Comprehensive Two Dimensional Gas Chromatography (GCxGC) and Baseline Correction

CSCE990 Informatics Seminar

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Overview

- Introduction
- Baseline Correction
- Methods
- Future work

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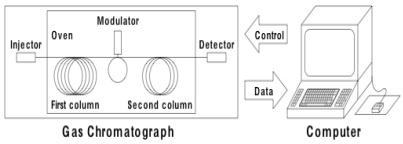
Introduction

Comprehensive two-dimensional gas chromatography separates chemical species with two capillary columns interfaced by a two-stage thermal desorption (Reichenbach et al, 2002)



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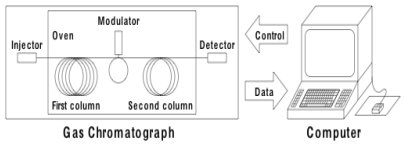
Introduction

- A modulator iteratively traps and collects analytes from first column and then releases (injects) them into the second column.
- Each second column separation is fast (e.g., using a short column) so that it finishes before the injection of the next modulation cycle.
- Modulators use thermal cycles (cold to trap and focus, hot to release) or valves (closed to trap and collect, open to release).



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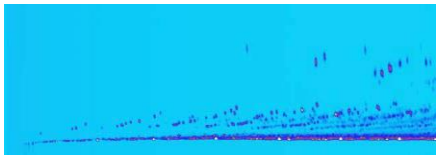
Introduction

GCxGC output image can be displayed in a two dimensional plane. X-axis,(left-to-right) is the elapsed time for the first column separation. Y-axis (bottom-to-top) is the elapsed time for the secondary column separation



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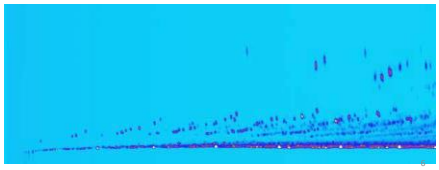
Introduction

Each pixel value indicates the rate at which molecules are detected at a specific time. Each resolved chemical substance in a sample produces a small blob or cluster of pixels with values that are larger than the background values.



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Introduction

The typical data processing sequence for a single chromatogram is:

1. Model and correct for signal baseline
2. Detect peaks
3. Distinguish and quantify peaks
4. Identify compounds
5. Quantify compounds
6. Report information

Analysis of multiple chromatograms may involve sample classification, chemical fingerprinting, sample cluster analysis, sample trend analysis, etc.

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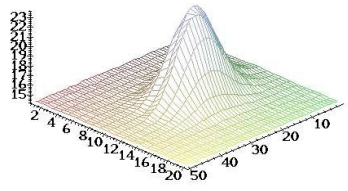
Baseline Correction

In Gas chromatography, the signal peak, induced by constituent compounds in the sample, rise above a base line level in the output.



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Baseline Correction

Baseline Level (under controlled environment):

1. Steady-state standing-current baseline in detector
2. Temperature-induced column-bleed

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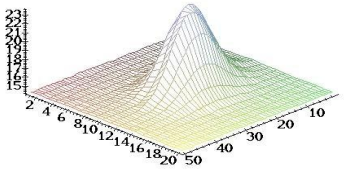
Baseline Correction



Example: In this isolated 3D peak rising to a maximum value of over 23 picoamps. But actual peak value is less than 10 picoamps. That means baseline of that region is more than 14 picoamps.

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Baseline Correction

Under typical controlled conditions, the baseline offset values change relatively slowly over time, forming a slightly curving baseline across the image. The signal and noise fluctuate more rapidly over time and so can be separated from the slowly varying baseline offset.

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Methods

General Approaches:

1. Estimating the baseline around each peak separately.
2. Estimating the baseline across the data comprehensively

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Methods

Comprehensive Baseline Method(Reichenbach et al.) :

1. Identify background region by locating data points with smallest value in second-column chromatogram.
2. The local means of the values from the data are taken as first estimates of baseline, and variance of the values taken as the first estimates of the noise distribution.
3. The signal processing filters are used to reconstruct the baseline as a function of the local estimates.
4. The baseline estimates is subtracted from the signal.

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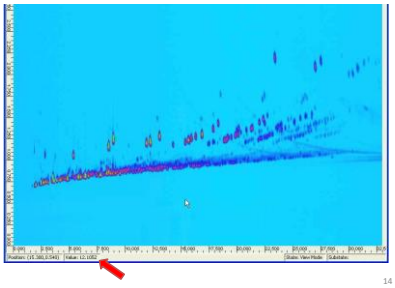
Methods

Before Baseline Correction



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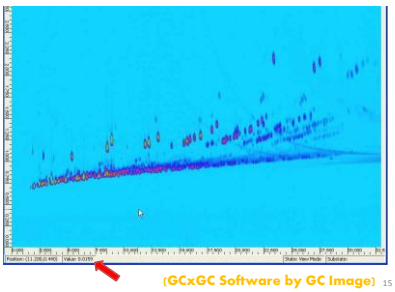
Methods

After Baseline Correction



(GCxGC Software by GC Image)

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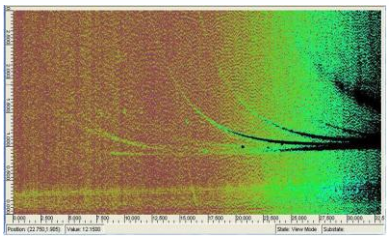
Methods



The image is for a *blank* run (*i.e.*, no sample) and the value range of the color map is set to be very small (13 picoamps to 15 picoamps) in order to highlight the small but clear increase in baseline value with time

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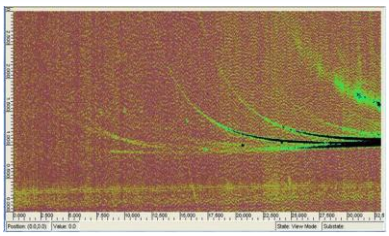
Methods



The same image after **Correct Baseline** (with a value range of -1 to 1). The rise in the baseline level has been removed.

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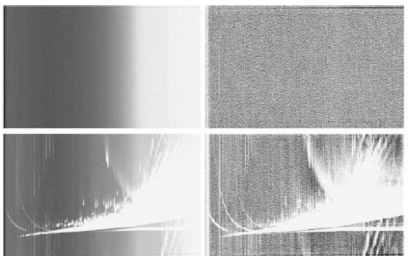
Baseline Correction



Baseline correction for a blank sample (top) and diesel sample (bottom), before baseline correction (left, with a grayscale range of 1.0 picoamp, 14.5 to 15.5) and after baseline correction (right, with a grayscale range of 0.1 picoamp, from −0.5 to 0.5).

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Future Work

- LCxLC has a much different baseline. The rapid second column gradient separation causes rapid changes in the baseline.
- Researchers at VCU are researching a method to correct LCxLC baseline by inferring the spectral characteristics of the baseline across a blank image (i.e., no analytes) then using distinct spectral characteristics to infer the baseline level in the LCxLC data. They uses a linear technique, but the method seems to require 3 components, which suggests the possibility of non-linear characteristics.

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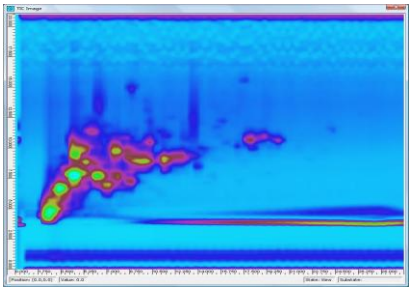
Future Work



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References

- S. Reichenbach. "Data acquisition, visualization, and analysis." In *Comprehensive Two Dimensional Gas Chromatography*, Ed. L. Ramos, pp. 77-106, Elsevier, 2009
- S. Reichenbach, M. Ni, D. Zhang, and E. Ledford. "Image Background Removal in Comprehensive Two-Dimensional Gas Chromatography." *International Symposium on Capillary Chromatography*, CDROM, 11p, 2002.
- S. Reichenbach. "Informatics for Comprehensive Multidimensional Chromatography"

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Thank You

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