PARTICLE INSTRUMENTS-

Particle Sizers

# Model 390069

Data Merge Software Module

For Merging and Fitting of SMPS<sup>™</sup> and APS<sup>™</sup> Data Files

User's Guide

P/N 1930074, Revision D April 2011



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# Model 390069

Data Merge Software Module

For Merging and Fitting of SMPS<sup>™</sup> and APS<sup>™</sup> Data Files

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# **Manual History**

The following is a manual history of the Model 390069 Data Merge Software Module (for merging and fitting of  $SMPS^{TM}$  and  $APS^{TM}$  data files) User's Guide (Part Number 1930074).

| Revision | Date           |
|----------|----------------|
| A        | July 2005      |
| В        | October 2005   |
| С        | September 2010 |
| D        | April 2011     |

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# **About This Manual**

# Purpose

This is a user's guide for installing and using the Model 390069 Data Merge Software Module (for merging and fitting of  $SMPS^{TM}$  and  $APS^{TM}$  data files).

# **Related Product Literature**

- Model 3936 Scanning Mobility Particle Sizer<sup>™</sup> (SMPS<sup>™</sup>) Spectrometer Instruction Manual, part number 1933796, TSI Incorporated
- Model 3034 Scanning Mobility Particle Sizer<sup>™</sup> (SMPS<sup>™</sup>) Spectrometer Operation and Service Manual, part number 1980842, TSI Incorporated
- Model 3321 Aerodynamic Particle Sizer<sup>®</sup> (APS<sup>™</sup>) Spectrometer Instruction Manual, part number 1930092, TSI Incorporated
- Aerosol Instrument Manager<sup>®</sup> Software for APS Spectrometers Manual, part number 1930064, TSI Incorporated)
- Aerosol Instrument Manager<sup>®</sup> Software for SMPS Spectrometers Instruction Manual, part number 1930104, TSI Incorporated

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# CHAPTER 1 Introduction

The Model 390069 Data Merge Software module<sup>\*</sup> offers researchers a consistent method of merging and fitting particle size distributions from two well-known TSI aerosol instruments, the Scanning Mobility Particle Sizer<sup>™</sup> (SMPS<sup>™</sup>) spectrometer and the Aerodynamic Particle Sizer<sup>®</sup> (APS<sup>™</sup>) spectrometer, to produce wide range composite particle size distributions, curves and statistics for analysis.

The Model 390069 Data Merge Software enables you to quickly and easily merge and fit SMPS and APS data files to produce particle size distributions covering all three modes of particles found in the atmosphere—nuclei, accumulation, and coarse mode aerosols. The software is designed to work with a variety of SMPS spectrometers and APS spectrometers that use TSI's Aerosol Instrument Manager<sup>TM</sup> software. As a result, wide particle size distributions ranging from 0.0025 to 20 micrometers can be created, depending on the SMPS system configuration.

With Data Merge Software you can:

- Process a set of SMPS distributions (samples) together to find the *average* of the entire set, *or* calculate a *set of averages*, each representing the average for a specific, regular time-interval.
- Process a set of APS distributions (samples) together to find the *average* of the entire set, *or* calculate a *set of averages*, each representing the average for a specific, regular time-interval.
- Convert APS data to "Mobility Diameter" units or SMPS data to "Aerodynamic Diameter" units.
- Merge an SMPS distribution with an APS distribution to form a Composite distribution. The Composite distribution can be expressed in Mobility or Aerodynamic Diameter units.
- Fit model functions (Lognormal or Rosin-Rammler) to the SMPS, APS and Composite data to produce an accurate estimate of the frequency size distribution from 0 to ∞ and produce statistics that can be used to *characterize* the distributions.
- Merge averaged distributions—Use the Averaging feature as a pre-process to Merging.

<sup>&</sup>lt;sup>\*</sup>Developed under agreement with Chimera Technologies, Inc.

- Save Averaging/Merge settings and sample lists to a file then later Restore those settings to duplicate or modify a processing session.
- Export data from any stage of the process to tab-delimited text files for input to other software.
- Export customized graphs to WMF, BMP, PNG, of JPG image files or to the Windows clipboard for inclusion in reports, presentations, websites, etc.

# Notations/Conventions Used in This Manual

- Throughout this manual when reference is made to "Windows," it implies Windows<sup>®</sup> 2000 or Windows<sup>®</sup> XP.
- Bold face type is used to indicate that you should perform the indicated action. For example "select the **File** menu" means that you should use the mouse and click on the menu called File.
- When instructions direct you to select items from a menu, a vertical bar (1) is used to separate the items you should select. For example, "select **File** | **Properties** | **Scheduling**" means you should click on the File menu, then select the Properties item, and then select the Scheduling tab.

# CHAPTER 2 Typical Workflow Overview

In this overview, a typical Data Merge Software module workflow is outlined. The workflow is presented in a logical sequence, but Data Merge Software is designed to be fully interactive—all options can be changed at any time during the process and results recalculated.

The input to Data Merge Software will be data from SMPS and APS data files created by Aerosol Instrument Manager<sup>®</sup> software. To do useful work, Data Merge Software module must have access to one or more of these SMPS/APS data files. The typical workflow would start by collecting your data files and moving them to the computer that will be running Data Merge Software module or by making them available via network connection.

Next you would use Data Merge Software module Browse or Search features to select samples from your data files that you wish to include in your averaging/merging process. Samples that you select are gathered into a "sample list".

At this point of the process, you might preview some or all of the samples in your sample list(s) and select any Data pre-processing options such as applying efficiency correction to APS data, applying multiple-charge correction to SMPS data, etc.

If Averaging is part of your process, you would next set up the averaging settings and enable averaging.

In preparation for Merging, you would next use on-screen cursors to "window" the SMPS and APS data to exclude "noise" in the tails of the distribution or otherwise focus on areas of interest within the data.

The next step in Merging would be to select merge settings. This includes setting up the fitting functions for the modes of the SMPS, APS and Composite data sets (up to 3 modes per set) and choosing SMPS channels per decade settings.

Once you have set the initial parameters for a Merge, you would initiate a Merge by clicking the Merge button. After the initial Merge, merging parameters, data windowing, data pre-processing, etc. can all be changed and the Merge recalculated with the changed parameters. This will often be an iterative process as you refine the parameters of the Merge.

After you are satisfied, you may wish to Export your results to a file to log them and to import them into other software programs.

Another option would be to export the plotted data graph image to the clipboard or a file for use in reporting.

You would typically save the Averaging/Merge sample lists and settings to a file so that you could easily restore the settings later and reproduce your results.

# CHAPTER 3 Installing the Software

This chapter describes the installation requirements for the Data Merge Software module and the installation procedure.

# Installation Requirements

To use this software you will need:

- PC with 300 MHz or higher processor clock speed recommended; 233 MHz minimum required (single or dual processor system);\* Intel Pentium/Celeron family, or AMD K6/Athlon/Duron family, or compatible processor recommended.
- Super VGA (800  $\times$  600) or higher-resolution video adapter and monitor.
- Microsoft Windows<sup>®</sup> XP, Vista<sup>®</sup> (32 bit), or Windows<sup>®</sup> 7 (32 or 64 bit) operating systems.
- A hard drive large enough to accommodate Windows, the Data Merge Software, and data files.
- A CD-ROM drive (for installing software from CD).
- 128 MB or more of random access memory (RAM).
- Keyboard and Mouse.
- A Microsoft Windows-compatible printer is optional.

# Installation

Install the Data Merge Software module as follows:

- **1.** Shut down (exit) all programs/applications on the Windows desktop.
- **2.** With the computer on and Windows running, insert the Data Merge Software CD-ROM in your CD drive to run the **setup.exe** from the CD.
  - **a.** If AutoPlay is enabled on your PC, the setup program will begin automatically and the introduction screen will be displayed on the Windows desktop.

- **b.** If AutoPlay is not enabled, select **Run** from the **Start** menu and type: D:\SETUP (where D is the letter corresponding to your CD drive) in the Open box and press **OK**.
- **3.** Follow the instructions as the setup program runs. When setup is complete, you should read the README.TXT file. The README.TXT file contains information that could not be included in this manual. If you decide not to read the file immediately, you can access the file later using a text editor such as Notepad.

The setup program creates a directory (folder) called "Data Merge Software Module" on your hard disk (assuming you accepted the default directory name). The directory contains the required program files, sample data files, and an electronic file of this manual.

You will find a "Data Merge Software Module" icon on your desktop and in the Start menu under **Program Files | TSI | DataMerge**.

*Note:* Before creating a TSI menu item, the setup program checks for an existing one. If one is present, it adds the icon only.

# CHAPTER 4 Software Operation

This chapter is designed to give you an introduction to the operation of the Data Merge Software module. Using it, you will:

- Start the program
- Select samples for processing
- Select and view samples
- Data averaging
- Data merge and fitting
- Save and restore settings
- Export results to a file
- Batch processing
- Quit the program

# Start the Program

To start the program, proceed as follows:

From the Windows desktop, press the **Start** menu and then select **Programs | TSI | Data Merge | Data Merge Software Module.** 

The Data Merge Software main interface screen appears as shown in Figure 4-1.



The Data Merge Software Module Main Interface Screen

# **Select Samples for Processing**

The first step in preparing to process data with Data Merge Software is to select samples found in your data files and collect them into a "sample list". Samples from multiple files can be collected together into a single sample list. Data Merge Software maintains two (2) main sample lists: the SMPS sample list and the APS sample list. There are a number of tools available to help you build your sample lists.

# **Search for Samples**

Use this feature to select samples based on a number of search criteria such as date range, day of week, and time of day.

Search for Samples button is located on the main interface screen between the SMPS and APS sample lists. Click the button to open the **Sample Search** dialog.

The first step in searching for data samples is to select the base folder for the search.



Click the **Look in**: button to select the base folder for the search. When the search is initiated, Data Merge Software module will search through the files found in this base folder.

If you select **Search Subfolders** by checking the box, Data Merge Software will search the selected base folder and also any subfolders found below the base folder. This can be useful if your SMPS and APS data files are organized into separate subfolders under a single base folder.



Use Begin Date and the End Date to select a range of dates for the sample search. Use the **All Dates** checkbox to easily include samples of any date in the search range. If you click **Find Folder Date Range**, Data Merge Software will determine the true date range of the files in the search folder(s) based on sample timestamp and fill in the Begin and End dates to reflect that range.

You can also select the days of the week that you want to include in the search criteria. When specific days of the week are selected, only samples from the specified days will be included in the sample search. Use the pull-down to quickly select **All Days**, **Weekdays**, Weekend Days or to clear the day-of-week selection.

You can narrow the search further by selecting a specific daily time-of-day range. For example, you can set the time-of-day range Between 7:00 AM and 9:00 AM.

Use the **Select Span** pull-down to quickly select a preset time-span such as 15 minutes, 30 minutes, 1 hour, 2 hours, etc. When you select a time span from the pull-down, the end time of the time range will change to reflect the selected span of time.

If **Lock to span** is checked, when you change the time in the first time range box, the second time will track it, maintaining the selected time span.

| Search Criteria                                   |  |  |  |
|---|--|--|--|
| Include data only within this range of dates:     |  |  |  |
| Begin Date: 7/ 6/2004                             |  |  |  |
| End Date: 7/ 6/2005                               |  |  |  |
| I All Dates                                       |  |  |  |
| Include data only from selected days of the week: |  |  |  |
| All Days 💽 🔽 Wednesday                            |  |  |  |
| 🔽 Sunday 🔽 Thursday                               |  |  |  |
| 🔽 Monday 🔽 Friday                                 |  |  |  |
| 🔽 Tuesday 🔽 Saturday                              |  |  |  |
| Include data only from selected daily time range: |  |  |  |
| Between 12:00 AM                                  |  |  |  |
| and 12:00 AM 븣                                    |  |  |  |
| or select span of 🛛 Full Day 🔍                    |  |  |  |
| 🔲 Lock to span                                    |  |  |  |
| Include only file names that include the text:    |  |  |  |
| fine (blank field matches all)                    |  |  |  |
| Include only data of type:                        |  |  |  |
| C SMPS C APS   Both                               |  |  |  |
|   |  |  |  |
| Create new list     Search                        |  |  |  |
| C Add to existing list                            |  |  |  |

Figure 4-2 Search Criteria Dialog Box

You can also filter the search based on the file name. Enter a string of text in the field labeled **Include only file names that include the text**:. Only files that contain that text in the file name will be included in the search. The matching is case-insensitive.

You can set the Search Criteria to search for SMPS data files, APS data files or Both. When SMPS and APS samples are well correlated, it is very convenient to search for both types of data in the same search.

When searching for samples, you can choose to **Create new list** or **Add to existing list**. Use this feature to build a list of samples that don't fit into a single criteria. For example, you could first search for samples between 8:00 AM-9:00 AM, then change your criteria to find samples between 5:00 PM-6:00 PM, select **Add to existing list** and search again to create a list that contains samples from both time ranges.



Once you have selected the appropriate criteria,

click the **Search** button to initiate the sample search. Data Merge Software will search through files located in the base folder (and subfolders if selected), apply the search filtering criteria to each file and each sample and then return a list of samples that match the search criteria in the Selected Files & Samples list.



Figure 4-3 Selected Files & Samples List

You can manually remove files or samples from the list by rightclicking the item and selecting **Remove**..from the context menu. This only removes the item from the list, it does not affect the data file.

<u>A</u>ccept List

Once you are satisfied with the contents of the sample list, click **Accept List**. Click **Cancel** to and return to the main screen

reject the new list and return to the main screen.

# **Browse SMPS/APS Files**

Another way to select samples for processing is to "browse" for data files and select samples manually. On the main interface screen, under each sample list, you will find these browse buttons:

Browse SMPS Files Browse APS Files

Software Operation

When you click the **Browse SMPS Files** or **Browse APS Files** button, you will be presented with a file/sample browser dialog (Figure 4-4).

| elect officio outripica         |  | 2 🛛                        |
|---------------------------------|--|----------------------------|
| Look in: 🔁 TSI_Lab_Tests        | . ← È 💣 ⊞·                             | -                          |
| Name 🔺                          | Size Type                              | Date Modified 🔨            |
| AC fine222.580                  | 193 KB 580 File                        | 6/30/2005 12:35 PM         |
| AC fine.580                     | 193 KB 580 File                        | 6/8/2005 5:07 PM           |
| Candle Smoke 2.1.580            | 1,428 KB S80 File                      | 12/2/2004 10:56 AM         |
| Candle Smoke 2.580              | 1,512 KB S80 File                      | 12/2/2004 1:00 AM 🗧        |
| Candle Smoke.580                | 577 KB S80 File                        | 1/31/2005 12:48 PM         |
| Incense in Smoke Chamber 2      | 757 KB S80 File                        | 11/30/2004 1:26 PM         |
| Incense in Smoke Chamber.580    | 423 KB 580 File                        | 1/31/2005 12:56 PM         |
| 🖬 Laskin 25psi 2.580            | 49 KB 580 File                         | 12/3/2004 4:40 PM          |
| 🔳 Laskin 25psi 3.580            | 13 KB 580 File                         | 12/3/2004 5:00 PM          |
| 🔳 Laskin 25psi.580              | 493 KB 580 File                        | 12/3/2004 4:17 PM 💦        |
| I advin Conservator COD         | 100 VD CON Ella                        | 10/0/004 10/E0 AM          |
| File name: AC fine.S80          |  |                            |
|                                 |  |                            |
| Files of type: AIM SMPS Data    |  | <b>_</b>                   |
| Recent Folders C:\Merge Data Se | ts\TSI_Lab_Tests                       | •                          |
| AC fine.S80                     |  | Total Samples in file: 16  |
| Sample Data                     |  | ~                          |
| 22000                           | ······································ | 4 13:44:43 Thu 1 of 16     |
| 2000                            | Ŭ 12/02/0/                             | 4 12:49:42 Thu 2 of 16     |
| 1000                            | 0 12/02/04                             |                            |
| £14000                          |  | 4 13:54:43 Thu 3 of 16     |
| 8_12000                         |  | 4 13:59:43 Thu 4 of 16 🛛 🧹 |
| 8 10000                         |  | Clear Selection            |
|                                 | Selected Sample,                       | cical Selection            |
| 4000                            | Llick + to add to list                 | 1                          |
| 2000                            |  |                            |
|                                 | Add All File Samples                   | OK Cancel                  |
| Hobes Deameer (nm)              |  |                            |
|                                 |  |                            |

Figure 4-4 Select SMPS Samples Dialog Box

The upper section of this screen presents a familiar file browser that you can use to browse to a specific folder. Use the Recent Folders drop-down to quickly jump to recently used folders. When you first start using the software, the Recent Folders list will be empty, but over time a listing of folders you've visited will be created for you to select from.

To add samples from a file to your sample list for processing:

- Select the file of interest with a single left-click. The first sample from the selected file will appear on the preview graph.
- Use the **up/down arrow buttons** or type a number into the Selected Sample field to select a different sample for previewing.
- Click the + button to add the sample you are previewing to your sample list.
- Click **Add All File Samples** to add *all* of the samples from the selected file to the list.

You can also view samples that have already been added to the sample list by selecting that sample item from the list.

When you right-click on samples in the list, a menu will pop-up that will give you an option to Remove a sample from the list. You can also click **Clear Selection** to remove all samples from the list. This only removes the items from the list, it does not affect the data file.

When you are done selecting samples, click **OK**. Click **Cancel** to dismiss the file browser and quit the sample selection process.

As a short-cut, if you simply want to select all samples from a single specific file, browse to the folder where the file is located, and double-click the file. This will automatically select all of its samples into the list and close the browser dialog, as if you had clicked **OK**.

### Save/Restore

You can also load samples into a sample list using the **Save/Restore** feature. Since this is a more advanced feature that involves saving and restoring other program settings, it will be described more completely in a later section of the manual.

# Select and View Samples

Once you have selected samples into one or both sample lists you can view them on the main screen graph. Left-click the sample from the list that you wish to view (Figure 4-5).

✓ Sync Lists → If Sync. Lists is checked and both lists have samples in them, making a selection in one list will also change the selection in the other list. When you select a sample from one list, the Sync. Lists feature will attempt to find the sample in the other list that most closely matches in time. This feature works best when the SMPS and APS sample times are well correlated.

When **Sync. Lists** is unchecked, you must select samples from each list individually.



**Figure 4-5** Data Merge Software Module Dialog Box

When you right-click a selection in a sample list (Figure 4-6), a context menu will appear. This allows you to view a sample from the list or remove it. When you choose to remove an item, this only removes the item from the list, it does not affect the data file.



#### Figure 4-6

Right-click a Selection in a Sample List

## Windowing the Data

Using the on-screen cursors, it is possible to define a region of interest for each data set (SMPS and APS). This windowing will affect the calculation of data statistics and also how the two data sets are merged and fitted.

To select a region of interest for each data set, simply drag the associated left and right cursors into the desired position. As the

cursor is being dragged, you will notice that the cursor position value is displayed above the moving cursor line.

## **Diameter Scale Units**

Most of the controls for Data Merge Software are accessed using the **Settings & Reports** button. The first page of the Settings and Reports property sheet is Graph Settings. Included on this screen are the controls for setting the Diameter Scale Units.



Figure 4-7 Diameter Scale Units Dialog Box

Within Aerosol Instrument Manager Software the diameter values for particle data is represented on two different scales. Diameters for SMPS data are expressed in Mobility diameter units and diameters for APS data are expressed in Aerodynamic diameter units.

To merge the two data types accurately, it is important that both data types use the same diameter unit. To accurately convert the data from one diameter unit to the other, it is important to provide a Density parameter and a Shape Factor parameter. Click the **?** button to see a table of densities and shape factors for common particle materials and geometric shapes. When both parameters are 1, there is no difference between the two scales.

An example of the effect of the Density parameter is shown in Figure 4-8 and 4-9 below.





Here APS data is being converted to Mobility Diameter using a Density parameter of 1



#### Figure 4-9

In this example, the Density parameter has been set to the assumed density for this material (2.65g/cm<sup>3</sup>)

To change the values for Density and Shape Factor, enter a new value into the associated text field. Click the **Apply** button to see the effect of new values on the plotted data.

Use the **Mobility Diameter/Aerodynamic Diameter** radio button controls to select the diameter scale unit for the plotted data.

# **Data Preprocessing Settings**

To access the Data Preprocessing controls, click **Settings & Reports** button and select the **Graph Settings** tab:

| □ Data Preprocessing           □ ✓           □ ✓           ▲ Apply APS Efficiency Correction | Apply SMPS Multiple Charge Correction | Obey File View Boundaries |
|--|---------------------------------------|---------------------------|
|  | Apply SMPS Diffusion Correction       | Gas Density (g/cc) 0.0012 |

#### Figure 4-10

Data Preprocessing Dialog Box

Use these controls to select options for data preprocessing (processing that is applied to the input data prior to merging).

#### Table 4-1

Descriptions of Data Preprocessing Settings

| Option                                      | Description  |  |  |
|---|--|--|--|
| Apply APS<br>Efficiency<br>Correction       | When this is selected, predefined corrections are<br>applied to the APS data to compensate for counting<br>inefficiencies in the lowest range of the APS device.<br>Applying the correction will generally give a more<br>accurate result.   |  |  |
| Apply SMPS<br>Multiple Charge<br>Correction | Applies a Multiple Charge correction to the SMPS<br>data. This is the same correction that is available in<br>Aerosol Instrument Manager Software. The Model<br>3034 SMPS device applies this correction internally,<br>so this setting will not affect data from that device.   |  |  |
| Apply SMPS<br>Diffusion<br>Correction       | If this box is selected (a checkmark indicates it is<br>selected), it enables a mathematical correction for<br>diffusion losses. It is especially important to use<br>diffusion loss correction when sizing aerosols smaller<br>than 100 nm, since in this size regime diffusion<br>becomes increasingly important.<br>This is the same correction that is available in<br>Aerosol Instrument Manager <sup>®</sup> Software. This<br>correction does not affect data from the 3034 SMPS<br>device.<br>Enter the carrier gas density. This will be used in the<br>calculation of the Diffusion Correction.<br>See Appendix G in the Aerosol Instrument Manager <sup>®</sup> |  |  |
|   | calculation of the Diffusion Correction.<br>See Appendix G in the Aerosol Instrument Manager <sup>®</sup><br>Software Manual for more information.   |  |  |

| Option                       | Description   |  |
|------------------------------|---|--|
| Obey File View<br>Boundaries | When this setting is unchecked (default), data is<br>read in from the data files ignoring any boundary<br>settings (cursor positions) set from within the<br>Aerosol Instrument Manager software—the entire<br>data set is available for use within Data Merge<br>Software.   |  |
|                              | When this setting is checked, Data Merge Software<br>will obey the boundary settings imposed by the<br>Aerosol Instrument Manager software and only use<br>the data within Aerosol Instrument Manager<br>software's defined view boundaries.  |  |
|                              | Aerosol Instrument Manager software saves one set<br>of view boundaries per data file, so you could use<br>Aerosol Instrument Manager software to pre-window<br>data for averaging. For example, the lower 2/3 of a<br>distribution from one SMPS file could be averaged<br>with the upper 2/3 of a distribution from another<br>SMPS file. |  |

# **Graph and Export Settings**

To access the Graph and Export Settings, click the **Settings & Reports** button on the main screen and select the **Graph Settings** tab (Figure 4-11).

| ſ | Graph and Export Settings |                         |                           |  |  |
|---|---------------------------|-------------------------|---------------------------|--|--|
|   | Show SMPS Data            | Show SMPS Fit           | Show SMPS Cursors         |  |  |
|   | 🔽 Show APS Data           | Show APS Fit            | Show APS Cursors          |  |  |
|   | 🔲 Show Composite Data     | Show Composite fit      | Hide data outside cursors |  |  |
|   | Plot Modes Summed         | O Plot Modes Separately | Disk Click on the secol   |  |  |
|   | 🔲 Use Log Y Scale         | Weight Number           | for additional settings   |  |  |
|   |                           | <u>\</u>                |                           |  |  |

#### Figure 4-11

Graph and Export Settings Dialog Box

These controls determine how the input and output data will appear on the graph and when exported to a file.

The **Show**...controls (**Show SMPS Data**, **Show SMPS Fit**, **Show SMPS Cursors**, etc.) determine which data sets or cursors are to be displayed on the graph (note that the Composite Data, SMPS Fit, APS Fit and Composite Fit will not be displayed on the graph until after a Merge has been initiated).

Normally, SMPS and APS data outside of the respective cursors will be shown in a light gray color. If **Hide data outside cursors** is selected, data outside of the cursors will not be shown on the graph at all. **Plot Modes Summed/Plot Modes Separately** affects the way that multi-modal fit data will be displayed on the graph—summed together into a single curve or plotted as separate curves.

When **Use Log Y Scale** is checked, the graph will be displayed with a logarithmic Y scale. *This setting does not affect exported data*.

Use the **Weight** drop down list to select the weighting for the data displayed on the graph. The choices are **Number**, **Diameter**, **Surface**, **Volume**, and **Mass**.

*Note*: The selected weighting will be used when the data is merged.

## **Data Hot-Spot Cursors**

When you click on a data point on the graph, a pair of cross-hair Hot-Spot cursors will appear and the data x and y values will be displayed. The Hot-Spot cursors can be dragged around the graph to show the x-y values for various points on the graph. To hide the Hot-Spot Cursors, right-click on the graph and select **Clear Hot-Spot Cursors** from the context menu that appears (See "Graph Context Menu" in the next section).

## **Graph Context Menu**

When you right click on the Graph window, a context menu will appear that allows you to set some additional properties of the graph, and allows you to export or print the graph image.



Figure 4-12 Graph Context Menu

| Option                    | Description  |
|---------------------------|--|
| Border Style              | Select border style for the graph.   |
| Font Size                 | Select or changes the font size for the graph.   |
| Plotting Method           | Select a plotting method for the graph.  |
| Grid Options              | Select grid options on the graph.  |
| Include Data<br>Labels    | Include data labels on the graph.  |
| Mark Data<br>Points       | Mark data points on the graph.   |
| Show Legend               | Show a legend on the graph.  |
| Maximize                  | Temporarily show the graph in a full screen mode.  |
| Log Y Scale               | Display the graph with a logarithmic vertical scale.   |
| Use Monochrome<br>Scheme  | Display the graph in a monochromatic scheme that works well with monochrome printers.                              |
| Export Graph<br>Image     | Export the graph image to the clipboard or to a file.  |
| Print                     | Print the graph image.   |
| Reset Merge               | Reset the current Merge. No new merge will be<br>performed on the data until the Merge button is<br>clicked again. |
| Clear Hot-Spot<br>Cursors | Hide Hot-Spot cursors that are visible on the graph display.   |

 Table 4-2

 Descriptions of Graph Context Menu Options

# **Data Averaging**

Data Merge Software can be used to average samples of the same type. SMPS samples can be averaged with other SMPS samples and APS samples can be averaged with other APS samples. You can perform averaging alone or as a pre-process to Data Merging.

You can average an entire list of samples to create a single average sample as the result or you can set an Averaging interval and create a list of averages representing the averages at regular time intervals.

## **Select Samples for Averaging**

Using "Search" or "Browse" methods described in the earlier sections, select 2 or more samples into one of the sample lists (SMPS sample list, or APS sample list). To perform averaging, you need to have at least two input samples in at least one of the samples lists.

# **Averaging Setup**

Averaging Setup

To access the Averaging Setup screen, click **Averaging Setup** on the main interface screen.

### Finding a Single Average for an Entire List

Select **Use Average of entire list** then click **OK**. Enable Averaging to see the result.

| Averaging Setup                     |        |
|-------------------------------------|--------|
| Averaging interval (hh:mm:ss)       | ОК     |
| (Use 00:00:00 for 24 hour interval) | Cancel |
| Use Average of entire list          |        |

#### Figure 4-13

Averaging Setup—Use Average of Entire List

### **Creating a List of Interval Averages**

Select an averaging interval by typing numbers into the Averaging interval time fields or by using the up/down arrow buttons. If possible, you should pick a value that is a multiple of the sampling frequency of the unprocessed list. For example, if the samples in the list represent one sample every 5 minutes, then the lowest practical averaging interval would be 10 minutes—this would average the samples together in groups of two. Setting the Averaging interval to 20 minutes would average groups of 4 samples, etc. When you have selected the averaging interval, click **OK**. Enable Averaging to see the result.



#### Figure 4-14

Select Averaging Interval using Averaging Interval Time Fields

# **Enable Averaging**

✓ Enable Averaging On the main screen, use the **Enable Averaging** checkbox to turn averaging on and off. When it is checked, the sample list will display one or more time-labeled samples that represent the average(s) of the original sample list. You can select the averaged samples for viewing just as you would regular file samples. When Enable Averaging is unchecked, the original sample

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list is again displayed. You can easily toggle back and forth between the original and the averaged list using this checkbox control.

#### Using "Obey File View Boundaries" Setting to Affect Averaging

Similar to Aerosol Instrument Manager software, Data Merge Software maintains a single set of cursor positions (or "view boundaries" as they are called within Aerosol Instrument Manager software) per sample list—you cannot set up different windowing per sample.

In some cases, it might be desirable to average one section (set of bins) of a particular distribution with a different section of another distribution. Since Aerosol Instrument Manager software saves one set of view boundaries per data file, you could use Aerosol Instrument Manager software to pre-window data for averaging. For example, the lower 2/3 of a distribution from one SMPS file could be averaged with the upper 2/3 of a distribution from another SMPS file.

To accomplish this, set the view boundaries of your data in Aerosol Instrument Manager software, save, and close your data files, select them into Data Merge Software and enable **Obey File View Boundaries** (found under **Setting & Reports | Graph Settings** tab).

# **Data Merge and Fitting**

Within the Data Merge Software, the terms "Merge" and "Merging" refer to the process of combining an SMPS distribution with an APS distribution to form a single "Composite" distribution and then fitting size distribution model functions to the measured data. The fitting provides an accurate estimate of the frequency size distribution from 0 to  $\infty$ . If sufficient data is available, the fitted functions provide an extrapolation of the frequency distribution function beyond the range of the measured data.

Utilizing the *Distribution Fitting and Merging (DFM) engine* licensed from Chimera Technologies, the Merge feature of Data Merge Software Module will:

- Fit multiple, independent size-distribution functions (i.e., multimodal fit) to individual component data sets (SMPS and APS).
- Combine multiple component data sets (SMPS and APS) into a single composite data set.
- Fit multiple, independent size-distribution functions to the Composite data set.

Data Merge Software provides an interface that allows you to perform data merging interactively so that you will be able to manipulate the appropriate parameters and quickly see the effect on the Merge result.

## **Fitting Modes and Models**

Data Merge Software will fit distribution model functions to the SMPS and APS input distributions and the Composite distribution that Data Merge Software creates by combining SMPS and APS distributions. The user selected weighting (Number, Diameter, Surface Area, Volume or Mass) is applied to the SMPS and APS data before it is passed to the fitting engine.

For each of these three data sets, Data Merge Software can fit up to three modes to the data. Some SMPS, APS distributions can be fit with reasonable accuracy with just a single mode (Figure 4-15).



Figure 4-15 Lognormal, Single Mode Fit

Other distributions are more obviously multi-modal (Figure 4-16).



Figure 4-16 Lognormal, 2 Mode Fit

For *each* of the three available modes, Data Merge Software can fit either a Lognormal function or a Rosin-Rammler function to the distribution.

# **Fitting Methods**

To setup the Data Merge Software Module for fitting, the types of distribution functions to use for each of the modes must be specified. The options are to either explicitly specify the distribution function for each mode (e.g., Lognormal, Rosin-Rammler, or none), or to select one of two *automatic* fitting methods for each mode and to let the Data Merge Software determine which distribution functions best represent the distribution.

The fitting method can be specified *separately for each mode*. That is, for the three modes available with the Data Merge Software, one mode could use the Full Automatic Fitting method, a second mode could use the Constrained-Automatic Fitting method, and the third mode could use the Constrained Fitting method.

Using the Constrained Fitting Method, you specify *exactly* which function (Lognormal or Rosin-Rammler) you want the Data Merge Software to fit to each mode of the distribution. The Data Merge Software module will perform the fit exactly as you have specified.

The two automatic fitting methods are

- Full Automatic Fitting (Full Auto)
- Constrained-Automatic Fitting
  - o Lognormal Automatic (Lognorm. Auto)
  - o Rosin-Rammler Automatic (R-R Auto)

With the Full Automatic Fitting method, the Data Merge Software determines two things

- The number of modes in the distribution
- The distribution function type used to represent each mode

With the Constrained-Automatic Fitting method, the Data Merge Software determines only one thing

• Whether additional modes of the type specified are needed (i.e., lognormal or Rosin-Rammler)

The Full Automatic Fitting method is convenient for automatically determining both the number and types of modes needed, however, it requires smoothed, accurate data to obtain reliable data fits. Also, because all possible combinations of distribution functions are tested, *it requires substantially more computational effort than the other fitting methods.* 

The Constrained-Automatic Fitting is convenient for areas of the distribution where modes may be transient. For example, if a measurement system is monitoring an aerosol downstream of a power plant, the time dependency of the modality of the particle size distribution will change depending on the wind direction and its tendency to direct aerosol from the power plant to the measurement instruments. For such a condition where the type of aerosol distribution emitted from the power plant is known but its appearance in the measured size distribution is time dependent, the Constrained-Automatic Fitting method will determine when that specific distribution function is needed in the specified part of the distribution.

#### Automatic Fitting Criteria (Auto Fit Target)

The fitting algorithm used in the Data Merge Software calculates a "Goodness of Fit" parameter that represents *the average difference between the fitted size distribution and the data*. The fitting algorithm determines the number of distribution functions to use and also determines the optimum fitting-function parameters for each distribution function by minimizing this fitting parameter. To use either of the automatic fitting methods, the Data Merge Software determines when the best fit has been obtained by requiring that the calculated fitting criterion be less than or equal to an Auto Fit Target criterion that you supply.

The Constrained-Automatic Fitting method tests whether the addition of the distribution function of the specified type and in the specified mode causes the calculated fitting parameter to fall below the target fitting criterion. The Full Automatic method tests whether the addition of a distribution function of any type and in the specified mode causes the calculated fitting parameter to fall below the Auto Fit Target fitting criterion, and then determines which distribution type best represents the distribution in the respective mode. The goal is to add distribution functions until the modal features of the data are represented. The goal is not to add modes to simply minimize the fitting parameter. Therefore, the target fitting criterion must be chosen so that it matches in some sense the uncertainty inherent in the data. Setting the Auto Fit Target fitting criterion too small will erroneously force either of the automatic fitting methods to use the maximum number of distribution functions allowed to fit the data.

Data with large interval-to-interval fluctuations caused either by statistical fluctuations in the sample data or by other random fluctuations in sampling conditions either requires the data to be smoothed by merging multiple intervals into a reduced set of intervals (reducing the channels per decade setting), or requires the use of a larger Auto Fit Target fitting criterion than data that does not suffer from such statistical fluctuations. That is, the goal of the automatic fitting methods is to add distribution functions so that each of the modes in the data are represented, but not to add distribution functions to try to represent fluctuations caused by either sampling artifacts or statistical fluctuations. Thus, the value of the Auto Fit Target fitting criterion used must be adjusted so that it reflects the quality of the data in each of the data sets. Experience is required to determine suitable values.

The Auto Fit Target criteria can be set separately for each of the component data sets (SMPS, APS) and for the Composite data set.

## Windowing Component Data

When preparing to perform a Merge, it is very important to properly window the component SMPS and APS component data sets. Excluding noisy sections of data in the tails of the component distributions is particularly helpful in creating an accurate and useful fit. Here are a few tips for effectively windowing the SMPS and APS component data:

- Use the "Log Y Scale" when windowing the data to more easily see where the tail data becomes stable
- Exclude noisy tails from the distributions. With the noise removed from the tails of the data, it will be much easier for the DFM to discover the true significant modes of the component and composite data.
- At the lower end of the APS range, the distribution may drop off due to counting inefficiencies at the lowest end of the scale. Cropping this low end drop off from that data may result in a more accurate result.



Figure 4-17 Windowing Examples

## **Merge Setup**

To access the settings that control the Merging process, click the **Settings & Reports** button on the main interface screen and select the **Merge Settings** tab.

| Settings and Reports   |
|--|
| Graph Settings       Merge Settings       Results of Last Merge       Data Statistics         SMPS Channels per Decade       APS Data Rescale Setting         • 64       32       16       8       4         SMPS Mode Fit Settings       APS Mode Fit Settings       Comp. Mode Fit Settings         1       Lognormal       1       Lognormal       1  |
| 2     None     2     None     2     None     2     None     2     None     2     None     3     None     1 |

Figure 4-18

Settings and Reports Dialog Box

# SMPS Mode Fit Settings, APS Mode Fit Settings, and Comp. Mode Fit Settings

This is where you will select the Fitting Method for each distribution and mode. For each of the three (3) available modes (1, 2, 3) there is a drop-down list where you will make your selections (Figure 4-19).

|   | SMPS Mode Fit Settings |               |          |  |  |  |  |  |
|---|------------------------|---------------|----------|--|--|--|--|--|
|   | 1                      | Full Auto 📃 💌 | Auto Eit |  |  |  |  |  |
|   | 2                      | None 🗾        | Target   |  |  |  |  |  |
|   | 2                      | None          | 0.005    |  |  |  |  |  |
|   | 5                      | Lognormal     |          |  |  |  |  |  |
| ľ |                        | Rosin-Rammler |          |  |  |  |  |  |
|   |                        | Lognorm. Auto |          |  |  |  |  |  |
| - |                        | R-R Auto      |          |  |  |  |  |  |
|   |                        | Full Auto     |          |  |  |  |  |  |

Figure 4-19 SMPS Mode Fit Settings Dialog Box

#### Table 4-3

Descriptions of SMPS Mode Fit Settings

| Option    | Description   |
|-----------|---|
| None      | Do not fit a function to this mode. You must fit at<br>least one mode of each distribution, so this selection<br>is not available for Mode 1. |
| Lognormal | Fit a Lognormal function to this data (Constrained Fitting method).   |

| Option        | Description  |
|---------------|--|
| Rosin-Rammler | Fit a Rosin-Rammler function to this data (Constrained Fitting method).  |
| Lognorm. Auto | Data Merge Software attempts to fit a Lognormal<br>function to this mode using the "Constrained-<br>Automatic Fitting" method described above. Data<br>Merge Software tries to determine if adding a<br>Lognormal mode will improve the overall Goodness<br>of Fit for the distribution.   |
| R-R Auto      | Data Merge Software attempts to fit a Rosin-<br>Rammler function to this mode using the<br>"Constrained-Automatic Fitting" method described<br>above. Data Merge Software tries to determine if<br>adding a Rosin-Rammler mode will improve the<br>overall Goodness of Fit for the distribution.   |
| Full Auto     | Data Merge Software attempts to fit a Lognormal, or<br>Rosin Rammler function to this mode using the "Full<br>Automatic Fitting" method described above. Data<br>Merge Software determines if adding a mode of <i>either</i><br><i>model type</i> (Lognormal or Rosin-Rammler) will<br>improve the overall Goodness of Fit for the<br>distribution and selects the type that produces the<br>best fit. |

*Note:* It is always necessary to fit at least one mode to each distribution (SMPS, APS, or Composite). Because of this, the setting for Mode 1 of each distribution cannot be set to "Lognorm. Auto" or "RR-Auto" until one of the other modes in that distribution is set to "Lognormal", "Rosin-Rammler", or "Full Auto".

## Auto Fit Target

As described earlier, the Constrained-Automatic and Fully Automatic fitting methods rely on an Auto Fit Target setting. Whenever one of the automatic fitting methods is selected for any of the modes, the Auto Fit Target edit box control will appear so that you can customize this setting. When none of the automatic fitting methods are chosen, the Auto Fit Target control is hidden.

#### **SMPS Channels per Decade Setting**

Data with large interval-to-interval fluctuations caused either by statistical fluctuations in the sample data or by other random fluctuations in sampling conditions may require the data to be smoothed by selecting a lower channels-per-decade setting. This setting is found in **Settings & Reports, Merge Settings** tab.

#### **APS** Data Rescale

Under normal conditions, SMPS and APS measurement systems give accurate and reliable concentration readings, allowing your SMPS and APS data to match and merge well. For the purposes of experimentation and correction of unusual conditions, Data Merge Software offers an option to rescale the APS data using an algorithm designed to mathematically match it to the scale of the SMPS data.

There are two automatic methods available for rescaling the APS data and a third "manual rescale" method that lets you scale both data sets by factors that you select:

- Use Overlap Summing Method—Sum the data in the overlapping region for each component data set (SMPS and APS), and rescale the APS data sets so that the sum of the distributions in the overlapping region for each of the data sets is the same. This option is labeled Use Overlap Summing Method.
- **Use Fit Estimate Method**—Use the fitted functions for each of the component data sets (SMPS and APS) to estimate the total for each data set in the overlapping region, and then use these two estimated totals to rescale the APS component data set.

If instead of an overlapping region there is a gap between two neighboring component data sets, then the fitted functions for each data set can be extrapolated into the gap, and estimates calculated for the total of each component data set in the gap. These estimated totals in the gap region for each component data set are then used to rescale the APS component data set.

• **Manual Rescaling**—When you select this method, you will be able to enter an arbitrary scaling factor for both data sets. As an example, if you took SMPS samples using a dilution of 100:1, you could set a scaling factor of 100 for the SMPS data to bring it into range with your APS data.

Note that if you set up your APS sample data in Aerosol Instrument Manager to use a Dilution/Efficiency file, Data Merge will read that setting from the APS data file and obey the dilution factor you had previously chosen. When Averaging is disabled, the dilution factor for the data will be shown in the title of the data graph like this:

#### AC fine.S80, sample 1, 12/02/04 13:44:43 32 c/d / AC fine.A21, sample 1, 12/02/04 13:44:44 (dil.:1.00)

Any manual scaling you select will be applied *after* the APS data has been scaled to compensate for the defined dilution factor.

The APS dilution factor and the SMPS and APS manual scaling factors will be recorded in the output file when you use the Batch Process or Export features.

## **Performing the Merge**

Once you have set the initial settings, you can initiate the merge by clicking the **Merge** button on the main interface screen.

The Setting and Reports screen is designed so that you can interactively change the various settings, apply them to the Merge and see the results. You should notice that once a Merge has been initiated, it will be recalculated as needed each time you move a cursor, change certain parameters or click the **Apply** button in the Settings & Reports screen. To clear this automatic re-merging, right click on the graph and select **Reset Merge** from the menu that appears. This will clear the current Merge.

When the Merge is performed, a summary status will appear under the graph indicating the **Goodness of Fit** for each of the 3 distributions. The Goodness of Fit value represents *the average difference between the fitted size distribution and the data*, so the fit is better as the Goodness of Fit value approaches 0.

To view more detail about the results of the merge, select the **Results of Last Merge** tab from the Setting and Reports screen. There you will find various details about each distribution and mode that was fit. Click the **view in browser** button to view the details as an HTML page in your browser.

Also located in the Setting and Reports screen is the **Data Statistics** tab. Here you will find extensive statistical information about the SMPS, APS and Composite data sets and each fitted function and mode. Click **view in browser** to view the statistics page as HTML in its own browser window.

Viewing the Merge Results and Data Statistics in a browser not only gives you the benefit of viewing the information in a larger window, it also allows you to use all of the features of the browser such as saving the information to an HTML file or text file.

#### **Merging Tips**

- Remember to window the data to exclude noisy tails and major differences between the SMPS and APS data.
- Set the appropriate **Density** and **Shape Factor** so that the data is converted accurately between Mobility and Aerodynamic diameter.
- Use the automatic fitting modes carefully—they rely on properly conditioned input data to produce accurate results.
- The Automatic fitting methods can be very useful for discovering the characteristics of a distribution, but can also take a substantial amount of processing time. Once you have used automatic fitting tools to help you characterize a

distribution, you might wish to use the fitting results to determine good function and mode settings for the **Constrained** or **Constrained-Auto** fitting methods. This will cut down on processing time as related distributions are fit.

• Data Merge Software can fit up to three (3) modes per data set. While this is sufficient to characterize most distributions, there may be times when you want to fit and plot more than three modes. In this case, it may be possible to perform several fits, each using the windowing tools to focus on a particular range of the distribution. You can then Export the data from these fittings, and combine modes externally for plotting in another software package.

# Save and Restore Settings

Data Merge Software allows you to save the settings of a Merge to a file. You can restore those settings later, to duplicate or modify a processing setup you've saved. The **Save/Restore** button is found on the main interface screen.

The Save/Restore feature will save and restore the SMPS and APS sample lists, the state of the Averaging Setup and most of the settings found under the Settings & Results screen.

## **Save Settings**



## Figure 4-20

Save Settings to File

- 1. Click **Save/Restore**, the Save/Restore menu will appear.
- 2. Select Save settings to file.
- **3.** Browse to the location where you wish to save the settings file, name the file and click **Save**.

## **Restore Settings**



Figure 4-21 Restore Settings From File

- 1. Click **Save/Restore**, the Save/Restore menu will appear.
- 2. Select Restore settings from file.
- **3.** Browse to the location where you have previously saved a settings file, select the settings file and click **Open**.

# Export Results to a File

Data Merge Software can export the results of Averaging and Merging to a tab-delimited text file appropriate for import into other software programs.

# **Export Settings**

The contents of the Export file are largely controlled by the **Graph and Export Settings**. This creates a WYSIWYG (What you see is what you get) relationship between the displayed graph and the Export file.



#### Figure 4-22

Graph and Export Settings Dialog Box

You can control which data sets will appear in the Export file using the **Show**..controls. For example, if **Show SMPS Data** is checked, the input SMPS data will be present in the Export file. If it is unchecked, it will not. The **Show SMPS Cursors** and **Show APS Cursors** do not affect the Export file, *however* the **Hide data outside cursors** control does have an effect. When the **Hide data**..control is checked, only the SMPS and/or APS data inside the respective cursor range will be included in the Export file. If Hide data..is unchecked, the entire data set will be included.

If you have checked **Show SMPS Data** and/or **Show APS Data** *and* **Hide data outside cursors** is *not* checked, the Export file will use Include Flags (one for each data bin) to indicate whether a data bin was inside or outside of the cursor area (Figure 4-23).

| SMPS INPUT DATA                            |          |          |          |          |          |          |          |          |
|--|----------|----------|----------|----------|----------|----------|----------|----------|
| Include Flag:                              | 0        | 0        | 0        | 0        | 1        | 1        | 1        | 1        |
| Low Boundary Diameter:                     | 13.82372 | 14.33013 | 14.85508 | 15.39927 | 15.96339 | 16.54817 | 17.15438 | 17.7828  |
| High Boundary Diameter:                    | 14.33013 | 14.85508 | 15.39927 | 15.96339 | 16.54817 | 17.15438 | 17.7828  | 18.43423 |
| Midpoint Diameter (x):                     | 14.07465 | 14.59024 | 15.12473 | 15.67879 | 16.25315 | 16.84855 | 17.46576 | 18.10558 |
| Data (y): AC fine.S80 1, 12/02/04 13:44:43 | 324.431  | 61.7316  | 117.778  | 56.1709  | 53.5764  | 0        | 48.9776  | 0        |

Figure 4-23 SMPS Input Data

A '**0**' in the Include Flag field indicates that the data was outside of the cursor range, a '**1**' indicates that it was inside the cursor range.

If any of the selections, **Show SMPS fit**, **Show APS fit** or **Show Composite fit** are checked, the Export file will include a set of X,Y coordinates for the selected fit data.

The Plot Modes Summed/Plot Modes Separately will also control how fit data is represented in the Export file. If you select **Plot Modes Summed**, then separate modes of a multi-modal fit will be pre-summed within the Export file. If **Plot Modes Separately** is selected, each mode of a multi-modal fit will be output separately.

The **Use Log Y Scale** setting has no effect on the Export file.

The Export file will also contain *all* statistics for the data you choose to include.

# **Exporting the Data**

- 1. Click Export
- 2. Browse to the location where you wish to save the data file
- **3.** Name the file and click **Save**.

# **Batch Process**

Batch Process

The **Batch Process** feature provides a convenient way for you to process an entire list of samples.

Batch process will step through each sample in a list or each sample pair in both lists, perform the desired processing then accumulate the results in an Export file that you specify.

The Batch Process is basically an automation of these steps:

- 1. Select a sample from the list (or sample pair from both lists).
- **2.** Allow previously set-up processing to occur.
- **3.** Log the results to the output Export file.

Step through this process for each sample in the list(s).

This means that you can use it to automate any process that Data Merge Software performs on samples.

#### **To Perform Batch Averaging**

If you have created a list of Interval Average samples, you can export them to a single file using Batch Process:

- **1.** Perform the averaging.
- **2.** Click **Batch Process**. Browse to the location where you wish to save the Batch Results file, name the file, and click **Save**.
- **3.** Batch Process will step through the list and export the listed samples to the selected file.

#### **To Perform Batch Merging**

- 1. Select samples into both sample lists.
- **2.** Setup all appropriate merge parameters and other settings manually and test the settings on one or more samples pairs in the lists. You must manually initiate a Merge at least once before beginning the Batch Process.
- **3.** Click **Batch Process**. Browse to the location where you wish to save the Batch Results file, name the file, and click **Save**.
- **4.** Batch Process will step through the entire list selecting sample pairs, performing a Merge and collecting the output into the Export file.

# How the Sync. Lists Feature Affects Batch Process

If only one sample list has samples in it, the Sync. Lists setting has no affect on Batch Process. Batch Process will simply choose the first sample from the populated list, and then step through each sample one-by-one.

When both lists are populated and Sync. Lists is *enabled*, then starting from the first item, Batch Process will *step through each entry in the SMPS list* and for each SMPS sample selected, allow the Sync. Lists algorithm to select a time-correlated sample from the APS list. The number of samples processed will depend solely on the number of samples in the SMPS list.

When both lists are populated and Sync. Lists is *disabled*, Batch Process will start by selecting the first item from **both lists** then through each item in both lists one-by-one *until* it reaches the bottom of the shortest list.

# Quit the Program

To end the program, click the "X" button in the upper right corner.



# APPENDIX A Calculations Used in Data Merge Software Module

This appendix details the equations that are used within Data Merge Software Module.

# Mobility/Aerodynamic Diameter Conversion

The fundamental equation relating aerodynamic diameter  $d_a$  to mobility diameter  $d_m$  is

$$d_a = d_m \left[ \frac{C(d_m)}{C(d_a)} \right]^{\frac{1}{2}} \left( \frac{\rho_p}{\chi \rho_o} \right)^{\frac{1}{2}}$$

Here  $\rho_p$  is the particle density,  $\rho_0$  the reference density 1 gram/cm<sup>3</sup>, and  $\chi$  is a dynamic shape factor. *C(d)* is the slip correction:

$$C_c = 1 + \frac{2\lambda}{D_p} (1.142 + .558e^{\frac{-0.999Dp}{2\lambda}})$$

 $\lambda$  = Mean Free Path = 6.65e-8

To change the coefficient that Data Merge Software uses for Mean Free Path in this equation, edit the DataMerge.ini file found in the Data Merge installation folder using Notepad or another text editor. Find the section **MergeEquations** and the key **MeanFreePath** and change it to the desired value. The default setting in the DataMerge.ini file looks like this:

```
[MergeEquations]
MeanFreePath=0.000000665000000
```

# SMPS Single and Multiple Charge Correction

For SMPS data, Single Charge correction is applied to the data automatically when it is converted from its raw form.

Choose the Multiple Charge Correction check box in the **Settings & Reports->Graph Settings** tab to enable a mathematical correction for particles with multiple charges.

These corrections are implemented using a charge correction table file. The default table holds values calculated for positively-charged particles measured using a Model 3080 Classifier with a negative High Voltage (HV). (*Note: This is the standard configuration.*) For negatively-charged particles (i.e., a positive HV is installed), the file **ChargeNEG.dat** is supplied in the directory in which DataMerge is installed. If you are measuring negatively-charged particles, you may edit the DataMerge.ini file (using a text editor such as Notepad) to include the correct file name:

#### [SMPS]

CHARGECORR\_FILE="C:\Program Files\TSI\Aerosol Instrument Manager\ChargeNEG.dat"

Refer to Aerosol Instrument Manager<sup>®</sup> Software for SMPS Spectrometers Instruction Manual (part number 1930104, TSI Incorporated) for further details of the single and multiple charge correction features.

# Why Are Diffusion Losses Important in the SMPS<sup>™</sup> Spectrometer?

To understand why we need a Diffusion Loss Correction, it is necessary to recall three facts:

- 1) When aerosol particles collide with a surface they adhere due to van der Waals force, electrostatic force and surface tension.
- 2) Diffusion is the primary transport mechanism for particles smaller than 0.1  $\mu$ m (100 nm).
- **3)** The smaller the particle the more rapid the diffusion.

Thus, if an aerosol particle diffuses to the wall of its measurement flow path, there will be diffusion losses, and the measured size distribution will under represent small particles. Since the Scanning Mobility Particle Sizer<sup>TM</sup> (SMPS<sup>TM</sup>) spectrometer measures particles in the size range of 2.5 nm–1000 nm, diffusion losses are unavoidable. They are however, quantifiable.

Diffusion losses are frequently characterized in terms of penetration

(P) through a tube:  $P = \frac{n_{out}}{n_{in}}$ 

Penetration is a function of the particle diffusion coefficient (D), length of the tube (L), and volumetric flow rate (Q). The Diffusion coefficient (D) is affected by temperature, gas medium, and particle diameter.



**Circular Tube Penetration Efficiency** 

Figure A-1 Circular Tube Penetration Efficiency [Gormley and Kennedy (1949)]

Note that the diffusion loss through a tube (for a fixed volumetric flow rate) is not a function of tubing diameter. The additional distance the particles must travel to the walls in a wider tube is offset by a longer residence time.

# How Can You Characterize Diffusion Losses in the SMPS<sup>™</sup> Spectrometer?

The Scanning Mobility Particle Sizing<sup>TM</sup> (SMPS<sup>TM</sup>) spectrometer can be broken down into five different flow paths for which an aerosol penetration can be calculated.

- $P_1$  = Penetration through the impactor inlet
- $\mathrm{P_2}$  = Penetration through the bi-polar neutralizer and internal plumbing
- $\rm P_{_3}$  = Penetration through the tubing to the Differential Mobility Analyzer (DMA) and CPC
- $P_4$  = Penetration through the DMA
- $P_5$  = Penetration through the CPC





The total penetration through the system is the product of the individual penetration values:

$$\mathbf{P}_{total} = \mathbf{P}_1 \mathbf{P}_2 \mathbf{P}_3 \mathbf{P}_4 \mathbf{P}_5$$

## Determination of P<sub>1</sub>

The penetration through the impactor assembly was determined experimentally using all three impactor sizes (0.0457 cm, 0.0508 cm, & 0.071 cm) and a variety of flow rates.  $P_1$  is dependent on the Reynolds number so it is affected by the flow rate and the gas properties of the working gas. When using an impactor, it is important to stay within the recommended flow ranges to achieve the highest accuracy for the Diffusion Loss Correction.

## Determination of P<sub>2</sub>

The penetration through the internal passages of the Model 3080 Classifier (including the Model 3077/3077A neutralizer) was determined experimentally at a variety flow rates.  $P_2$  is a function of the particle diffusion coefficient and flow rate.

# Determination of P<sub>3</sub>

Penetration through the connecting tubing was calculated using Gormley and Kennedy's equations for penetration through a circular tube<sup>1</sup>.

*Note:* Diffusion Loss Correction was designed for use with CPCs in "high flow mode" where this option is available.

# Determination of P<sub>4</sub>

Penetration through each of the Differential Mobility Analyzers (Model 3085 and Model 3081) was determined using published data<sup>2.3.4</sup> on the transfer functions for these DMAs and was also validated experimentally.

# Determination of P<sub>5</sub>

 $P_5$  is the counting efficiency of the CPC and includes penetration inside the CPC, activation efficiency and optical detection efficiency.

Note: All of the experiments were performed using air at Standard Temperature & Pressure (STP) as the working gas. Since diffusion losses are a function of the particle diffusion coefficient (D) and D is a function of the working gas properties, the use of different working gases and/or conditions will result in an error in the calculated diffusion loss. It is possible to input gas properties in the software to increase the Diffusion Loss Correction accuracy, but other working gases and conditions have not been experimentally verified.

# **Fitting Model Functions**

When a Merge is performed, fitting parameters Param. A, Param. B, and Param. C are reported within the software on the Results of Last Merge report screen. They are also reported in files exported using the Export feature.

## **Lognormal Model Function**

A = Param. A, B = Param. B, C = Param. C

$$y = \frac{A}{\left(\sqrt{2\pi} \cdot \ln(C)\right)} \cdot exp\left[-\frac{1}{2} \cdot \left(\frac{\ln\left(\frac{x}{B}\right)}{\ln(C)}\right)^{2}\right]$$

## **Rosin-Rammler Model Function**

A = Param. A, B = Param. B, C = Param. C, Zero = 1e-32 (small number added to avoid going to 0)

$$y = A \cdot C \cdot \left(\frac{x}{B + Zero}\right)^{C} \cdot \exp\left[-\left(\frac{x}{B + Zero}\right)^{C}\right]$$

# Normal Statistics Calculated from Data

These statistics are calculated for SMPS and APS input data and the Composite (merged SMPS and APS) data. They are reported on the **Data Statistics** report screen. They are also reported in files exported by the Batch Process and Export features.

| Normal Statistics Calculated from Data  |   |                                 |                                 |                                  |                                 |  |  |
|---|---|---------------------------------|---------------------------------|----------------------------------|---------------------------------|--|--|
| Weighting<br>Statistic  | Number  | Diameter                        | Surface Area                    | Volume                           | Mass                            |  |  |
| Concentration   | $n = \frac{c}{tQ}\frac{\phi}{\eta}$   | $d = D_p n$                     | $s = \pi D_p^2 n$               | $v = \frac{\pi D_p^3 n}{6}$      | $m = \rho v$                    |  |  |
| Total Concentration   | $N = \sum_{l}^{u} n$  | $D = \sum_{l}^{u} d$            | $S = \sum_{l}^{u} s$            | $V = \sum_{l}^{u} v$             | $M = \sum_{l}^{u} m$            |  |  |
| Mode  | $D_p(n_{\max})$   | $D_p(d_{\max})$                 | $D_p(s_{\max})$                 | $D_p(v_{\max})$                  | $D_p(m_{\rm max})$              |  |  |
| Median ( $\widetilde{x}$ )  | D <sub>p</sub> (N / 2)  | $D_p(D/2)$                      | D <sub>p</sub> (S / 2)          | D <sub>p</sub> (V / 2)           | D <sub>p</sub> (M / 2)          |  |  |
| Mean ( $\overline{x}$ )   | $\frac{\sum_{l}^{u} nD_{p}}{N}$   | $\frac{\sum_{l}^{u} dD_{p}}{D}$ | $\frac{\sum_{l}^{u} sD_{p}}{S}$ | $\frac{\sum_{l}^{u} v D_{p}}{V}$ | $\frac{\sum_{l}^{u} mD_{p}}{M}$ |  |  |
| Geometric Mean $(\bar{x}_g)$<br>$exp\left[\frac{\sum_{l}^{u} n \ln D_p}{N}\right]$ substitute <i>d</i> , <i>s</i> , <i>v</i> , <i>m</i> and <i>D</i> , <i>S</i> , <i>V</i> , <i>M</i> in place of <i>n</i> and <i>N</i> for other weightings  |   |                                 |                                 |                                  |                                 |  |  |
| Geometric Standard<br>Deviation ( $\sigma_g$ )  | netric Standard<br>ation ( $\sigma_g$ ) $exp\left[\frac{\sum_{l=1}^{u}n\left[\ln D_p - \ln \overline{x_g}\right]^2}{N}\right]^{\frac{1}{2}}$ substitute <i>d</i> , <i>s</i> , <i>v</i> , <i>m</i> and <i>D</i> , <i>S</i> , <i>V</i> , <i>M</i> in place of <i>m</i><br>and <i>N</i> for other weightings |                                 |                                 |                                  |                                 |  |  |
| Geometric Standard<br>Deviation ( $\sigma_g$ ) $\left[ \sum_{l}^{u} n \left[ \ln D_p - \ln \overline{x_g} \right]^2 \right]^{\frac{1}{2}}$ substitute d, s, v, m and D, S, V, M in place of<br>and N for other weightingsNote: In all cases above, $D_p$ is in Mobility Diameter units. |   |                                 |                                 |                                  |                                 |  |  |

The symbols used in the formulas are defined as:

*c* = particle counts per channel S = total surface area concentration*n* = number weighted concentration per channel V =total volume concentration *s* = surface area weighted concentration per M = total mass concentrationchannel Q = sample flow rate v = volume weighted concentration per channel t = sample timem = mass weighted concentration per channel  $\rho$  = particle density  $\eta$  = sample efficiency factor per channel  $ln = natural \log log$  $\phi$  = sample dilution factor exp = base of natural log (e)  $D_p$  = particle diameter (channel midpoint) l = lower channel boundary*C* = total particle counts u = upper channel boundaryN =total number concentration

# Statistics Calculated from Fitting Parameters

These statistics are calculated for fitted data sets and are calculated using the parameters from the fitted model functions (Param. A, Param. B, Param. C).

These tables show the statistics as they are calculated when Number weighting is selected. When another weighting is selected, the parameters and equations from the first column will apply to the selected weighting. Statistics for the other weightings (those not selected) will be calculated based on the mathematical relationships defined by the equations shown here. Statistics for the selected weighting will be the most accurate and comprehensive.

# Lognormal Function Statistic Calculations

| Statistics Calculated from Fitting Parameters: Lognormal Model |   |   |   |   |  |  |  |  |
|--|---|---|---|---|--|--|--|--|
| Weighting<br>Statistic   | Number<br>(Selected Weighting)  | Diameter  | Surface Area  | Volume/Mass   |  |  |  |  |
| Median   | В   | $B \cdot \exp(\ln(C)^2)$                                      | $B \cdot \exp(2 \cdot \ln(C)^2)$                      | $B \cdot \exp(3 \cdot \ln(C)^2)$  |  |  |  |  |
| Geometric Mean   | В   |   |   |   |  |  |  |  |
| Geometric<br>Standard Deviation                                | С   |   |   |   |  |  |  |  |
| Geometric Mode   | В   | $B \cdot \exp(\ln(C)^2)$                                      | $B \cdot \exp(2 \cdot \ln(C)^2)$                      | $B \cdot \exp(3 \cdot \ln(C)^2)$  |  |  |  |  |
| Arithmetic Mean  | $B \cdot \exp\left(\frac{1}{2} \cdot \ln(C)^2\right)$   | $B \cdot \exp\left(\frac{3}{2} \cdot \ln(C)^2\right)$         | $B \cdot \exp\left(\frac{5}{2} \cdot \ln(C)^2\right)$ | $B \cdot \exp\left(\frac{7}{2} \cdot \ln(C)^2\right)$   |  |  |  |  |
| Arithmetic<br>Standard Deviation                               | $B \cdot \sqrt{\exp(\ln(C)^2) \cdot \left(\exp(\ln(C)^2) - 1\right)}$                                       |   |   |   |  |  |  |  |
| Arithmetic Variance  | $B^{2} \cdot \left[ \exp\left(\ln(C)^{2}\right) \cdot \left(\exp\left(\ln(C)^{2}\right) - 1\right) \right]$ |   |   |   |  |  |  |  |
| Total Concentration  | A   | $A \cdot B \cdot \exp\left(\frac{1}{2} \cdot \ln(C)^2\right)$ | $A \cdot \pi \cdot B^2 \cdot \exp(2 \cdot \ln(C)^2)$  | Volume:<br>$A \cdot \frac{\pi}{6} \cdot B^3 \cdot \exp\left(\frac{9}{2} \cdot \ln(C)^2\right)$<br>Mass ( $\rho$ = particle<br>density):<br>$\rho \cdot A \cdot \frac{\pi}{6} \cdot B^3 \cdot \exp\left(\frac{9}{2} \cdot \ln(C)\right)$ |  |  |  |  |

A = Param. A, B = Param. B, C = Param. C

= Equation unknown

| Statistics Calculated from Fitting Parameters: Rosin-Rammler Model |  |   |   |  |  |  |  |
|--|--|---|---|--|--|--|--|
| Weighting<br>Statistic   | Number<br>(Selected Weighting)   | Diameter  | Surface Area  | Volume/Mass  |  |  |  |
| Median   | $d_0 \cdot \ln(2)^2$   |   |   |  |  |  |  |
| Geometric Mean   | $d_0 \cdot \exp\left(\frac{-\gamma Euler}{C}\right)$   |   |   |  |  |  |  |
| Geometric Standard<br>Deviation                                    |  |   |   |  |  |  |  |
| Geometric Mode   | $d_{_0}$   | $d_0 \cdot \left(1 + \frac{1}{C}\right)^{\frac{1}{C}}$                                      | $d_0 \cdot \left(1 + \frac{2}{C}\right)^{\frac{1}{C}}$                                      | $d_0 \cdot \left(1 + \frac{3}{C}\right)^{\frac{1}{C}}$   |  |  |  |
| Arithmetic Mean  | $d_0 \cdot \Gamma\left(1 + \frac{1}{C}\right)$   | $d_{0} \cdot \frac{\Gamma\left(1 + \frac{2}{C}\right)}{\Gamma\left(1 + \frac{1}{C}\right)}$ | $d_{0} \cdot \frac{\Gamma\left(1 + \frac{3}{C}\right)}{\Gamma\left(1 + \frac{2}{C}\right)}$ | $d_{0} \cdot \frac{\Gamma\left(1 + \frac{4}{C}\right)}{\Gamma\left(1 + \frac{3}{C}\right)}$  |  |  |  |
| Arithmetic Standard<br>Deviation                                   | $d_0 \cdot \sqrt{\Gamma\left(1 + \frac{2}{C}\right) - \Gamma\left(1 + \frac{1}{C}\right)^2}$         |   |   |  |  |  |  |
| Arithmetic Variance  | $d_0^2 \cdot \left(\Gamma\left(1 + \frac{2}{C}\right) - \Gamma\left(1 + \frac{1}{C}\right)^2\right)$ |   |   |  |  |  |  |
| Total Concentration  | Α  | $A \cdot d_0 \cdot \Gamma\left(1 + \frac{1}{C}\right)$                                      | $A \cdot \pi \cdot d_0^2 \cdot \Gamma\left(1 + \frac{2}{C}\right)$                          | Volume:<br>$A \cdot \frac{\pi}{6} \cdot d_0^3 \cdot \Gamma\left(1 + \frac{3}{C}\right)$<br>Mass ( $\rho$ = particle density):<br>$\rho \cdot A \cdot \frac{\pi}{6} \cdot d_0^3 \cdot \Gamma\left(1 + \frac{3}{C}\right)$ |  |  |  |

## **Rosin-Rammler Function Statistic Calculations**

 $\overline{A}$  = Param. A, B = Param. B, C = Param. C,  $d_0$  = Param. B + Zero (1e-32)

Euler's constant  $\gamma = 0.57721566490$ 

= Equation unknown

 $\Gamma$  = Euler's Gamma Function:

Polynomial approximation to Euler's Gamma function Gamma(1+x) = x! for real x from Handbook of Mathematical Functions, ed. Abramowitz & Segun, 6.1.36

Polynomial approximation for Gamma(1+x) when  $0 \le x \le 1$ When x is outside this range, use the recursion relation Gamma(1+x) = x\*Gamma(x) Note that the function is singular for x = -1, -2, -3,...

 $\begin{array}{ll} Gamma(1+x) = 1+b1*x + b2*x^2 + ... + b8*x^8 + epsilon(x) \\ where the coefficients are \\ b1 & -0.577191652 \\ b2 & 0.988205891 \\ b3 & -0.897056937 \\ b4 & 0.918206857 \\ b5 & -0.756704078 \end{array}$ 

- b6 0.482199394
- b7 -0.193527818
- b8 0.035868343

and the maximum error abs(epsilon(x)) <= 3E-7

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# APPENDIX B DistFit<sup>\*</sup> Particle Data Conversion and Fitting Program





**DistFit** is used to manipulate particle size distribution data and to fit multimodal distributions to the data, such as lognormal and Rosin-Rammler distribution functions.

# **Data Conversion**

**DistFit** can convert between the many moments and weightings of size distribution data unique to the aerosol field. For example, a measured number size distribution can be converted to a mass distribution. The measured particle size might be aerodynamic diameter, yet it is more common to display the geometric diameter. **DistFit** does such data conversions, including data smoothing.

# **Data Merging**

**DistFit** can merge multiple component data sets into a single, composite data set. For example, two instruments might be used to measure different size ranges of an aerosol. DistFit can be used to merge two such component distributions into a single, composite distribution.

<sup>\*</sup>DistFit Particle Data Conversion and Fitting Program is a product of Chimera Technologies, Inc.

Chimera Technologies, Inc. 15051 Zodiac St. NE Forest Lake, Minnesota 55025, USA Tel/Fax: 651-464-7771 info@ChimeraTech.com http://www.DistFit.com

# **Data Fitting**

**DistFit** can fit multimodal distribution functions to the data and contains both automatic and manual fitting methods, thus giving the user control over all aspects of the fitting procedure. Multiple data sets in a subdirectory can be automatically fit and a report of the fitted functions can be produced for each data set.

# **Data Reporting**

**DistFit** can produce reports of the data, including measures of central tendency, fitted functions, goodness of fit, and submicron/supermicron fractions. Respirable fractions, and PM (particulate matter) fractions are planned for a future version.



# **DistFit Features**

## **Data Input**

- **DistFit** formatted files
- Free-format ASCII files (up to 1000 data points)
- Instrument data files (e.g., for TSI SMPS™ and APS™ spectrometers)

## **Data Types**

- Classified
- Frequency
- Cumulative less-than and greater-than

## Moment Data (size data)

- Geometric diameter
- Aerodynamic diameter

# Weighting Data (measured data)

- Number
- Length
- Surface Area
- Volume
- Mass

# **Data Manipulation**

- Superimpose, add, average, or subtract multiple data sets
- Merge multiple data intervals (i.e., data smoothing)
- Merge multiple data sets (e.g., TSI SMPS and APS spectrometers)

# **Multimodal Curve Fitting**

- Fit selected range of data set
- Include/exclude individual data points
- Include/exclude "0" data

#### **Curve** Fitting

- o Full automatic fit
- $\circ \quad \text{Constrained automatic fit} \\$
- o Manual, constrained fit
- $\circ$  Number of modes in fit: 1 to 3

# **Data Reports**

- Measures of central tendency (standard deviation, mean, median, and mode sizes)
- Fitted function parameters and fitting criterion
- Interval-by-interval comparison of discrete and analytical data **Size Classifications** 
  - o Supermicron/submicron fractions
  - o Respirable fraction
  - $\circ~$  PM fractions (1, 2, 5, and 10  $\mu m)^{\text{Error! Bookmark not defined.}}$

# **Fit Reports**

- Summary of fit parameters
- Summary of fitted parameters for each mode
- Fitting criterion

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