Application Note AN-D-001

Metrohm IC Driver for OpenLab CDS

OpenLab controlled dual channel cation and anion analysis with automated Inline Eluent Production

OpenLab CDS is the newest generation of Agilent's chromatography data systems, combining chromatography and mass spectrometry in a single software platform.

The release of the Metrohm IC Driver 1.0 for OpenLab enables the full integration of Metrohm IC instruments in OpenLab CDS. The integration provides a single software solution for IC-MS hyphenation. OpenLab-based laboratories profit by saving time and costs for user trainings, validation, and software without any loss of the robustness and flexibility for which Metrohm is well-known.

This application focuses on the simultaneous analysis of cations and suppressed anions with a dual channel Metrohm IC operated by OpenLab CDS. The implemented automated Inline Eluent Production enables continuous operation without manual intervention, improving retention time stability. A soft drink was chosen as the example matrix in which to measure cations and anions, since these are important parameters for food safety and quality analyses. A long-term stability test confirms the expectations about repeatability, robustness, and quality for Metrohm devices.

EXPERIMENTAL

To guarantee food safety and quality, the determination of major cations and anions is of special interest for the beverage industry. The task for the present study was the analysis of major cations and anions in a soft drink within one determination by an ion chromatography system, operated with Agilent OpenLab CDS.

Major cations and anions are analyzed with a dual channel IC setup (Figure 1) based on a 4-point calibration in the mg/L range. To assure appropriate analyses, the sample is diluted in ultrapure water and mixed with ethanol to guarantee sample stability.

The complete Metrohm IC configuration is controlled by OpenLab CDS (Figure 1). The acquisition method contains component-specific control parameters and time settings for the configured instrument setup:

- IC start parameters: e.g., recording time, flow rate, column temperature, etc.
- IC time program: e.g., injection and data analysis
- Sample processor start parameters: e.g., peristaltic pump speed
- Sample processor time program: e.g., sample preparation or transfer

Special «Event wait» commands allow synchronization and timing. In addition to the common chromatographic control parameters, automatic eluent production is included in the method. With a 941 Eluent Production Module, eluents are automatically prepared from an eluent concentrate – either commercially available (e.g., Merck) or self-prepared – allowing maximum analysis flexibility. The eluent production is triggered by sensors. In OpenLab CDS, up to four sensors can be controlled in parallel with this module, either with empty- or full-mode monitoring, depending on the purpose. Thus, the module can not only be used for eluent production, but also for monitoring the water supply, concentrate, or waste levels.

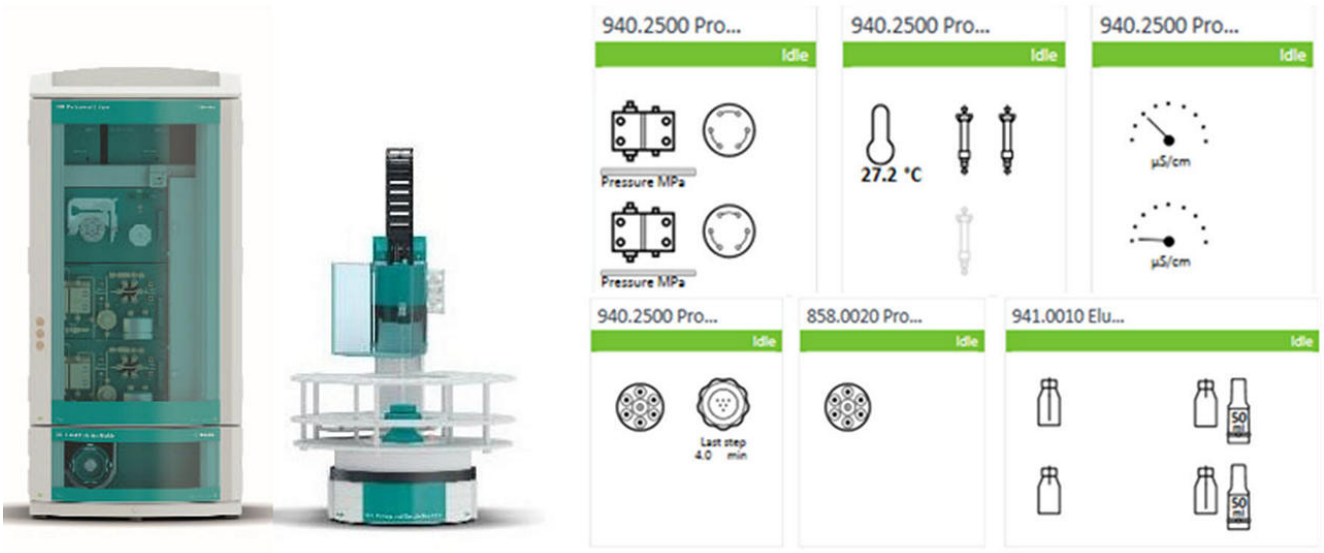

Figure 1. (L) Setup for cation and suppressed anion analysis with a Metrohm 940 dual channel IC (940 Professional IC Vario TWO) and Inline Eluent Production with a 941 Eluent Production Module and (R) configuration in OpenLab.

RESULTS

Multiple injections of the standards (cation standards shown in Figure 2) and sample (Table 1) showed only small variations in the peak areas. RSDs ranging from 0.1–1.1% prove the proper repeatability and robustness are achieved from the dual channel system.

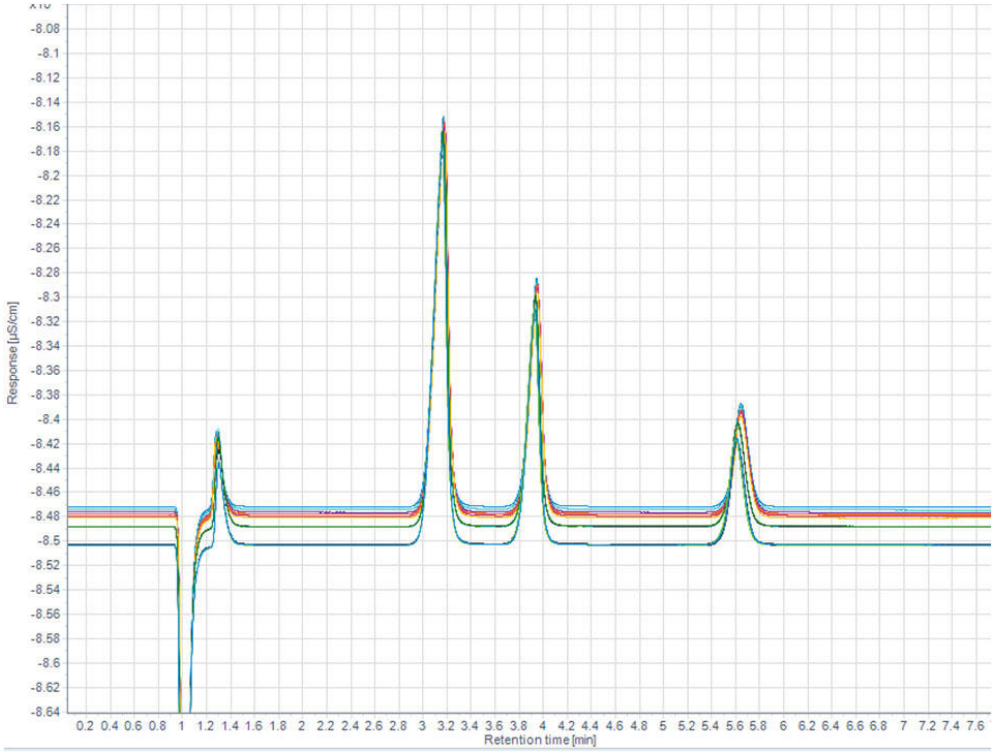

Figure 2. Repeat analyses (n = 100) of a mixed cation standard (lithium 10 mg/L, sodium and potassium 20 mg/L).

Data quantification is based on linear regression of the peak areas (Figure 3). As major components of the soft drink, K^+, Ca^{2+}, PO_4^{3-}, Cl^-, Mg^{2+}, and NO_3^- are found following a decreasing concentration order (Table 1). These concentrations meet the FDA recommendations for bottled soft drinks (21CFR165.110). As expected, the concentrations for other anions fall well below the critical levels cited by the FDA of 1.4–2.4 mg/L F^- (depending on air temperature), 10 mg/L NO_3^- (as N), and 250 mg/L SO_4^{2-}.

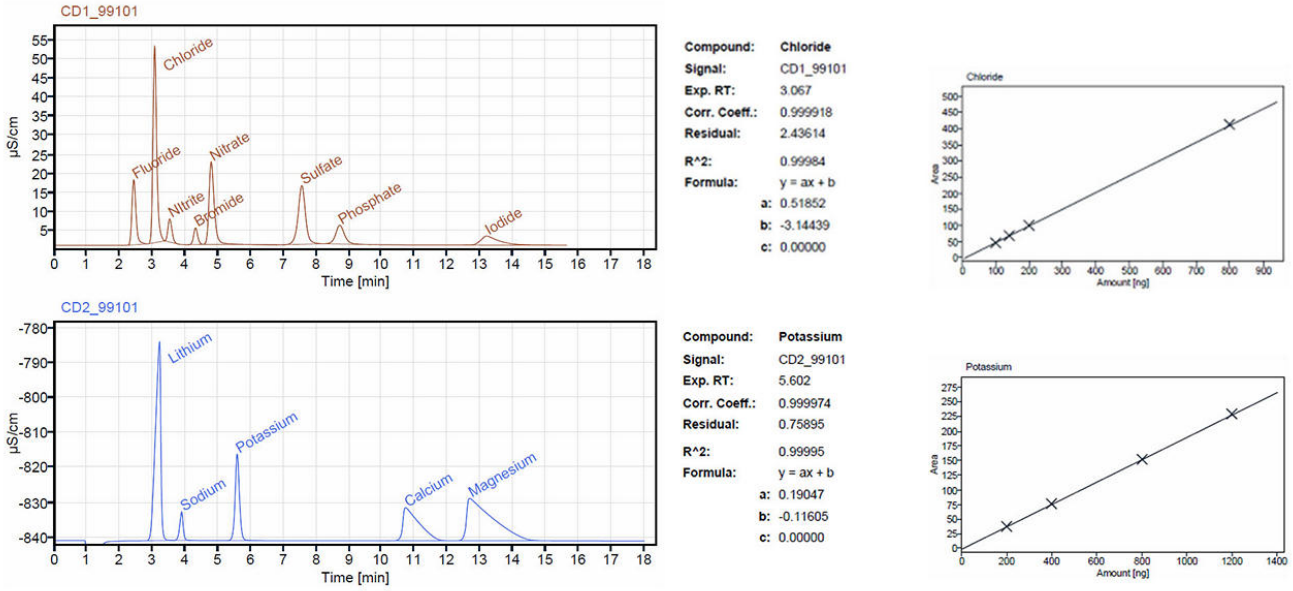

Figure 3. (L) Chromatograms for mixed standards for anions (red) and cations (blue) analyzed with a dual channel IC (940 Professional IC Vario TWO) operated by OpenLab CDS and (R) example calibration curves for chloride and potassium based on the evaluation of the peak areas. The chromatograms show anion and cation conductivity tracks determined with a Metrosep A Supp 17-150/4.0 and a Metrosep C4-150/4.0 column, respectively. The calibration curves show response data for the peak areas versus the concentration amounts in ng. Considering the injection volume (here, 20 µL), the concentrations can be converted into mg/L units.

Table 1. Repeatability of double injections for selected cations and anions in the soft drink sample. The concentrations are determined as amounts in ng and are converted into mg/L units through dividing by the injection volume (20 µL) and multiplication with the dilution factor (3).

Analyte	Conc. amount (ng)	Conc. (mg/L)	RSD (%)
K^+	905	135.8	0.1
Ca^{2+}	172	25.8	0.1
PO_4^{3-}	145	21.8	0.1
Cl^-	99	14.9	0.8
Mg^{2+}	81	12.2	0.2
NO_3^-	59	8.9	1.1

CONCLUSION

The Metrohm Driver 1.0 for OpenLab CDS opens the path for IC analyses performed for a variety of applications across different sectors (e.g., food industry, water and environmental monitoring). The implementation of features beyond the usual IC functionalities such as automation, sample preparation, and suppression, massively improve the ion analytics in OpenLab.

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