Retention time correction in gas chromatography by modelling concentration related effects

Highly reproducible retention times ($t_R$) are a basic requirement for automation of peak assignment in complex gas chromatograms. Drifting retention times are handled best by frequent updates, based on reference peaks, even for every chromatogram, if a sufficient number of reference peaks is always present. The updates may be interpolated for peaks between the reference peaks. Some refinements of this concept have been reported as well as alternative concepts, including pattern recognition algorithms to achieve ultimate precision. However, there are applications causing additional challenges requiring special measures. One is the effect of concentration on $t_R$ of individual peaks, becoming relevant, where - in addition to high complexity and variability in composition - a wide concentration range has to be covered. The analysis of fatty acid methyl esters (FAME) is such an application. A model describing concentration related effects on $t_R$ was drawn up and found to work best for this purpose. The precision of peak alignment could be improved by more than an order of magnitude, allowing reliable automation of routine analysis.

Biography

Rudolf Kapeller received his DPhil in Chemistry from the University of Innsbruck. He worked as Analytical Chemist at the Bundesstaatliche bakt.-serol. Untersuchungsanstalt and since 8/1985 at the Austrian Agency for Health and Food Safety – Institute for Food Safety in Linz; from 5/1996 to 12/2015 as Head of the Institute. He has been the author of various publications in the field of analytical chemistry and food safety. His research interests include Analytical Chemistry in the field of Food Safety, Chemometrics, Statistics, Method Validation and Automation.

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