

Accepted Manuscript

Title: Modelling of retention in analytical supercritical fluid chromatography for CO₂ - methanol mobile phase

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PII: S0021-9673(13)00994-1

DOI: <http://dx.doi.org/doi:10.1016/j.chroma.2013.06.069>

Reference: CHROMA 354468

To appear in: *Journal of Chromatography A*

Received date: 29-5-2013

Revised date: 26-6-2013

Accepted date: 27-6-2013

Please cite this article as: M. Leško, D.P. Poe, K. Kaczmarek, Modelling of retention in analytical supercritical fluid chromatography for CO₂ - methanol mobile phase, *Journal of Chromatography A* (2013), <http://dx.doi.org/10.1016/j.chroma.2013.06.069>

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1 **Modelling of retention in analytical supercritical fluid chromatography for** 2 **CO₂ - methanol mobile phase**

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8 **Abstract**

9 Mathematical modelling of the chromatography process requires knowledge of the
10 isotherm model. Therefore a necessary step in calculations is estimation of the isotherm
11 model parameters. In this study the inverse method has been successfully used to estimate the
12 linear isotherm model parameters in supercritical fluid chromatography (SFC). Estimation
13 was based on measured retention times of experimental band profiles. The solute was
14 n-octadecylbenzene. The mobile phase was carbon dioxide-methanol, 95/5% v/v, and the
15 column was 250 mm x 4.6 mm i.d. packed with 5 – micron Luna C18(2) particles. The
16 experiments were done for outlet pressures from 100 bar to 150 bar at different flow rates and
17 different sets of experimental conditions: (1) column operated under convective air (CA); (2)
18 column operated in still air conditions. Moreover in the latter thermal mode were considered
19 two cases. In the first case the temperature of the oven air was different from the inlet
20 temperature of the mobile phase. In the second case the temperature of the oven air was the
21 same as inlet temperature of the mobile phase. The column efficiency was also analysed.

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23
24 Key words: Supercritical fluid chromatography; Inverse method; Isotherm model;
25 Heat balance; Mass balance, Column efficiency

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