

COMPETITIVE ADSORPTION OF SAMPLE SOLVENT AND ANALYTE IN SUPERCRITICAL FLUID CHROMATOGRAPHY

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Abstract

Supercritical fluid chromatography (SFC) has gained increased attention in the fields of theoretical research, purification processes and separation sciences over the last few years due to the latest technological advancements. The method is well-known for being capable of faster separations and reduced solvent consumption compared to liquid chromatography (LC) while also achieving high efficiency. Due to the nature of carbon-dioxide serving as mobile phase, eluent strength is well-tunable by adjusting temperature, pressure and the amount of organic modifier. However, SFC is considered a complementary technique besides liquid and gas chromatography since there is always a trade-off in terms of the advantages [1].

Recently, Gritti experienced an anomaly in the retention behaviour of alkylbenzenes using a heavily modified Waters ACQUITY UPC² System [2]. These small molecules are ideal for studying the processes taking place in the chromatographic column. Therefore, the aim of this work is to study the retention of several *n*-alkylbenzenes on an alkylamide stationary phase using a standard UPC² System and assessing the effect of different sample solvents on chromatographic efficiency. The results show that even a small amount of methanol overloads the column and a competitive adsorption takes place between the analytes and the sample solvent. This is indicated by the changes in column efficiency, retention factors and peak widths. The selected experimental conditions guarantee that the density of the mobile phase does not change significantly along the column, so the phenomenon can be modeled as in LC. The concentration of the analytes is negligible compared to the amount of methanol – but their adsorption is influenced by the solvent – while the adsorption of methanol remains unaffected by the alkylbenzenes. The competition was described by determining the single-component adsorption isotherms for both the analytes and the solvent then competitive isotherms were calculated. The solvent effect was modeled by a numerical method created in-house where the differential mass balance equation was integrated using the Rouchon algorithm. The experimental observations were confirmed by *in silico* experiments and further cases involving hypothetical analytes were studied as well.

References

- [1] Tarafder, A.: *Trends Anal. Chem.* **81** (2016) 3-10.
- [2] Gritti, F.: *J. Chromatogr. A* **1468** (2016) 209-216