

Chromatography Toolkit for LabVIEW

WillStein Software

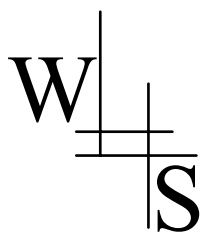
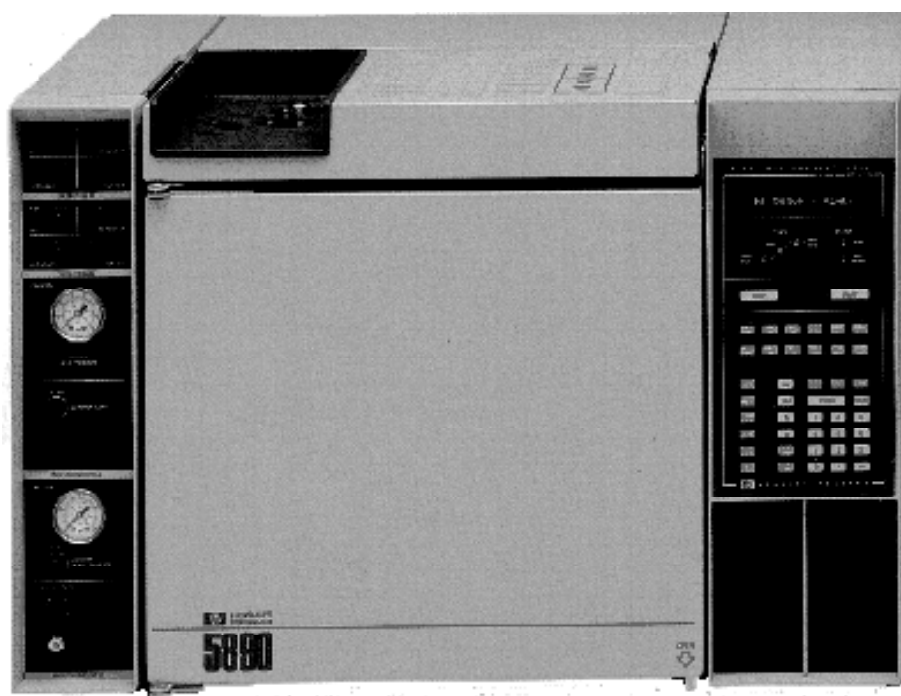
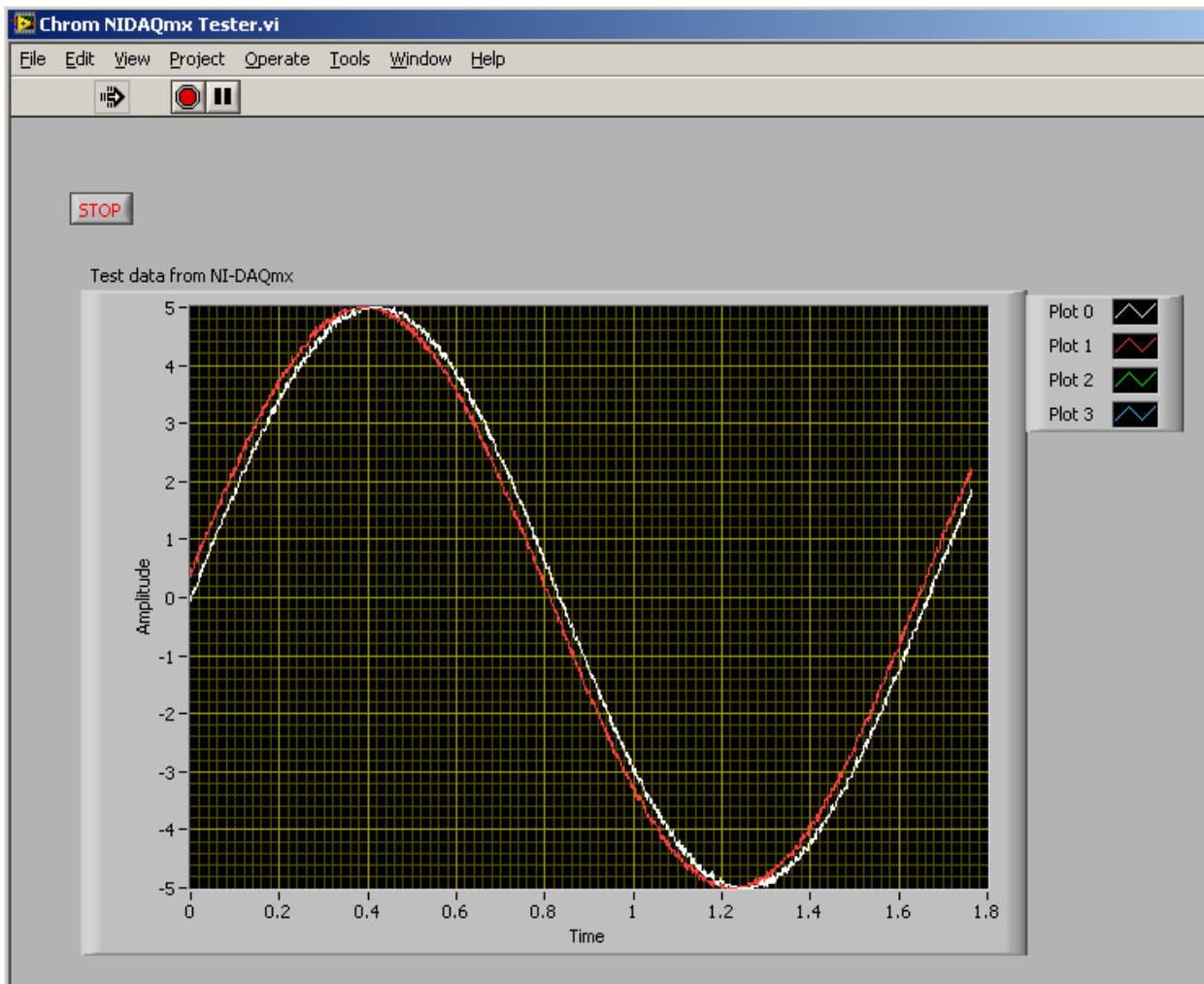


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Please e-mail or send any comments regarding the software or the manual to the above address.

Version Number of Software: 2.3.0

What is the Chromatography Toolkit?

The Chromatography Toolkit is a chromatography data system written specifically for LabVIEW. It can acquire data, automatically detect peaks, and display results in real time.

Both a turnkey chromatography system and a peak detection library are provided in the toolkit. The flexibility of LabVIEW allows the turnkey system to be modified by the end user to provide functions specific for that lab or pilot plant. For example, the peak areas found by the peak detection VI could be used to provide real time feedback control for a distillation column.

The "Chromatography Toolkit.vi" can be used out of the box as a complete chromatography system. It provides data acquisition from National Instrument DAQ cards, real time graphs, peak information, and data storage and retrieval. Data can be acquired from up to 4 channels at once in a single chromatogram, or 4 chromatograms of one signal each. Instructions are provided to allow the user to write their own data acquisition modules. Add on modules are available which provide data acquisition for the HP 5890 and Agilent 6890.

The "Peak Detection.vi" can be used independently of the Chromatography Toolkit.vi in a user's own custom application. The algorithm is capable of dealing with curved baselines, fused peaks, and shoulders typical in chromatographic applications. Data are sent to the vi in "chunks" to provide real time processing, or in one large batch for post analysis.

Getting Started

System Requirements

The Chromatography Toolkit requires LabVIEW 7 or greater for either Windows 2000 or Macintosh OS X. Either the LabVIEW Base Package or the Full Development Package can be used. Any computer or o

Installation

GC WorkMate/LV consists of one main program and several sub-vi's. The main program is named "GC WorkMate/LV.vi" which is located in the Chrom.llb. Several additional VI libraries are used to organize the subroutines.

- Macintosh: A CD-ROM is provided with the VI Libraries. Copy the entire "Chromatography Toolkit" folder to your hard drive.
- Windows: A CD-ROM is provided with the VI Libraries. Copy the entire "Chrom" directory to your hard drive.
- Internet: If you receive the software or an update via the internet, then decode the individual libraries and place them into a common directory as described above.

To start the main program in LabVIEW:

Double click on "Chrom.llb". This will automatically load "GC WorkMate/LV.vi".

Internet Note: Macintosh

The toolkit has been stuffed and binhexed using Stuffit Deluxe. A free utility called Stuffit Expander can be used to decode the toolkit. Stuffit Expander can be from Aladdin Software at <<http://www.aladdinsys.com/>>.

Internet Note: Windows

The toolkit has been zipped and then uuencoded. Use Aladdin Expander for Windows or another Zip utility to decode the toolkit. Aladdin Expander is free and is available from Aladdin Software at <<http://www.aladdinsys.com/>>.

Internet Note: PDF files

The instructions are provided as a PDF file. This can be viewed using the free program called Adobe Acrobat Reader. This can be obtained from <<http://www.adobe.com/>>.

Demo Version

The demo for GC WorkMate/LV can be downloaded from our web site at <www.willstein.com>. This download consists of a data file and the vi library.

Differences from the Main Version

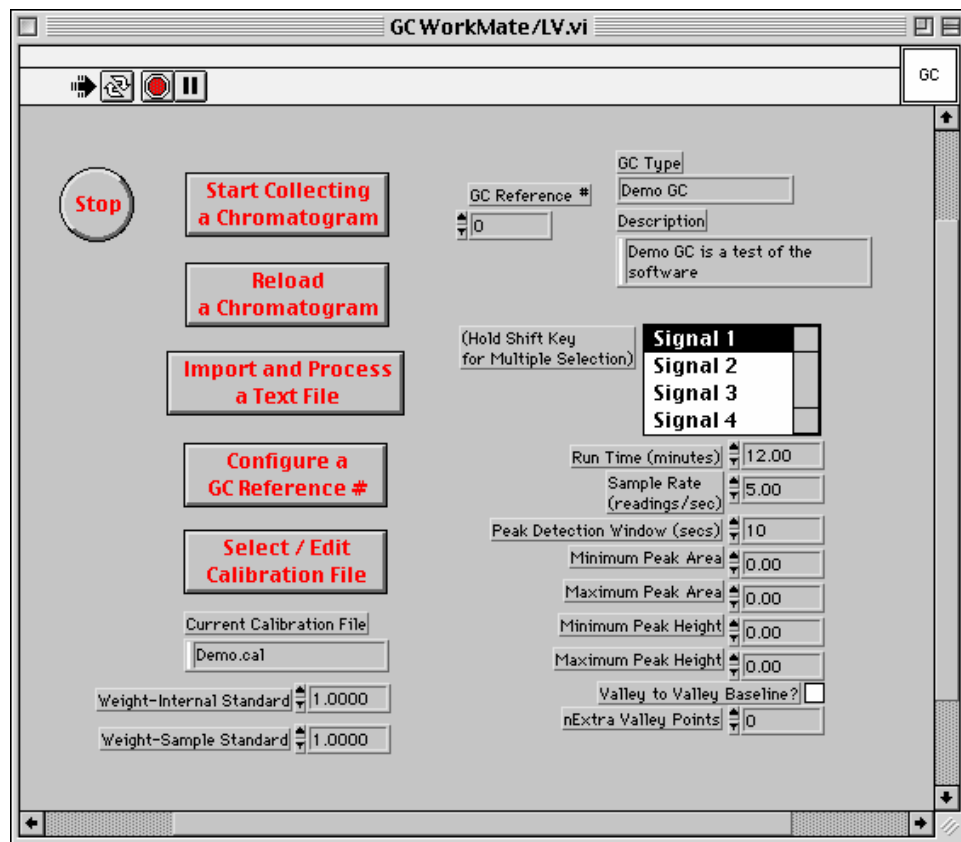
The demo version provides simulated data acquisition from a “Demo GC”. This demo reads in previously acquired data from the hard drive in order to simulate an actual chromatogram. The full version provides data acquisition routines for the MIO boards from National Instruments. Add on modules are also available for the HP 5890 and Agilent 6890.

Also, the full version provides block diagrams for all vi’s except the peak detection vi’s. This allows you to create your own programs by examining these examples.

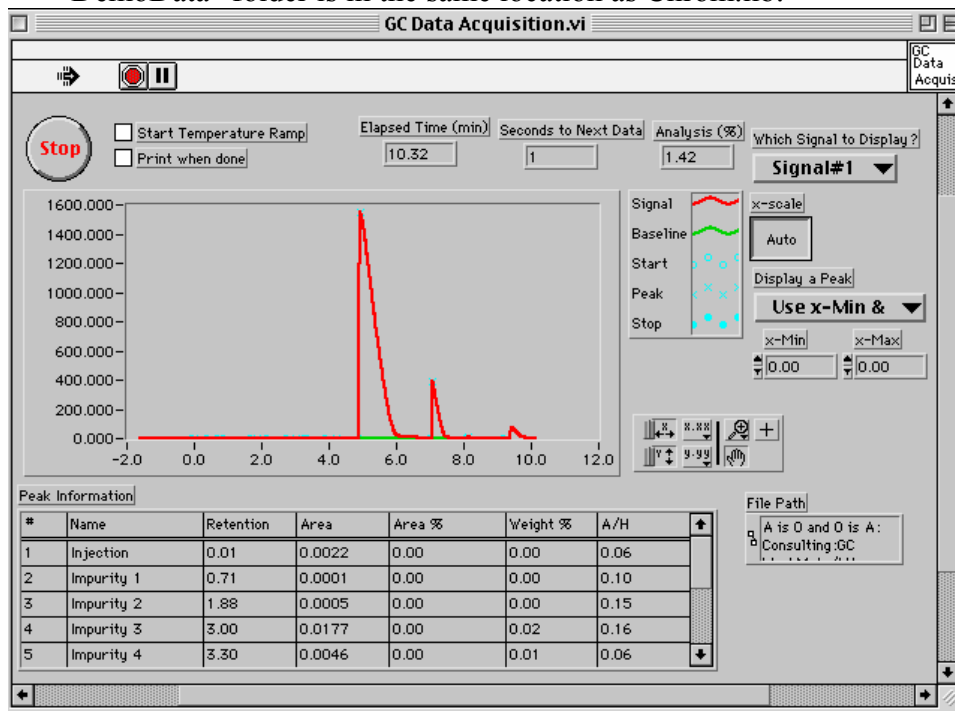
Please look over the remainder of this manual for more information on the full version of the program. You can also purchase the software for a 30 day no risk trial period.

Running the Demo

- 1) Double click on Chrom.llb in order to load the main program. The main program is entitled “GC WorkMate/LV.vi”, and is shown below.



- 2) Click on the “Run” arrow in order to execute the LabVIEW program.
- 3) Press the “Start Collecting a Chromatogram” button in order to start the demo. The following screen will appear. You will be prompted for a file name in order to store this chromatogram. If the chromatogram does not appear, then check to make sure that the “DemoData” folder is in the same location as Chrom.llb.



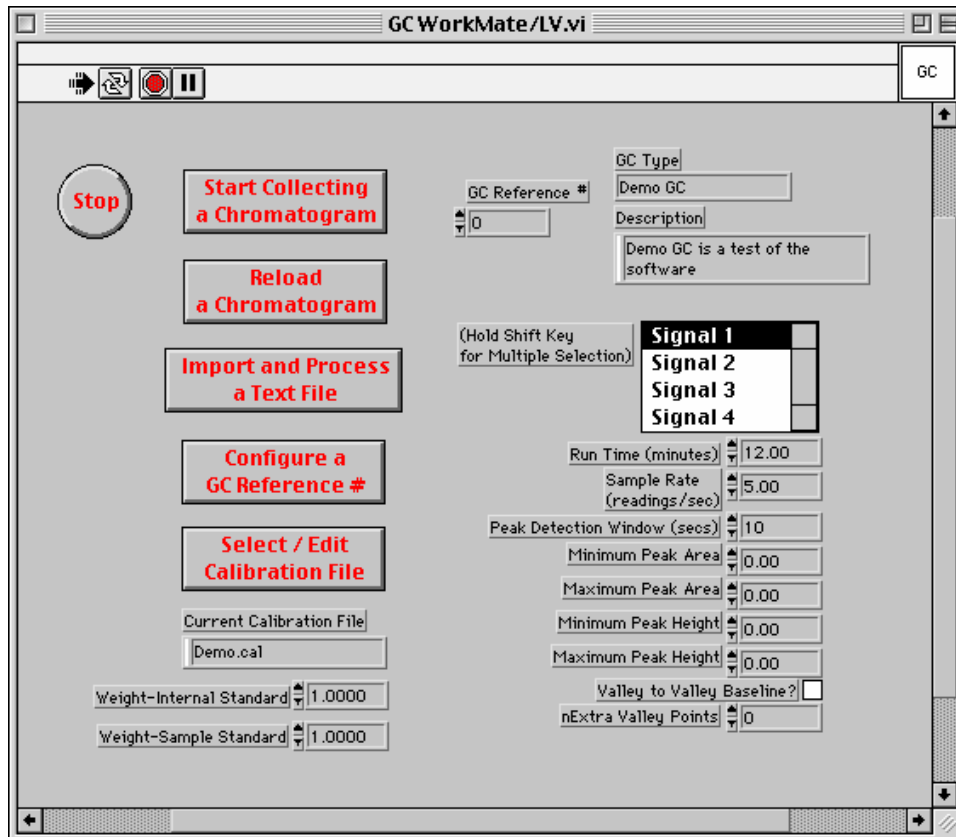
- 4) Notice that the peaks are automatically detected and added to the Peak Information list.
- 5) The demo is configured to run 5 times faster than real time in order to speed things up.

Running the Chromatography Toolkit

See the section “Running the Demo” for an introduction into using this software.

The Chromatography Toolkit has several screens that are visible to the user. GC WorkMate/LV.vi is the main starting point. The other windows “popup” as the result of pressing buttons on the main screen.

Load the main program, GC WorkMate/LV.vi by double clicking on Chrom.llb. The following display will be shown. This vi does not do any processing on its own. Instead, it provides a central launching screen to select various options.



Press the “Run” button on the LabVIEW toolbar in order to activate the program. The “Run” arrow will be filled in when successful. The buttons contained in the program itself will then execute the actions described below.

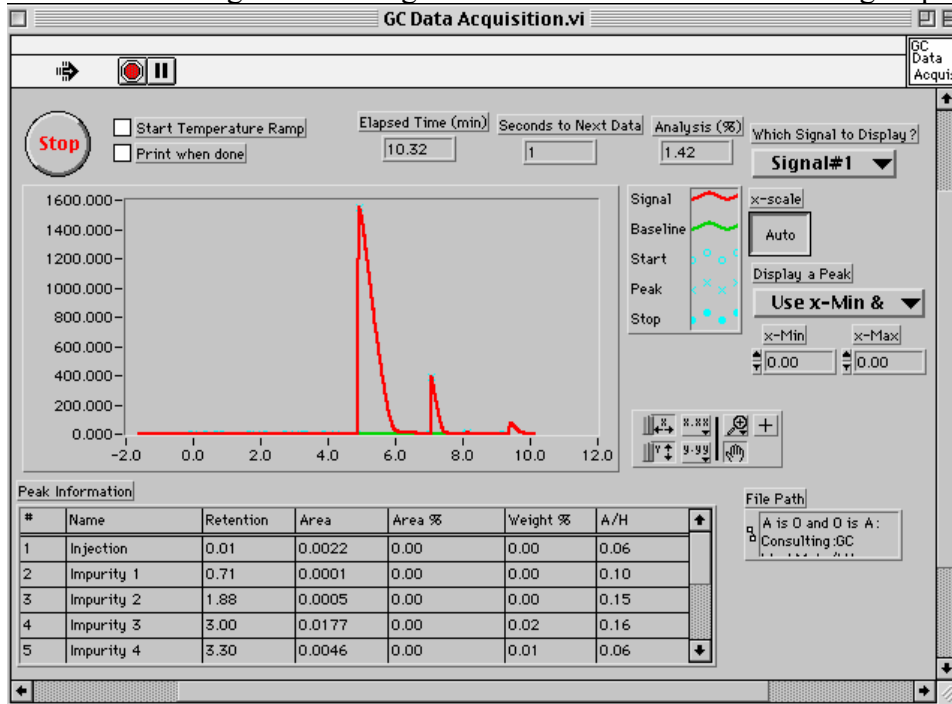
This vi consists of several objects.

- 1) The Stop button is used to stop the LabVIEW program. This will turn off the “Run” button, but it will not exit LabVIEW.

- 2) The “Start Collecting a Chromatogram” button is used to start the data collection.
- 3) The “Configuration” items are used to specify the various parameters needed by the data collection and peak detection. Default settings are provided for the demo.
Advanced: This can be modified by the user to acquire data at a given time interval, or in response to some other action in the lab.
- 4) The “Reload a Chromatogram” is used to load a previously collected chromatogram into the display window. Various regions of the chromatograph can then be examined in finer detail.
Note: This feature only loads data files created by GC WorkMate/LV. See the “Import and Process Text File” to import your own data files created in by other software.
- 5) The “Import and Process Text File” button is used to load in an ASCII data file containing data that you wish to process with the Peak Detection routines. This is described in a section later in this manual.
- 6) The “Configure a GC Reference #” is used to define a configuration for a particular type of GC.
- 7) The “Select/Edit a Calibration” is used to handle calibration data.

Start Collecting a Chromatogram

Pressing the “Start Collecting a Chromatogram” button results in the following display:



The following sections provide more detail about this screen.

General Controls

- 1) The “Stop” button is used to stop the data acquisition before the allotted time has elapsed.
- 2) “Start Temperature Ramp” sends the start signal to either the HP 5890 or Agilent 6890. The time axis will reset so that time zero corresponds to injection.
- 3) “Print When Done” will send the final output to the printer for an automatic report.

Display Controls

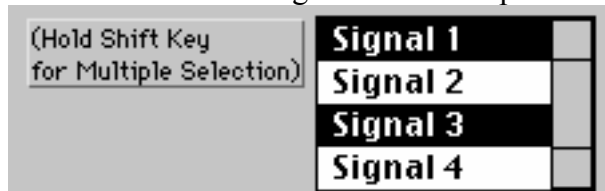
- 1) “Which Signal to Display” is used when more than one signal is being acquired at a time.
- 2) The “x-scale” options allow a subset of the data to be displayed in order to examine the finer details of a chromatogram.
 - a) The “Auto/Manual” toggle button controls whether the entire chromatogram is displayed, or just a subset. “Auto” will always display the entire chromatogram. “Manual” allows the “x-min” and “x-max” controls to specify the range of data to view.
 - b) The “Display a Peak” popup menu can be used to set the “x-min” and “x-max” controls to the start and stop time for a given peak. This provides an easy means to examine a specific peak. Peaks are added to this menu automatically as they are detected. Alternatively, the “x-min” and “x-max” can be entered manually.

Indicators

- 1) The graph shows the signal, baseline and peaks during the data acquisition.
- 2) The “Peak Information” table provides a summary of the peaks that are found. This is only a subset of the information calculated for each peak. The user is free to customize this display to show whichever information they need, such as the peak start/stop times, the full width at half maximum (FWHM), etc. This is described later in this manual under “User Customization of GC Workmate/LV”. Peak names are included if a calibration file was provided.
- 3) “Elapsed Time” shows the current amount of data that has been acquired. This will lag behind your watch since data arrive in chunks during the data acquisition. “Seconds to Next Data” indicate when this next chunk will arrive. For example, the HP 5890 always sends 60 data points at a time. Therefore, at 5 readings per second, new data will arrive every 12 seconds.
- 4) “Analysis %” indicates the amount of time that the peak detection algorithm requires. Normally this is only a few percent indicating that most of the CPU time is available for other processing.

Collecting Data From More Than One Signal

Select more than one signal by holding the shift key down while clicking on the signal list on the main screen. These signals should be previously defined for the current GC Reference #.



During data collection, one signal is displayed at a time.

Collecting Data From Multiple GC's/HPLC's

Data can be acquired from up to four instruments at a time. See information on the specific type of hardware below for configuration information. To start:

- Select the signal or signals for collection.
- Press the “Start Collecting a Chromatogram” button.
- A data collection window will then appear. You can then click on the main window or use the LabVIEW Windows menu to select the main window.
- Select a different signal and again press the “Start Collecting a Chromatogram” button.
- Use the LabVIEW Windows menu to view the desired window. Up to four data acquisition windows can be created and run independently.

- Note: The signal selection is used to determine which data acquisition to open. Be sure to select different signals before pressing the “Start Collecting a Chromatogram” button.

- **Note: Test this feature in the Demo mode before trying to collect actual data.**

Demo

No special configuration is required for the Demo GC. Use this mode before trying to collect actual data.

NI-DAQ and NI-DAQmx

<<< This section needs to be updated. Contact WillStein Software if you would like to use this feature.>>>>

HP 5890 and Agilent 6890

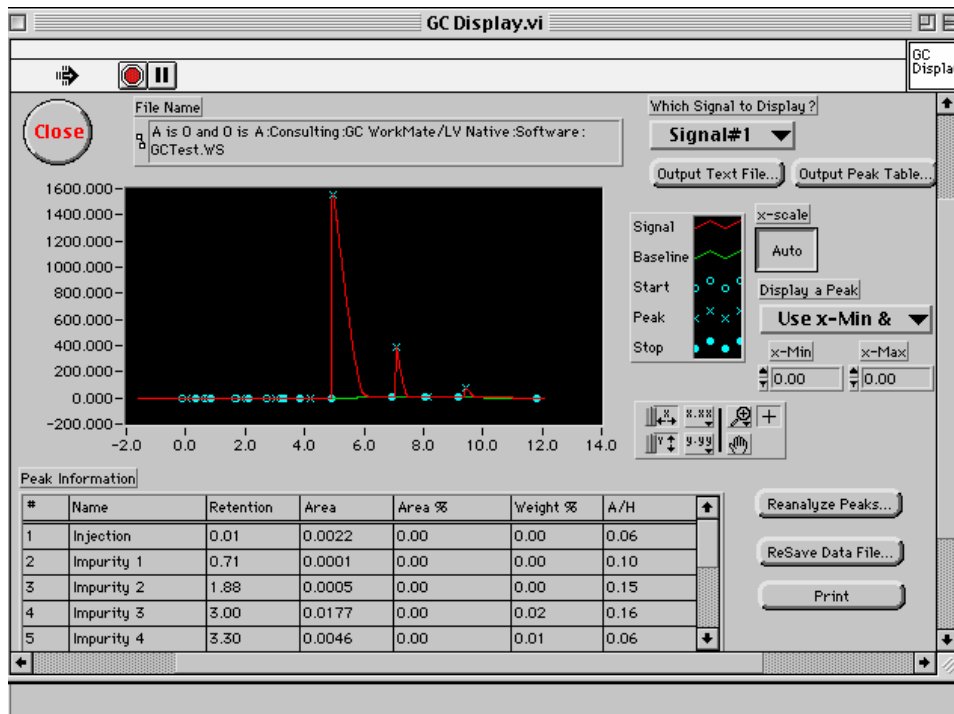
These modules have not yet been converted to allow acquisition from more than one instrument at a time. Contact WillStein Software if you need this functionality.

Different Types of Hardware

You can acquire data from different types of hardware at the same time. For example, HP 5890 and NI-DAQmx configurations can be used simultaneously.

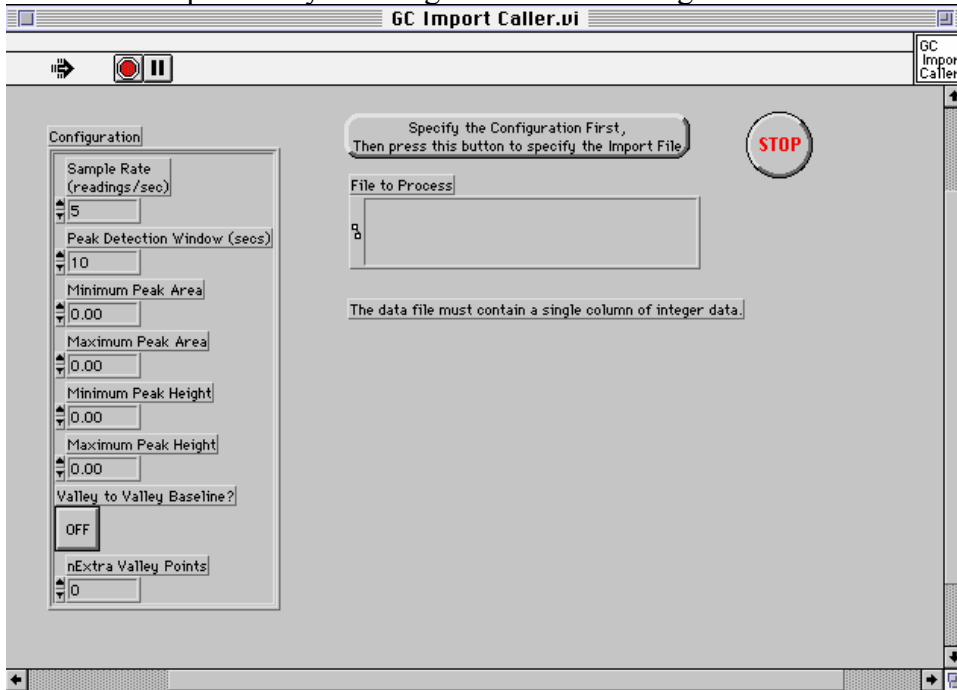
Reloading Existing Data

Press the “Reload a Chromatogram” button on the main GC WorkMate/LV.vi screen. You will be prompted to locate a data file that was previously created with GC WorkMate/LV. This file will then be opened into a window named “GC Display.vi”. This is very similar to GC Data Acquisition.vi, and functions in the same way.



Importing a Text File

Press the “Import and Process Text File” button on GC WorkMate/LV.vi in order to display the following screen. Enter in the configuration information, especially the Sample Rate. Then, press the button to specify a data file to import. The data file should be a single column of ASCII data separated by a carriage return or a carriage return/line feed.

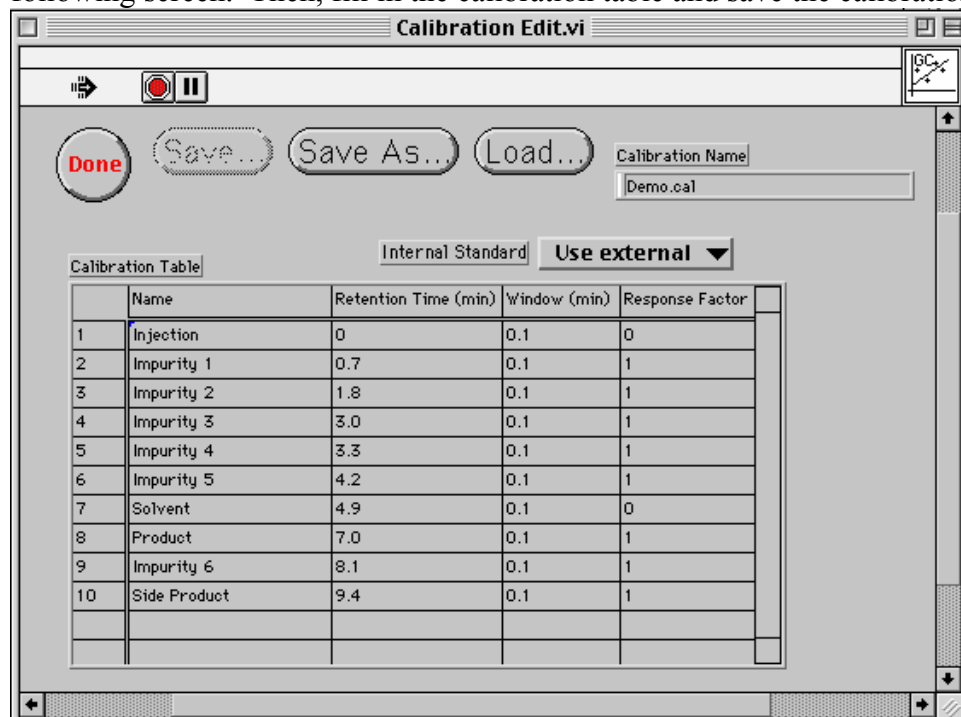


The data will then be processed and displayed in its own window. The option will be given to save the baseline that was created, or to save the peak information.

This vi also serves as an example for using the Peak Detection routines in your own custom vi's.

Working with Calibrations

Press the “Select/Edit a Calibration” button on GC WorkMate/LV.vi in order to display the following screen. Then, fill in the calibration table and save the calibration.



The Retention Time and Window are used to identify a given peak. The actual retention time must be within +/- the “window” value in order to be identified. For example, in the above table, any peak with a retention time between 0.6 and 0.8 minutes will be identified as Impurity 1.

The Response Factor is used to calculate the weight percent of each peak. There are two ways in which this is done.

External Standard

The simplest method is to use an External Standard in which case the following formula applies. Note that the weight percent will always add up to 100% even if there are non-volatiles or if some peaks are missed.

$$\text{Weight Percents: } Wt\%_i = 100\% * \frac{\text{Area}_i * RF_i}{\text{Total}}$$

Where:

- Area_i Area of the “i-th” peak.
- RF_i Response factor for the peak
- Total Total of the numerator used to normalize the quantities.

You must run a calibration mixture in order to calculate the response factors. The following example shows the calculations involved.

Compound	Calibration Concentration (%)	Retention Time (min)	Window (min)	Area	Area %
Methane	1.00	0.55	0.1	0.0004	3.2
Ethane	0.99	0.76	0.1	0.0022	17.6
Propane	1.01	1.34	0.2	0.0032	25.6
iso-Butane	1.00	2.35	0.3	0.0035	28.0
n-Butane	1.00	3.39	0.4	0.0032	25.6
Carrier Gas	95.00			ignored	

First, notice that the “window” is made larger for the later peaks since there is greater separation at higher retention times.

Second, the Response Factor is calculated as follows:

$$\text{RF (Methane)} = 1.00 \text{ wt\%} / 3.2 \text{ area \%} = 0.31$$

$$\text{RF (Ethane)} = 0.99 \text{ wt\%} / 17.6 \text{ area \%} = 0.056$$

$$\text{RF (Propane)} = 1.01 \text{ wt\%} / 25.6 \text{ area \%} = 0.039, \text{ etc}$$

Notice that either the Area or Area% can be used as long as you are consistent.

These Response Factors can then be used to analyze an unknown sample as follows. Again assume that the carrier gas accounts for 95% of the total.

Compound	Area	Area %	Response Factor from calibration	Area% * RF	wt %
Methane	0.0046	29.3	0.313	9.17	3.7
Ethane	0.0051	32.4	0.056	1.82	0.7
Propane	0.0035	22.6	0.039	0.89	0.4
iso-Butane	0.0019	12.2	0.036	0.44	0.2
n-Butane	0.005	3.5	0.039	0.14	0.1
Carrier Gas	Ignored			ignored	
Total	0.0156	100%		12.45	5.0

First, the Area is normalized into an Area %. The Area % is then multiplied by the response factors calculated previously. The total of 12.45 is then used to normalize this value into the wt % as follows:

$$\text{Methane} = (9.17 / 12.45) * 5\%$$

Note that this calculation is normalized to 5% instead of 100% in order to account for the carrier gas.

Internal Standard

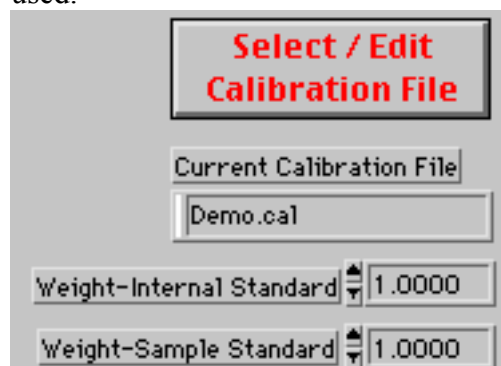
An internal standard requires additional information. Note that the areas are not normalized to 100%.

Weight Percents:
$$Wt\%_i = 100\% * RF_i * \frac{Area_i}{Area_{ISTD}} * \frac{Weight_{ISTD}}{Weight_{Sample}}$$

Where:

- Area_i Area of the “i-th” peak.
- Area_{ISTD} Area of the internal standard peak.
- Weight_{Sample} Weight of the sample.
- Weight_{ISTD} Weight of the internal standard in the sample.
- RF_i Response factor for the peak

The weight of the sample and internal standard must be provided when an internal standard is used. This is specified on GC WorkMate/LV.vi. This can be ignored if an external standard is used.



The following shows an example for performing this calculation. Roughly 1 gram of sample is added to 9 grams of solvent with 0.5 grams of an internal standard. The internal standard is used to provide a known quantity to compensate for injection volume, detector response, etc.

The following shows the calibration data:

Compound	Known wt %	Area Counts	Area %	Response Factor
Methanol	20.0%	1000	11.8%	1.00
Ethanol	30.0%	2000	23.5%	0.75
Propanol	50.0%	3000	35.3%	0.83
Internal Standard		2500	29.4%	
Total	100.0%	8500	100.0%	

The Methanol response factor was calculated as:

$$RF = (1000 / 2500) * (1 \text{ gram} * 0.20 / 0.5 \text{ grams}) = 1.0$$

An unknown sample can then be analyzed as shown in the following example. Assume the following quantities: 1.1 grams of sample and 0.55 grams of internal standard.

Compound	Area Counts	Response Factor	Calculated wt%
Methanol	3000	1.00	62.5%
Ethanol	2000	0.75	31.3%
Propanol	1000	0.83	17.4%
Internal Standard	2400		
Total			111.1%

The sample calculation for Methanol is as follows:

$$\text{Methanol wt\%} = 100\% * (3000 / 2400) * (0.55 / 1.1) = 62.5\%$$

Controlling Data Acquisition Parameters

The first few parameters on GC WorkMate/LV.vi control the data acquisition for the GC.

Parameter	Description
GC Reference #	This reference number refers to a specific configuration of equipment. This is described in more detail below.
Signal Menu	This menu selects data acquisition for one or more signals. Holding down the shift key allows more than one signal to be selected at a time. At least one signal must be selected at all times, so a signal must be selected before unselecting all signals.
Run Time (minutes)	This is the amount of data acquisition time for the chromatograph.
Sample Rate (readings/second)	This is the number of samples taken per channel per second. More RAM is required for larger sample rates, but the signal will be more accurate. In general, the sample rate should be chosen so that all peaks have at least 50 data points.
Peak Detection Parameters	These are described in a later section. The main peak detection parameter is “Peak Detection Width” which specifies the number of seconds that you expect for a typical peak width. This can be smaller than the actual peak width in order to not miss any peaks. The smaller this peak is, the more peaks will be identified. At some point, “noise” might start to be identified as a peak if this value is set too small.

GC Reference # 0

GC Type Demo GC

Description Demo GC is a test of the software

(Hold Shift Key for Multiple Selection)

Signal 1	
Signal 2	
Signal 3	
Signal 4	

Run Time (minutes) 12.00

Sample Rate (readings/sec) 5.00

Peak Detection Window (secs) 10

Minimum Peak Area 0.00

Maximum Peak Area 0.00

Minimum Peak Height 0.00

Maximum Peak Height 0.00

Valley to Valley Baseline?

nExtra Valley Points 0

Specifying Data Acquisition Hardware

GC WorkMate/LV.vi supports data acquisition from several types of hardware. The following sections provide more detailed information about each type of hardware.

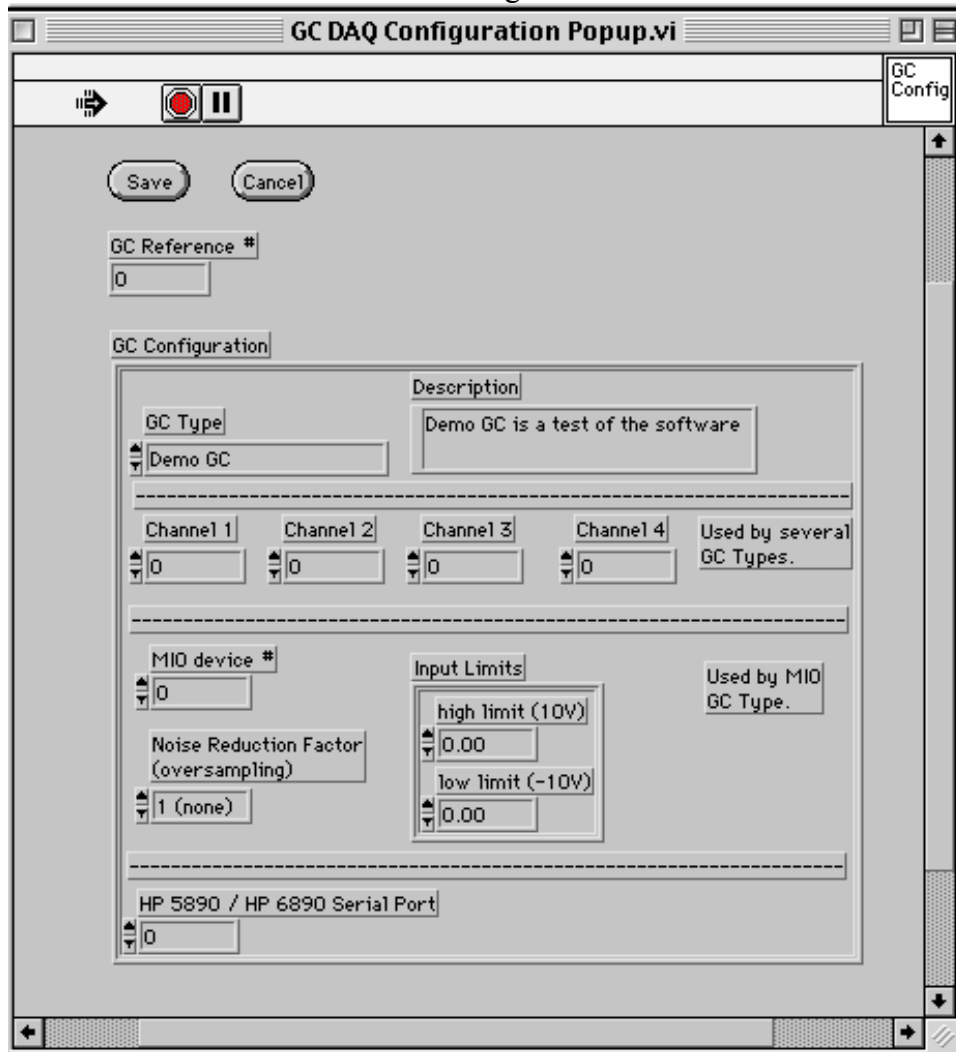
- Demo GC: This simulates data acquisition by reading in data from a previously collected data file.
- MIO: Any of National Instruments MIO boards can be used for either a Macintosh or Windows.
- HP 5890: HP provides two options for communicating with a computer.
 - The more common option is part number 19257A. This board is often pre-installed and is used for the ChemStation software from HP. You can recognize this option since both an RS-232 and an HPIB (also known as GPIB and IEEE-488) connection are provided.

- The less common option is an RS-232 board, part # 19254A, and only provides an RS-232 connection.
- Agilent 6890: This chromatograph has a built in RS-232 port, which can communicate with GC WorkMate/LV.vi. This module is available for an additional cost.
- Customer Supplied: This slot is provided to allow the end user to write their own data acquisition module. This is described in more detail below.

Defining a GC Reference Number

Press the “Configure a GC Reference Number” on the main front panel. This brings up the following display. Note that not all parameters are needed for all types of GC’s.

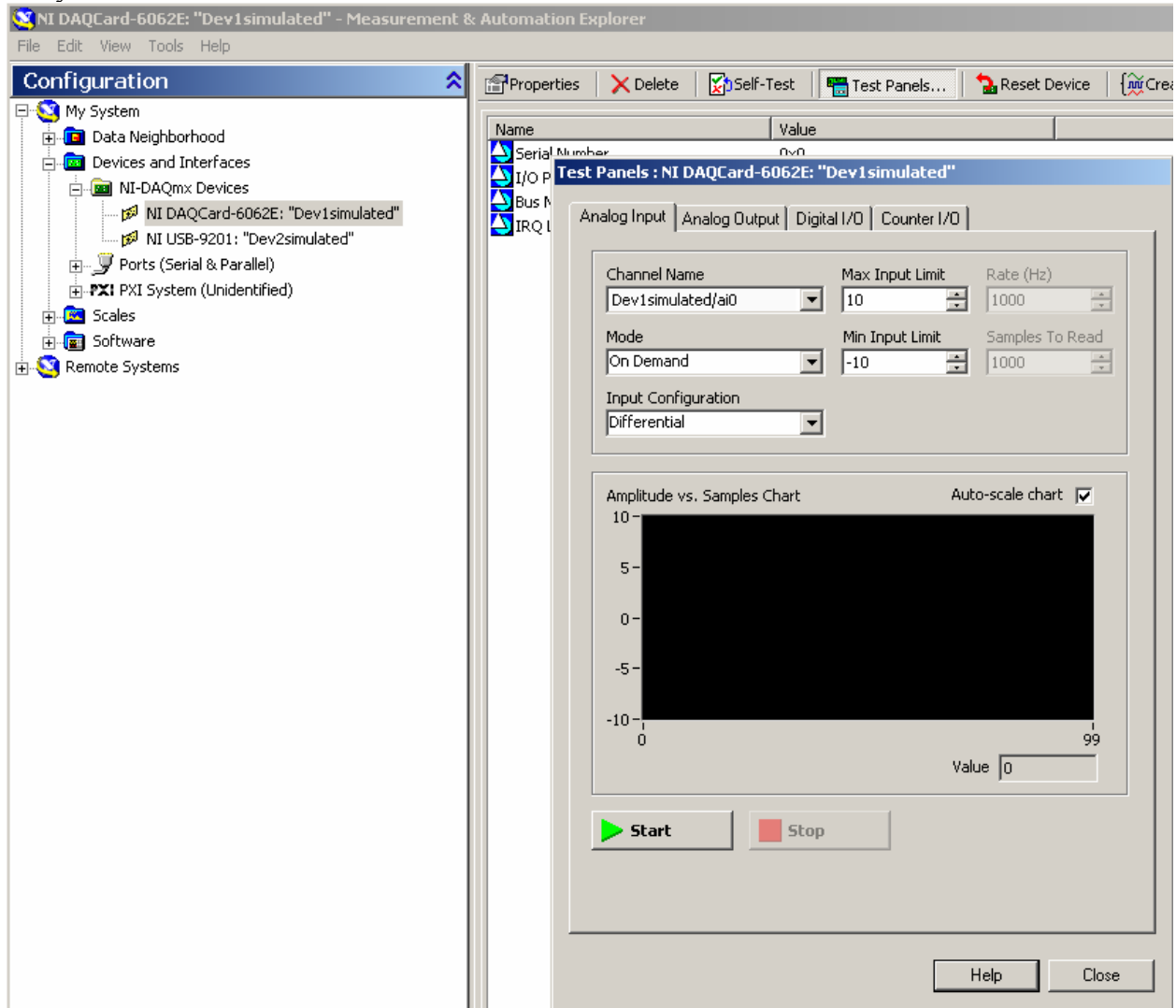
Change the “GC Reference #” to the desired value. If you only have one GC, then you can define the configuration for GC Reference #0. If you have more than one GC, you can use different reference numbers for the different configurations.



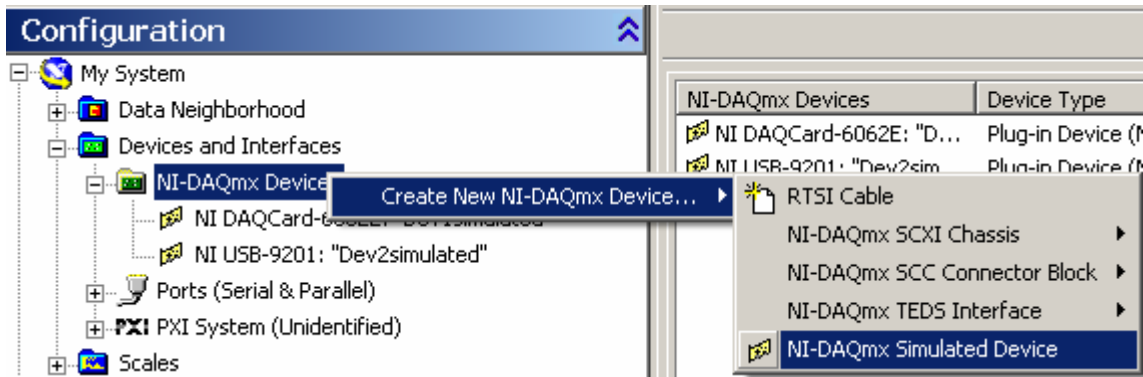
Using National Instruments Boards using the new NI-DAQmx interface

Consult the reference manual for the given National Instruments board for installation instructions. Note that LabVIEW requires drivers in order to communicate with NI-DAQmx boards. NI-DAQmx drivers are generally provided on a separate CD from LabVIEW. Consult your LabVIEW or NI-DAQmx documentation and create a simple test program to verify that LabVIEW can communicate with your board.

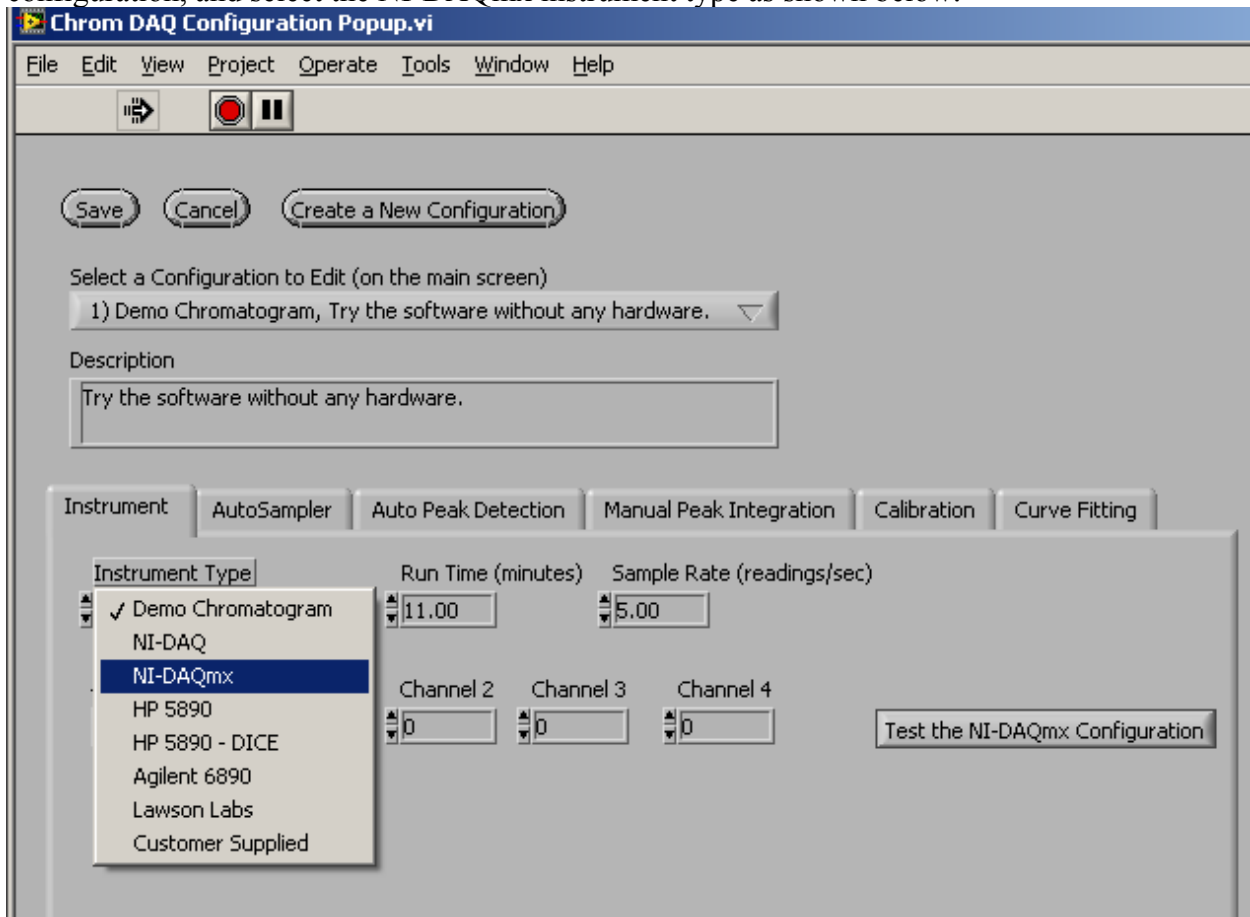
Use the Measurement and Automation Explorer program provided by National Instruments to test your initial installation.



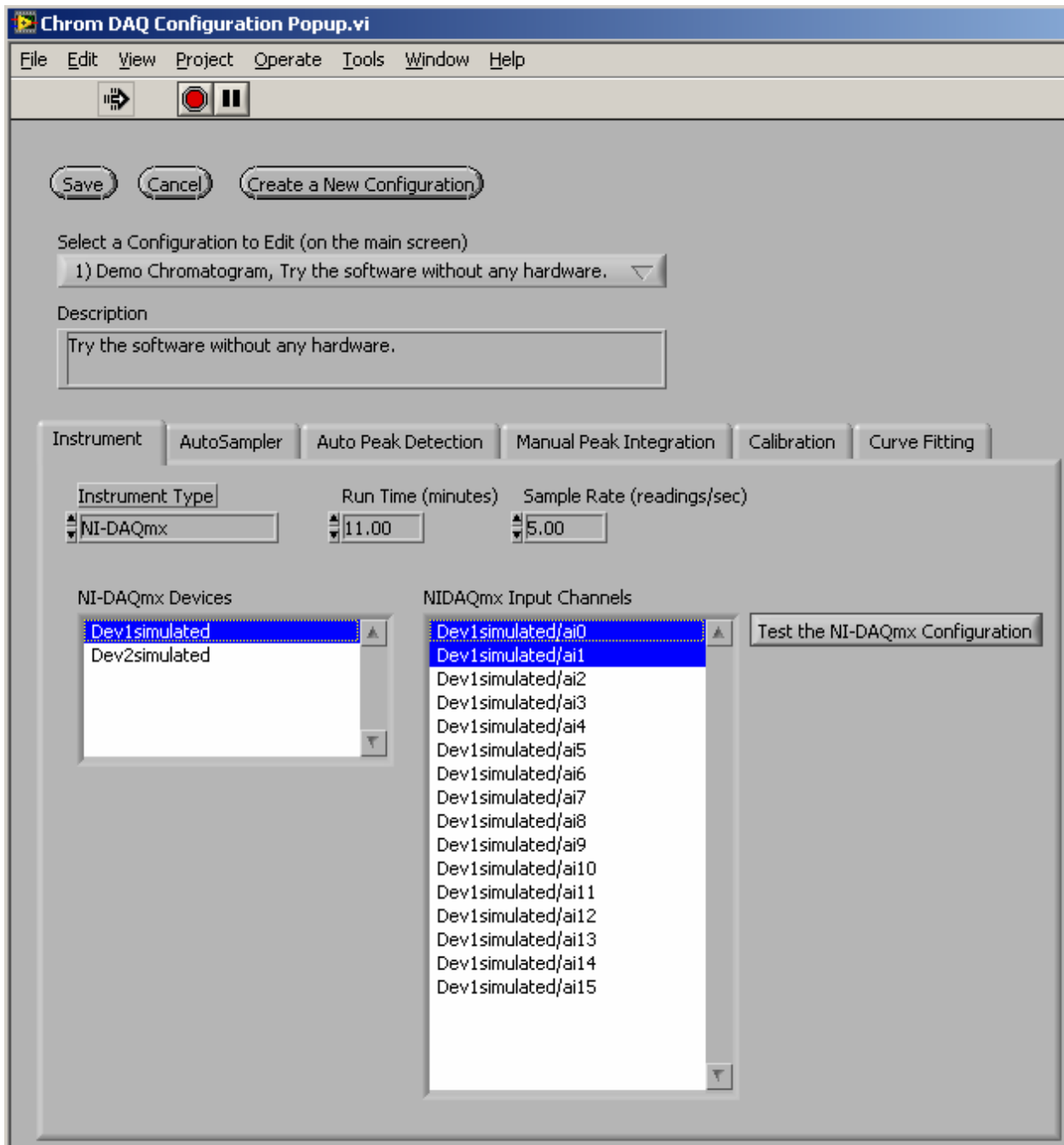
Note that you can even create a simulated NI-DAQmx device by right clicking as shown below. This will allow you to test the software on another computer that is not connected to your device.



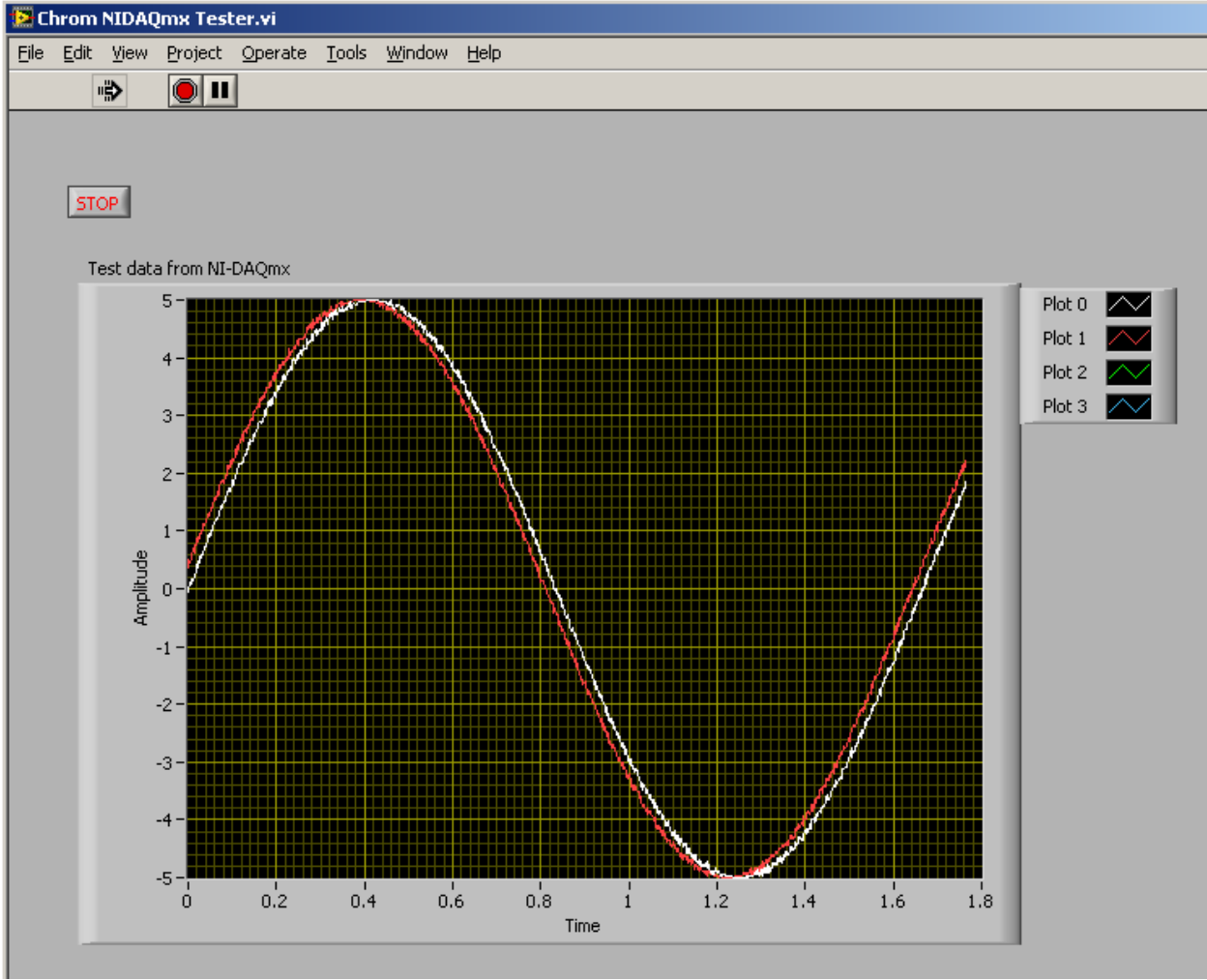
You can then open the Chromatography Toolkit once you have tested the communication. Edit a configuration, and select the NI-DAQmx instrument type as shown below.



The available NI-DAQmx devices and channels are listed. Select one or more channels for use by this configuration as shown below. Also specify the Sample Rate and Run Time.



Click on the “Test the NI-DAQmx Configuration” button in order to test the system. You can connect a battery or some other signal source in order to verify that you have the correct channels connected.



Using National Instruments MIO Boards using the old NI-DAQ interface

Consult the reference manual for the given National Instruments board. Assign the board an MIO Device #, and enter this number in a GC Reference Number. Also enter the channels that are connected to the GC, and the Input Limits. The Input Limits are used to specify the gain for the data acquisition.

Refer to your MIO Manual for the following information:

- Defining the MIO Device #.
- Information on the available gains. In general, the Input Limits should be as small as possible in order to have the largest possible gain.
- Information on the available channels. Some boards support data acquisition only when the channels are specified in a certain order, and not when they are present in a random order. Refer to your data acquisition manual that came with your board for more information.

Testing a National Instruments NI-DAQ Board

You can use the “GC DAQ MIO Tester.vi” that comes with the Chromatography Toolkit to test the various parameters described above before you start trying to acquire data. This vi provides an error message in the case the software is configured incorrectly.

Double click on the “GCDAQ.llb” library.

Using a Hewlett-Packard HP 5890 GC

WillStein Software provides an add on module for the HP 5890. This module is capable of starting a run and acquiring the data directly over an RS-232 connection. This requires an RS-232 board from Hewlett-Packard, but no additional data acquisition hardware is required on the computer.

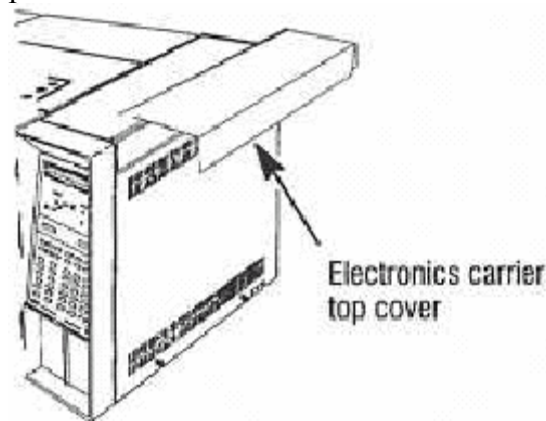
Types of RS-232 Boards available for the HP 5890

HP provided two types of RS-232 boards for the HP 5890. Different configurations are required for these different boards. You must first determine which board that you have installed. The more common option is the “DICE” board, which provides both an RS-232 and a GPIB connection on the back side of the HP 5890. The “Single RS-232” board only provides an RS-232 connection.

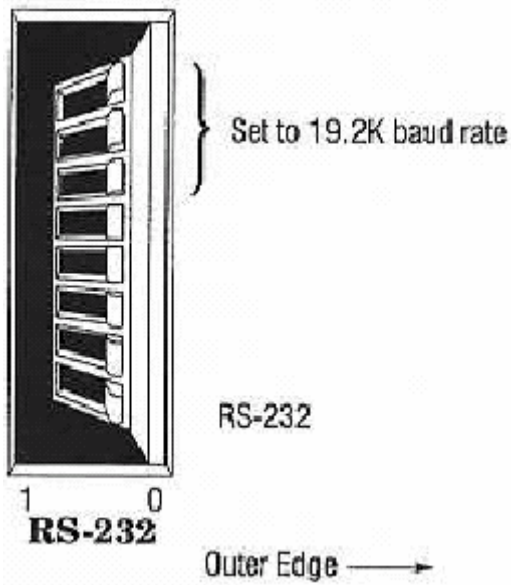
“DICE Board” - Setting the Baud Rate on the HP 5890

The RS-232 parameters are controlled by dip switches on the RS-232 board itself

First, turn off the power on the HP 5890, and then locate the board by opening the right side panel.



Set the dip switches so that they are all pointing to the right (away from the GC itself).



“DICE Board” - Serial Cable

This can also be made up from a 9-25 pin standard cable with a null modem inserted.

DB-9 Female	DB-25 Male
1,6	20
2	2
3	3
4	6, 8
5	7
7	5
8	4
9	Blank
Shield	Shield, 1

Note for reference, a standard DB-9 Female to DB-25 Male cable is:

DB-9 Female	DB-25 Male
1	8
2	3
3	2
4	20
5	7
6	6
7	4
8	5
9	22
Shield	Shield, 1

“Single RS-232 Board” - Setting the Baud Rate on the HP 5890

The RS-232 interface transfers data at a specified baud rate (baud = bits per second). This baud rate must be identical for both the sender and the receiver. The maximum baud rate for an RS-232 connection is 19,200. However, Chromatography Toolkit is normally configured for 9600 baud. This is more reliable than the maximum rate and does not significantly effect the performance of the connection.

The HP 5890 sets the baud rate and two other control parameters (ST and HR settings) a single command. Note that, the ST and HR controls prevent the GC from being used from its keyboard, and only allow a remote computer to adjust the operating parameters. These controls are not used in Chromatography Toolkit, and must be bypassed. With this in mind, the baud rate may be selected as discussed on page 4-2 of the RS-232 manual. The instructions for 9600 baud are given below.

- 1) Press CLEAR and PERIOD on the HP 5890 keypad. The LED display should read “CALIB AND TEST [0-9]”.
- 2) Press “3” to select the third calibration/test command. The LED display should read “CONFIGURE NETWORK”.
- 3) Press “ENTER”. The LED display should read “GLOBAL ADDR: ##,##”. Note that “LOCAL” may appear instead of “GLOBAL”; this is irrelevant. Also a number may appear instead of the “##” to indicate the current configuration.
- 4) Press “25” and then press “ENTER” to set the baud rate to 9600 with both HR and ST bypassed. GC WorkMate is preset to use 9600 baud.
- 5) This setting will not take effect until the HP 5890 is restarted. Therefore, either turn the HP 5890 off and then on again, or, press “CLEAR-PERIOD-5-ENTER” to reset the electronics.

“Single RS-232 Board” - Cable Specification

The HP 5890 RS-232 board provides a 25 pin male cable that must be connected with your own cable. The pin connections are as follows:

- 2: Transmit
- 3: Receive
- 7: Ground

Note that a null modem will be required in order to reverse pins 2 and 3. A null modem can be built into the cable that you use.

Macintosh Cable

You can purchase a standard modem cable and attach a null modem/gender changer. Or, you can use a cable with the following pinouts:

Mac Din 8	DB 25 Female
3	2
5	3
4,8	7

Windows Cable, Black Box #BC01900 (as of 9/2001)

You can purchase a standard modem cable and attach a null modem/gender changer. Or, you can use a cable with the following pinouts:

DB9 Female	DB 25 Female
2	2
3	3
5	7

25 Pin Cable Stub (Agilent part 19242-60500)

The following table shows the connections for this cable in case you need to make your own cable.

25 Pin Connector	Color	Function	12 Pin Connector (#1 is at the top left)
1	Silver	Ground	4 (also connect to shield)
2	Blue	Transmit	5
3	Red	Receive	1
7	Green	Ground	3

Using an Agilent 6890 GC

WillStein Software provides an add on module for the Agilent 6890. This module is capable of starting a run and acquiring the data directly over an RS-232 connection. No additional hardware is required since the 6890 has a built in RS-232 connection.

Cable Specification

Windows:

- HP part number G1530-60600
- Black Box part number EYN257H-00060FF
- Standard Female to Female null modem cable.

Female DB-9

1	DCD	Input
2	RxD	Input
3	TxD	Output
4	DTR	Output
5	GND	
6	DSR	Input
7	RTS	Output
8	CTS	Input
9	RI	

Female DB-9

4	DTR	
3	TxD	
2	RxD	
6	DSR and 1 DCD	
5	GND	
4	DTR	
8	CTS	
7	RTS	
	No connection	

Macintosh

Female DB-9

1	DCD	Input
2	RxD	Input
3	TxD	Output
4	DTR	Output
5	GND	

Macintosh DIN 8

1	HSKo	
3	TxD -	
5	RxD -	
2	HSKi	
4, 6, 8	GnD, TxD +, RxD+	

6	DSR	Input	1	HSKo
7	RTS	Output	2	HSKi
8	CTS	Input	1	HSKo
9	unused			

User Customization of GC WorkMate/LV

The diagrams are hidden for the Peak Detection routines and can not be modified by the end user. However, there are a number of ways for end users to customize GC WorkMate/LV.vi in order to fit into their lab.

List of vi's for Customization

The following is list of vi's which might need to be modified or which might serve as templates for your own custom application.

- GC WorkMate/LV.vi
- GC Data Acquisition.vi
- GC Display.vi
- data acquisition
 - GC DAQ Init.vi
 - GC DAQ Pump.vi
 - GC DAQ Dispose.vi
 - GC DAQ Start Button.vi
 - GC DAQ Validate.vi
- GC Peak Information.vi

Calling GC Data Acquisition.vi from your own program

Controlled Start of Data Acquisition

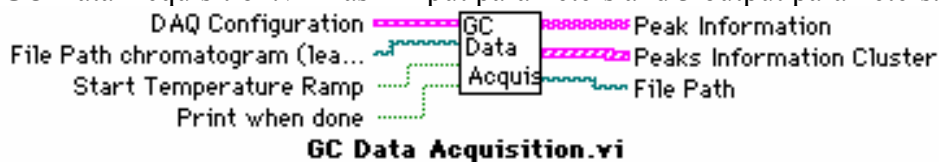
“GC Data Acquisition.vi” can be used directly in your own vi's. In this way, data collection could be initiated by a user defined event, such as a specified time interval, a valve opening, a temperature reaching a critical value, etc.

Real Time Process Control

Similarly, the results of the data acquisition could be used to control a chemical reactor, distillation column or some other process operating in a lab or pilot plant. In this way, the peak information can be used for feedback to a real time process control loop.

How To Do It

“GC Data Acquisition.vi” has 4 input parameters and 3 output parameters.



Inputs

- The “DAQ Configuration” cluster described in “Controlling Data Acquisition Parameters”.

- The second input is a path to the file to store the results. If this path is empty, you will be presented with a dialog asking where you would like to store the data file. You can avoid this dialog by providing a path to store the new data file. You can use any LabVIEW commands to generate this path automatically.
- The “Start Temperature Ramp” Boolean is used send the start signal to the GC. This is provided for the HP 5890 and Agilent 6890. Other GC’s require user customization.
- The “Print when done” Boolean will cause a printout to be generated at the end of the run.

Outputs

- The “Peak Information” output provides the table of peak information that is shown in real time.
- The “Peak Information Cluster” is a Cluster Array. Each array element contains a cluster of information about a given peak such as its retention time and area.
- The “File Path” provides the name and location of the data file containing the data.

Display or Use the Full Peak Detection Information

Only a subset of the peak information is displayed for each peak. The user can customize the display to show more of this information. Also, the user could use the full peak information for creating a report or doing other calculations.

Using the Peak Detection Library in Your Own Program

“GC Import and Process.vi” serves as an example for using the Peak Detection Library in your own vi’s. This vi loads a text file and calls the peak detection library in order to process the file. Use this vi as a template for processing your own data. Comments are provided in this program to illustrate the steps required.

User Defined Data Acquisition

Use the Peak Detection.vi for Other Applications

Peak Detection.vi is self contained, and can be utilized in other applications separately from GC WorkMate/LV. Therefore, a user can create their own LabVIEW program from the ground up and use Peak Detection.vi at the appropriate place. Alternatively, the data acquisition modules in GC WorkMate/LV.vi can be modified for the users own hardware. See the next section entitled “Modify the Data Acquisition Modules” for more information about the latter option.

Note: Be sure to include “Peak Detection Init.vi” in your custom program when you use “Peak Detection.vi”.

Modify the Data Acquisition Modules

GC WorkMate/LV provides data acquisition modules for a Demo GC and the MIO Series data acquisition boards. Add-on's are also available for RS-232 connections to the HP 5890 and Agilent 6890. The user is free to create their own data acquisition modules to support their own specific data acquisition hardware. The appendix provides a general outline of the data acquisition routines followed by a more specific discussion to allow the end user to create their own modules.

Peak Detection Reference

The Configuration cluster on the GC WorkMate/LV.vi screen contains the parameters controlling the automatic peak detection.

Configuration

GC Reference #	GC Type
0	Demo GC
Signal 1	(Hold Shift Key for Multiple Selection)
Signal 2	
Signal 3	
Signal 4	
Run Time (minutes)	11.00
Sample Rate (readings/sec)	5
Peak Detection Window (seconds) (ie, expected peak width)	30
Minimum Peak Area	0.00
Maximum Peak Area	0.00
Minimum Peak Height	0
Maximum Peak Height	0
Valley to Valley Baseline?	<input type="checkbox"/>
nExtra Valley Points	0

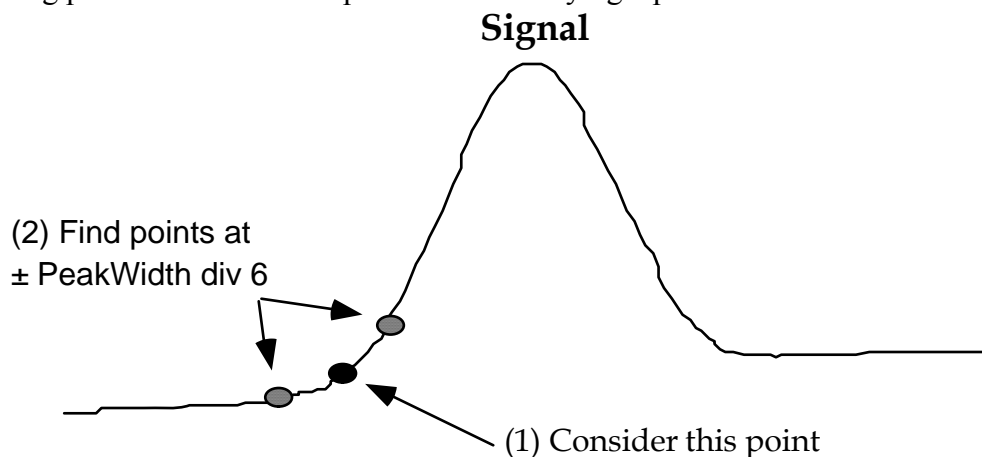
Parameter	Description
Peak Detection Window (seconds) (ie, expected peak width):	This is the most important parameter in the peak detection analysis. It should be set to the approximate width of your expected peaks (ie, the Full Width at Half Maximum). If this parameter is too small, then noise will start to be detected as peaks. If this parameter is too large, then some peaks will be overlooked.
Minimum Peak Area:	This is used to reject small peaks in order to reduce the likelihood of including noise in the peak table.
Maximum Peak Area:	This is used to reject large peaks, such as solvent peaks, from the peak table.
Minimum Peak Height and Maximum Peak Height:	In these two cases, the height is used to reject peaks instead of the area.
Valley to Valley Baseline? and nExtra Valley Points:	These parameters are used to control the method of drawing the baseline when peaks are found. See the examples for more information.

How are peaks determined?

Peaks are identified by examining the first and second derivative of the signal. A peak has a positive initial slope and a positive initial second derivative (negative peaks are handled analogously). A peak is recognized when the first and second derivatives are positive for a certain number of consecutive points.

The “Peak Width” parameter is used for two purposes. It first specifies how the first and second derivatives will be calculated. Secondly, it specifies the number of consecutive points that the first and second derivatives must be positive.

The following picture illustrates the process of identifying a peak.



First, the first and second derivatives must be evaluated at every point in the chromatogram. This is done by finding two additional points centered around the first point (ie, go forward by Peak Width div 2 and backward by Peak Width div 2). The first derivative is calculated as: $\text{first derivative} = (\text{last point} - \text{first point})/\Delta t$. The second derivative is calculated as: $\text{second derivative} = (\text{last point} - 2 * \text{mid point} + \text{first point})/(\Delta t * \Delta t)$.

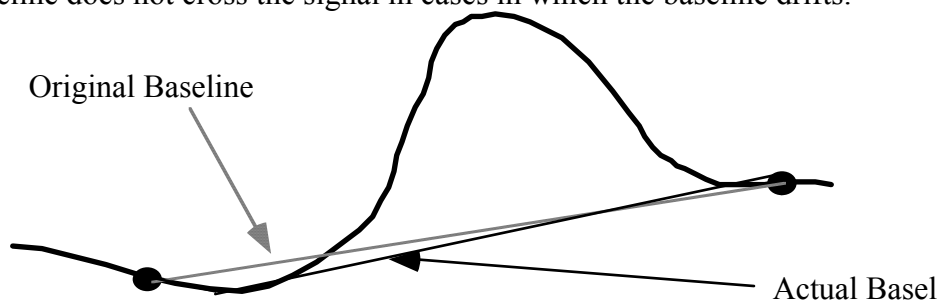
Secondly, a peak is recognized when both the first and second derivatives are positive for (Peak Width div 6).

The end of a peak is determined when the first and second derivatives return to “zero” after the peak maximum. A “zero” value is identified when the derivatives fluctuate from a positive value to a negative value a few times.

GC WorkMate also searches for overlapping peaks on the downslope of the current peak. If the first and second derivatives are again positive for Peak Width div 6, then a new peak is identified. The “Valley to Valley” parameter is then used to determine the baseline of the group of peaks as described below.

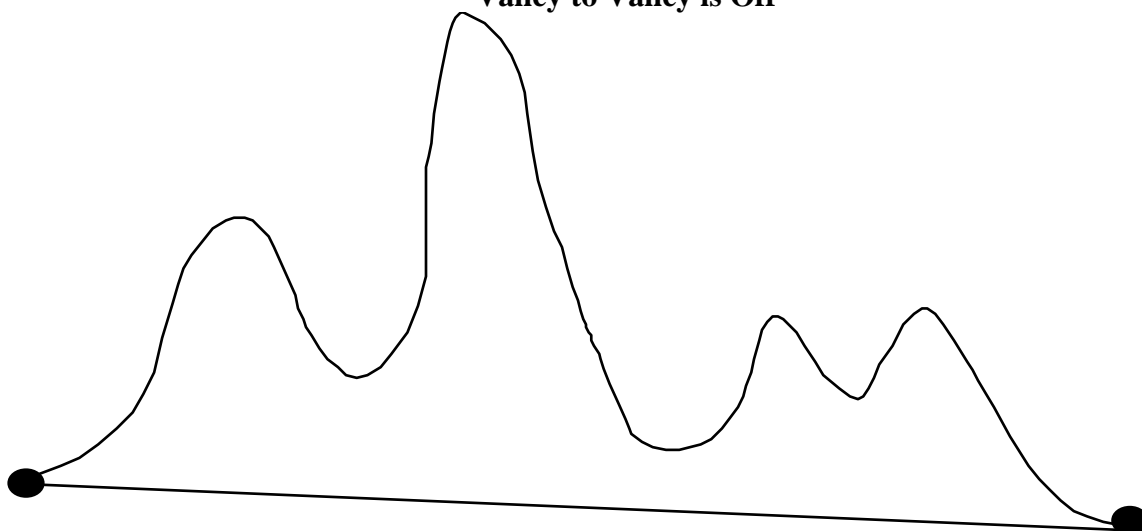
Constructing the Baseline

The baseline is constructed from the beginning to the end of a peak. GC WorkMate also insures that the baseline does not cross the signal in cases in which the baseline drifts.



There are two options in the case of overlapping peaks. If “Valley to Valley” is off, then the baseline is constructed from the beginning of the first peak to the end of the last peak in the group of poorly resolved peaks.

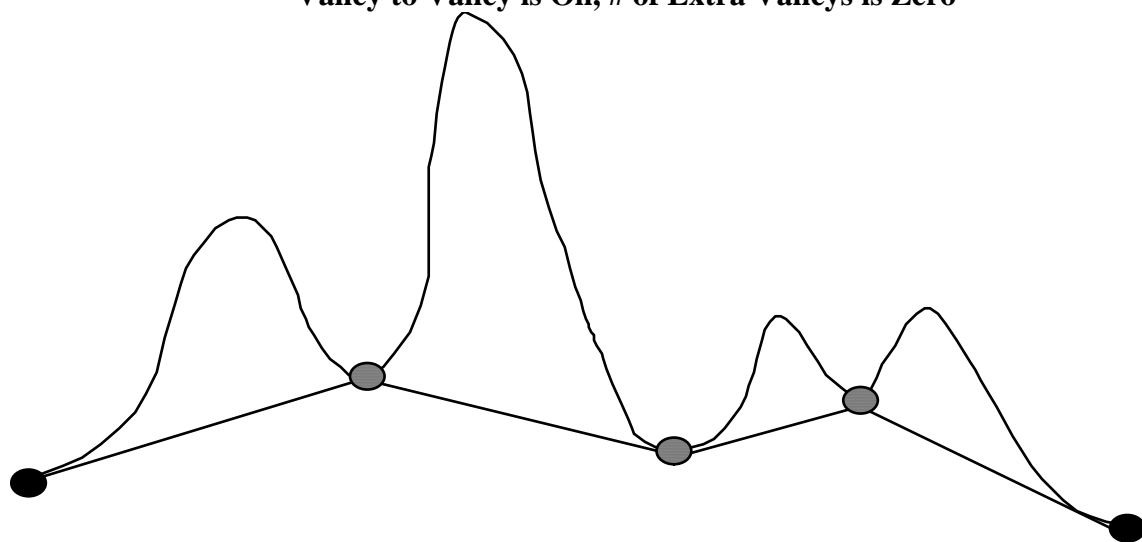
Valley to Valley is Off



If “Valley to Valley” is on, then the intermediate valley points are examined. “# of Extra Valleys” further refines this process as described below.

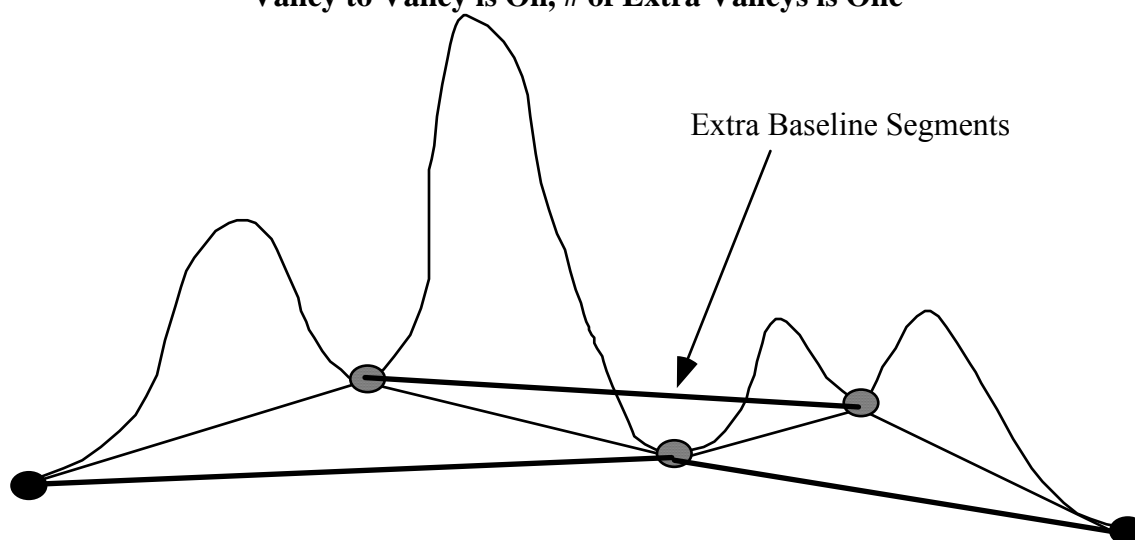
First, if “# of Extra Valleys” is equal to zero, then the baseline directly connects each valley point as shown below.

Valley to Valley is On, # of Extra Valleys is Zero



If the “# of Extra Valleys” is greater than zero, then additional valley points are connected. The final baseline is then the minima of the original valley points and these “extra” baseline segments. If “# of Extra Valleys” is one, then every other valley point is connected. If “# of Extra Valleys” is two, then every third valley point is connected, etc. This feature is useful when you have a large number of overlapping peaks.

Valley to Valley is On, # of Extra Valleys is One



Using the Optimum Sampling Rate

The "Peak Width" parameter and the Sampling Rate (readings per second) are interrelated. First, you should insure that you have at least 50 data points on each peak. For example, if a peak is 0.25 minutes wide, you can use a sampling rate of 5 readings per second. However, if your peaks are very narrow and are only a few seconds wide, then you should use 20 readings per second (or greater if your GC supports it).

Once you have specified the sampling rate, you can then choose an appropriate Peak Width parameter. The same rule then applies, choose a "Peak Width" parameter so that roughly 50 points are present on each peak. The Peak Width parameter can safely be less than the actual peak width, but it should not be significantly greater than the actual peak width.

Data Transformation Reference

The Data Transformation module provides a method for filtering or transforming data before data analysis.

During Data Acquisition

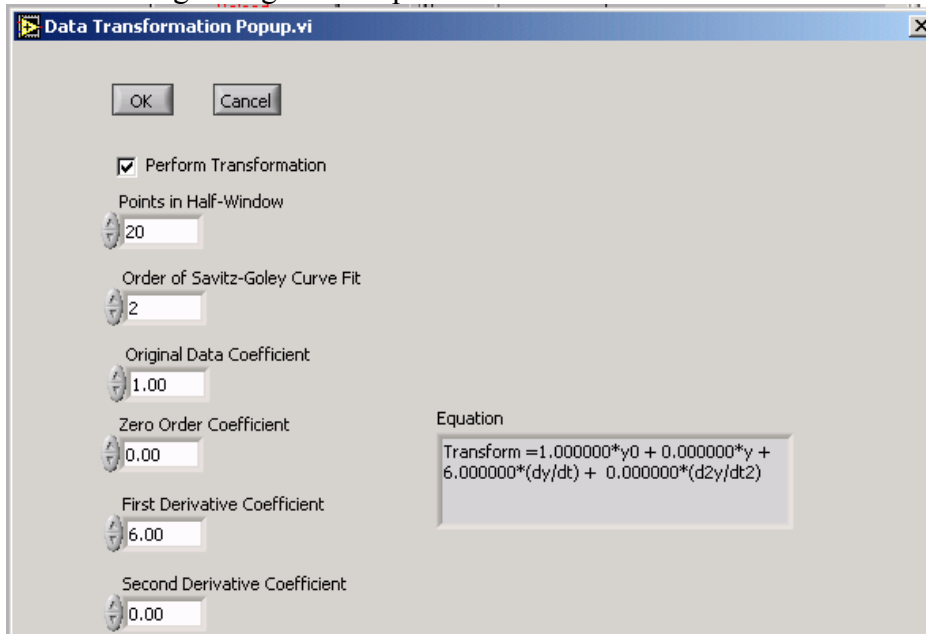
Currently, the software assumes that Signal 1 is being transformed and the result is placed in Signal 2. In this way, both the original signal and the transformed signal are maintained. Contact WillStein Software if you require the transformation of multiple signals.

During Import and Process

The data signal is transformed and replaced. The original data file serves as the backup of the original data.

Parameters

The following dialog lists the parameters available for the data transformation.



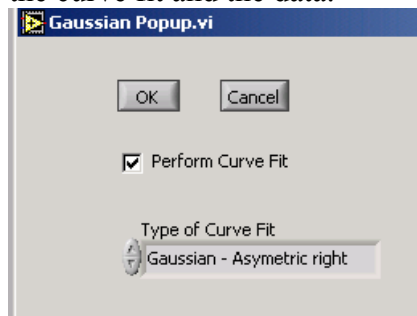
Parameter	Description
Points in Half-Window	This specifies the size of the window used in the Savitz-Goley curve fit described below. Example: 20 means that each transformation uses 20 points to the left of the current point, 20 points to the right, and the current point itself for a total of 41 points in the Savitz-Goley curve fit
Order of Savitz-Goley Curve Fit	For each point the data file, the specified number of points is fit to a polynomial of the specified order. Example: an order to 2 means that a

	<p>quadratic polynomial is fit. This curve fit can then be used to estimate the first or second derivative at the current point.</p> <p>This curve fit is then repeated for each and every point in the data file.</p>
Coefficients	The following coefficients define which terms will contribute to the result of the transform.
Original Data Coefficient	The value of the original data point is used in the calculation.
Zero Order Coefficient	The zero order result of the Savitz-Goley curve fit is used in the calculation. This corresponds to the average of the points in the window. This is the same as the moving average of the original signal, so this will provide some filtering compared with using the original data point.
First Order Coefficient	The first derivative with respect to time is used in the calculation.
Second Order Coefficient	The second derivative with respect to time is used in the calculation.
Equation	This field shows a description of the resulting transformation.

Curve Fit Reference

The Curve Fit module is used to fit a theoretical curve to the experimental data, such as a Gaussian peak shape.

The following dialog is used to specify the Curve Fit parameters. The only parameter is the Type of Curve Fit since the program will choose the initial guesses for the curve fit parameters from the peak detection algorithm. The software then minimizes the square of the error between the curve fit and the data.



Types of Equations and References

See the following references for more details:

- Data Analysis and Signal Processing in Chromatography, Attila Felinger, Elsevier, 1998, ISBN 0-444-82066-3.
- Dependence of Chromatogram Peak Areas Obtained by Curve-Fitting on the Choice of Peak Shape Function, Mindy L. Phillips and Robert L. White, Journal of Chromatographic Science, 1997(35), p75-81.
- Chromatographic Integration Methods, Norman Dyson, Royal Society of Chemistry, 1990, ISBN 0-85186-587-9

Gaussian

The following equation is used for the Gaussian Curve Fit:

$$c(t) = H * \exp\left(\frac{-(t - t_r)^2}{2 * \sigma^2}\right)$$

- H = Height
- t_r = retention time
- σ = standard deviation
- $Area = H * \sigma * \sqrt{2\pi}$

Gaussian - Asymmetric

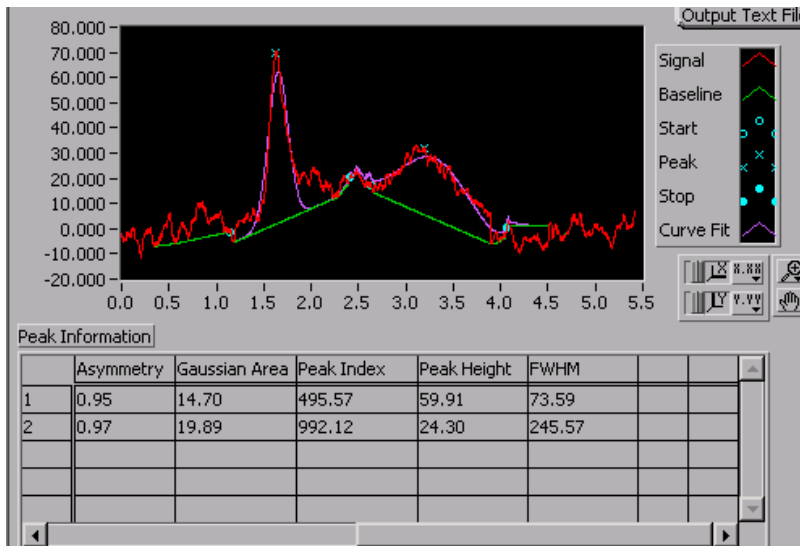
The following equation is used for the Gaussian - Asymmetric Curve Fit:

$$c(t) = \frac{A\sigma\sqrt{2\pi}}{2\alpha_1} * \left[\exp\left(\frac{\sigma^2}{2\alpha_1^2} - \frac{t-t_r}{\alpha_1}\right) \right] * \left[1 + \operatorname{erf}\left(\frac{t-t_r}{\sigma\sqrt{2}} - \frac{\alpha}{\alpha_1\sqrt{2}}\right) \right]$$

$$\text{Area} = A * \alpha * \sqrt{2\pi}$$

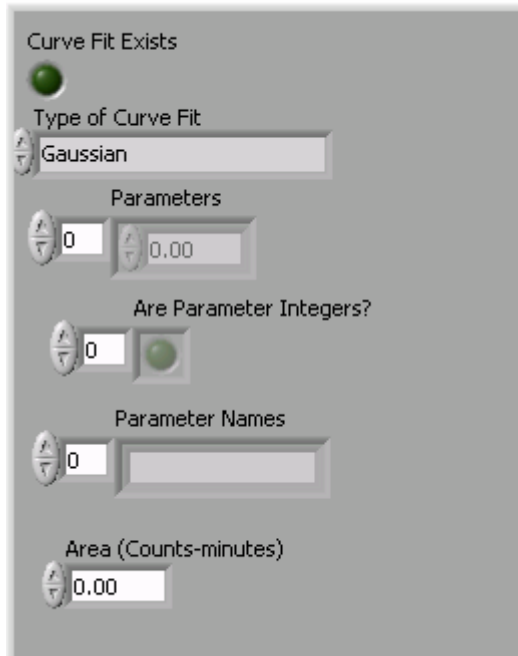
Results

Results of the curve fit are reported in two ways. First, the peak table is expanded as shown below. The Area, Peak Index, Height, and FWHM are listed for a Gaussian peak. FWHM stands for Full Width at Half Maximum, and is measured in minutes. Peak Index is the location of the peak, measured in the number of data points from the beginning of the file. Other curve fit equations show the parameters used in the curve fit.



Finally, the peak detection cluster contains the parameters used for the curve fit. The Parameter Names field identifies the parameters.

Curve Fit Parameters



Using in your own programs

Gaussian.llb contains two examples.

Curve Fit Example.vi can be used in your own LabVIEW programs. It takes an array of data and several parameter clusters, and then outputs the data transformation and curve fit results.

Curve Fit Example from File.vi reads in a single column of data from an ASCII file and feeds it to Curve Fit Example.vi.

Tips

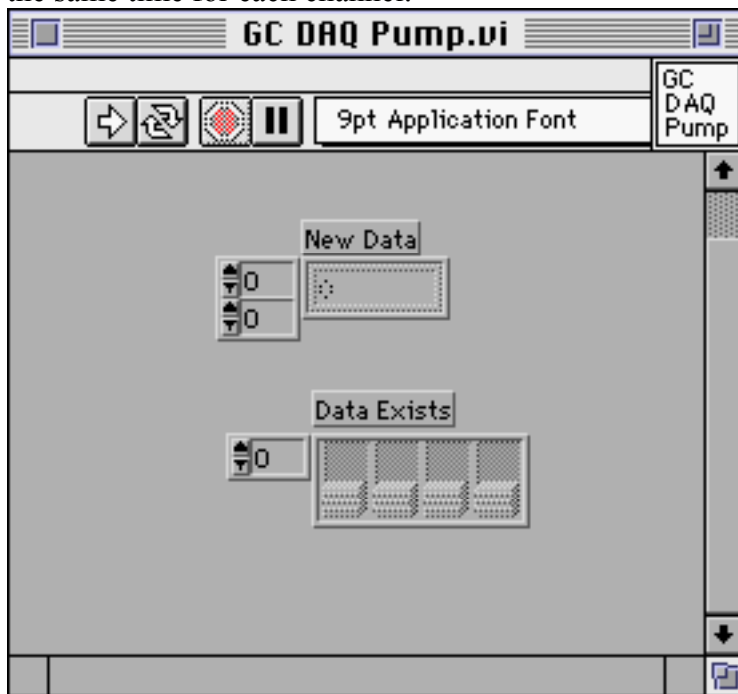
The following are some tips for using the curve fit algorithm.

- Specify the “Minimum Peak Area” in order to reject small peaks that are not meaningful. These peaks are probably irrelevant to your analysis and they will slow down the curve fit algorithm.
- The Gaussian curve fit executes faster than the asymmetric Gaussian.
- When using the curve fit in real time, insure that the data acquisition is buffered to allow for the extra time required for the curve fit.

Appendix

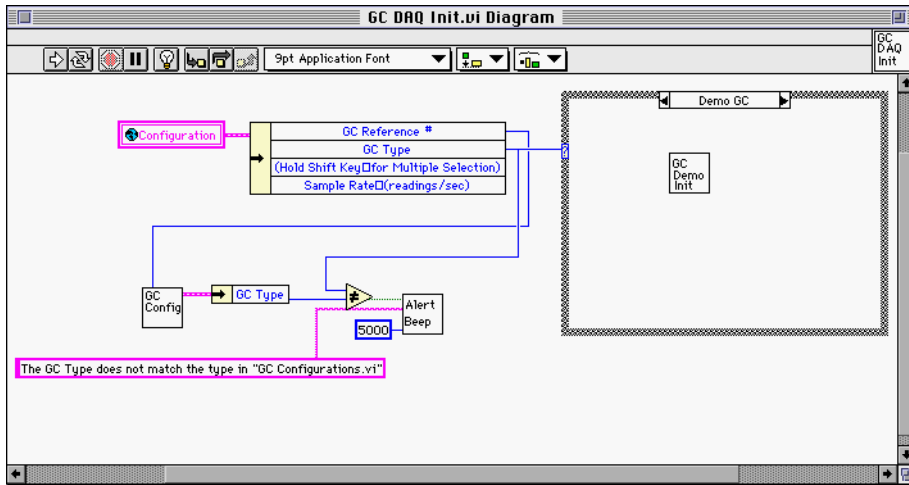
User Defined Data Acquisition VI's for Data Collection

GC DAQ Pump.vi is used to call the appropriate data acquisition routines as specified by the configuration associated with a GC Reference Number. This vi is responsible for filling in the “New Data” and “Data Exists” arrays. New Data is a two dimensional array; one dimension specifies the channel and the other specifies the samples within each channel. The “Data Exists” array is a Boolean array specifying if data is available for the given channel since not all types of GC's return data at the same time for each channel.

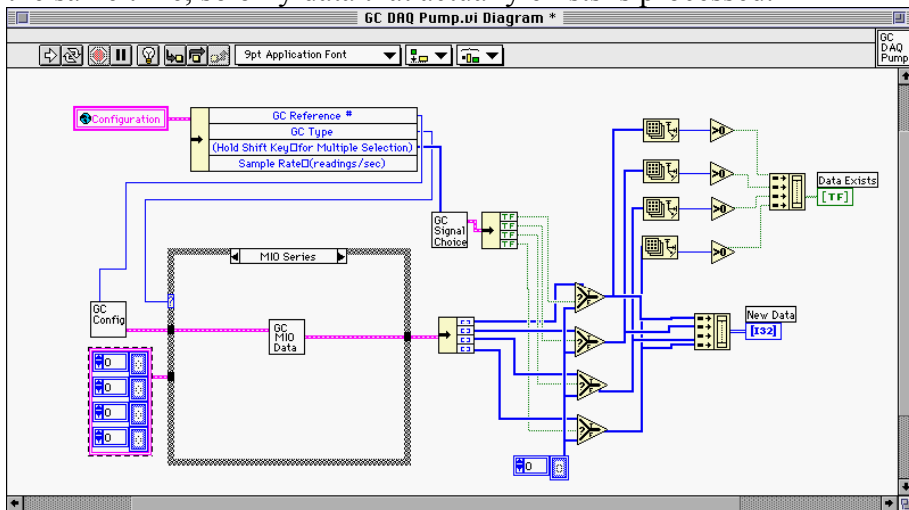


GC DAQ Init.vi and GC DAQ Dispose.vi are called automatically before data acquisition starts and after it finishes, respectively. These routines provide a convenient location to put these one time procedures required for your own data acquisition.

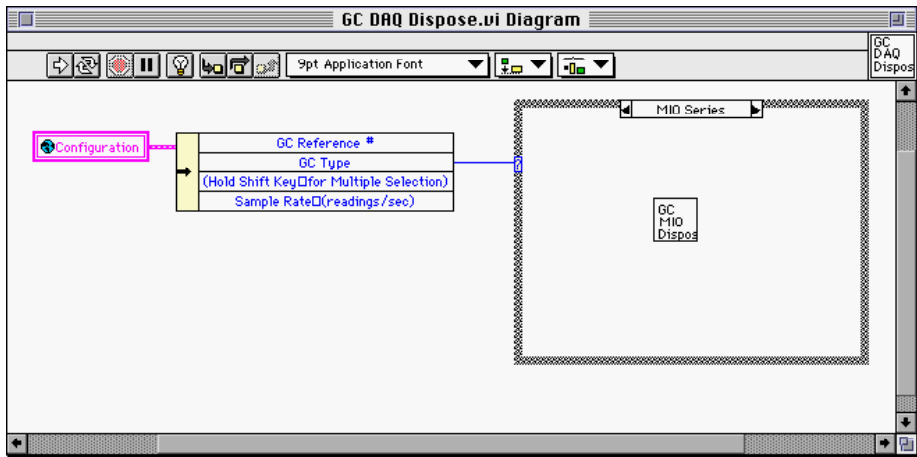
GC DAQ Init.vi is called once prior to starting the data acquisition. It has no parameters on the Front Panel. The Block Diagram checks what type of GC is used, and calls the appropriate initialization routine through the Case Structure. Add your own module under the “Customer Supplied” case element.



GC DAQ Pump.vi is responsible for acquiring data and “pumping” it into the peak detection routine. This again does its actual work by calling a subvi for the appropriate type of GC. Also notice that the “Data Exists” array is filled in automatically based on both the configuration and the available data. For example, data can be acquired from all four channels specified on an MIO board, but data will only be processed for those channels selected on the GC WorkMate/LV.vi front panel. Also, some GC’s may not return information from all channels at the same time, so only data that actually exists is processed.



GC DAQ Dispose.vi is called once after a chromatographic run is complete. Again, the GC Type is used to select the appropriate subvi to execute. For example, the data acquisition is stopped for the MIO board in order to prevent the buffer from being overrun.



Registration Form

WillStein Software

Mail To: 1723 Elmwood Avenue, Wilmette, IL 60091, or

eMail To: willstein@willstein.com

It is important that you return this registration card in order to receive future updates. **PO's normally do not contain your name or address, so this is the only way to insure that you will receive future updates.**

Product Name: Chromatography Toolkit for LabVIEW
Platform / Operating System: _____
Purchase Date: _____
Name: _____
Company Name _____
Address _____

City, State, Zip Code _____
Country _____
Phone Number _____
Fax Number _____
e-mail address _____

What were some of the factors that lead you to purchase this product????

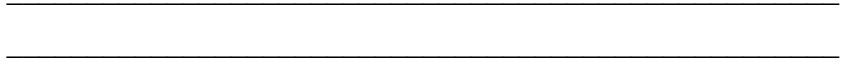
- _____ Demo version from the web site
_____ 30 day trial period
_____ Recommendation from another user

Other: _____

What is your intended use for this product????

- _____ Peak Detection library with my own custom application
_____ Use as is, out of the box.

Please describe your application: _____



Licensing Agreement

The Basics:

The Chromatography Toolkit for LabVIEW is licensed for use on a single computer. Multiple computers or multiple LabVIEW licenses require individual copies of this software.