An Introduction to LECO's Comprehensive Two-Dimensional Gas Chromatography (GCxGC) with ChromaTOF® Software

LECO Corporation; Saint Joseph, Michigan USA

NOTE: This document is intended to provide an introduction to LECO's GCxGC systems. Suggestions and recommendations are intended to help new users familiarize themselves with the technique and how the ChromaTOF® software is utilized. Many advanced parameters and options in GCxGC-related Methods are not addressed in this document. It is not designed and is not intended as a substitute for attendance at the LECO GCxGC Training Course. Methodology and Method Content are discussed at a level intended to enable a new user to begin system familiarization at a basic level.

Introduction

Comprehensive Two-Dimensional Gas Chromatography (GCxGC) is a technique that utilizes two columns of different selectivities, connected in series, to increase chromatographic resolution and peak capacity. The columns are joined by a modulator. The purpose of the modulator is to collect segments of effluent from the first column or first dimension, focus it into a narrow plug, and rapidly inject it onto the second column, or second dimension, where a rapid separation is performed every cycle, or modulation period. The technique is "comprehensive" in that the modulator functions in such a fashion that all effluent from the first dimension column is transferred onto the second dimension column.

In the most commonly used system configuration, a longer column, often 10 to 30 m in length, with a non-polar stationary phase, such as polydimethylsiloxane, is used in the first dimension. A shorter, generally 0.5 to 2 m, narrower bore column with a polar stationary phase, often a wax, is used in the second dimension. The conditions used are such that the elution bands at the end of the first dimension are significantly wider than would be observed under conditions optimized for a single column separation. This is done in order to obtain modulations across a band, often referred to as "slices", in much the same way as data points are obtained across a traditional 1D GC peak. As these elution bands exit the first dimension column, they enter the modulator, where they are focused into a narrow plug and injected onto the short second dimension, where a second rapid separation is performed. Figure 1 shows a conventional 1D GC peak and the same peak run in GCxGC. The second dimension column is usually of a narrower bore than the first dimension column in order to increase velocity on the second column. This is necessary because each second dimension separation must be completed before the next cycle of the modulator. The signal, as seen from the detector, is that of a series of short second dimension chromatograms, one for each modulation period.
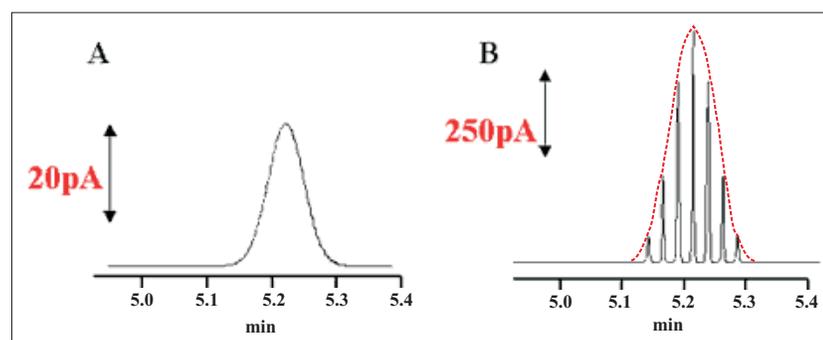
Figure 1: (A) A peak, run in conventional 1D GC, as detected by an FID. (B) The same peak, run in GCxGC with a thermal modulator, as detected by an FID. The peak has now been divided into seven slices by the modulator. Note that the shape of the unmodulated peak (the dashed red line) has been maintained after modulation. Another advantage of GCxGC, specific to thermal modulation, is the increase in signal intensity due to focusing of the peaks that occurs as part of the modulation process.

Visualization and interpretation of the chromatogram is extremely difficult in this format. At this point, the data processing software (ChromaTOF) converts the linear trace into a matrix. Figure 2 shows the process of converting the linear trace, showing five modulations of a single 1st dimension peak, into a two-dimensional matrix. Before the individual second dimension chromatograms are separated, a single retention time is associated with each data point, (Ex. the red peak in Figure 2A has a retention time of 72.4 seconds). Within the modulation, the red peak has a retention time of 2.4 seconds. When the matrix is formed, modulations have 1st dimension retention times increasing in increments of modulation period (5 seconds in this case). The red peak's 1st dimension retention time would be 70 seconds, and its 2nd dimension retention time would be 2.4 seconds. For the blue peak in the next modulation, its 1st dimension retention time would be 75 seconds, and its 2nd dimension retention time would be 2.4 seconds. The 1st dimension retention time identifies which modulation the peak occurs in and the 2nd dimension retention time identifies a peak's retention time within the modulation. The peak can be approximated in 3D in this matrix view. The peak's shape in the 2nd dimension can be taken directly from the linear trace. The peak's shape in the 1st dimension is approximated by traces across the individual modulations (see Figure 1B). These two sets of traces can then be combined to form a wire frame 3D representation of the GCxGC peak (see Figure 2D).

Technical Brief

A)

t_r (s)

B)

Masses: TIC

C)

2nd Dim t_r (s)

1st Dim t_r (s)

D)
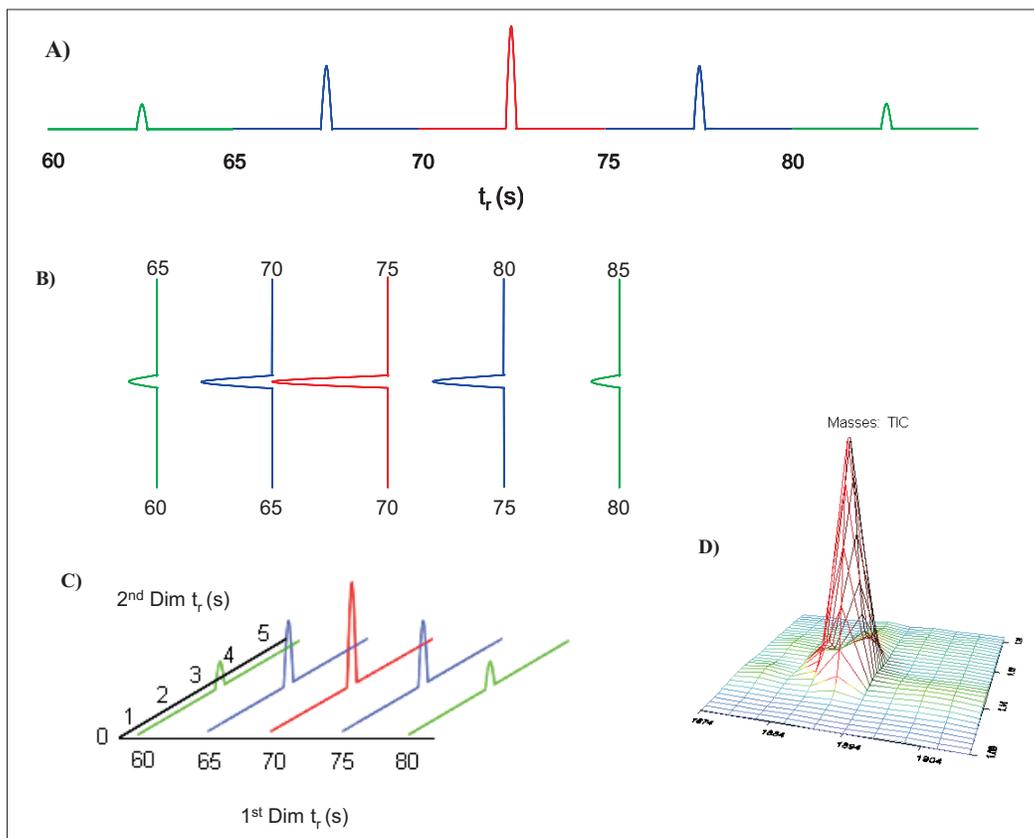
Figure 2: (A) The linear trace as seen by the detector. Each color segment of the trace represents an individual second column separation associated with a single cycle of the modulator. The trace shown in this figure corresponds to data collected using a 5 second modulation period. (B) The linear trace is then divided into its individual second dimension separations. (C) The individual second column separations arranged by 1st dimension retention time on the x-axis and by 2nd dimension retention time on the y-axis. The intensity of the detector signal is displayed on the z-axis. (D) A wire frame 3D approximation of a peak generated by ChromaTOF from data similar to that shown in (C).

By applying a color-scaled surface to the wire frame, a 3D chromatogram is generated, with retention times on the x- and y-axis, and detector response on the z-axis. Figure 3 shows a section of an actual 3D chromatogram. In ChromaTOF, this is referred to as a "Surface Plot". The more common way to view these chromatograms in ChromaTOF is a two-dimensional representation known as a "Contour Plot". In the Contour Plot, the viewpoint of the observer is as if they were looking directly down the z-axis. In this view, signal intensity is represented by a scaling of color.

A)   Masses: TIC

B)   Masses: TIC
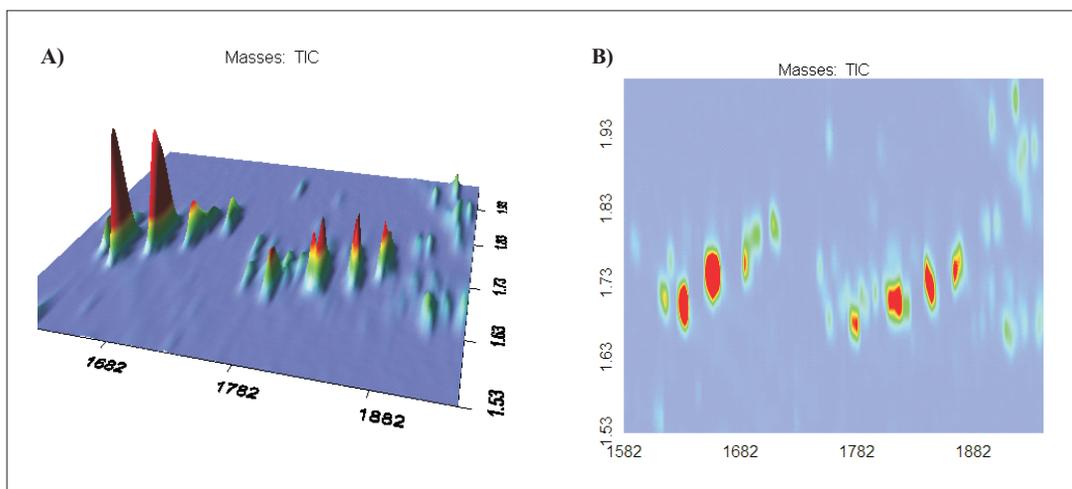
Figure 3: (A) A Surface Plot of a portion of a GCxGC chromatogram. (B) A Contour Plot of the same region displayed in (A).

ChromaTOF for GCxGC

ChromaTOF is LECO's proprietary software package for chromatography. ChromaTOF version 4.22, the most current version as of this time, will be shown. Some features and software layout may be different or absent if using a different version of the software. Three methods will be covered relating to the collection and analysis of GCxGC data, they are the

GC, MS, and DP Methods. Parameters of a method will be covered in a "top down" fashion, as they appear in the method. Before working through the methods, it is critical to establish that the correct column configuration is specified. Many method parameters are calculated according to information specified in these fields (i.e., flow, maximum temperature limits, etc.). Column configuration is found under the "Instrument/Gas Chromatograph/Column Configuration" pull-down menu (see Figure 4).

The fields for the column configuration of the instrument are shown in Figure 5. These would be the correct configuration entries for a 20 m x 0.25 mm I.D. x 0.25 μm df Rxi-1ms primary column and a 1.25 m x 0.10 mm I.D. x 0.10 μm df BPX-50 secondary column, operated in GCxGC mode, with the connection of the two columns occurring at the base of the modulator. It is essential that any changes that are made to the column configuration (i.e., trimming length from the column, changing column length, changing stationary phase, etc.) be updated in the Column Configuration to reflect the current configuration of the system. *(Note: The column internal diameter is entered in μm, not the mm value given on the column box.)
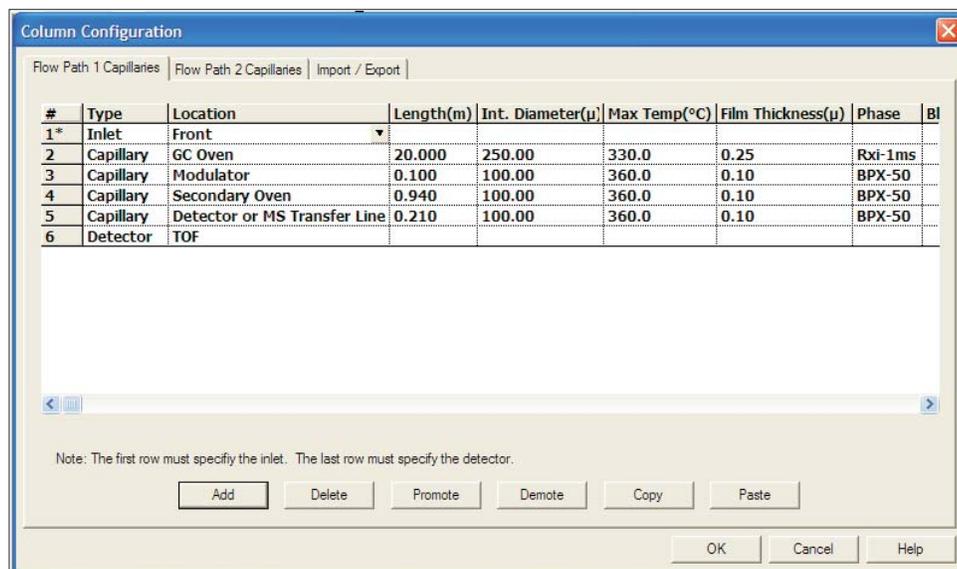
Figure 5: The correct Column Configuration entries for a 20 m x 0.25 mm I.D. x 0.25 μm df Rxi-1ms primary column and a 1.25 m x 0.10 mm I.D. x 0.10 μm df BPX-50 secondary column, operated in GCxGC mode, with the connection of the two columns occurring at the base of the modulator.

GC Method

The GC method covers parameters necessary for operation of the GC. These include system configuration, oven temperature programs, inlet parameters, etc., as well as parameters specific to modulator operation in the GCxGC mode.

At the top of the GC Method, the first piece of information that must be confirmed is the identification of the type of GC that is being used. The choices available in ChromaTOF v. 4.22 are the Agilent 7890, the Agilent 6890, the Shimadzu GC-2010 and a Generic GC. Immediately below the GC type are two options, one for LTM columns and one for GCxGC. The box for GCxGC must be checked. Figure 6 shows this portion of the GC Method as it would look for an Agilent 6890 operating in GCxGC mode.
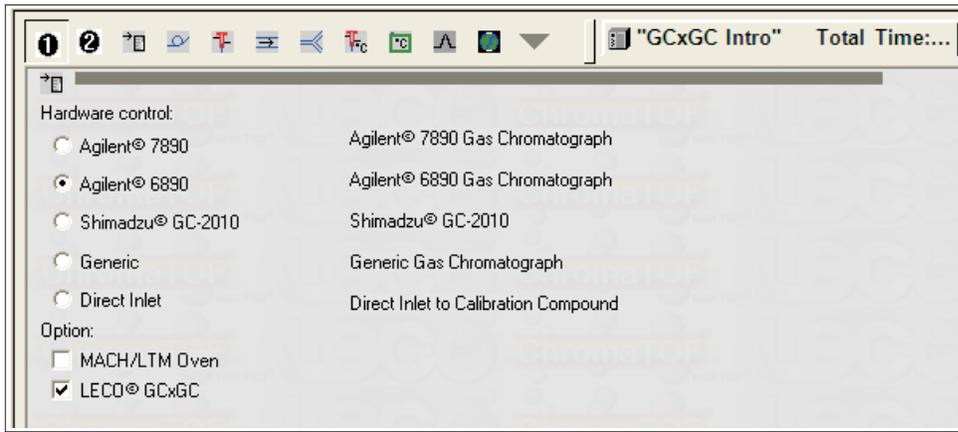
Figure 6: A portion of the GC Method as it would look for an Agilent 6890 operating in GCxGC mode.

The next section of the GC Method is the Column Configuration section. At the top of this section is a colored indicator with a dialogue box. Its purpose is to give a quick indication of any problems in the Column Configuration. A green indicator means there are no detected problems. A yellow indicator means a problem has been found, but this problem does not prevent the system from operating. A red indicator means a problem has been found, and the system cannot function until this problem is resolved. When a yellow or red indicator is present, the problem will be indicated in the dialogue box. The column configuration defaults to the global configuration of the system at the time the new GC Method was created. If the global configuration has been changed since the creation of the GC Method, the method can be updated by right-clicking and selecting "Use Global Column Configuration" (see Figure 7). This will update the Column Configuration to match the Instrument Global Settings.
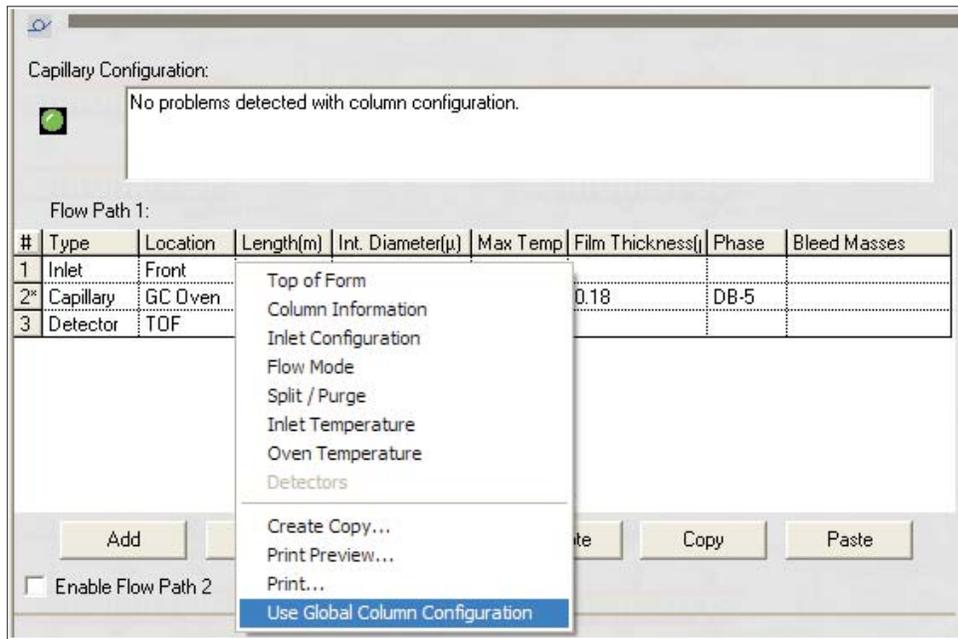
Figure 7: If the global configuration has been changed since the creation of the GC Method, the method can be updated by right-clicking and selecting "Use Global Column Configuration".

The next section of the GC Method relates to the carrier gas and inlet set-up. Use the pull-down menus to select the correct settings for the instrument in question (see Figure 8). The example shown is for a system using helium carrier gas with a Split/Splitless inlet operated in Split mode. It is important to note that the Active Inlet Location must match that specified in the Global Column Configuration.
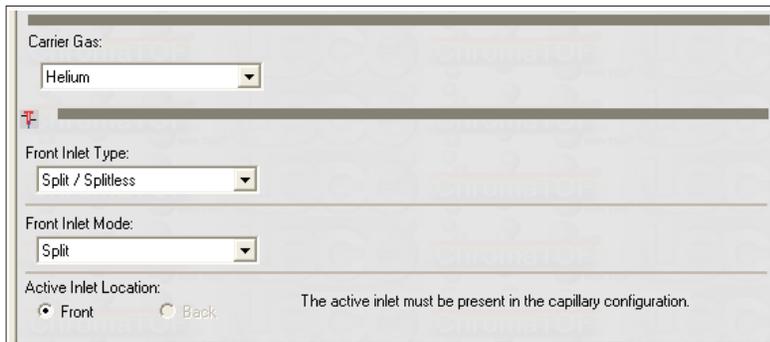
Figure 8: The section of the GC Method relating to the carrier gas and inlet set-up.

The next section of the GC Method is the Column Flow Mode section. At the top of this section is a colored indicator with a dialogue box, similar to that found in the Column Configuration section of the GC Method. Immediately below is a check box enabling the use of "Corrected constant flow via pressure ramps". Note that when this box is selected, the pull-down menu for column mode disappears. It is critical that Corrected Constant Flow be used in GCxGC mode. The reason for this is that in the LECO GCxGC, a column ensemble is used. This column ensemble consists of two columns with different inner diameters. The GC's Electronic Pressure Controller (EPC) is only capable of handling a single column's parameters. In order to obtain correct flows for the system, ChromaTOF calculates a "virtual column" using the information in the GC Method Capillary Configuration and generates a pressure ramp program for the EPC. This pressure ramp program allows the system to maintain a constant flow during the course of the analysis. Failure to utilize Corrected Constant Flow is one of the most commonly seen sources of problems with GCxGC methodology.
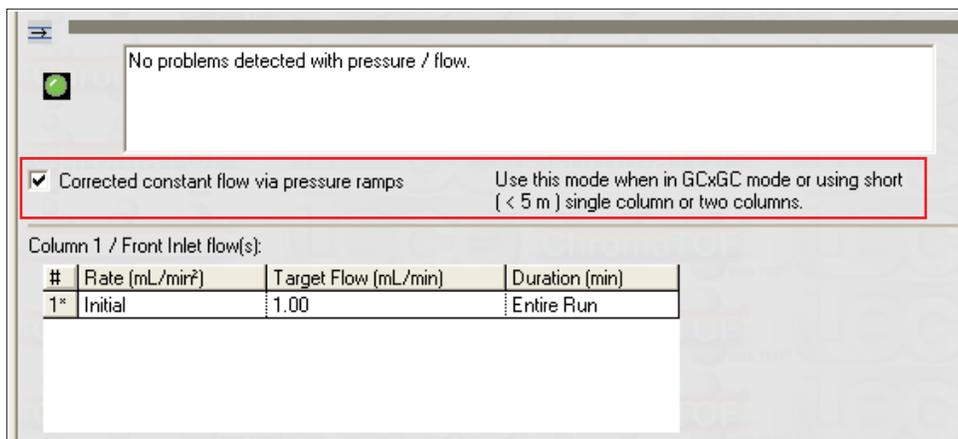
Figure 9: The Column Flow Mode section of the GC Method. The "Corrected constant flow via pressure ramps" box must be selected for GCxGC methods.

The next section of the GC Method is the Oven Programming section. At the top of this section is a colored indicator with a dialogue box, similar to that found in the Column Configuration section of the GC Method. The GC oven temperature program is entered under "oven temperature ramp" (see Figure 10). In GCxGC, it is most common to utilize ramp rate in between 5°C/min and 12°C/min and in some cases, as fast as 20°C/min. The check-box for "Enable Secondary Oven" must be checked. The second dimension column is housed in the Secondary Oven. The term used in GCxGC to describe the temperature relationship between the Primary Oven and the Secondary Oven is called the "Column Offset". The Secondary Oven's temperature program differs from that of the Primary Oven in its initial and final temperature. This difference is the Column Offset and is a positive number for LECO's GCxGC. In the example shown in Figure 10, the Column Offset is +5°C. The Secondary Oven's temperature program is identical to that of the Primary Oven except that its initial and final temperatures are 5°C higher. In ChromaTOF, there is no field to enter the desired Column Offset; it must be accounted for in the values you enter into the oven temperature programs. Column Offsets of +5°C to +15°C are most commonly used. The Column Offset is adjusted to modify retention in the second dimension. It can be decreased to increase retention in the second dimension, or it can be increased to decrease retention in the second dimension.
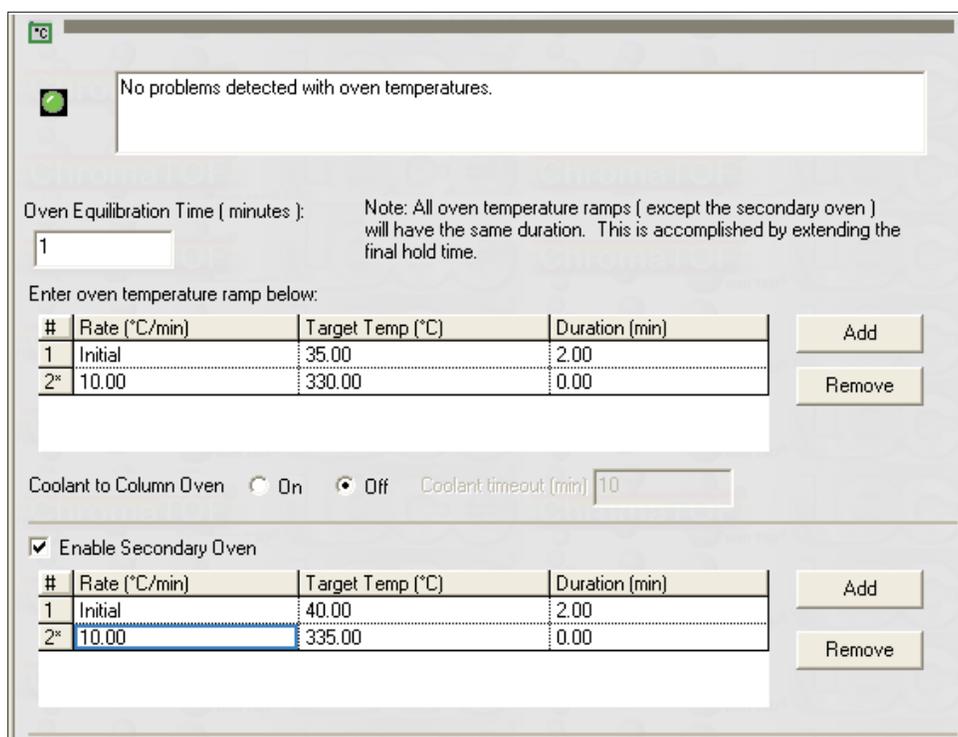
Figure 10: An example of the Oven Programming section of the GC Method. In this example, a +5°C Column Offset is utilized.

The GCxGC Parameters section is where modulator specific criteria are established. The first step is to ensure that the check-box labeled "Modulator Enabled" is selected. Immediately below this is where the Modulator Offset is established. The modulator serves two distinct functions, trapping segments of primary column effluent and acting as the injector for the secondary column. As with a conventional GC inlet, it is beneficial for the temperature of the inlet to be higher than that of the analytical column. This allows for the transfer of relatively narrow injection plugs from the inlet to the column. In thermally modulated GCxGC, this is accomplished by maintaining the modulator, and its associated hot jets, at an elevated temperature in relation to that of the secondary column. The difference in temperature between the modulator/hot jets and the secondary oven is referred to as the Modulator Offset. In the case of LECO's thermally modulated GCxGC, the modulator is located in the primary oven with the secondary oven located on top of the modulator housing. Because of this configuration, the temperature differential between the primary oven and the modulator/hot jets is actually the sum of Column Offset and the Modulator Offset. This sum of offsets is the value that is entered into the "Modulator Temperature Offset" field in ChromaTOF. LECO recommends a Modulator Offset of +15°C as a starting point in method development. In the example shown in Figure 10, a +5°C Column Offset is specified. If the LECO recommended Modulator Offset of +15°C were used, the value entered into the Modulator Temperature Offset would be "20". This corresponds to the sum of the two offsets (see Figure 11).

The "Purge Pulse Time" setting provides the ability to pre-chill the cold jets before operation of the cold jets commences. The default value is "0" and this value should be sufficient the majority of the time. It may be necessary to enter a different value, for example, if the dead time of the primary column were very short, the start of modulator cycling was delayed to some point after injection, or it was necessary to modulate very volatile species such as butane. In that case, a value between 1 and 10 seconds would be entered. If a value of "5" were entered, the colds jets would turn on for 5 seconds immediately prior to the start of modulator cycling.

The "Modulation Timing" section establishes the timing of the various segments of the overall modulator cycle. The "Start" and "End" correspond to the initiation and termination of modulator operation. The default values are "Start of Run" and "End of Run". The "Modulation Period" refers to the amount of time necessary to complete a full cycle of both stages of the modulator. As a general rule of thumb, it is desirable to make the Modulation Period as short as possible, while obtaining sufficient separation on the secondary column and avoiding wrap-around. Modulation Periods of less than 2 seconds should be avoided due to temperature lag. The most common values for Modulation Period are between 4 and 7 seconds. For a 5 second Modulation Period, each stage of the modulator would comprise 2.5 seconds. This time is then subdivided again into the "Hot Pulse Time" and "Cool Time". The Cool Time corresponds to the amount of time that the modulator is focusing analytes. The Hot Pulse Time corresponds to the time that the modulator is functioning as the injector for the secondary column. Only the Hot Pulse Time is entered by the user. The Cool Time is calculated by the software by subtracting the Hot Pulse Time from the modulator stage duration and assigning the used portion of the modulator stage duration as Cool Time. Hot Pulse Times between 0.60 s and 0.80 s should be sufficient for the majority of applications. It is important to remember that there must be a compromise between the performance of the focusing and injecting functions of the modulator. Increasing the Hot Pulse Time to improve injection performance will decrease focusing performance and vice versa.

Figure 11: An example of the GCxGC Parameter section of a GC Method. In this example, a +5°C Column Offset and a + 15°C Modulator are utilized along with a 5 second Modulation Period using an 800 ms Hot Pulse.

DP Method

The Data Processing (DP) Method covers parameters necessary for analyzing the data collected by the GCxGC. Some of these include computing the baseline, establishing criteria for finding peaks, calculating the area and height of peaks, and on GCxGC systems equipped with a Time-of-Flight Mass Spectrometer (TOFMS), and a library search of the spectra against a library for analyte identification. Examples shown will assume the GCxGC is equipped with a TOFMS.

When a new DP Method is created, the only content the method will display is a selection of 16 un-checked boxes (see Figure 12). In this example, only the 4 most commonly used tasks will be discussed (see Figure 13). The remaining available tasks will be covered in the Training Class.
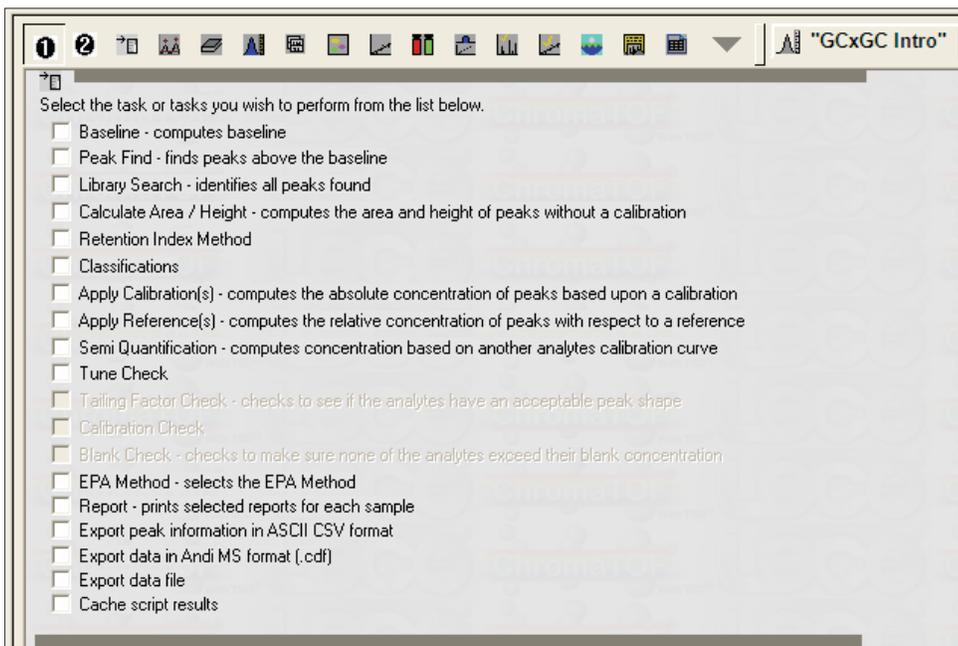
Figure 12: The selection of available tasks in a new DP Method.
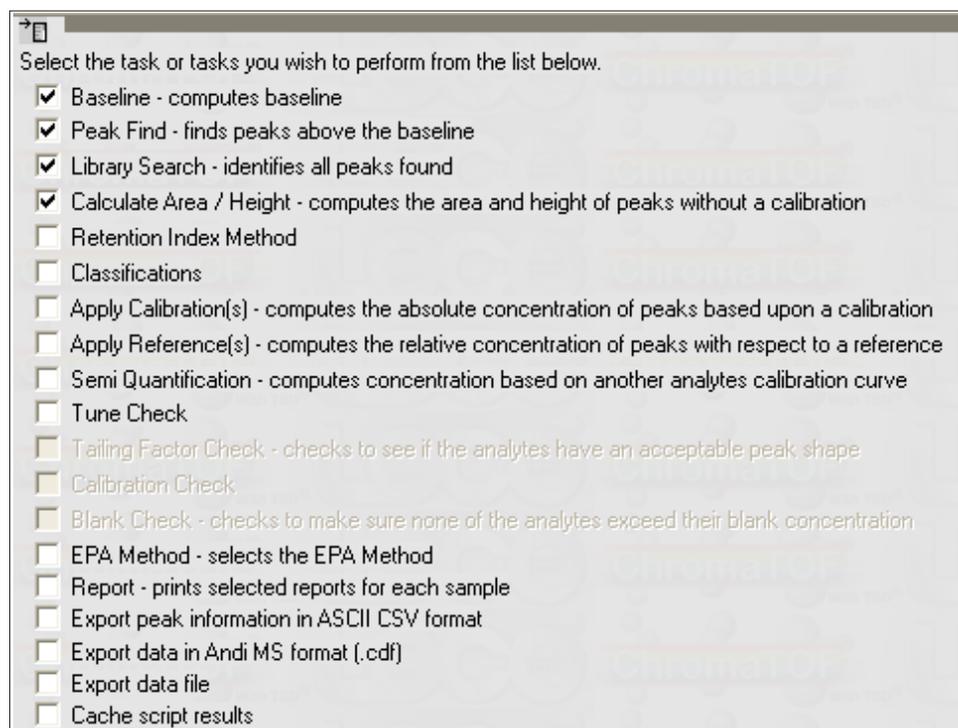
Figure 13: The selection of available tasks in a new DP Method with the 4 most commonly used tasks (Baseline, Peak Find, Library Search, and Calculate Area/Height) selected.

It is usually beneficial to use an unprocessed data file to assist in developing the DP Method. The linear trace is used to determine peak widths in both the primary and secondary dimensions.

In the Baseline section, ChromaTOF calculates the baseline for the chromatogram. The first criterion that must be entered is to specify what portion(s) of the chromatogram the baseline should be calculated for. The default values that ChromaTOF populates the fields with are to calculate baseline from "Start of Run" to the "End of Run". The next field establishes the Baseline Offset. This establishes where the baseline will be drawn in relation to the noise. The default value is 1.0, which draws the baseline just above the noise. The most commonly used values are 0.5 and 1.0 with analyst preference determining the choice. The final information in this section is determining how data smoothing will be performed. The default setting is "Auto". In the pull-down menu, the analyst can specify "No Smoothing", a specific number of data points (3 to 49) to smooth, or "Auto". The "Auto" setting determines the number of points to smooth by using the expected peak width value from the Peak Find, and is described in the next section. Figure 14 shows an example where the baseline is calculated through the middle of the noise—from the start of the run to the end of the run—and automated smoothing is used.

Figure 14: An example of the section of the DP Method pertaining to calculation of the baseline.

The next section of the DP Method relates to the Peak Find task. The first information requested is the expected baseline peak width in the second dimension. The expected peak width should be in accordance with the minimum expected peak width for the analysis. The most effective way to determine this value is to examine an unprocessed data file that the new method will be used to process. The first step is to select an unprocessed data file in Acquired Samples, then display the chromatogram for that sample (see Figure 15). Zoom in to a single modulation early in the chromatogram and locate a narrow, well-shaped peak. This peak should be representative of the narrowest peaks you want the Peak Find algorithm to identify as a peak. Peaks narrower than this peak will be considered noise. Zoom in on this peak in order to determine its width at baseline. The peak shown in Figure 16 shows a baseline width of approximately 0.100 seconds. This is the value that will be entered as the expected peak width in the DP Method (see Figure 17). If peak widths are expected to increase significantly during the run, it is possible to specify an expected peak width at two different points during the run. This option is covered in the training class. Immediately beneath this section is an entry for the "Maximum number of unknown peaks to find". The default value is 100,000. The value's basic starting point should be greater than or equal to the number of peaks the analyst expects to see in the run. Further strategies for utilizing this field are covered in the training class.
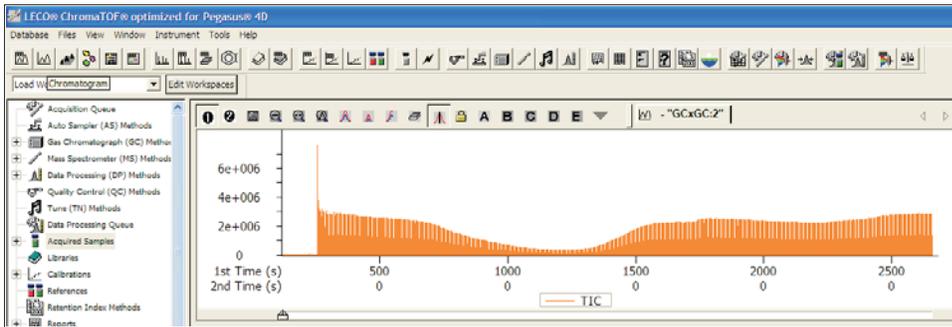
Figure 15: An example of the linear trace chromatogram for an unprocessed sample.
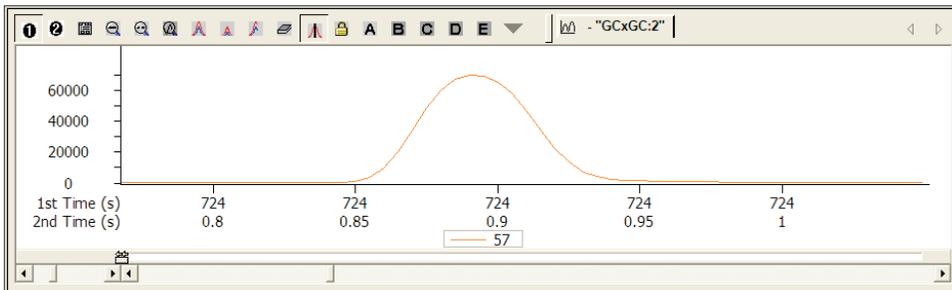
Figure 16: An example of a single peak in the linear chromatogram. In this example, the peak has a baseline peak width of approximately 0.100 seconds.

Figure 17: An example of the expected peak width section of the DP Method where the minimum peak width for the peak find algorithm is 0.100 seconds, and the analyst expects to see 5000 peaks in the run.

The next section of the DP Method relates to segmented processing of the data. Segmented processing allows for the processing of selected portions of the data. The default setting specifies that Peak Find process from the "Start of Run" to the "End of Run" and specifies the minimum S/N ratio for the Peak Find algorithm to assign a peak. The use of multiple lines in this table allow the analyst to either turn on/off Peak Find at different times during the run or change the minimum S/N requirement throughout the run. There are two other fields in the table—masses and apexing masses. These fields will be covered in the Training Class. An example of the segmented processing portion of the DP method utilizing Peak Find throughout the chromatogram with a minimum S/N of 100 is shown in Figure 18.

Figure 18: An example of the segmented processing section of the DP Method. In this example, Peak Find searches the entire chromatogram for peaks with a minimum S/N of 100.

The next section of the DP Method is the GCxGC parameters section. The GCxGC Parameters check-box must be checked in order for the GCxGC parameters to be visible in the method. The "Match Required to Combine" field is an important criterion in how the peaks in the individual second dimension chromatograms, or slices of a component, are combined into a single peak. The "Match Required to Combine" describes the minimum spectral similarity between peaks in adjacent slices in order for them to be combined into a single GCxGC peak. The default value is 600.

Figure 19: An example of the "Match Required to Combine" field in the GCxGC parameters section of the DP Method with a minimum spectral similarity of 600 required in order for the peaks to to be combined.

The next field allows for an analyst-specified amount of second dimension retention time shift for slices of a peak. In a temperature-ramped oven program, the last slice of a peak will elute at a higher temperature than the first slice. This will result in the last slice having a slightly shorter second dimension retention time than that of the first slice. For slices of the same peak, the shift will always be to an earlier second dimension retention time. If this option is selected, the default setting is to allow for a 0.100 second shift earlier in the second dimension (see Figure 20). This feature is more relevant with larger, wider first dimension peaks that are modulated into 5 or more slices. The more slices a peak is modulated into, the larger the shift to earlier second dimension retention times will be.

Figure 20: An example of allowed second dimension Retention Time Shift in the GCxGC parameters section of the DP Method.

The next section of the GCxGC parameters section of the DP Method concerns the expected peak width in the first dimension. Since there is no detector at the junction of the primary and secondary columns, this value must be extrapolated from the linear trace of second dimension chromatograms from an unprocessed run. Because the modulator collects and focuses segments of effluent from the first column, retention times in the first dimension can only be approximated in increments of modulation period. The method for extrapolating the first dimension peak width is to identify how many slices a peak has been divided into, and multiply that number by the modulation period. In this example, a single analyte chromatogram will be used. In Figure 21A, the linear trace of second dimension chromatograms is shown. By drawing a line connecting the apexes of the second dimension peaks (Figure 21B), we can approximate the shape of the first dimension peak. The first dimension peak was modulated into 7 slices in Figure 21A. If the modulation period for this separation was 5 seconds, the extrapolated first dimension peak width would be 35 seconds.
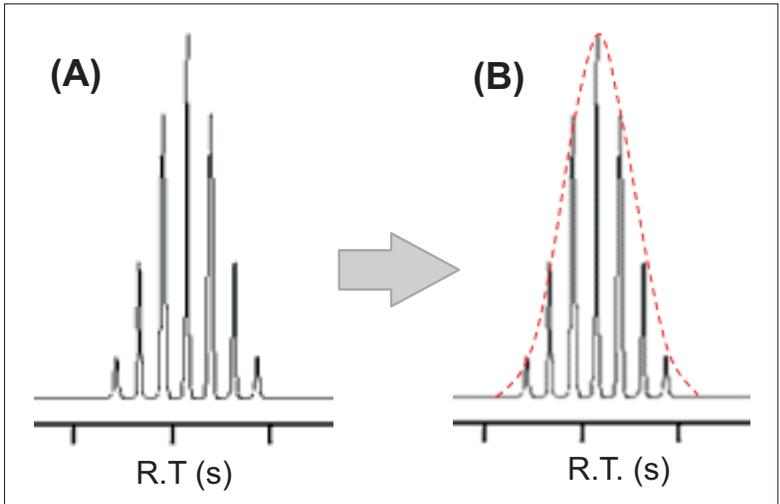
Figure 21: An example of the procedure for extrapolating the first dimension peak width from the linear trace of second dimension chromatograms. In (A) the linear trace of second dimension chromatograms for a single analyte is shown. By drawing a line connecting the apexes of the second dimension peaks (B), we can approximate the shape of the first dimension peak. The first dimension peak was modulated into 7 slices In Figure 21A. If the modulation period for this separation was 5 seconds, the extrapolated first dimension peak width would be 35 seconds.

If peak widths are expected to increase significantly during the run, it is possible to specify an expected peak width at two different points during the run. This option will be covered in the training class. Following the field for expected peak width in the first dimension, there is a field for the minimum S/N required for a sub-peak to be considered part of a peak. This field sets the S/N criterion for the earliest and latest sub-peaks of the overall peak, which are generally the smallest sub-peaks. An example where 25 second wide first dimension peaks were expected is shown in Figure 22. The minimum S/N for Sub-peak setting will be covered in the training class.

Figure 22: An example of the expected first dimension peak width in the GCxGC parameters section of the DP Method, where 25 second wide first dimension peaks were expected.

The Integration Approach dictates how the integration of peaks are performed. The Traditional method is the default, and will be discussed here. The Adaptive method will be covered in the training class. In the Traditional Integration Approach, each sub-peak is individually integrated and the area reported for a peak is equal to the sum of the areas of its sub-peaks. Figure 23 shows the Integration Approach Menu.

Figure 23: An example of the Integration Approach of the GCxGC parameters section of the DP Method.

The remaining content of the DP Method is specific to instruments equipped with a mass spectrometer. The first section is the Library Search, and is only applicable to Pegasus 4D's with the TOFMS. This section will not be visible on a GCxGC-FID system. The first section relates to the library search mode. The default mode is a Normal search in the Forward mode. Other modes will be discussed in the training class. The entry for "number of library hits to return" is where the analyst can specify how many library hits will be in the Hit Table for that peak. In the example shown in Figure 24, the top 10 library hits by spectral similarity will be returned in the Hit Table. The number of hits returned can be increased, but the size of the data file will increase proportionately.

Figure 24: An example specifying a Normal Forward Library Search returning the top 10 library hits by similarity.

The next section of the Library Search is where specific spectral requirements for the search are entered. The first piece of information is which mass range the Library Search should be performed on. In general, the best approach is to use all masses collected (*) in the field. The Minimum and Maximum Molecular Weights Allowed should be set to the range that was specified in the Mass Spectrometer (MS) Method. Additional strategies for Library Searching will be covered in the training class. The Mass Threshold setting allows the analyst to filter individual m/z peaks below certain abundance from both the library and caliper spectra. The entry entitled "Minimum similarity match before name is assigned" allows the analyst to assign a threshold for naming peaks. In order for a peak to be assigned the name associated with the first entry in its Hit Table, the peak's spectrum must have a similarity greater than, or equal to, the specified value, when compared against the library spectrum. Peaks that have a similarity less than the specified value, when compared against the library spectrum, are assigned a peak identification of "Unknown". When a peak is identified as Unknown, it does not mean that this peak cannot be identified. It merely means that the peaks similarity to the library spectrum did not meet the criterion specified by the analyst. Determining the necessary similarity is important, as the cut-off value is absolute. If the threshold is 700, a peak with a similarity of 699 will be identified as an "Unknown" peak. In Figure 25, an example is shown where all masses collected are searched; the peak's spectra are compared against the library spectra over the range of m/z from 35 to 350. An ion in the peak's spectrum or the library spectrum must have a relative abundance of at least 20 (2.0% of base peak's intensity) to be considered in the similarity score, and the peak's spectrum must have a similarity greater than, or equal to 700, when compared against the library spectrum for a name to be assigned to the peak.

Figure 25: An example of the Library Search section of the DP Method where all masses collected are searched; the peak's spectra are compared against the library spectra over the range of m/z from 35 to 350. The base ion of the peak's spectrum must have a relative abundance of at least 20, and the peak's spectrum must have a similarity greater than, or equal to 700, when compared against the library spectrum for a name to be assigned to the peak.

The final area of the Library Search section of the DP Method is where the libraries to be used in the Library Search are specified. The only libraries that can be selected are libraries that have been loaded and recognized by the ChromaTOF software. These can include user generated libraries as well as commercially available libraries like those available from NIST or Wiley. Only the libraries specified in the DP Method will be used in the Library Search. Figure 26 shows an example where the mainlib and replib from NIST will be used in the Library Search.

Figure 26: An example where the mainlib and replib from NIST will be used in the Library Search.

Figure 27: An example where the Unique Mass is utilized for the area/height calculation.

The last section of the DP Method is where criteria for area/height calculation is specified. The default setting for this field is "U", which specifies that the Unique Mass be used for area/height calculations. Use of the Unique Mass is optimal for ChromaTOF's deconvolution algorithm. It is also possible to use specific masses, the Apexing Masses, or the Total Ion Count. The example shown in Figure 27 utilizes the Unique Mass for the area/height calculation.

Conclusions

This document is intended to provide an introduction to LECO's GCxGC systems. Suggestions and recommendations are intended to help new users familiarize themselves with the technique and how the ChromaTOF software is utilized. Examples in this work are not put forth as suggested methods for customer use. They are examples of how methods are created and how criteria in the method are determined. LECO strongly suggests that users attend the GCxGC training class as soon as possible after installation of their GCxGC instrument.