Ezchrom Elite Client/Server
Chromatography Data System (Version 3.3.2 SP1)

DEPARTMENT OF ENVIRONMENTAL PROTECTION
CHEMISTRY SECTION
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1. SCOPE AND APPLICATION

1.1. EZChrom Elite Client/Server is a chromatography data system package from Scientific Software, Inc., that is used throughout the Chemistry Section as a data acquisition tool. Data acquired by EZChrom may be processed using Target Chromatography software, Masshunter Quant software or the EZChrom package itself. It runs on the Florida DEP network.

1.2. This SOP will address basic background information related to Data Acquisition, and take the user through a chronological set-up of an EZChrom acquisition run sequence.

1.3. To get more information on the options discussed below see the REFERENCE in Section 11.

1.4. This SOP does not address Data Processing part of the software.

2. EZCHROM ACCESS

2.1. The chromatographic hardware (i.e., GC, -, IC, etc.) must be hard-wired to an EZChrom Server data interface, which controls data transfer from the instrument to the network computer system. An EZChrom Server may have up to eight channels; only one chromatographic detector may be interfaced to each channel.

2.2. EZChrom may be accessed from a Client PC or from an EZServer, which operates under installed EZChrom Elite software.

2.3. Log on is accomplished by opening an instrument configured in the EZChrom Elite Enterprise. To do this click on EZChrom Shortcut present on your desktop or go to Start/Programs/Chromatography and click on EZChrom Elite. The EZChrom Elite Enterprise screen will appear. First click on the EZ Server of interest. This will display the instruments which are hooked up to that server. Double click on the instrument you want to open. This will display a Login box. Enter your user name. Choose the domain as FloridaDEP. Choose the instrument name (ex. GC_ECD_3.i.). Enter your password: the same one you are using to login to the DEP Network (FloridaDEP domain). This will open the instrument. To open an instrument, its status has to be “available”. If the status is “busy” it means another client is operating that instrument and it cannot be operated by a second client. In this case the only option is to “open offline”. This will allow you to create a method or a sequence on that instrument but not to run it.

3. CONFIGURATION

3.1. Configuring EZChrom Elite Client/Server is the process of defining the system and its hardware. A System Administrator performs this task.

3.2. Enterprise Configuration.

3.2.1. This involves defining the EZChrom Elite Client/Server enterprise location and instrument. FL DEP ENTERPRISE is configured as:

FL DEP ENTERPRISE

- GC Lab 303
- GC Lab 303 EZ Server 1 (currently not used)
- GC Lab 303 EZ Server 2

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- GC Lab 303 EZ Server 3
- GC Lab 303 EZ Server 6

3.3. Interface Configuration

3.3.1. The system communication hardware is set up, such as A/D boards etc. In FL DEP ENTERPRISE there are two configured interfaces: CIO/DIO and SS 420 A/D.

3.4. Instrument Configuration

3.4.1. Each instrument to be used on the system must be configured. This is carried out by a System Administrator or designee and involves defining the type of instrument and type and number of detectors, etc. As an example of that is the configuration of a HP 7890 hooked up to EZ Server 2:

3.4.2. HP7890 Configuration. An example is GC_ECD_1.i, EZ Server2:

- Instrument Name: GC_ECD_1.i
- Instrument Type: Generic System
- External Events:
- Name Source Configuration
- Trigger SS420 Board: 2, In2, State: Closed
- Detector Name: D1
- Detector Model: Analog
- Acquisition Source: SS420
- Board: 2, Analog Input: Chan C
- Y-Axis Units: Volts
- Y-Axis Multiplier: 1e-006
- Detector Name: D2
- Detector Model: Analog
- Acquisition Source: SS420
- Board: 2, Analog Input: Chan D
- Y-Axis Units: Volts
- Y-Axis Multiplier: 1e-006

Each type of instrument in the Enterprise will have its own configuration.

4. CLIENT/SERVER OPERATION

4.1. When operating EZChrom Elite in a Client/Server mode there will be one or more Client Workstations along with one or more EZServers configured on the network. All instruments are physically attached to the EZServers. The EZServers acquire the data and can control instrumentation. The client workstations are where the users of the systems develop methods and sequences, and perform all operations of the system, including submitting data acquisition runs and sequences to the EZServers.

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5. DATA ACQUISITION USING EZSERVERS

5.1. When a run sequence is started from a client workstation the run is submitted to the EZServer where the instrument is attached. Once a run is submitted, the EZServer assumes control over the acquisition and control functions. All methods and sequences are copied to the EZServer when a run sequence is submitted to the server. If the network goes down, the EZServer will continue to run with the files it has on its hard disk.

5.2. As the user who submitted the run sequence, you will have access to the Run, Extend Run, or Stop Sequence functions. If you are not the user who submitted the run, you can view the run (if you have the instrument rights), but you cannot stop or modify a sequence that has been started by another user.

5.3. Once you have submitted a sequence to an EZServer from a client workstation, you can modify the method. You must save the file (File/ Method/Save) in order for the changes to be used for subsequent sequence runs that use this method. The user who submitted a sequence to the EZServer may add or remove runs from the submitted sequence from a client workstation. In order for sequence changes to take effect, the sequence must be saved (File/Sequence/Save).

6. DATA FILE STORAGE

6.1. When running samples, the file is stored locally on the EZServer first. At the end of each run the file is copied to its final destination on the Server. If this operation is not successful, an error log is generated. A watchdog program that periodically checks the network monitors this error log. As soon as the network is up, the files queued on the local drive are copied to the Server.

6.2. After acquisition the data is stored on ***Ezchrom on 'Tlhlabapp'*** in the appropriate folder for the instrument e.g.\\tlhlabapp\EzChrom\GC_ECD_1\Data. If dual detectors are used data files from both detectors are stored here as two sets of data. (These files can be re-exported to Target).

6.3. If Target is being utilized for processing of the data the data files are stored on ***'Target data on 'Tlhlab1'*** in the appropriate folder for the instrument e.g.\\tlhlab1\TargetData\GC\GC_ECD_1.i\Detector_A (and/or Detector_B) in the form of .cdf files. This raw data can be processed using the Target Chromatography Data System.

6.4. If Masshunter is used for data processing the data is exported to either the Masshunter processing computer (FID) or the "NPD Masshunter data" folder on the DEP network (within the GCGroup folder on TLHLAB5).

7. DATA FILE STRUCTURE

7.1. A data file is created whenever a sample run is acquired. The file contains the following information:

7.2. File information header. This contains information such as the date and time of acquisition, sample ID etc.

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7.3. Raw data points for the run saved for each detector channel (a chromatogram). The raw data points are saved in binary format.

8. CREATING DATA ACQUISITION METHODS

8.1. There are two types of data acquisition methods to be created for FL DEP ENTERPRISE INSTRUMENTS. These are methods for instruments configured "without remote instrument control" (using analog output signal) and methods for instruments configured "with remote instrument control" (using digital output signal). No instruments are currently connected using digital output signal.

8.2. Creating a Data Acquisition Method For The / Shimadzu GC 2010 / Agilent 6890/Agilent 7890 (without remote instrument control-analog signal output)

8.2.1. Click on Instrument Wizard tab. In the Instrument Wizard box click on the button labeled "Create or modify a method". The Method Wizard will appear. Select the "Create a new method" to start creating the acquisition method. Click on D1 tab (front detector). Click on the box adjacent to "Acquisition channel on". Set the Sampling Frequency to10 Hz. Set the run time as in the GC temperature program. Set an acquisition delay if needed. Click on blue right arrow until you get to Advanced Method Options dialog box. Select on the toolbar D1 (Detector 1/Front). Click on the box adjacent to Export Enabled. Choose from the drop down list "Chromatogram". Choose from "Parameters to export" "AIA (*.CDF) and click on right green arrow to move this parameter into the "Export this parameter" box. Select for Field separator: <Tab>. Enter the Path for exporting files for D1: eg.\\tlhlab1\TargetData\GC\GC_ECD_1.i\Detector_A.

8.2.2. Do the same for D2 (rear detector). All parameters will be the same. This time the Path to export data is: \\tlhlab1\TargetData\ GC\GC_ECD_1.i\Detector_B.

8.2.3. Click the Trigger tab and select the Trigger Type as "External". Save the method." File/Method\Save as "in the \\tlhlab1\ EzChrom\Gc_ecd_1\Method \ as ex. for ECD_1.met. Both channels have the same acquisition parameters, the only difference is the data export path.

8.3. Creating A Data Acquisition Method For The HP 6890 / (with remote instrument parameters control-digital output signal). Example only. No instrument currently uses this protocol.

8.3.1. If you have the Instrument digital output signal option installed, and your instrument is configured as an HP6890, the instrument control functions appears as part of the Instrument Setup window. Click on Instrument Wizard tab. In the Instrument Wizard box click on the button labeled "Create or modify a method". The Method Wizard will appear. Select the "Create a new method" to start creating the acquisition method. Enter appropriate values for each parameter displayed in the following windows: Temp/Inlet Temp / Inlet Pressure/Signals/"Det Type" Front/"Det Type" Back/Autosampler /Trigger. Click on each tab to open the window and set values for both channels Front and Back. Click on blue right arrow until you get to Advanced Method Options dialog box. Select on the toolbar, D1 (Detector 1/Front). Click on the box adjacent to Export Enabled. Choose from the drop down list "Chromatogram". Choose from "Parameters to export" "AIA (*.CDF) and click on right green arrow to move this parameter into the "Export this parameter" box. Select for Field separator: <Tab>. Enter

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the Path for exporting files: \\tlhlab1\TargetData\GC\GC_ECD_3.i\Detector_A. Save the method as Front Channel Method (ex. HPCF_3F.met =**H**ewlett **P**ackard, **C**onstant **F**low, instrument **3**, **F**ront). Keep the same parameters for Back channel D2 (Detector2/Back). This time the Path to export data is: \\tlhlab1\TargetData\GC\GC_ECD_3.i\Detector_B. Save the method as Back Channel Method (ex. HPCF_3B.met =Hewlett Packard, Constant Flow, instrument 3, Back).

9. CREATING A DATA ACQUISITION SEQUENCE

9.1 In order to be able to create two sequences one for each channel of the same instrument, set the number of Towers to 2. The following modification has to be done in the "Registry Editor": Click on Start/Run: RegEdit. Go into HKEY_LOCAL_MACHINE/Software/Chromatography System/C:/EZChrom Elite/Debug

- Right click on the far right side and select 'New' from drop down menu
- Choose 'DWORD Value'
- Rename "New Value #1" to NumTowers
- Double click on 'NumTowers' and in the Value Data field, type "2"
- Exit the Registry
- Open the instrument and then open a sequence that uses dual channel
- Check for 'Dual, Front, Rear" option. This will create in the sequence window two tabs: "Front Tower" and "Back Tower" for two acquisition channels.

9.2 Creating a run sequence

9.2.1 If you are using an autosampler to inject samples, you must define the samples and how they are to be acquired and analyzed. This is done using a sample Sequence.

9.2.2 To create a new sequence, click the File/Sequence/New command. The Sequence Wizard dialog box will appear. Create first the sequence for the Front Tower. Type the Method name to be used for acquisition, or select the name from a list of available methods by clicking the File Open button in the Method column. Both Front and Back Towers use the same acquisition method: ex. ECD_1.met.

9.2.3 Click "For Acquisition" button. Leave the Sample amount/Internal Standard amount/and Multiplication factor at their default values. Click "Next". The "Sample ID" field is for identification of the samples. Click the blue right arrow and select the "User name"<U>. In the "Data path" enter the path where you want the data to be stored, or select an existing path by clicking the "File Open" button. For "Data File" click the blue right arrow, and select "Increment Number"<01>. This will allow you to create a set of data using the date the sequence you intend to run, incremented by one for each sample. Ex. for Front Channel 081507F01etc (August 15, 2007, Front channel, Sample #01, etc). For number of unknown runs in sequence, enter 3. Leave the other fields at default values. Click "Next" to continue. Leave "Calibration / Report windows" unchanged, since we do not use EZChrom for data processing. Click "Next". Click "Finish". In this moment the Sequence Wizard will prompt you to create a Sequence for Back Tower. Enter the same as for Front Tower. Enter the same method name for the two channels.

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Click “Finish”. A sequence spreadsheet will appear, with “Front” and “Back” tabs, three rows for samples, and method name you specified. Click on “Front” tab. Enter Sample ID names for all samples in the Sequence. To create new lines in the sequence use down arrow. Right click on Method ID in the first cell in the Sequence and chose “Fill down”. This will spread the Method ID to all samples you entered. Click on first cell for Data File. Enter the Data File as Sequence Date followed by Tower name F or B, ex. 081507F<01>. Right click on this field, and chose “Fill down”. In the dialog box: “Increment Data File” click OK. This will create automatically for each sample a different Data File number to prevent duplication (no sequence will start if there are duplicate file name data). Do the same for the Back Tower using this time B for Back channel instead of F. Name the first sample in the Back Channel Sequence. Here there are two possibilities: (1) name the first injection as “No Sample” if you choose to keep idle the Back tower while the Front one is injecting the first on Autosampler tray, and (2) give a real name (ex. ISO-8) for the first injection if you choose the Back tower to inject the first vial (filled with ISO-8), while the Front tower is injecting the second vial. Have the last vial in the tray filled with ISO-8 for the last injection in the Front or leave it idle. Save the Sequence as DATA.seq in the “Instrument/Sequence” subdirectory (ex. 081507.seq).

10. RUNNING A SEQUENCE FILE

10.1. To start acquiring data using the sequence you have just created, click the “Sequence Run” button on the toolbar, or do a right-hand mouse click in the sequence spreadsheet, and select “Run Sequence”. Choose for Tower Mode “Dual” to run simultaneously in two channels. Click on “Start” button. Click on” Window/Tile horizontally”. Your monitor screen will be split into 2 or 3 subscreens: First will display real time data acquisition for Detector 1, second for Detector 2 (if present), and third will show the Run Sequence Status on the Sequence spreadsheet.

10.2. To schedule a run click the “Sequence Run” button on the toolbar. In the bottom left hand corner of the screen click the clock icon under “begin run” box. This will give you three options of when to schedule the run; the first option is to begin immediately, the second option is to begin after a specified amount of minutes, the third option is to begin at a specified date and time. Continue as described in section 10.1.

10.3. To queue a run sequence when a different sequence is running click the “Sequence Run” button on the toolbar. Browse and find the sequence run file that you would like to queue in the “sequence information” box. Schedule the run as above and hit submit run. The run queue can be viewed by clicking on Control/ Run Queue or by clicking the run queue icon on the toolbar. In the run queue window you can make additional changes to the start time by right clicking on the sequence file and picking “change begin time”.

10.4. A sequence can be modified and saved while it is running by going after editing to File/Sequence/Save or by using the save icon on the toolbar.

10.5. To stop a Sequence click on “Stop sign” on toolbar and choose to

1) “Stop current run only” This will stop the run immediately and start the next run in the sequence as soon as the instrument has equilibrated.

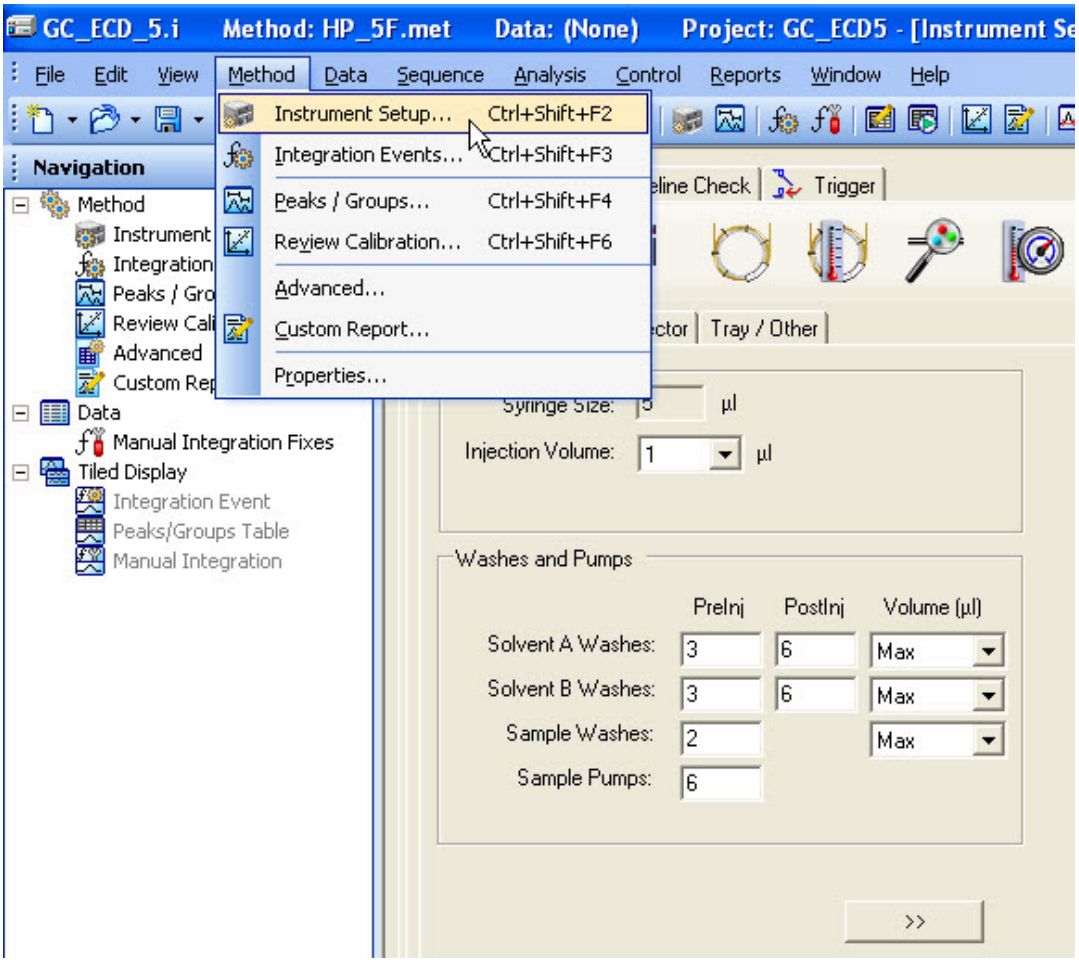
2) “Stop current run and sequence run” This will stop the current run and the sequence immediately.

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3) “Stop sequence after current run completes” This will stop the sequence as soon as the current run has completed.

4) “Stop all run queue items you submitted” This will stop the current run, the sequence and all sequences submitted under your name in the run queue.

5) “Stop all run queue items” This will stop the current run, the sequence and all sequences submitted by any user in the run queue.



11. REFERENCES

11.1. EZChrom Elite Client / Server-Chromatography Data System for Windows 7; Version 3.3.2 SP2, Build 3.3.2. 1037; SN 02091900234

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APPENDIX OF CHANGES

09/13/2010 Section 11 of the SOP was edited to reflect changes in the software, from version 3.2.1 to version 3.3.2 SP1.

07/29/2014 Removal of digital control due to re-wiring during the Windows -7 EZchrom software upgrade.

07/05/2018 EZChrom data processing with Masshunter added.

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