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Control Charting on the HP 3396/93 Integrators Using HP Peak-96 and Microsoft® Excel

Application Note 228-122

Data Handling

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Abstract

HP Peak-96 and Microsoft® Excel are used to demonstrate the control charting process on an HP 3393 or HP 3396 Integrator. A sample Excel macro is included.

Introduction

EPA regulations require that statistical analysis be performed on integrator data to ensure that instruments are performing properly. Among the requirements is quality control charting for which the analyst is required to observe trends in data over a period of time. The purpose of this application is to provide an example of how to use HP Peak-96 in conjunction with Microsoft® Excel (hereafter referred to as Excel) for the control charting process.

HP Peak-96 Information Manager is a PC-based communications package that manages data from one to four integrators. HP Peak-96 provides a systematic method for storing the data and is able to convert integrator files to the standard ASCII format required by other applications. Control charting can be accomplished by using these HP Peak-96 functions to prepare integrator files to be read by a spreadsheet application for further analyses.

Microsoft® Excel is a spreadsheet program that runs in the Microsoft® Windows environment. Using Excel, macros can be created to automatically perform statistical analysis on data acquired from an integrator and exported by HP Peak-96. The macro included in this application demonstrates Excel's capability to analyze integrator data for the purpose of control charting.

Setting Up with HP Peak-96

Several steps are involved in setting up the files for control charting. The first is to create the directory C:\Control. The macro searches this directory for the files to be control charted. The directory can be created by typing `MKDIR Control` at the MS-DOS® prompt from the root directory. The following steps should be done with HP Peak-96 loaded on the PC and the sequence loaded on the integrator with the correct calibration file.

Before Generating the Data

If at all possible, the next two steps should be done before the files that are to be control charted have been generated. If the files have already been generated, skip to the next section, which explains the procedure for that instance.

The first step is to edit the method using either integrator commands or the HP Peak-96 remote keyboard. In the section labeled Print & Post-Run List Options, specify that the postrun report be stored on the host computer (H). In the Report Options section, specify that no uncalibrated peaks be reported (figure 1).

The second step is to set the data prefix for the HP Peak-96 Autoname function. This function renames the integrator files that are stored on the PC using a data prefix and the current run number. Although the Series II integrators also carry an autoname application, this must not be used, because it increments

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the files differently than HP Peak-96. To specify the data prefix for the HP Peak-96 Autoname function:

1. Select the appropriate integrator.
2. Select DATA ACQUISITION, then SETUP PC.
3. Press ENTER at the Generate New Prompt.
4. Change the Data Prefix by typing in a new prefix up to 5 characters long (figure 2).

The files will be stored in the drive and path listed here. To change the place of storage, type the new drive and path in the appropriate fields. When the changes have been made, press ESC.

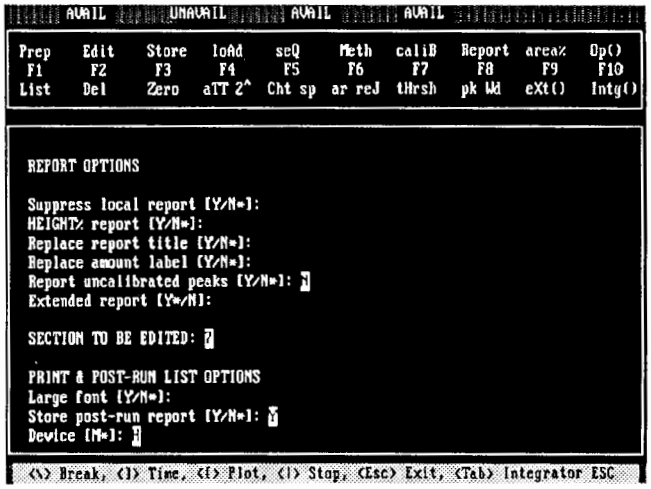

Figure 1. Editing the method using the HP Peak-96 remote keyboard.

If the Data Was Generated Previously

Control charting is still possible if the files have already been generated; however, the file manipulation described in the preceding section must be done manually. First, all the files to be control charted must be transferred to the PC. This can be done using the HP Peak-96 Utilities Transfer function. Then the files must be renamed to be consistent with the HP Peak-96 autonaming function. This means all the file names must contain the same prefix and a suffix that is an integer between 1 and 999. This can be accomplished using the HP Peak-96 File Rename function to rename each file. More information on these functions can be found in the HP Peak-96 User 's Guide.

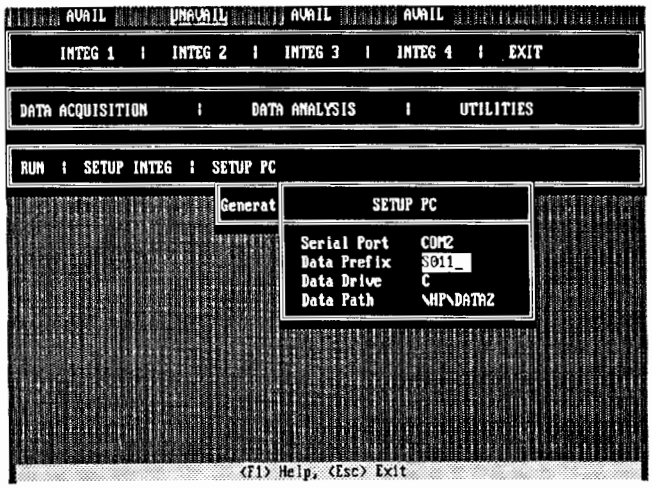

Figure 2. Setting the data prefix for the HP Peak-96 Autoname function.

After Generating the Data

When all the data to be control charted has been generated, the next step is to create a file, Names.ASC, that contains the names of all the compounds in the calibration table. The control charting macro requires this file to organize the data retrieved from the report files. A short basic program, Names.BAS, is provided to generate this file. The program can be downloaded from the PC by using the HP Peak-96 Utilities Transfer function. Alternatively, the code can be typed in directly, provided the integrator has BASIC. The code for the program is listed in figure 3. Once stored on the integrator, the program can be assigned a key that will automatically execute the program when pressed. This is done by typing `AS 7 M:Names.BAS` at the system prompt which will assign the program Names.BAS to function key 7.

```
>LIST
   5   ! PROGRAM TO GET CALIBRATED COMPONENT NAMES
  10
  15   ASSIGN "m:NAMES.BAS",7
  20   CREATE "M:NAMES.UA1",-1
  30   OPEN #1: NAME "M:NAMES.UA1"
  40   PRINTER IS #1
  50   WHEN EXCEPTION IN
  60     FOR I=1 TO 500
  70       PRINT NAME$(I)
  80     NEXT I
  90   USE
 100     IF EXLINE(70) THEN
 110       CLOSE #1
 120       END
 130     END IF
 140   END WHEN
 150   END

>
```

Figure 3. BASIC code for Names.BAS.

When executed, the program gets the compound names from the current calibration table and stores them in the file Names.UA1 on the PC. The alternative to running this program is to create the file by using a text editor and manually typing in the compound names, one per line, to match the calibration table order.

The files to be control charted must be converted to standard ASCII format by using the HP Peak-96 Export function. This is done by the following steps:

1. Select the appropriate integrator.
2. Select UTILITIES, then FILES.
3. Select the option to Export.
4. Select the Text option.

   The screen will display the names of all the report and text files (figure 4). Select Names.UA1 along with the report files to be control charted by pressing [F5] for each selection. Because the macro reads in every file it finds within the user-specified range, be certain that only the files to be control charted are exported. Press ENTER when the selections have been made.
5. Type `C:\Control` as the directory in which to export the files.

The final step before loading Excel is to rename stray files. The macro determines which files to open by the file name prefix and the starting and ending suffix numbers specified during execution. To include files with different names, the files must be renamed before running the macro. Any files that fall within the range that are not needed for this application should also be renamed or deleted at this time.

After completing the above steps, the files are ready to be read into Excel for control charting.

Control Charting with Microsoft® Excel

The included macro, Control.XLM, demonstrates Excel's capability for control charting. The macro is capable of reading up to 250 ESTD/ISTD, extended or short, calibrated report files from HP 3396 Integrators, or short calibrated report files from HP 3393 Integrators. The macro reads in files from the specified range, extracts the necessary data from each file, stores the data in a results sheet, and creates charts that display changes in the data over time.

To run Control.XLM, load Excel and open the macro. The macro is opened by selecting the Open option in the File pull-down menu and choosing "Control.XLM" from the directory in which it is stored. If desired, the macro can be opened automatically each time Excel is loaded by editing the WIN.INI file. To do this, load WIN.INI into a text editor and page down to the section labeled [Microsoft Excel]. Insert a line in this section and type `open=C:\Control\Control.XLM`. When opened, the macro can be run by pressing [CTRL] and [r] at the same time.

The macro begins by opening the Names.ASC file. It then copies up to 500 names from this file to a new worksheet, Results.XLS. These names become the headers for the data retrieved from the integrator report files.

The macro then prompts the user for the files to be control charted. A dialog box prompts for the file name prefix, the starting suffix number, and the ending suffix number (figure 5). The macro searches the C:\Control directory for files with the specified prefix within the specified range and reads them in one at a time.

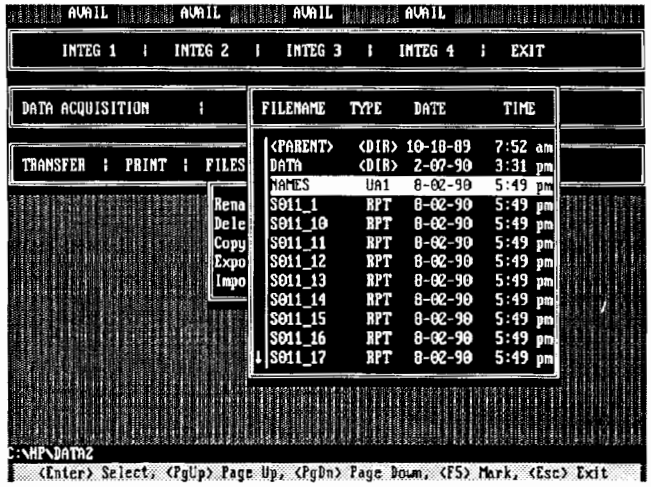

Figure 4. Exporting files from HP Peak-96.

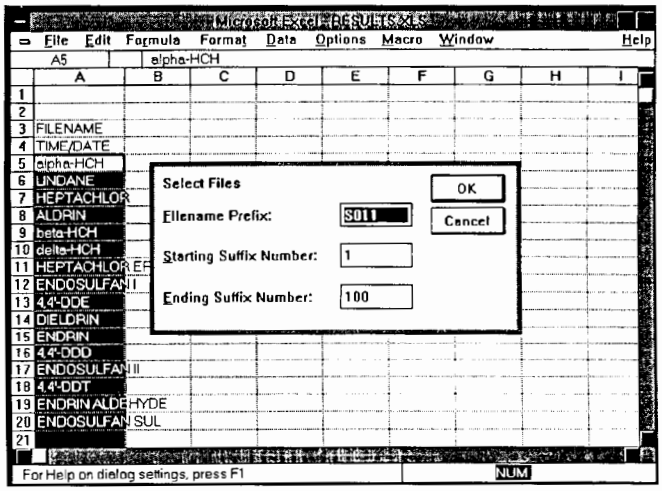

Figure 5. Prompt to input file names. Created by the FilenameBox dialog box code in Control.XLM.

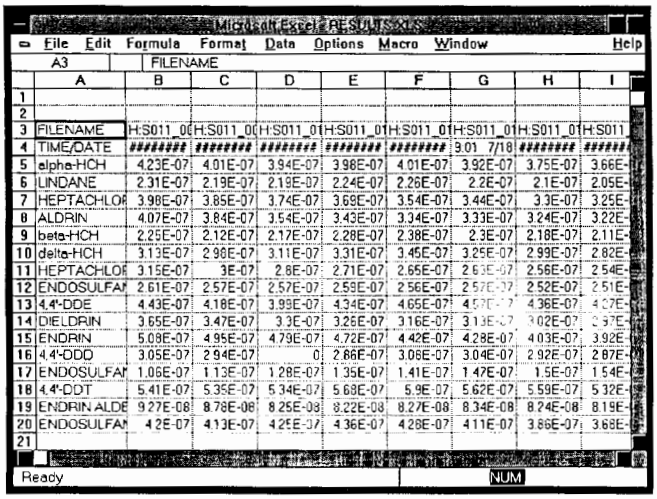

Figure 6. Example of the results sheet generated by Control.XLM.

For each file, the macro parses the data and calculates the response factor (RF) for each compound in the report. The file name, date and time, and the RFs for each compound are then copied to the results sheet. A sample results sheet is shown in figure 6.

When all the files have been processed the user is given the option to view a chart showing the changes in RF over time for specified compounds. The dialog box allows the user to view one compound, view four compounds, or return to the results sheet (figure 7).

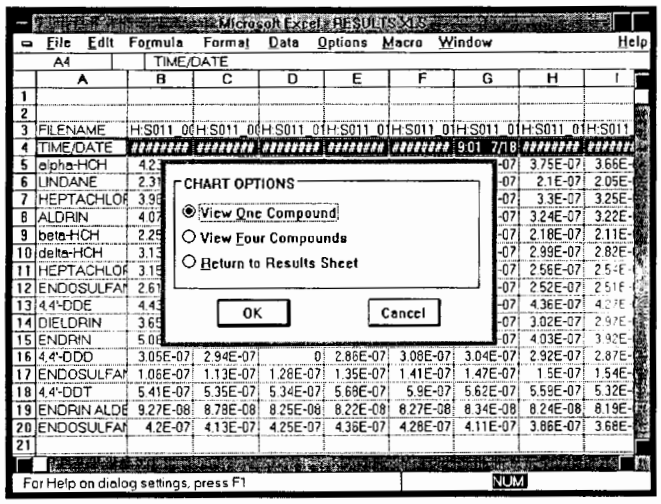

Figure 7. Prompt for chart options. Created by the ChartBox dialog box.

If the option to view one compound is chosen, a dialog box appears to prompt the user to input the name of the compound to be charted. A compound name box will display a list of all the compounds in the results sheet (figure 8). The user may select a name from the box or type in the name as it appears in the calibration table. When the name has been entered, the macro displays a chart showing the RF of the compound over time. A 20% window is calculated and plotted with the RF so that the variance may be seen more clearly. This is useful in determining if the compound is staying within EPA specifications. An example of this chart can be seen in figure 9.

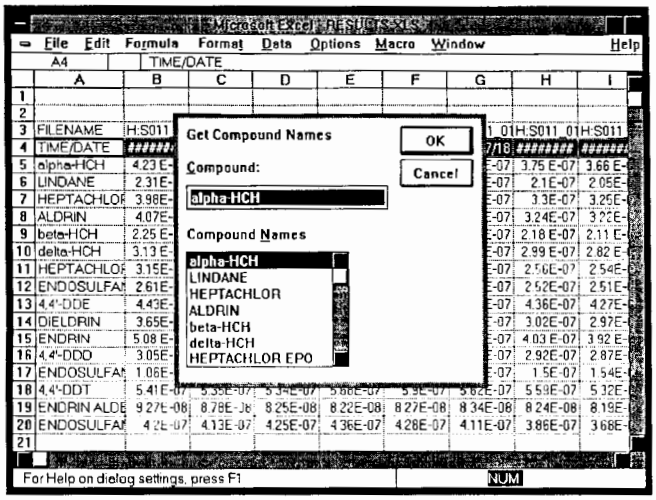

Figure 8. Prompt to input name of compound to be charted. Created by the View1Box dialog box.

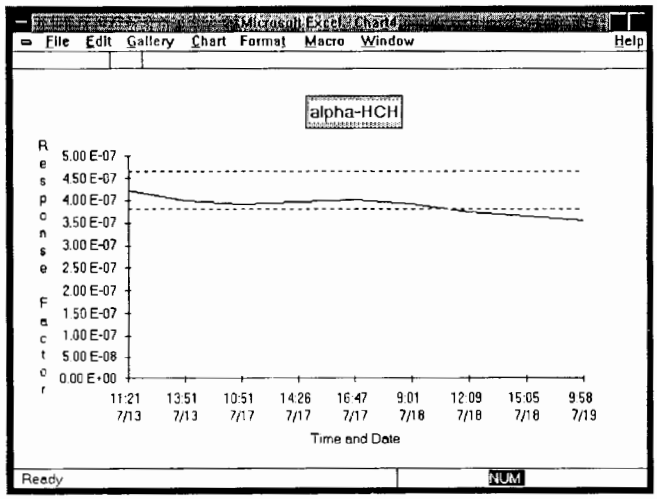

Figure 9. Example of a chart displaying one compound.

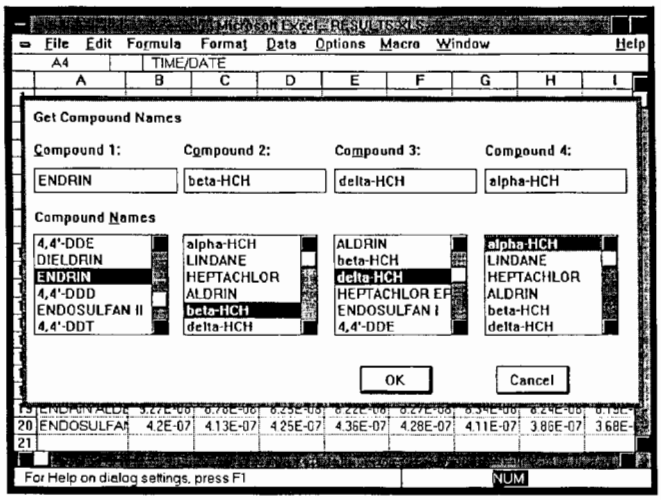

Figure 10. Prompt to input the four compound names to be charted. Created by the View4Box dialog box.

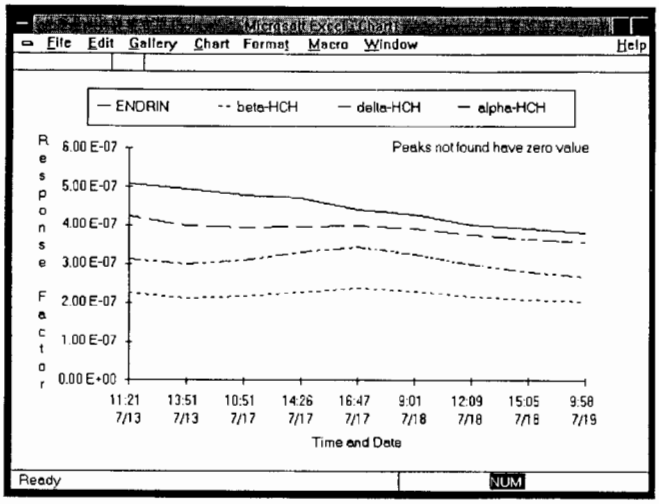

Figure 11. Example of a chart displaying up to four compounds.

If the option to view four compounds is chosen, a dialog box appears to prompt the user to input the names of the four compounds to be charted. The user may either type in the compound names or choose from name boxes that display the names of the compounds in the results sheet (figure 10). Fewer than four compounds may be viewed by selecting the same compound twice. When the compounds are entered, the macro displays a chart showing the RFs for the specified compounds over time. This can be useful in viewing degradation in compounds or viewing the changes in one compound in relation to others. Figure 11 shows an example of this chart.

The macro stops after a chart is displayed. More charts may be viewed by pressing [CTRL] and [c] at the same time. This combination may be pressed for the chart options anytime after the results sheet has been generated. Updating the results sheet automatically updates the existing charts.

Appendix A lists the macro code for Control.XLM. Documentation and suggestions for modification are included.

Summary

The control charting process demonstrates how to use HP Peak-96 in conjunction with Microsoft® Excel to analyze integrator data. HP Peak-96 is used to set up the files; Microsoft® Excel is used to perform the analysis.

To summarize, the steps to set up the files for control charting are as follows:

1. Create a directory, C:\CONTROL.
2. Edit the report options in the method.
3. Set the autoname function in HP Peak-96.
4. Run a basic program, Names.BAS, on the integrator.
5. Export the files to be control charted.
6. Rename stray files.

Excel is then loaded to perform the analysis. The macro, Control.XLM, reads in the files and extracts the necessary data. Calculations are performed on the data and the results are stored in a results sheet. After all the files have been processed, the macro displays the control charts showing the changes in specified compounds over time.

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