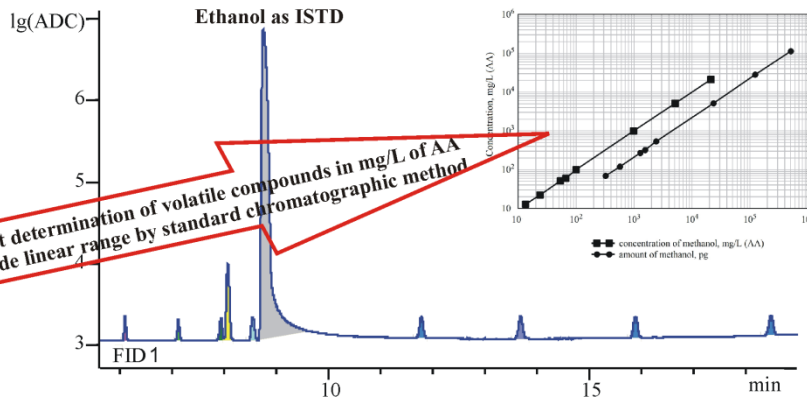




ETHANOL AS INTERNAL STANDARD FOR QUANTITATIVE DETERMINATION OF VOLATILE COMPOUNDS IN SPIRIT DRINKS

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Theoretical background

The IS method is applied, where the GC calibration includes measuring of relative detector response factors RRF_i for every analyzed compound relative to IS. RRF_i are calculated from the chromatographic data for standard solutions with known concentrations of analyzed compounds and IS. They may be expressed by the following equation:

$$RRF_i = R_{F_i} / R_{F_{IS}} = \frac{C_i^{st}(sol) / C_{IS}^{st}(sol)}{A_i^{st} / A_{IS}^{st}} = \frac{A_{IS}^{st} \cdot C_i^{st}(sol)}{A_i^{st} \cdot C_{IS}^{st}(sol)}$$

where $R_{F_{IS}}$ is the detector response of the internal standard component A_{IS}^{st} and A_{Et}^{st} are the peak areas of the i -th compounds and IS, respectively, for a standard solution. $C_i^{st}(sol)$ and $C_{IS}^{st}(sol)$ are the concentrations of the i -th compound and IS, respectively, expressed in mg/l

$$\text{In the case of ethanol-IS} \quad RRF_i = \frac{A_{IS}^{st} / C_{Et}^{st}}{A_i^{st} / C_i^{st}} = \frac{A_{IS}^{st} \cdot C_i^{st}}{A_i^{st} \cdot \rho_{Et}}$$

where A_{Et}^{st} and A_i^{st} are the peak areas of ethanol in the standard solution and the analyzed sample, respectively. C_i^{st} and C_{IS} are the concentrations of the i -th compound and IS, expressed in mg/L (AA). $\rho_{Et} = 789300$ mg/L is the known density of ethanol.

Then the concentration C_i of the i -th sample compound relative to absolute alcohol has the form:

$$C_i = RRF_i \cdot \frac{A_i}{A_{Et}} \cdot \rho_{Et}$$

$$\text{Finally:} \quad C_i = RRF_i \cdot \frac{A_i}{A_{Et}} \cdot \rho_{Et} = C_i^{st} \cdot \frac{A_{Et}^{st}}{A_i^{st}} \cdot \frac{A_i}{A_{Et}}$$

$$C_i = \frac{\sum_{l=1}^N \sum_{j=1}^M (S_{ij}^{st} / S_{Etij}^{st}) \cdot C_{ij}^{st}}{M \cdot \sum_{l=1}^N \sum_{j=1}^M (S_{ij}^{st} / S_{Etij}^{st})^2} \cdot \frac{A_i}{A_{Et}}$$

where C_{ij}^{st} are the concentrations of the i -th compound of the l -th level of the calibration compound, respectively; S_{ij}^{st} and S_{Etij}^{st} are the areas of the i -th compound and ethanol of l -th level of the calibration compound, respectively. N is the number of calibration compounds. M is the number of measurements of each calibration compound.

Main idea

The concentration C_i of the i -th component in the sample is directly expressed in mg/L (AA).

Additional **measurements of the volume content of ethanol** in the sample **are not required**.

The procedure of the **IS introduction** into the analyzed sample **is not needed**, since ethanol is the main component of the sample and is already contained in it.

Substantial simplification of the whole measurement procedure as well as **improves the reliability** of obtained data.

Proposition

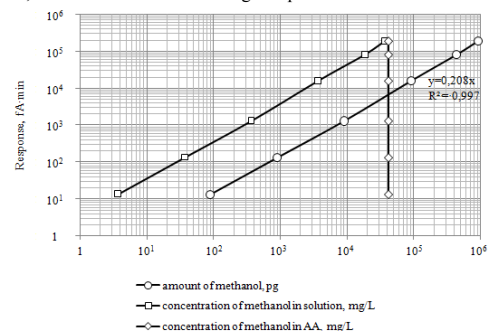
➤ **History of alcohol production** has period for thousands of years and seemingly here all the methods of its quality control are well-known and one can not offer anything new. Thousands of testing laboratories all over the world carry out gas chromatographic (GC) analysis of volatile compounds in spirit drinks day-and-night. Acetaldehyde, methyl acetate, ethyl acetate, methanol, 2-propanol, 1-propanol, isobutyl alcohol, n-butanol and isoamyl alcohol are the main volatile compounds that should be determined in spirit drinks according to the standards and regulations. Concentrations of these compounds expressed in milligrams per litre of absolute alcohol are traditionally calculated using the internal standard (IS) method or external standard (ES) method.

➤ **We propose the new methodical approach** of using ethanol as internal standard in GC analysis of volatile compounds in spirit drinks in daily practice of analytical and testing laboratories.

➤ **We propose a significant simplification of the analysis**. Namely, since ethanol is the main component in the alcohol products, we regard it as IS without introducing of any additional substances in the sample.

Experimental results

The standard ethanol-water (96:4) solution of volatile compounds: acetaldehyde, methyl acetate, ethyl acetate, methanol, 2-propanol, 1-propanol, isobutyl alcohol, n-butanol, isoamyl alcohol was analyzed after dilution with water in the ratios 1:1, 1:9, 1:99, 1:999, and 1:9999 for the following components:



The first line is the detector response versus the amount of the compound. The second and the third ones are the detector response versus the concentration of the compound, expressed in mg per litre of solution and in mg per litre of absolute alcohol. A corresponding linear dependence is added. Even after dilution with water in the ratio 1:999, the difference between the measured concentrations of all compounds and their values calculated using the gravimetric method does not exceed 7.7%. With the dilution 1:9999 there are peaks of methanol and ethanol only. Other compounds significantly are less than level of detection. But the relative discrepancy of measured concentrations of methanol does not exceed 6.6%. The rest of the components have similar graphs.