

**XV REUNIÓN CIENTÍFICA  
SOCIEDAD ESPAÑOLA DE CROMATOGRAFÍA  
Y TÉCNICAS AFINES · SECyTA 2015**

*XV SCIENTIFIC MEETING  
OF THE SPANISH SOCIETY OF CHROMATOGRAPHY  
AND RELATED TECHNIQUES · SECyTA2015*

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**ESTIMATION OF COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHIC RESPONSE FROM ONE-DIMENSIONAL GAS CHROMATOGRAPHY DATA**

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Optimization of a separation in comprehensive two-dimensional gas chromatography (GC×GC) requires the selection of an appropriate set column, and the optimisation of their respective dimensions, temperature programs and flow rates. Until not so long ago, a time consuming trial and error process was the only way to select the columns and chromatographic conditions for the two GC dimensions. During the last few years, several attempts have been proposed to estimate the chromatographic response in GC×GC [1-4]. Although most of these methods are helpful contributions, some of them focussed exclusively on the retention time estimation and do not consider the effect of peak width, also essential for a correct prediction of the chromatographic separation capability. Others are based on theoretical formulas not applicable to the extreme experimental conditions used in GC×GC, or are only valid for specific types of compounds or stationary phases: these models cannot be corrected for different separation problems.

In this work, modelization of retention time and peak width has been carried out from experimental 1D GC data in order to estimate the response in GC×GC separation for different column sets operated under different flows and temperatures.

Several theoretical and experimental models are proposed for estimation of <sup>1</sup>D and <sup>2</sup>D retention time and peak width; in experimental models, 1D GC data are required together with information on column characteristics and operation conditions. Models for hold-up time, retention factor and peak width were first validated in 1D GC from the fit between experimental and calculated data. Their validation in GC×GC was carried out by using *n*-alkanes and a mixture of disaccharides as their trimethylsilyl oxime derivatives. Comparison of experimental and estimated data showed good results for retention time in both first and second dimension. Peak widths presented, however, some errors, caused by the no consideration on estimation of the effect of the modulator or the rather unusual chromatographic conditions used.

The developed programme is very versatile as it can be used for the calculation of the chromatographic response of compounds with different polarity and volatility, analysed under different pressures and temperature ramps, and with different sets of columns.

[1] J.V. Seeley, E.M. Libby, K.A.H. Edwards, S.K. Seeley, *J. Chromatogr. A* **1216** (2009) 1650.

[2] F.L. Dorman, P.D. Schettler, L.A. Vogt, J.W. Cochran, *J. Chromatogr. A* **1186** (2008) 196.

[3] Y. Zhao, J. Zhang, B. Wang, S.H. Kim, A. Fang, B. Bogdanov, Z. Zhou, C. McClain, X. Zhang, *J. Chromatogr. A* **1218** (2011) 2577.

[4] S. Zhu, S. He, D.R. Worton, A.H. Goldstein, *J. Chromatogr. A* **1233** (2012) 147.

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