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Updating chromatographic predictions by accounting ageing for single and tandem columns

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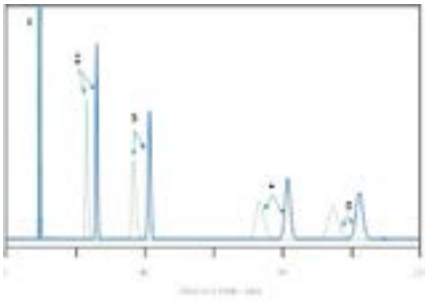
Model-based chromatographic optimizations provide the best separation conditions efficiently. Unfortunately, with the routine usage, columns inevitably suffer some deterioration and, as a result, actual chromatograms may differ from the forecasted expectancies; new optimal separation conditions are then needed, but unfortunately, models are not valid anymore. The chromatographer could then decide repeating the whole modelling process, but this solution is undesirable and too time consuming, particularly when several coupled columns are involved. We propose a shortcut to correct time and peak profile predictions. The original models are corrected by introducing parameters accounting the deterioration, obtained using a small subset of compounds, selected from those studied in the training set before the column had suffered performance decline. The ageing parameters are not solute dependent. These are fitted in such a way that they minimize the discrepancies between the data predicted with the original retention models for the brand-new column and the experimental data measured for the aged column. The approach was developed and tested to predict the chromatographic behaviour of 15 sulphonamides, analysed with individual and tandem columns, using isocratic and gradient elution. From the gathered information, predictions more in line with the deteriorated performance were forecasted for the whole family of compounds analysed with that column (or set of coupled columns). The results suggest that, whenever the columns keep sufficient performance, we can take advantage of the extensive experimental work carried out when the system was initially modelled with the brand-new columns. With this information and a minimal extra experimental effort, accurate enough predictions in the degraded situation are possible. The full modelling of the chromatographic behaviour is thus only made with the brand-new columns. The agreement between predicted and experimental chromatograms in the aged columns was excellent.



Recent Publications

1. Ortiz-Bolsico C, Torres-Lapasió JR, Ruiz-Angel MJ and García-Alvarez-Coque MC (2013) Comparison of two serially-coupled column systems and optimization software in liquid chromatography for resolving complex mixtures. Journal of Chromatography A 1281:94-105.
2. Alvarez-Segura T, Torres-Lapasió JR, Ortiz-Bolsico C and García-Alvarez-Coque MC (2016) Stationary phase modulation in liquid chromatography through the serial coupling of columns. Analytical Chimica Acta 923:1-23.
3. Ortiz-Bolsico C, Torres-Lapasió JR and García-Alvarez-Coque MC (2013) Simultaneous optimization of mobile phase composition, column nature and length to analyse complex samples using serially coupled columns. Journal of Chromatography A 1314:39-48.
4. Ortiz-Bolsico C, Torres-Lapasió JR and García-Alvarez-Coque MC (2014) Optimization of gradient elution with serially-coupled columns: Part I: Single linear gradients. Journal of Chromatography A 1350:51-60.

5. Ortiz-Bolsico C, Torres-Lapasió JR and García-Alvarez-Coque MC (2014) Optimization of gradient elution with serially-coupled columns: Part II: Multi-linear gradients. Journal of Chromatography A 1373:51-60.

Biography

Tamara Alvarez-Segura completed her Master degree in Experimental Techniques in Chemistry in 2014, at the University of Valencia. She is now performing diverse research activities in the Department of Analytical Chemistry to get her PhD degree. She has received two Pre-doctoral fellowships. During her Master studies, she began her collaboration with María Celia García-Alvarez-Coque and José Ramón Torres-Lapasió in the field of the modulation of the selectivity in HPLC, using serially coupled columns and other strategies to analyse complex samples. She has written 11 research articles and presented several communications in international meetings. The PhD period included a three-month stay (September to November 2017) in the Analytical Chemistry Department at the University of Barcelona (Spain), under the supervision of Prof Martí Rosés, working in the field of Hydrophilic Interaction Liquid Chromatography (HILIC).

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