全二维气相色谱在石油生物标志物定量中的应用

许强[1]，鲁杰[1]，Alan G. Marshall[1,2]，Mark Merrick[3]，Joseph Binkley[3]，Michael Mason[3]
廖玉宏[4]，潘银华[4]
1. 新能源研究所，佛罗里达州立大学，塔拉哈西，FL 32310
2. 化学与生物化学系，佛罗里达州立大学，塔拉哈西，FL32306
3. 美国力可（LECO）公司，St. Joseph，MI
4. 有机地球化学国家重点实验室，中科院广州地球化学研究所 广州 510640

化石燃料来源于古老的活体有机质的深度埋藏。在沉积盆地形成和演化的地质历史过程中，一些有机分子在经受了物理化学作用改造后仍能保留原有的碳骨架结构。我们称这些分子为生物标志化合物，并常常将它们与石油和煤的成因和沉积环境联系起来。生物标志化合物中的甾烷和藿烷已经普遍被用于获取诸如母源、形成年代、成熟度和生物降解程度等地球化学信息。

甾烷和藿烷传统上使用气相色谱-质谱（GC-MS）或气相色谱-双质谱联用（GC-MS-MS）在离子碎片特征峰m/z 191和m/z 217上进行分析，以区分干扰定量测量的重叠部分[1,2]。生物标志化合物的相对丰度则利用色谱峰的强度进行评估，这类似于“半定量”。对应定量而言，气相色谱与火焰离子检测器（FID）联用是一种更为可取的方法，它能够提供所有碳氢化合物种类及其异构体一致的响应。

全二维气相色谱（GC×GC）与火焰离子检测器（FID）联用作为一种新型的分析方法[3]，不仅能够在分离上解决甾烷和藿烷在色谱上重叠的问题，而且提供了更加精确的定量数据，从而获得更可靠的生物标志化合物分布的信息。在本报告中，我们将会具体地展示全二维气相色谱（GC×GC ）火焰离子检测器（FID）联用与气相色谱-质谱（GC-MS）的半定量结果的对比优势。

References:

1. "GC/MS in the Petroleum Industry", C. S. Hsu and D. Drinkwater in "Current Practice in GC/MS (Chromatogr. Sci. Series, Vol. 86)", Chapter 3, W. W. A. Niessen, ed. New York: Dekker Marcel, 2001; pp. 55-94.

2. "Biomarker Analysis for Petroleum Exploration", C. S. Hsu, C. C. Walters, G. H. Isaksen, M. E. Schaps and K. E. Peters in "Analytical Advances for Hydrocarbon Research", Chapter 9, New York: Kluwer Academic/Plenum Publishers, 2003; 223-245.

3. "Chromatographic Analysis of Fuels", F. P. Di Sanzo in "Analytical Advances for Hydrocarbon Research", Chapter 9, New York: Kluwer Academic/Plenum Publishers, 2003; 113-146.

(English Translation)

Comprehensive Two-dimensional GC (GCxGC) for Quantitation of Petroleum Biomarkers

Chang S. Hsu[1], Jay Lu[1], Alan G. Marshall[1,2], Mark Merrick[3], Joseph Binkley[3] and Michael Mason[3], Yuhong Liao[4], Yinghua Pan[4]

1. Future Fuels Institute, Florida State University, Tallahassee, FL 32310
2. Dept. of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306
3. LECO Corporation, St. Joseph, MI
4. Guangzhou Institute of Geochemistry, Chinese Academy of Sciences

Fossil fuels are derived from deeply buried ancient living organisms. Some of the molecules in these organisms retain their basic carbon skeletons after physicochemical transformation during the geological history of sedimentary basin. These molecules, know as biomarkers, are used to relate the origin and depositional environment of petroleum and coals. Among the biomarkers, 4-ring steranes and 5-ring hopanes have been commonly used for obtaining geochemical information, such as source, age, maturity and biodegradation.

Hopanes and steranes are traditionally analyzed by GC-MS or GC-MS-MS from their characteristic fragment ions of m/z 191 and 217 to resolve from overlapping components that interfere quantitative measurement.[1,2] The relative abundances of these biomarkers are estimated from the peak intensities as "semiquantitation". A more desirable method for quantitation is to use GC flame ionization detector (FID) that is known to provide uniform response across all hydrocarbon classes and isomers.

A new analytical method, comprehensive two-dimensional GC (GCxGC), [3] resolves overlapping components from steranes and hopanes, providing much more accurate quantitation data, thus, more reliable information on biomarker distributions. This improvement can be important for integrated basin assessment utilizing biomarkers. In this presentation, we will demonstrate the use of GCxGC FID and its comparison with the GC-MS semi-quantitation results.

Proc. The 13th National Meeting on Geochemistry in China, Nanning, China. October 31-November 3, **2011**, p. 780.