
**Rate of Adsorption Option
for the
ASAP 2020**

Operator's Manual

V1.02

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CHAPTER 1

GENERAL INFORMATION

- Organization of This Manual
- Description

GENERAL INFORMATION

This manual is intended as a supplement to your current ASAP 2020 Operator's Manual and addresses the operation of the Rate of Adsorption software designed for use in the Microsoft Windows® environment.

The Rate of Adsorption option allows you to use the ASAP 2020 software to collect ROA data, and then ROA software to view the data.

This program provides any ASAP 2020 user the ability to display in tabular and graphical form, the ROA data collected by the ROA functions in the ASAP 2020 software. These functions are enabled by selecting **Collect ROA data** on the ASAP 2020 Analysis Conditions dialog box.

The Rate of Adsorption option comes complete with the following items, the:

- Rate of Adsorption software
- Operator's manual

Organization of This Manual

This manual contains the following chapters.

Chapter 1 **General Information.** Provides an overview of the ROA program.

Chapter 2 **Installation.** Provides system requirements and installation instructions for the ROA software.

Chapter 3 **User Interface.** Provides software interface.

Chapter 4 **Ordering Information.** Contains ordering information.

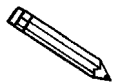
Appendix A **Error Messages.** Lists the error messages displayed by the ROA program and provides a cause and corrective action for each.

Appendix B **Format of Exported Data.** Contains the format and description of exported data.

Index Provides quick access to a subject matter.

Conventions

This manual uses the symbol shown below to identify notes of importance.



Notes contain important information pertinent to the subject matter.

Description

The Rate of Adsorption (ROA) display program for the ASAP 2020 allows you to measure how rapidly and how much of an increment of gas is removed from the space above a sample as it is bound into an adsorbed, absorbed, or chemisorbed form that no longer contributes to the pressure observed above the sample. There are two elements to this measurement: rate of removal and amount removed.

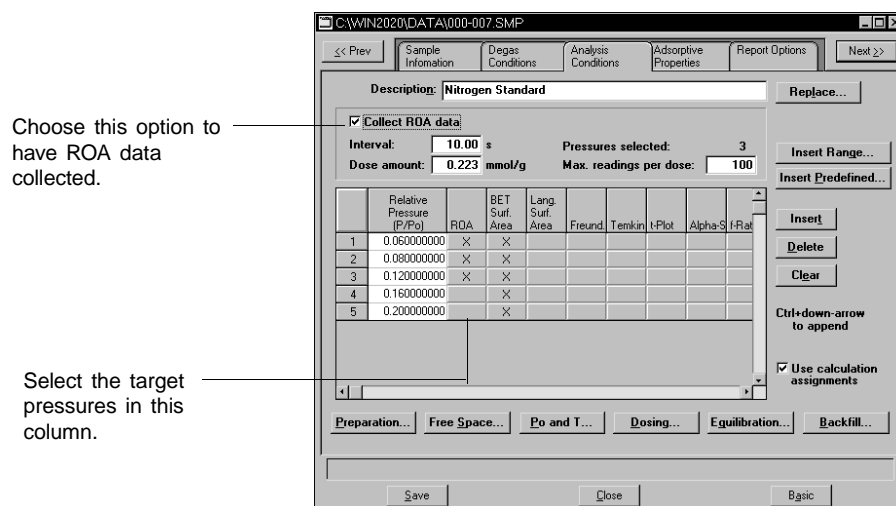
This removal rate and amount removed are governed by many variables which may be difficult to sort out. These include:

- total surface area
- ability to dissipate the heat of sorption
- tortuosity of the path leading to the sorption site
- surface to volume ratio of the sample
- presence of pores marginally able to permit passage of the adsorbate molecules

Most researchers would use ROA to determine relative ease of access of gases to the sorbing surface. Others might find ROA useful for observing the progress of the very slow processes of absorption or diffusion. ROA data is useful in applications that depend upon materials which exhibit proper rates of uptake. These include catalysts for chemical and petrochemical production, membranes for separating gases of differing molecular size, and air and water purification devices.

In adsorption, ease of access to a surface usually implies a well-branched pore structure with large main pores from which the smaller pores branch off, and from which in turn, even smaller pores branch. On the other hand, absorption, and also diffusion processes, usually involve molecular wandering through the poreless structure of a solid. The number of collisions per unit time tends to govern the rate at which a gas penetrates into a solid. Thus, important information about the structure of a solid may be available from observing the uptake rate.

While Chapter 3 covers use of the ROA software in detail, the first item on the Analysis Conditions dialog box shows where you must select or deselect collection of ROA data.



If **Collect ROA data** is selected, an ROA column is added to the Pressure table. This allows you to select the target relative pressures to be included. For each ROA check box selected, the 2020 program records rate of adsorption data for all doses applied in reaching that pressure.

Dosing Methods

Since the collection of ROA information changes the operation of the 2020 program, it is worth comparing it to normal dosing behavior.

Normal Dosing

Consider an experiment consisting of three relative pressures. Two measurements have been completed as shown in the following table:

| Target Relative Pressure | Actual Relative Pressure | Absolute Pressure | Volume Adsorbed |
|--------------------------|--------------------------|-------------------|-----------------|
| 0.10000000 | 0.097621435 | 72.09072 | 51.8960 |
| 0.20000000 | 0.200204767 | 147.8530 | 61.3624 |
| 0.30000000 | | | |

Next pressure to be measured. →

The ASAP 2020 will attempt to reach the next target relative pressure of 0.3 as quickly as possible by estimating the volume adsorbed at the new pressure using the previous measurements. It will then apply a dose based upon that estimate (in this example approximately 10 cm³ STP). If the estimate is too low, the 2020 will quickly detect this fact and apply more gas. Once enough gas has been applied to insure a measurement near the target pressure, the 2020 will allow the system to reach equilibrium before recording the final pressure and volume adsorbed. The resulting collected data would be as follows:

| Target Relative Pressure | Actual Relative Pressure | Absolute Pressure | Volume Adsorbed |
|--------------------------|--------------------------|-------------------|-----------------|
| 0.10000000 | 0.097621435 | 72.09072 | 51.8960 |
| 0.20000000 | 0.200204767 | 147.8530 | 61.3624 |
| 0.30000000 | 0.301772141 | 222.8614 | 70.3245 |

ROA Dosing

If the target relative pressure of 0.3 were selected for ROA data collection, the operation would be completely different. A fixed amount of gas *as specified by the experimenter, rather than estimated by the 2020*, is applied to the sample. Once the dose fully equilibrates, the pressure and volume adsorbed are recorded. If the resulting pressure does not exceed the target, the process is repeated. For example, if the ROA dose amount were set to 5 cm³ STP, the following measurements could result.

| Target Relative Pressure | Actual Relative Pressure | Absolute Pressure | Volume Adsorbed |
|--------------------------|----------------------------|----------------------|--------------------|
| 0.10000000 | 0.097621435 | 72.09072 | 51.8960 |
| 0.20000000 | 0.200204767 0.243758757 | 147.8530 180.0199 | 61.3624 65.9373 |
| 0.30000000 | 0.312624148 | 230.8758 | 70.5122 |

Extra ROA measurement. →

The first ROA dose equilibrated at relative pressure 0.2437 and *an extra data point was recorded for the isotherm*. The second ROA dose equilibrated above the target pressure, so no additional doses of gas were necessary.

Data Collection

In addition to changing the dosing methodology, selecting a pressure for ROA analysis causes the rate at which the dose is adsorbed to be recorded. As soon as the sample valve is opened, the ASAP 2020 begins recording the pressure in the sample tube. The cumulative volume adsorbed is calculated and saved in the ROA results file.

Three parameters are provided for controlling the data collection: **Dose amount**, **Interval** and **Max. readings per dose**.

Dose amount

This is the fixed quantity of gas to be applied to the sample for adsorption. The portion of gas actually adsorbed depends upon the slope of the isotherm at that point.

Interval

This refers to your desired frequency of taking readings of sample tube pressure. The interval is actually the spacing between readings and may range from 0.1 to 99.0 seconds. A single entry consisting of time, pressure, and volume adsorbed is recorded in the ROA data file for each reading made. Time refers to the number of seconds elapsed since the start of the dose.

If the sample adsorbs the dose quickly, a small interval may be used to resolve clearly the rapid change in pressure. If the adsorption process is much slower, a larger interval would be appropriate to prevent redundant readings.

Max. readings per dose

This parameter limits the total number of readings which will be saved in a file for a single dose. For example, let's assume the interval is set to 0.1 second to resolve the rapid change in pressure immediately after the sample valve is opened. Let's also assume you are interested in only the first 20 seconds of the process even though 200 seconds are required for the dose to reach full thermal equilibration. Then you would limit the readings per dose to 200 (20 seconds x 10 intervals of 0.1 second each) to avoid collecting large amounts of useless data.

CHAPTER 2

INSTALLATION

- System Requirements
- Installing the Software

INSTALLATION

This chapter describes how to install the ROA program.

The ROA software kit includes the following items:

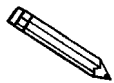
- One CD containing the software program
- Operator's manual

Notify Micromeritics immediately if your kit is incomplete.

System Requirements

Your system must meet or exceed the following requirements before you can install the DataMaster software:

- Pentium 333MHz computer (or equivalent)
- CD-ROM drive
- 128 megabytes of main memory
- 1-gigabyte hard drive
- SVGA monitor (800 x 600 minimum resolution)
- Windows 2000 or Windows XP Professional



To ensure safe operation and recovery after a power failure, *Windows must start automatically when your computer is turned on.* See *Turning the System Off* in Chapter 3 for comments regarding power failures.

Installing the Software

The ROA software is supplied on a CD. Perform the following steps to install the software:

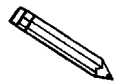
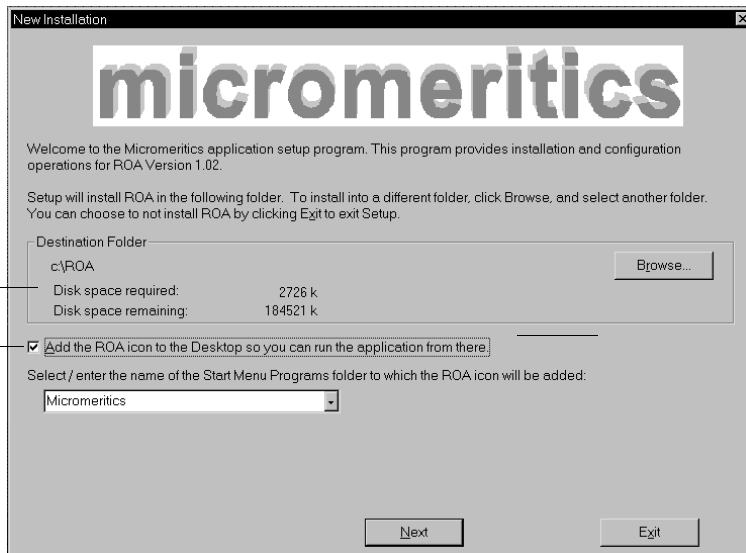
1. Insert the program CD into the CD-ROM drive.
2. Select **Start** from the Status bar, then **Run** from the Start menu.
3. Enter the name of the drive designator, followed by **setup**. For example:

e:setup

4. Click ; the New Installation dialog box is displayed.

Displays the amount of current disk space and the amount required for installation of the application. Also displays the directory into which the application will be installed.

Select to add the DataMaster icon to your desktop for quick access to the application.



You may cancel the installation at any time by selecting . If you do so, you must start the installation program from the beginning.

The Destination Folder group box displays the amount of current disk space, the amount of disk space required for the application, and the directory into which the application will be installed. If you wish to install the application into a different directory, click to choose the directory.

For convenience in running the application, you can add an icon to your desktop by selecting the checkbox just below the Destination Folder group box.

5. The ROA icon is added to the Micromeritics folder by default. If you prefer a different folder, enter or select one from the drop-down list.
6. Click to complete installation of the ROA program; the Installation complete dialog box containing the Readme file is displayed.
7. Use the scroll bar if you want to read the contents of the file, then click to close the dialog box.
8. Remove the ROA program CD and store in a safe place.
9. Double-click on the ROA icon to begin the program.

Using the Setup Program for Other Functions

After initial installation of the ROA program, the application setup program is also used to:

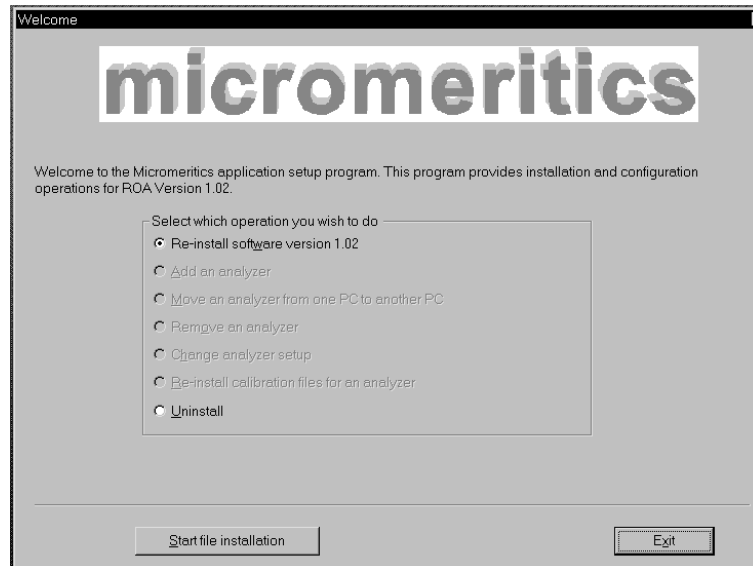
- Upgrade software
- Uninstall the ROA program

To start the application setup program:

1. Ensure that the analysis program is not operating.
2. Insert the CD into your CD-ROM drive.
3. Select **Start** from the Status bar.
4. Select **Run** from the start menu.
5. Enter the drive designator of the CD-ROM drive, followed by **setup**. For example: **e:setup**.

Alternatively, you can click , navigate to your CD-ROM drive, and select **setup.exe**.

- Click **OK** ; the setup Welcome screen showing the options available is displayed.



- Choose the desired option.

Reinstalling the Software

When you install a software upgrade, the system installs all of the application files that do not already exist on the computer. There are three types of subsequent installation; the software version controlled by the setup program is:

- a later version than the version installed on the computer
- the same version as the version installed on the computer
- an earlier version than the version installed on the computer

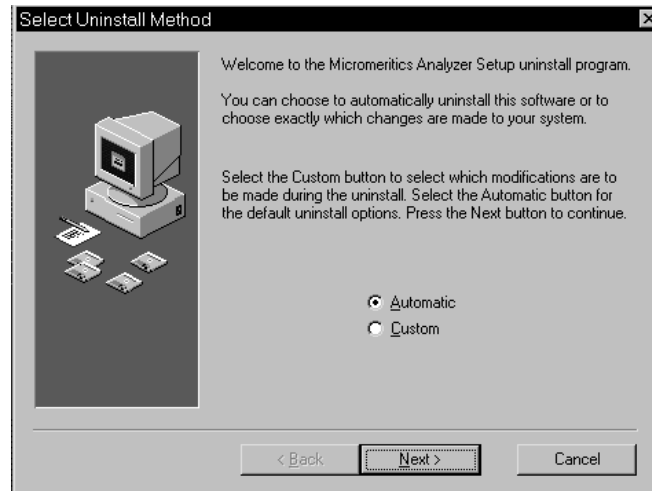
The setup program automatically detects which type of installation applies and customizes the selection in the Setup dialog accordingly.

- Start the Setup program. Choose the software option; remember, only the applicable option will display; it will be one of the following:
 - Upgrade software to version (number) from version (number)
 - Reinstall software version (number)
 - Downgrade software to version (number) from version (number)
- Click **Start File Installation** ; the application installs the software and redisplay the setup Welcome dialog. If no other operations are desired using this dialog, click **Exit** to close the dialog.

Uninstalling the Software

When you uninstall the ROA program, the application removes the ROA program; it does not remove data files. Perform the following steps to uninstall the program:

1. Start the Setup program. From the Setup dialog, select **Uninstall**, then click **Next**; the Select Uninstall Method dialog is displayed.



3. Choose one of the following:
 - **Automatic:** click **Next**; the system uninstalls the program automatically and the setup Welcome dialog redisplay.
 - **Custom:** click **Next**; a series of dialogs is displayed, allowing you to choose the files you wish to uninstall. After all files are selected and uninstalled, the setup Welcome dialog redisplay.
4. Click **Exit** to close the Welcome dialog.

CHAPTER 3

USER INTERFACE

- ROA Main Menu
- Using the ROA Option

USER INTERFACE

This chapter provides information on the options available from the main menu of the ROA program and operating instructions.

ROA Main Menu



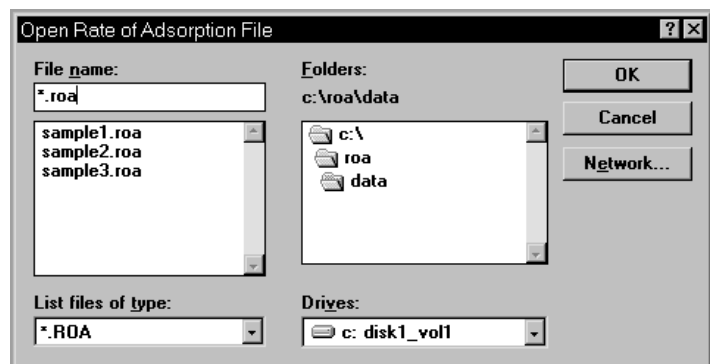
File



The options on this menu are used to open collected ROA data files, save files, and exit the ROA program.

Open

Displays the Open Rate of Adsorption File dialog, allowing you to select a file for which you wish to see collected ROA data.



Network...

This push button is available only if you are attached to a Novell network or run Windows for Workgroups. It provides for network management.

Save

Save is enabled only after the Sample Information dialog is modified. It permits you to save a file using the same name.

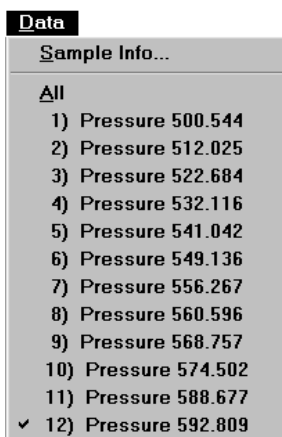
Save As

Save As permits you to save a file under a different name.

Exit

Exit takes you out of the ROA program.

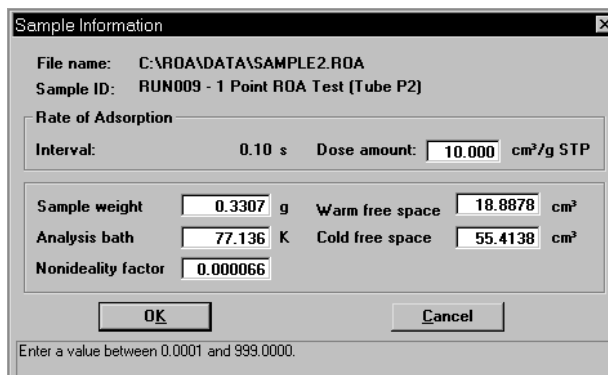
Data



Data is used to modify the sample information and to specify which pressure points (for which ROA data was collected) should be reported by the ROA program. You can select **Sample Info**, **All** (points), or **an individual point**.

Sample Info

Displays the Sample Information dialog.



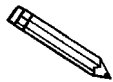
Sample Info*(continued)*

Using the Sample Information dialog, you can change any of the enabled parameters.

All parameters affect the computation of the specific volume adsorbed. When **OK** is selected, the volume adsorbed is re-computed for all readings and the results are reflected in the tabular and graphical output. Depending upon the amount of data, the re-computation may take several seconds. Making changes to this dialog enables the **Save** selection on the **File** menu.

All

Selecting **All** generates tabular and graphical output of the collected ROA data for *all pressure points of this sample*. When you select All, a check mark will appear next to it and be removed from wherever it was before.



When reports are produced with a destination of *Report to Screen*, a different display window is created for each data point. To avoid cluttering the screen and exhausting Windows resources, reports are produced for only the first 10 data points. Reports for additional data points must be individually selected.

Individual point

Selecting an **individual point** generates tabular and graphical output for just that pressure point's collected ROA data. When you select an individual point, a check mark will appear next to it and be removed from wherever it was before.

Reports

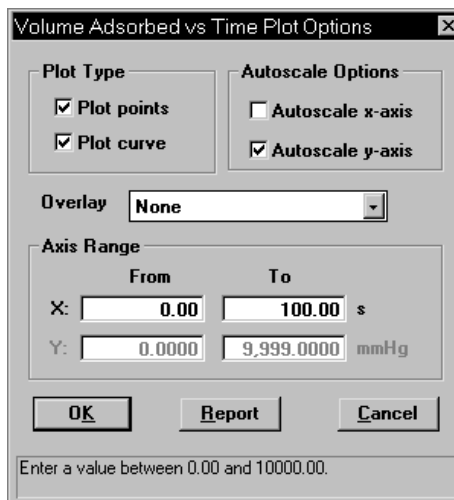


Report to Screen
Report to Printer
Report to Printer/Plotter

Select one of these three choices to specify which location should receive the output. Whichever you select will get a check mark next to it and the other choices will have the check mark removed. Selecting **Report to Screen** or **Report to Printer** causes all output to go to the designated location, screen or printer, respectively. Selecting **Report to Printer/Plotter** causes tabular output to go to the printer and graphs to go to the plotter.

Pressure vs Time
Vol. Ads. vs Time
dV/dt
dV/dLog (t)

Selecting any one of these four generates a graph with the data as defined by the selection title to appear. (If you want all four to appear, select **All** as described later.) A plot options dialog like the following will appear for whichever of the four is selected.



Pressure vs Time
Vol. Ads. vs Time
dV/dt
dV/dLog (t)
(continued)

The plot options dialog which appears will be exactly like this one and might vary only by title. For example, if your selection happened to be dV/dt, the title would be “dV/dt Plot Options.” The fields you can adjust are as follows:

Plot Type

Choices: Plot points, Plot curve (or both)

Select either or both. Selecting **Plot points** results in graphs with the data points noted but no lines (curves) connecting them. **Plot curve** results in curves showing without the data points noted. Selecting both results in both points and curves being displayed.

The proximity of data points and how much data must be plotted will determine the practicality of plotting one or the other or both.

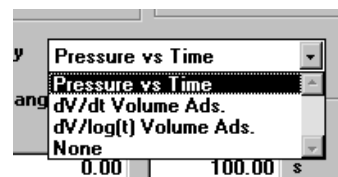
Autoscale Options

You can select or d-select to autoscale the X-axis and the Y-axis. If you select autoscale for an axis, the ROA program determines an appropriate scale for the axis in question.

If you deselect autoscale for an axis, the **Axis Range** fields are enabled so that you can enter a scale.

Overlay

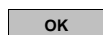
Select this to see a drop-down list of choices available.



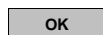
These may be used to overlay a second graph on top of the one selected under **Reports**. For each of the four graphs which may be selected from the Reports menu item, one of the other three may be overlaid on top of it.

Axis Range

These fields are enabled when you deselect Autoscale, allowing you to specify a range for scaling.

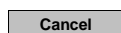


Click if you are just setting up your report options, but do not wish to run the report at the current time. The options you select will be saved.

For instance, if your Reports choice is **All** and you have a number of varying specifications for each report (autoscale, overlays, etc.), you should set the options for each graph on its plot options dialog and select , graph type by graph type. Then when you are done specifying all the options for each of the graphs, you can return to the Reports drop-down list and select **All** to run the graphs and tabular report.



Click to run this particular graph at the current time.



Click to cancel whatever selections you just made on this plot options dialog.

Tabular

Select this option for tabular data only.

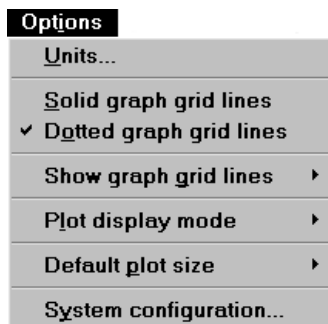
All

Select this to get all four graph types plus tabular data for the pressure points selected on the Data drop-down list described earlier.

Cancel

Select this to cancel any reports which are being generated within the ROA program and to close all of the active report displays. You must cancel any reports that have begun printing or that are queued in the Windows Print Manager from the Print Manager window.

Options



Units

Displays the Unit Selections dialog box allowing you to choose the way in which certain criteria are to display.



Solid graph grid lines Dotted graph grid lines

Allows you to choose whether to use solid or dotted lines when you choose to show graph grid lines.

When you choose dotted graph grid lines, the screen output actually displays as solid; however, dotted lines display when printed to a printer.

Show graph grid lines

The options on this cascading menu allow you to choose what type of lines to display on graphs, or you can choose to have none displayed.

Choices: None, Horizontal, Vertical, Both

Plot display mode

Select this to see two drop-down choices.

Square

Sizes the plot on the screen so it is always square.

Fill to fit

Sizes the plot on the screen so it fills the whole window.

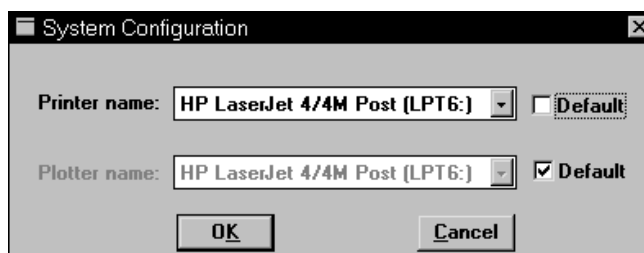
Default plot size

Select this to make a choice of the horizontal and vertical dimensions of plots printed on *printers or plotters*. The selection here does not apply to output on your screen.

Some laser printers have insufficient memory to contain the whole image prior to printing. If this occurs, you will see an appropriate message. Select a smaller plot size and try to print again.

System configuration

Select this to display the system configuration dialog.



Use this dialog to select the printer and plotter to be used for printing graphical and tabular ROA output. The device selected for the plotter will be used only if the destination for the report is printer/plotter. In this case the tabular reports are sent to the printer and graphs are sent to the plotter. Note that tabular data can go only to a screen or a printer.

The defaults will be whatever printer and plotter you have assigned as your system printer and plotter.

Both the printer and plotter have a drop-down list containing printer/plotter options.

Help



About

Displays information about the ROA program

Windows



Tile

Resizes all open windows and arranges them side by side so that the contents of all open windows are visible.

Cascade

Resizes all open windows and arranges them in a stacked fashion. The active window is positioned on top of the stack. Each window's title remains visible, making it easy to select other windows.

Arrange Icons

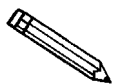
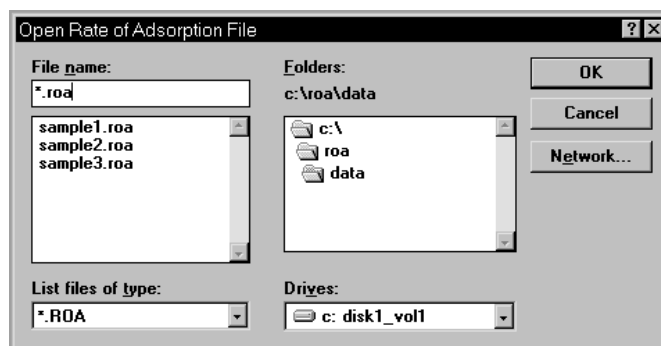
Arranges the symbols for all minimized windows in an orderly manner.

The Windows menu also displays all open files; the active window is preceded with a check mark (✓)

Using The ROA Program

The ROA program is activated through the ASAP 2020 analysis program. To activate ROA program:

1. From the ASAP 2020 menu, select **Reports, Rate of Adsorption**.
2. From the ROA menu, select **File** and **Open** to display the Open Rate of Adsorption File screen.



Remember that the ROA program *only displays* in tabular or graphical form the data that has already been collected; the actual data is collected by the ASAP 2020 program.

3. Select a file for which you wish to see collected ROA data. In this example, we'll select **Sample1.roa**.

A *Report in Progress* message appears indicating the file is being opened. The ROA program will pause briefly while this message is displayed. Then an Analysis Log will appear for the last point in the ROA data.

Report - Target Pressure 0.732

Sample ID: RUN010 - Alumina (krypton) Tube B2
File Name: C:\ROA\DATA\SAMPLE1.ROA

Sample Weight: 1.1253 g Warm Freespace: 16.6788 cm³
Analysis Bath: 77.100 K Cold Freespace: 43.2740 cm³

Analysis Log

| Time (s) | Pressure (mmHg) | Volume Adsorbed (cm ³ /g STP) | dV/dt Volume Adsorbed (cm ³ /g-s STP) | dV/dLog(t) Volume Adsorbed (cm ³ /g-s STP) |
|----------|-----------------|------------------------------------------|--------------------------------------------------|-------------------------------------------------------|
| 0.000 | 0.93475 | 0.0923 | 0.0013 | 0.0095 |
| 5.010 | 0.85725 | 0.0990 | 0.0009 | 0.0151 |
| 10.020 | 0.80425 | 0.1035 | 0.0005 | 0.0149 |
| 15.030 | 0.77375 | 0.1061 | 0.0003 | 0.0120 |
| 20.040 | 0.75625 | 0.1076 | 0.0002 | 0.0089 |
| 25.050 | 0.74625 | 0.1085 | 0.0001 | 0.0065 |
| 30.070 | 0.74025 | 0.1090 | 0.0001 | 0.0045 |
| 35.080 | 0.73675 | 0.1093 | 0.0000 | 0.0030 |
| 40.090 | 0.73475 | 0.1095 | 0.0000 | 0.0017 |
| 45.100 | 0.73375 | 0.1096 | 0.0000 | 0.0009 |
| 50.110 | 0.73325 | 0.1096 | 0.0000 | 0.0010 |
| 55.120 | 0.73275 | 0.1097 | 0.0000 | 0.0012 |
| 60.130 | 0.73225 | 0.1097 | 0.0000 | -0.0001 |
| 65.140 | 0.73225 | 0.1097 | 0.0000 | 0.0000 |
| 70.150 | 0.73225 | 0.1097 | 0.0000 | 0.0000 |
| 75.160 | 0.73225 | 0.1097 | 0.0000 | 0.0015 |
| 80.170 | 0.73175 | 0.1098 | 0.0000 | 0.0000 |
| 85.180 | 0.73175 | 0.1098 | 0.0000 | 0.0000 |

<< Prey Next >> Close Print Header

Click **Header** to remove the header and allow more of the report to display in the window. Simply click **Header** again to reinstate the header portion.

- Select **Data**, and all the pressure points for which ROA data were collected for this sample appear as follows.

File **Data** Reports Options Help Windows

Sample Info...

ROA V1.0

1 Point ROA Test (Tube P2)

Analysis Log

| Volume Adsorbed (cm ³ /g) | dV/dt Volume Adsorbed (cm ³ /g-s) | dV/dLog(t) Volume Adsorbed (cm ³ /g-s) |
|--------------------------------------|----------------------------------------------|---------------------------------------------------|
| 199.6910 | 0.0500 | -0.0050 |
| 199.6960 | 0.0000 | 0.0000 |
| 199.6960 | 0.0000 | 0.0000 |
| 199.6960 | 14.2300 | 11.3896 |
| 201.1190 | 111.9800 | 115.5505 |
| 212.3170 | 22.7699 | 28.7567 |
| 214.5940 | 23.5101 | 35.1177 |
| 215.9450 | 6.2900 | 10.8463 |
| 217.5740 | 7.2099 | 14.0950 |
| 218.2950 | 2.0399 | 4.4582 |
| 218.4990 | 2.9601 | 7.1511 |
| 218.7950 | 0.9200 | 2.4345 |
| 218.8870 | 1.3001 | 3.7398 |
| 219.0170 | 0.6100 | 1.8955 |
| 219.0780 | 0.8699 | 2.9032 |
| 219.1650 | 0.3601 | 1.2848 |
| 219.2010 | 0.7399 | 2.8102 |
| 219.2750 | 0.1901 | 0.7659 |

<< Prey Next >> Close Print Header

- Choose one of the following:
 - Select **Sample Info** to manipulate any parameters before producing output.
 - Select **All** to include ROA data for *all* pressure points for which ROA data was collected
 - Select an individual point to see ROA data for that point only.

6. Select **Options** to specify plot options.
7. Select **Reports** and the accompanying selections from the Reports drop-down list.
 - a. Choose whether the output should go to the screen, printer, or printer/plotter.
 - b. Select **All** or any of the four graphs or tabular report.
8. If you selected a particular graph from the Reports list, select the plot options for that graph, specifically:
 - points or curve plot type
 - autoscale options
 - overlay (if any)
 - axis range if autoscale was not selected.
9. To obtain the output displayed, select either:
 - on the Plot Options dialog of a particular graph, or
 - **All** from the Reports menu item.

A sample of graphical output with overlays is shown in Figure 3-1.



Always make sure you exit the ROA program and Windows before turning off the computer. Failure to do so could result in loss of data.

Power Failure in Computer or Instrument

ROA is a display program which runs in your computer and loss of power to it does not affect data collection in the ASAP 2020. A computer power failure which occurs while running the ROA program will result in loss of any changes to the sample information. If ROA data are being collected by the ASAP 2020 program, power must be restored to the computer immediately.

ROA data will be held for only a short time in the instrument controller. If the computer does not restart soon enough after the power failure, some ROA data will be lost.

If an **instrument power failure** occurs, data already collected by the instrument will be retained, but new data will not be collected.

You may not exit the ASAP 2020 program while instruments are collecting ROA data. An analysis must first be suspended before the ASAP 2020 will accept an exit request.

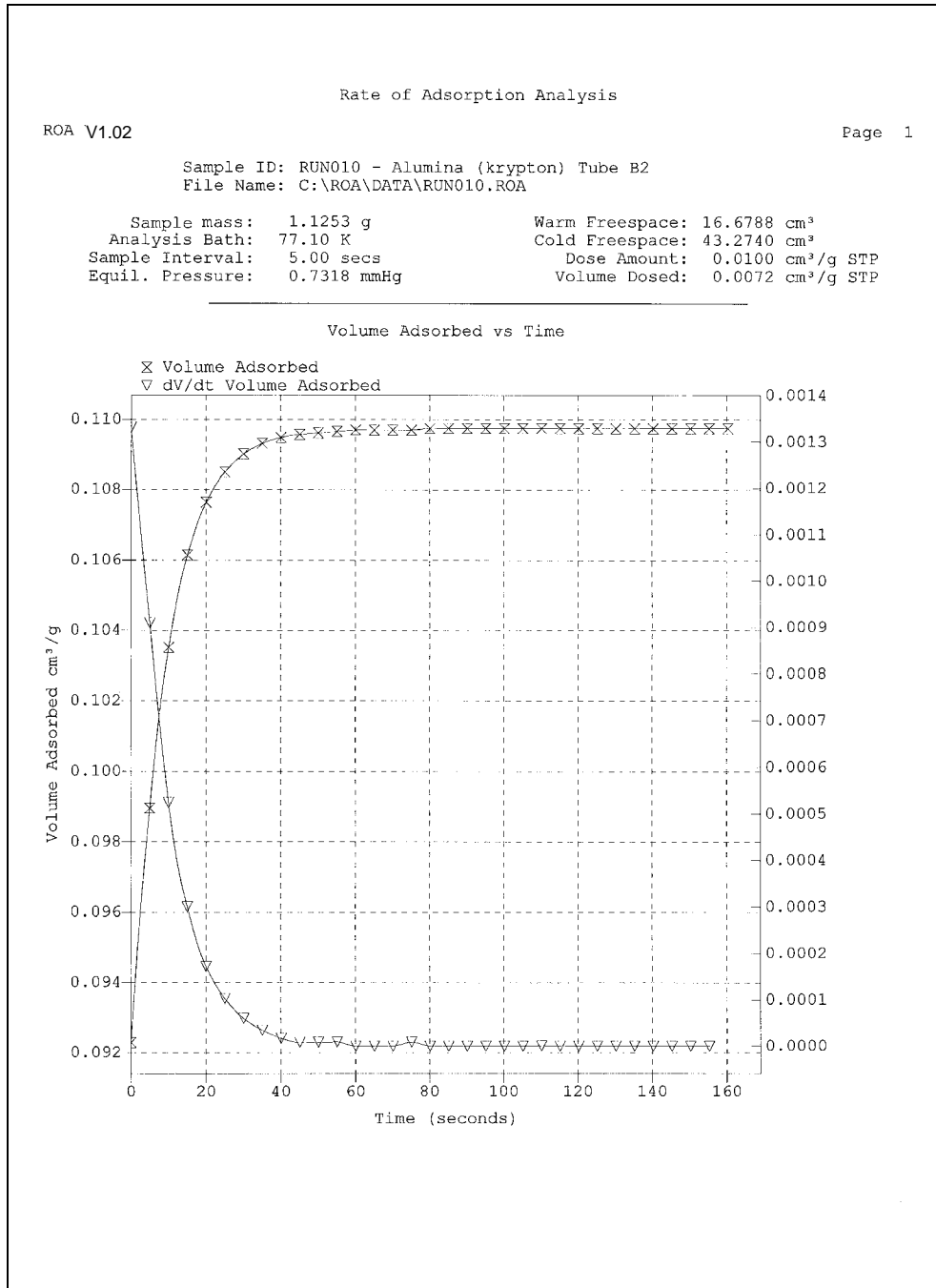


Figure 3-1. Example of Graphical Output

CHAPTER 4

ORDERING INFORMATION

ORDERING INFORMATION

| Part Number | Description |
|--------------|--------------------------------------------------|
| 202-20821-00 | ROA Kit; includes software and operator's manual |
| 202-42821-00 | Operator's manual |

APPENDIX A

ERROR MESSAGES

ERROR MESSAGES

This appendix contains the error messages which may be encountered during operation of the ROA program.

6200- Error parsing the contents of (file name). All data could not be loaded.

Cause: An error occurred while reading the contents of (file name). There is an error in the format of the entered data. All data up to the error has been loaded.

Action: Examine the file with the editor used to create it. Look for a typographical error in the text following the point at which the ROA program stopped loading data

6201- Invalid parameter (label) found. Value was ignored.

Cause: An invalid parameter was found in the header of the ROA file being loaded.

Action: Examine the file with the editor used to create it. Inspect the parameters at the start of the file. Remove the parameter named in the error message.

6202- Error!! More than (number) pressure entries stored for target pressure (pressure). Some data was discarded.

Cause: The ROA program only loads (number) measurements for a single pressure point. Additional entries are ignored.

Action: The ROA program functions with up to 1000 measurements; additional entries are ignored. Another analysis package must be used if more than 1000 measurements are to be collected.

6203- Do you wish to save the changes to the file (file name)? (yes, no)

Cause: Changes have been made to the current ROA data file. These changes will be lost if the file is not saved before a new file is loaded.

Action: Select **Yes** to save the changes; otherwise, select **No**.

6204- File (file name) contains no ROA data.

Cause: The file selected for analysis is empty.

Action: If the analysis is in progress, wait until the first ROA pressure has equilibrated.

6205- This operation will produce <number> display windows. Do you wish to proceed? (Yes, No)

Cause: You requested a report for **All** data points with **Report to Screen** selected as the destination. A report display window will be created for each data point in the loaded file.

Action: Usually **All** is selected when the destination is **Report to Printer**. Select **Yes** to proceed with the reports on the screen or **No** if you wish to change the destination.

6206- Only the first 10 data points will be reported to the screen. Report the remainder by selecting them individually.

Cause: You requested a report for **All** data points with **Report to Screen** selected as the destination. A report display will be created for *only* the first 10 data points to avoid overloading the screen.

Action: To produce a screen report for the additional data points, you must individually select each point. To produce reports on all of the data points at once, select **Report to Printer** as the destination.

APPENDIX B

FORMAT OF EXPORTED DATA

FORMAT OF EXPORTED DATA

The ASAP 2020 Front End (FE) stores the collected ROA data as comma delimited ASCII text so that it can be used by the ROA program as well as with spreadsheets or other custom developed analysis techniques. The ASCII text contains the following entries:

| | |
|-----------------|---------------|
| “Sample ID” | “<sample id>” |
| “Sample Weight” | xxx.xxx |
| “Analysis Bath” | xxx.xxx |
| “Warm FS” | xxx.xxx |
| “Cold FS” | xxx.xxx |
| “Interval” | xxx.xx |
| “Dose Amount” | xxx.xx |
| “Nonideality” | xxx.xx |

| | | |
|--------|---------|---------------------------------------------------|
| Point | 1 | //An index |
| Target | xxx.xxx | //Pressure table target pressure for point 1 |
| Dose | xxx.xxx | //Quantity of gas dosed in cm ³ /g STP |

//For Point 1, a table of Time, Pressure, and Cumulative specific volume adsorbed by the sample is created. Time is reported in seconds and refers to time elapsed since the start of the dose. Pressure is reported in mmHg and Cumulative specific volume adsorbed is reported in cm³/g STP.

| | | |
|--------|------------|------------------------|
| <time> | <pressure> | <cum. spec. vol. ads.> |
| ” | ” | ” |
| ” | ” | ” |
| etc. | etc. | etc. |

//Up to Point n

| | | |
|--------|---------|---------------------------------------------------|
| Point | n | //An index |
| Target | xxx.xxx | //Pressure table target pressure for point n |
| Dose | xxx.xxx | //Quantity of gas dosed in cm ³ /g STP |

//For Point n, a table of Time, Pressure, and Cumulative specific volume adsorbed by the sample is created. Time is reported in seconds and refers to time elapsed since the start of the dose. Pressure is reported in mmHg and Cumulative specific volume adsorbed is reported in cm³/g STP.

| | | |
|--------|------------|------------------------|
| <time> | <pressure> | <cum. spec. vol. ads.> |
| ” | ” | ” |
| ” | ” | ” |
| etc. | etc. | etc. |

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