Abstract

Quantification of major components by gas chromatography with flame-ionization detector (GC-FID) is established in routine laboratory practice. The FID detector is considered as universal detector for gas chromatography (GC), but it does not provide a response for a wide range of compounds and GC-FID analysis provides only quantitative data. The coupling of gas chromatography with mass spectrometry is a powerful analytical tool that provides not only quantitative data but also qualitative data on the structure of substances. When quantified by GC-MS, the detector oversaturation is a problem as it is a highly sensitive detector (at ppb level). One way to avoid oversaturation of the detector is to significantly dilute the solutions, which causes a decrease in the sensitivity of the method. Another approach to bypass detector saturation is to interrupt detection during solvent elution. For quantification of the major components of solutions, only the first method of bypassing detector saturation can be applied, but it is a labor-intensive process that increases the measurement uncertainty. The interruption of detection during solvent elution is not applicable for the purpose of quantifying major components, so a new approach of quantifying major components of solutions using M+1 ions was proposed and subsequently validated. These ions are provided by the heavy nuclides of common elements, especially carbon ^{13}C, whose natural abundance is around 1,07 %. Quantification of these ions will lead to a significant reduction in the signal of the main components, thus circumventing the problem of detector saturation. To evaluate the quantitative GC-FID and GC-MS analysis, an external standard method was used, where the major components content of the solutions was calculated from the regression equation of the calibration curve. Furthermore, a quantification method was proposed using a modified dependence of the ratio of the peak areas of the components to the weight fraction of each component. Eight pairs of commonly used solvents were selected for the preparation of major constituent calibration solutions and comparison of the metrological properties of GC-MS with GC-FID, and the ethanol abundance in 17 alcoholic beverages was determined for the application of the newly developed method in practice.