
- AQS requests
- File uploads
- Unit conversion
- Data aggregations
- Time series and data editing
- Scatter plots
- Bar charts (fingerprint)
- Screening checks
- Data exports and summary statistics

Overview

Idea exchange to prioritize features

Sonoma Technology, Inc.

National Association of Clean Air Agencies

EPA
Office of Air Quality Planning and Standards
New VOCDat Design

Overview

**EPA Data Mart**
- VOC, speciated PM, air toxics
- Meteorological data
- Ozone, PM mass, NOx, etc.

**VOCDat Website**
- Accessible from AirNow-Tech
- Import raw data files
- Request AQS data from Data Mart
- Edit null data codes
- View time series & scatter plots
- Screen data not meeting user-specified criteria
- Query data below MDL
- Output summary statistics
- Output AQS files

**User Data Files**
- AQS, PerkinElmer (*.txt), csv crosstab
- Single site at a time
- Limited date range

**Data Management System**
- Store user-specific data; delete after 6 months
- Calculate basic statistics, sum of values, etc.
- Perform unit conversions via lookup table

**Output Files**
- Data in AQS, csv crosstab format
- Summary statistics, screening results in .csv
- Save high-resolution graph images

Data Mart web service:
Select site, species category, date range
General Workflow in VOCDat

1. Add data to VOCDat
   - Data Dashboard
     - crosstab
     - aqs
     - txO

2. Explore data with graphs
   - Time Series
   - Scatter Plot
   - Bar Chart

3. Export data and statistics
   - Data Export
     - aqs
     - csv
Next Steps (1)

- Complete testing and release to AirNow-Tech
- Review feedback forms
- Identify & prioritize features for future phases
- Decide on a new name!

VOCDat release planned for late August!
# Next Steps (2)

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<th>Original VOCDat</th>
<th>New VOCDat (Phase 1)</th>
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<tr>
<td>Import data (AQS, TX0, ASCII)</td>
<td>✓</td>
</tr>
<tr>
<td>Export data (AQS, csv)</td>
<td>✓</td>
</tr>
<tr>
<td>Calculate aggregates (aromatics, carbonyls, paraffins, olefins, unidentified, sum of target compounds)</td>
<td>✓</td>
</tr>
<tr>
<td>Prepare data graphs (time series, scatter plot, fingerprint plot)</td>
<td>✓</td>
</tr>
<tr>
<td>Perform on-screen editing of data qualifier and null codes</td>
<td>✓</td>
</tr>
<tr>
<td>Perform QC screening checks</td>
<td>✓</td>
</tr>
<tr>
<td>Graph in elution order</td>
<td>✓</td>
</tr>
<tr>
<td>Easily change parameters on time series</td>
<td></td>
</tr>
<tr>
<td>Convert units on graphs</td>
<td></td>
</tr>
<tr>
<td>Apply user-defined scaling factors</td>
<td></td>
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<tr>
<td>Calculate weight percent</td>
<td></td>
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Next Steps (3)

Additional feature ideas from user feedback

- Data tables
- Additional import/export file formats
- Append to existing data sets
- Import multiple sites at once
- Secondary Y-Axis on time series
- Regression equations on scatter plot
- Edit data from scatter plot
- Custom aggregates on demand
- Stacked bar graphs
- Collocated/replicate data and precision/bias statistics
- Save graph setting for future use
- And more!
ATAQDat
(Analysis Tool for Air Quality Data)

ADAPT
(Air Data Analysis Program Tool)

NEWDat

MyDat

MyAirDat

Aeris
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Getting Started with VOCDat

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Background

• VOCDat was originally developed for the PAMS community to validate VOC data and prepare data for AQS submission.
• VOCDat was also used to analyze carbonyls, air toxics, and speciated PM$_{2.5}$.
• Evolution of desktop operating systems motivated the transition to a web-based application.

Timeline:
- 1995: Desktop VOCDat released
- 1995-2005: Updates and use by air quality community
- 2014: Transition to web application
To access VOCDat you must log in to AirNow-Tech. Use an Internet browser to navigate to http://airnowtech.org. This takes you to the AirNow-Tech home page.
AirNow-Tech Login

To enter, choose **Log In** in the upper right corner of the main page, above the navigation options.
To login, enter the credentials for an existing AirNow-Tech account and choose **Log In** or **Request an AirNow-Tech Account**.
To enter VOCDat, choose **VOCDat** from the **Tools** menu in the navigation options.
On your first visit, you will see the VOCDat Welcome page, to which you can return by clicking **VOCDat** at the top of any page.

1. **Add data to VOCDat**
   
   *Upload your AQS, crosstab or TXO-formatted files to store your data in the VOCDat server*

2. **Explore data with graphs**
To navigate VOCDat, use the **Manage**, **Explore**, **Export**, or **Help** links that appear at the top of each screen.

1. **Add data to VOCDat**
   - **Upload your AQS, crosstab or TXO-formatted files to store your data in the VOCDat server**

2. **Explore data with graphs**
Add Data to VOCDat

To get started using VOCDat, choose **Add data to VOCDat** from the Welcome screen or click **Manage**, then **add data**.

1. **Add data to VOCDat**

Upload your AQS, crosstab or TXO-formatted files to store your data in the VOCDat server

2. **Explore data with graphs**
Two options are available for adding data to VOCDat: file **Upload** and making an **AQS Request**.
To upload your own data files, select **Upload** from the menu of options and then complete the form.

Data in VOCDat are stored in data sets. Name your data set first.

Upload data in AQS format, crosstab format, or Perkin Elmer (*.tx0) format.

Upload your file with this button. Check the status by clicking **Manage**.
To add AQS data to VOCDat, choose **AQS Request** from the menu of options and then complete the form.

Data in VOCDat are stored in data sets. Name your data set first.

Make your request with this button. Check the status by clicking **Manage**.
The **Manage** page provides a summary of the data sets you have uploaded or requested from AQS. Add more data with the **add data** link.

Check the status of your data sets here. Once the status says “Available for use” the data are ready for graphing on the **Explore** page.
The **Explore** page provides three graph types: time series, scatter plot, and bar charts.

- Show and hide different graphs by clicking these icons.
- Zoom in and out on the graphs by dragging your mouse.
- Export graph images with this menu.
To create a time series, click the **Time Series** icon at the top of the **Explore** page. To add series to the graph, click the **add data** icon.
Select parameters from your available data sets. To draw the graph, click the **Minus** icon to close the menu.
Create a Time-Series Graph

Change the date range or y-axis minimum/maximum using the settings below the graph. Then click the **Graph** button to update the graph.
To edit data quality codes, first click on a point on the graph. Use the **Shift** or **Control** keys to select multiple data points.
Click on the **edit data** icon and choose to either **Update Null Codes** or **Update Qualifier Codes** from the menu. Select a single null code or up to ten qualifier codes.
To apply the selected code(s), click either the **Apply Qualifier Code/Null Code** button or the **Apply Qualifier/Null Code(s) to All Species** button.

Apply to all parameters in the data set with the same date/time as the selected data point(s).

Apply to only the selected data point(s).
Create a Scatter Plot

To create a scatter plot, click the **Scatter Plot** icon at the top of the **Explore** page. To add data to the plot, click the **plus** icon.
Select parameters from your available data sets. To draw the graph, click the **minus** icon to close the menu.
Create a Scatter Plot

Change the date range, parameters plotted on each axis, or axis minimum/maximum using the settings below the graph. Then click the **Graph** button to update the graph.

Set the date range of data to include in the graph and change the settings for the x-axis and y-axis.
To create a bar chart, click the **Bar Chart** icon at the top of the **Explore** page. To add data to the chart, click the **plus** icon.
Select parameters from your available data sets. To draw the graph, click the **minus** icon to close the menu.
Create a Bar Chart

Change the date range or y-axis minimum/maximum using the settings below the graph. Then click the **Graph** button to update the graph.
To toggle through time, click the +1 hour or -1 hour links.
The Export page provides the ability to set up custom screening checks, export data to a file, and export summary statistics to a file.

Set up custom screening checks for data quality control.

Export data or summary statistics to a file.
To help assess data quality, set up screening check(s) on the **Export** page. Name your file and then click **Export** to download a file with any data records that failed the screening check(s). Click the **add new check** icon to set up multiple checks.

Select from five types of screening checks.
To export data from VOCDat, choose either the Export Data or Export Summary Statistics radio button. Click Select data for export to specify the data to export. Optionally for data file export, choose to include missing data or perform data method detection limit substitutions.
More information is available about the following:

- **EPA AQS**
  [http://www.epa.gov/ttn/airs/airsaqs/](http://www.epa.gov/ttn/airs/airsaqs/)

- **EPA Datamart**
  [http://www.epa.gov/ttn/airs/aqsdatamart/](http://www.epa.gov/ttn/airs/aqsdatamart/)

- **PAMS Data Validation and Analysis**
  [http://www.epa.gov/ttnamti1/pamsworkbook.html](http://www.epa.gov/ttnamti1/pamsworkbook.html)

- **VOCDat User’s Guide - coming soon!**