Instructions for SonicData
Data Collection for the HP GC

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INTRODUCTION

The SonicData hardware and software interfaces were developed by Joseph A. Counsil and Benjamin Stauffer. This is an open-source project, and more information and a free copy of this software can be found at http://sonicdata.sf.net. This combination of a simple hardware interface and software replaces the old thermal-paper integrator, thus allowing the user to save, process, and print data using modern equipment and methods. The data is saved in a simple tab-delimited text file, thus allowing it to be opened and processed in Excel, or many other data-analysis programs.

GENERAL OPERATING PROCEDURE

1. Turn on the GC and set the temperature program as needed (injector, detector, and oven temperatures, and temperature program profile if not running an isothermal analysis).

2. Turn on the gas valves above the bench, and all except the AUX valve on the GC top-left panel.

3. Turn on the main valves at the nitrogen and hydrogen gas tanks at the end of the laboratory bench.

4. Depress the "ignite" button on the GC top-left panel to ignite the detector flame. It is sometimes necessary to gently blow a puff of air across the top of the detector to get the flame to ignite. To monitor whether the flame is ignited, press the "Signal 1" button once or twice until you see a number displayed on the GC display panel. If that number is non-zero, and is greater than 25 units, then the flame in the FID is ignited. You may verify this by turning off the hydrogen valve and observing that the signal display falls to zero or nearly zero (if you do this, remember to re-ignite the flame). You may also check for flame ignition by briefly holding a cool glass bottle directly above the detector, and you should observe some water condensation on the outside of the bottle.

5. Open the "AUX" flow valve on the GC top-left panel.

6. Allow the GC to equilibrate for at least 15 minutes before use.

7. Inject the sample, and as simultaneously as possible press the "Start" button on the GC (if you have set up a non-isothermal oven temperature program), and press the "Start Collection" button as detailed below in the SonicData software.

8. When the temperature program (or your estimated run time) is complete, you must click on the "End Collection" button in the SonicData software and save your data file as detailed below.

9. When finished, please remember to close all gas valves and turn off the GC. Also, remember to log out of the PC if you have logged into your personal account.

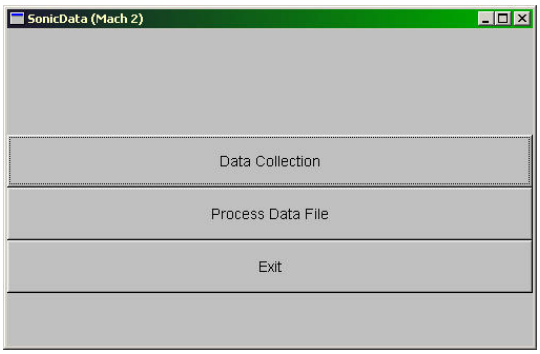
DETAILED SOFTWARE INSTRUCTIONS

This workstation uses a standard Windows XP campus install, and is on the network. It is set up to print to the laser printer near the UV-Vis spectrophotometers on the next laboratory bench. PLEASE DO NOT USE THIS WORKSTATION FOR WEB BROWSING, E-MAIL, ETC. It is ONLY intended to be used for data collection from the HP GC.

When you save your data and report files as shown below, please save them to the DESKTOP so you will not lose track of where they are located. When your work is complete, please copy the data files to your own media (e.g., USB drive, floppy, or through the network to your own DFS account). PLEASE REMOVE YOUR DATA FROM THIS PC after you have finished saving it to your own media.

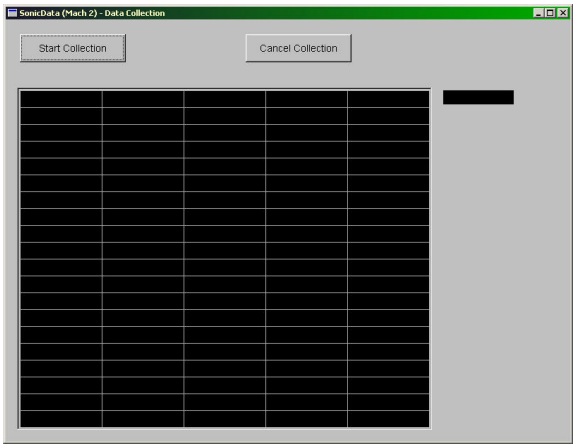
1. Log into the PC as "chemuser" with a password of "chem-241" on the "Log on to:" field of "this computer" (if it is not already logged into that account). You may also log in to your private DFS (campus) account, but please remember to log out when you are finished using the instrument.

2. Double-click on the "SonicData" icon. This will open the initial SonicData program window:



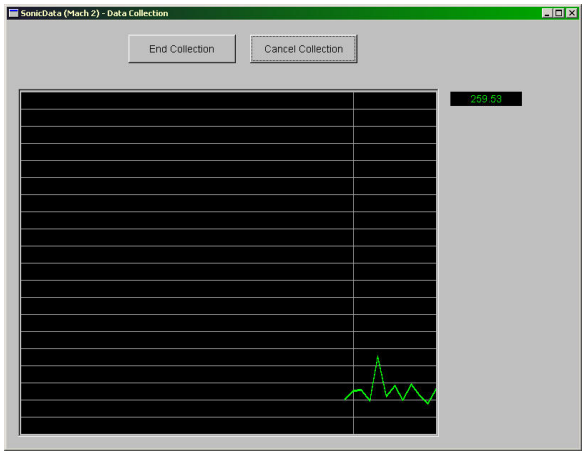
3. To begin the data collection process, click on the "Data Collection" button. To process an old data file (detailed in following sections), click on the "Process Data File" button. To exit, you may click the "Exit" button, the "X" box in the upper-right corner of the window, or simply press the "Esc" key on the keyboard. NOTE: The "Esc" key will exit ANY window or process in SonicData.

4. In the Data Collection window, as shown below, you may either press the "Start Collection" button or cancel the collection to return to the main window. When you click on the "Start Collection" window, the data collection process will begin immediately.



NOTE: When you start collection, if in a few seconds you do not see a number greater than zero displayed in the small black window to the upper-right of the plot area, then quickly press the "Cancel Collection" button, return to the Data Collection window and click "Start Collection" again. Occasionally the data collection process fails and must be restarted. This is a "bug" in the program which needs to be repaired.

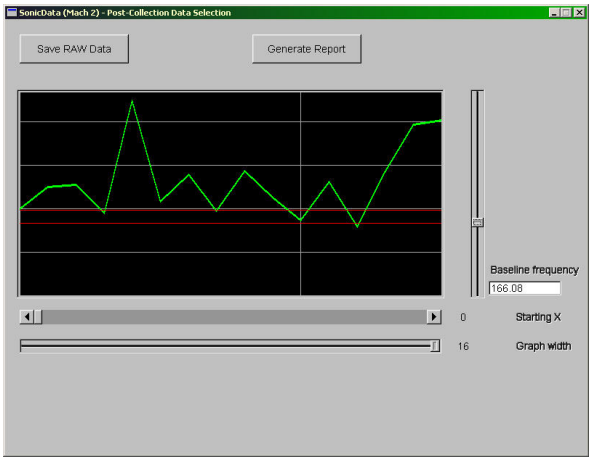
5. When the data collection starts, the collection window should look something like this:



Notice that you see both a numeric and plot display if the data collection has successfully begun.

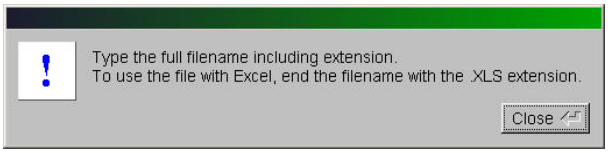
When your GC data collection is complete, you must manually stop the data collection process in SonicData by pressing the "End Collection" button. If you press the "Cancel Collection" button (or press the "Esc" key on the keyboard), your data will NOT be saved.

6. After the "End Collection" button is pressed, this window will be displayed:



This window presents several options as follows:

A) "Save RAW Data" - saves the unmodified original data set if you have not changed the "Starting X" and "Graph width" sliders. This function will save the modified data set if you have changed the scale by changing the "Starting X" and "Graph width" sliders. When you click on this button, the following information box will appear:

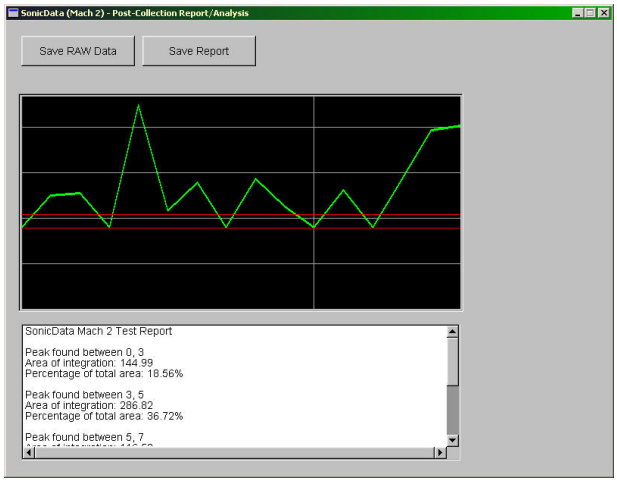


When you close this informational prompt, the standard Windows file-dialog box will appear. As mentioned in this information box, if you give the data file an "XLS" extension (e.g., "data1.xls"), it will allow you to later double-click on the file icon and it will automatically open in Excel. Alternatively, you could give the file a name such as "data1.txt" which would make it a simple text file, and a double-click on its icon will open the file in Windows Notepad.

NOTE: Since SonicData does not yet have the capability to print directly, you will need to open the data files in Excel, generate a graph, and print the graph from Excel.

B) "Generate Report" - will perform an integration on the data as shown in the display window. To adjust the baseline clipping level and peak threshold for the integration function, use the "Baseline frequency" slider to the right of the data display window. The lower horizontal red line is the baseline clipping level, and the upper horizontal red line is the integration peak threshold. Signals which pass below the baseline clipping level will be truncated and ignored, and signal peaks must exceed the peak threshold or they will be truncated from the data set and ignored. Click on the "Generate Report" button to display the integration report window as shown below.

7. When a report is generated, the following report windows is displayed:



A) "Save RAW Data" - This button saves the modified (zoomed, baseline-clipped) data set upon which the integration was performed. This is NOT the original collected data set. This function is otherwise similar to the "Save RAW Data" function in the original data collection windows as shown earlier.

B) "Save Report" will save the integration peak/area report which is displayed in the lower window. When this button is clicked, the following information window displays:

When this window is closed, a standard Windows file-dialog box appears. It is best to give the file extension of ".txt" (e.g., integration1.txt). This will allow the file icon to be double-clicked to open in Windows Notepad, then printed.

8. You can process a previously-collected data file by pressing the "Process Data File" button on the main window. When you click on this button, a Windows standard file-dialog box will open allowing you to select a raw data file to open and process in the same way as presented in the post-collection display window as detailed in item 6 above.