Database Management of the SpectrAA 600/800 System

Application Note

Atomic Absorption

Authors

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Introduction

The new generation SpectrAA 600/800 software stores information about methods, sequences, label files and results in an industry standard database for flexibility in manipulation and convenience of third party access. In fact, the SpectrAA 600/800 software automatically stores data sets with the option of signal graphics with every autorun performed. If the size of the database is allowed to grow unchecked, then system operation may become slower. Operations such as recalculating edited data, transferring of data, report generation and eventually even sample analysis may take longer to complete. As with most storage systems, regular database maintenance will ensure continued smooth operation.

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Guidelines for Database Maintenance

The following guidelines have been generated as an aid to users in gaining the best possible long term performance from their system.

Optimum Operating Speed

1. The CONFIG.SYS can be modified to create a Random Access Memory (RAM) disk which must have a size of at least 80 K. The following example creates a RAM disk of 128 K accessed as drive "E", assuming the hard disk already contains a C and D drive. These two lines should then be entered at the bottom of the CONFIG.SYS.
   SET SPECTRAA_DICTIONARY =E:\
   DEVICE=C:\OS2\VDISK.SYS 128,128,64
   The effect of these two lines is to place some of the frequently used database index files in a high speed RAM disk.
2. Ensure the SpectrAA is installed on a High Performance File System (HPFS) partition.
3. If HPFS is used, then the size of the cache in the CONFIG.SYS can be increased from 1024 to 2048 as shown in the example below.

   IFS=C:\OS2\HPFS.IFS /CACHE:2048 /
   CRECL:32 /AUTOCHECK:CD

   where, in this case, the AUTOCHECK parameter shows that both C and D are HPFS partitions.

Deleting Signal Graphics From Stored Data Sets

If they are no longer required, it is recommended that all the signal graphics should be deleted, by using the delete facility in the Administration window of SpectrAA. The delete facility dialog box allows the operator to delete signal graphics and/or results from one or all of the stored data sets. Once a data set is highlighted, it can be deleted from the database by selecting the delete button as shown in Figure 1. This will reduce the overall disk space requirements. In addition, transfer of results to and from the SpectrAA database is slower with signal graphics than without.

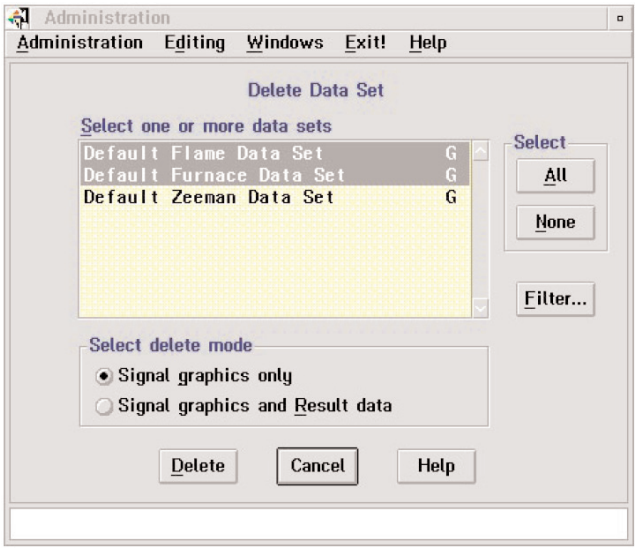

Figure 1. Deleting signal graphics from the SpectrAA database.

Transferring and Storage of Data

Once all the data files have been collected and reports have been generated, the analyst must decide whether the data needs to be retained for archival purposes. If the data is no longer required then it should be deleted from the SpectrAA database using the SpectrAA delete facility in the Administration window. If data files need to be archived, then the format is very important. If data editing, plot or report generation facilities are likely to be required at a later stage, the data files must be exported in the SpectrAA format so that the data can be imported back into SpectrAA. In all current versions, this will lead to several files with the same name but differing extensions (for example, Results.CTL, Results.SIG, ...). These files collectively constitute the exported data.

Data files should be transferred to a separate directory on the hard drive, using the SpectrAA "transfer to disk" facility in the Administration window (Figure 2). One or more data sets can be transferred under one file name by highlighting the required data sets and selecting the transfer button. Note: transferring data straight to a network directory from within SpectrAA usually takes longer than to a local hard disk. Once all the relevant data files have been transferred onto the hard drive, they can be compressed under one file name to simplify

housekeeping using one of the many widely available file compression utilities (for example, PKZIP, from PK ware, Inc. However , make sure that your compression program supports HPFS long file names if you use them). Generally large savings in disk space can be achieved (typically 75% to 85% compression). Not only does archiving files in compressed format save disk space, but it also saves valuable time in transferring data files from hard disk onto floppy disk when preparing backup files.

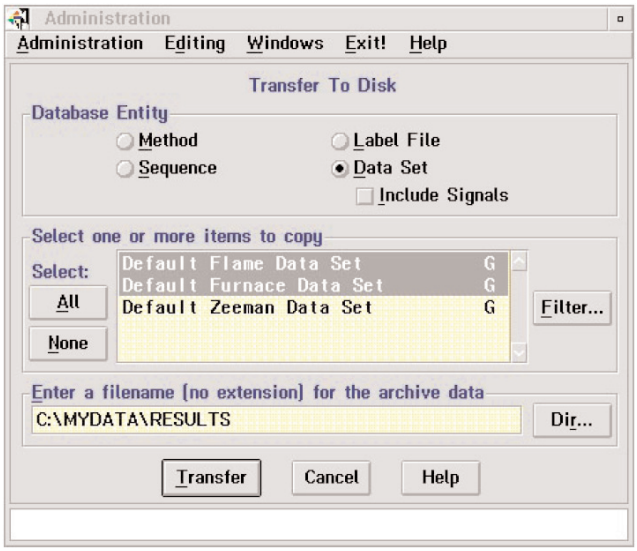

Figure 2. Transferring data files to a separate directory on the hard drive.

Exporting Data for Third Party Access

Alternatively, results can be exported as .PRN files (comma separated format) or written to disk in an ASCII text (.TXT) format, from the Reports window of SpectrAA. Once all the required data sets and report options have been selected, the results can be output under one file name as shown in Figure 3 and Figure 4. The .PRN file can then be imported into a spreadsheet or database utility program. These software packages would enable the analyst to perform a wide range of intensive mathematical calculations and customized report formatting. In the same way, the .TXT report could be incorporated in a word processing document.

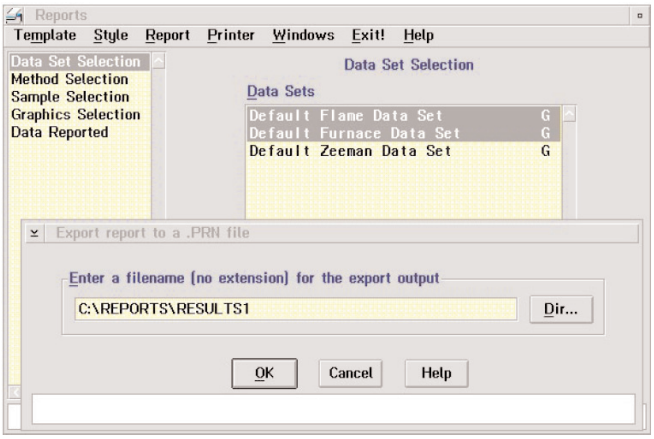

Figure 3. Exporting results as .PRN files.

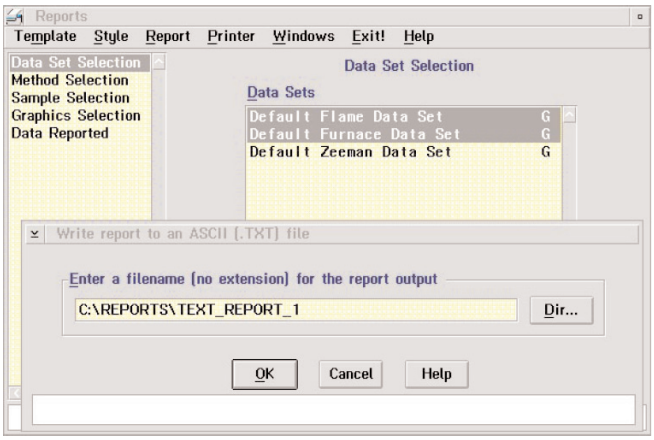

Figure 4. Exporting results in an .TXT format.

Maintaining the SpectrAA Database Regularly

Once the data files have been manipulated and archived onto the hard drive, they should be deleted from the SpectrAA database to ensure the efficiency of the system is maintained. It is recommended that at least once a week all data sets should be checked and those that are no longer needed be deleted. An overview of the transfer options available for maintaining the SpectrAA database is shown schematically in Figure 5.

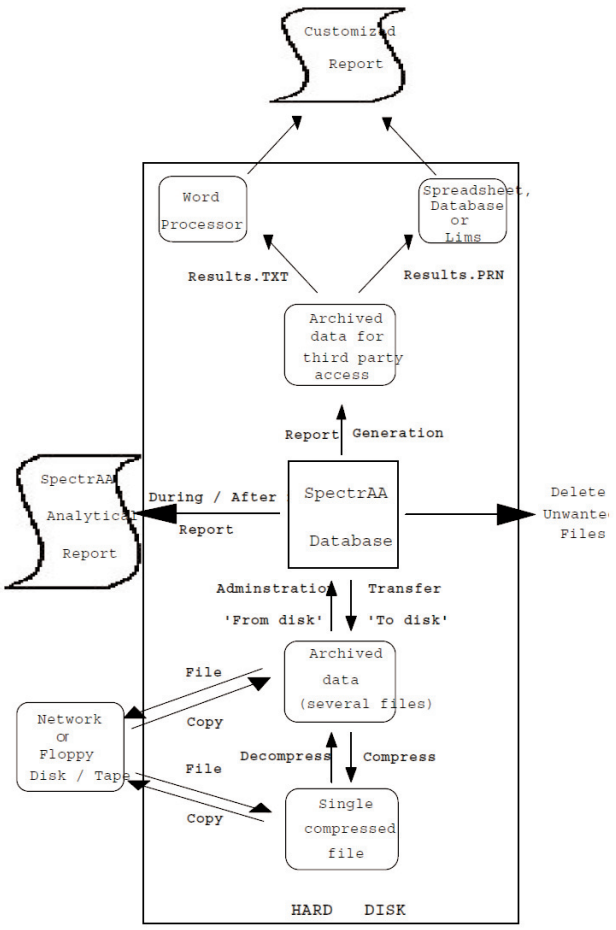

Figure 5. An overview of the transfer options available for maintaining the SpectrAA database.

Summary

Utilisation of data in the SpectrAA database can be more efficient if unwanted files are deleted. As with all storage systems, regular maintenance is required for continued smooth operation.

Acknowledgments

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Note: The contents of this document apply to versions up to, and including, 2.02. Software details and performance characteristics may change in later versions.

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