Multi-type Smart Templates™ with Peak Sets, Areas, and Meshes for Comprehensive Two-Dimensional Gas Chromatography (GCxGC)

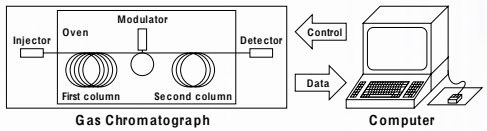
Stephen E. Reichenbach,[1] Daniel E. Hutchinson, [2] Qingping Tao,[2] Edward B. Ledford, Jr.,[3] Stella B. Cabanban,[4] Hung A. Pham,[4] Wayne E. Rathbun,[4] Haiyan Wang[4]
[1]University of Nebraska – Lincoln; [2]GC Image, LLC; [3]Zoex Corporation; [4]UOP LLC, a Honeywell company

Challenge

Automated comprehensive analysis.

Methods

Multi-type Smart Templates™ with peak sets, areas, and meshes for comprehensive two-dimensional gas chromatography (GCxGC).



GCxGC

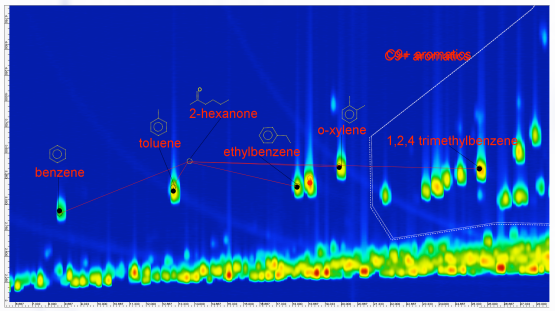
Comprehensive two-dimensional gas chromatography (GCxGC) cycles a thermal modulator (from Zoex Corporation) to progressively trap analytes from the first column and then release them into the second column. The fast separation in the second column completes during each modulation cycle. The detector operates at high speed to generate multiple data points across each peak in each modulation cycle. The sequential data from the detector is re-ordered as a two-dimensional array in which each successive second-column separation is presented as a bottom-to-top column of data points in the two-dimensional array.

Multi-type Smart Templates

Templates describe the 2D retention-time pattern of expected peaks. The template pattern is matched to the pattern of detected peaks to identify analytes.

Multi-type Templates include objects such as geometric shapes, text labels, and chemical structure diagrams. Shapes, such as polygons and meshes, are useful to define peak sets and regions.

Smart Templates utilize rules pertaining to the retention-times, computed statistics, and mass spectra in order to better match peaks and automate analysis.



Template Matching

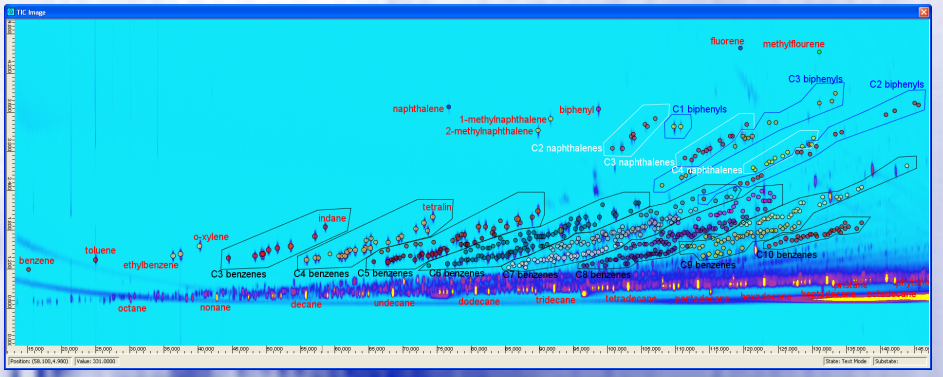
This example illustrates a 2D chromatogram from a diesel sample. The overlay shows the matching between a template created from the retention-time pattern of peaks observed in a gasoline sample (shown with open circles) to peaks detected in the diesel sample (indicated by filled circles). The matching is imperfect (i.e., the open and filled circles are not perfectly aligned), because different columns were used, but the matching is sufficient to accurately identify analyte peaks.

Graphical Elements

Graphical elements in the template are copied into the analyzed image, including polygons and other shapes, text labels, and chemical structure symbols.

The graphical elements have color specifications that can be used to visually highlight different attributes of peaks. In this example, the peak for 2-hexanone (which was an internal standard in the gasoline sample, but is not present in the diesel sample) is indicated with a white circle and the peaks for compounds calibrated to 2-hexanone are indicated with black circles and lines indicating the referenced internal standard.

Graphical elements are geometrically transformed in the retention-time plane to account for the transformation of the template peak pattern to fit the pattern of detected peaks in the analyzed sample.



Rules for Smart Peak Recognition

Some peaks may be surrounded by other peaks making correct identification more difficult. Rules written with CLIC™ can constrain peak pattern matching to ensure correct identifications. For example, the n-paraffins are detected amidst many other peaks, but have a larger response. A rule requiring a threshold response percent for each n-paraffin peak can be used to ensure correct identifications during peak pattern matching. For GCxGC-MS data, rules pertaining to the mass spectra can ensure correct identification. For example, a threshold match factor for NIST MS Search could be required for identification.

Peaks and Peak Sets

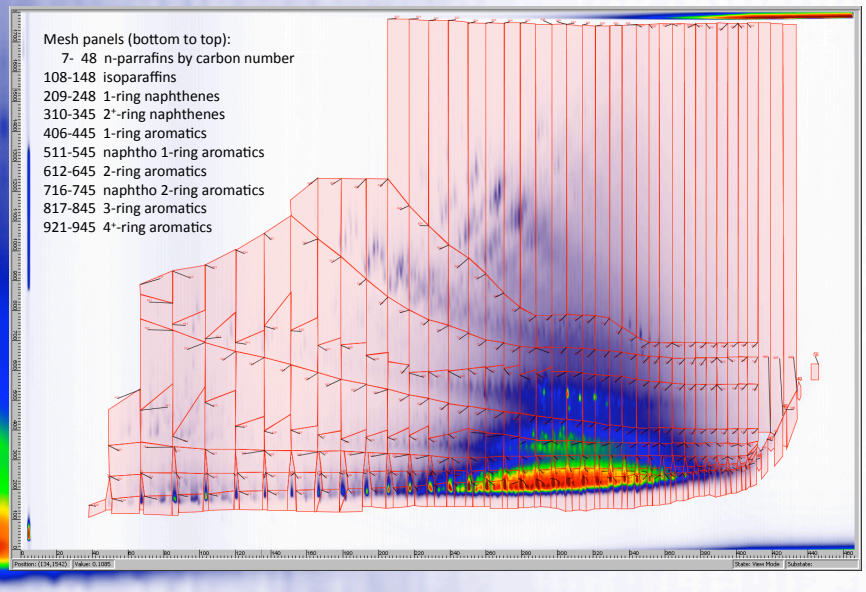
Peaks that can be reliably detected and identified can be quantified and reported individually and can be specifically identified as members of peak sets to be reported in aggregate. For example, two methyl naphthalene peaks are reliably detected and can be reported in aggregate as the C1 naphthalenes peak set. Detection of individual peaks for larger molecules becomes more difficult. Polygons and other shapes can be used to select peaks for aggregation. For example, a polygon can be drawn to delineate the C2 naphthalenes for aggregated reporting.

Smart Peak Sets

Some groups of peaks overlap, so simple shapes, such as polygons, may not be able to separate peak sets. CLIC rules can be associated with shapes to distinguish peaks. For example, the C4 naphthalenes and C2 biphenyl groups overlap, but can be distinguished by mass spectral rules.

Areas

Even GCxGC may yield some chromatographic regions with unresolved chemical mixture (UCM). If peak detection is unreliable, polygonal regions can be integrated and reported as areas, aggregating total response within the region.



Meshes

Meshes provide a complete tiling of chromatographic regions without gaps or overlaps. Mesh panels (the individual polygonal regions within a mesh) can be used to define peak sets (for peak aggregation), smart peak sets (with rule-based peak aggregation), or areas (to report total response within the region). Meshes are powerful structures for automated, comprehensive reporting.

University of Nebraska Lincoln

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Software for Multidimensional Chromotography

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