Chromeleon CDS Workflow for Determination of Inorganic Anions in Drinking Water According to U.S. EPA Method 300.1

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Disinfection Byproduct, EPA Method 300.1, Ion Chromatography, Water Analysis, Chromeleon 7.2 CDS

Goal
Demonstrate the use of a complete Chromeleon CDS solution for determination of inorganic anions in drinking water according to U.S. EPA Method 300.1.

Introduction
The determination of common inorganic anions and oxyhalides in drinking water is one of the most important ion chromatography (IC) applications worldwide. IC has been approved for compliance monitoring of inorganic anions in United States (U.S.) drinking water since the mid-1980s, as described in U.S. Environmental Protection Agency (EPA) Method 300.1.[1] Many other industrialized countries have similar health and environmental standards and a considerable number of regulatory IC methods have been published worldwide (e.g., in Germany, France, Italy, and Japan). In addition, many standards organizations, including the International Organization for Standardization (ISO), American Society for Testing and Materials (ASTM), and American Water Works Association (AWWA), have validated IC methods for the determination of inorganic anions in drinking water.[2,3]

The concentrations of some anions in drinking water are regulated due to their toxicity. For example, high levels of fluoride can cause skeletal and dental fluorosis, and nitrite and nitrate can cause methemoglobulinemia, which can be fatal to infants. Ozonation of drinking water containing bromide can result in the formation of the disinfection byproduct bromate, a potential human carcinogen even at low µg/L concentrations. Other common anions, such as chloride and sulfate, are considered secondary contaminants and can affect odor, color, and certain aesthetic characteristics in drinking water.

U.S. EPA Method 300.1
EPA Method 300.1 describes in detail the entire analytical process for determination of common inorganic anions and oxyhalides in drinking water. This includes descriptions of the practical execution of the analysis, like equipment, supplies, reagents, and standards, and procedure for collecting, preservation and storage of water samples. To generate reliable results when using IC in environmental analysis, quality control (QC) is essential. EPA Method 300.1 provides detailed instructions on the QC procedures to be implemented, consisting of three parts:

- Initial demonstration of performance (outside scope of presented solution)
- Assessing laboratory performance within every analysis batch
- Assessing analyte recovery and data quality

Finally, the procedures for calibration, standardization, data analysis, and calculations are described.

The laboratory's challenge is to correctly execute the guidelines as described in the EPA method, including calculating and assessing the final results. Often data is manually transferred to an external spreadsheet which is a time consuming and error prone process. Additionally, there is often poor control over these spreadsheets with no automatic tracking or versioning available.

This technical note presents a complete Thermo Scientific™ Dionex™ Chromeleon™ 7.2 Chromatography Data System (CDS) workflow solution to perform the determination of inorganic anions according to the requirements as described in EPA Method 300.1.

Experimental

The experimental conditions for execution of U.S. EPA Method 300.1 are described in several application documents, which are listed in Table 1.

Because of the variety of Thermo Scientific™ Dionex™ instruments and columns to perform successful analysis according to EPA Method 300.1, the Chromeleon workflow solution does not contain an instrument method and run parameters.

Table 1. Overview of application documents describing analysis according to U.S. EPA Method 300.1.

Application Document	Title	EPA Method 300.1 Part	Thermo Scientific™ Dionex™ Columns
AN133	Determination of Inorganic Anions in Drinking Water by Ion Chromatography	A	IonPac AS4A-SC, Analytical, 4 × 250 mm IonPac AG4A-SC, Guard, 4 × 50 mm
AN154	Determination of Inorganic Anions in Environmental Waters Using a Hydroxide-Selective Column	A	IonPac AS18 Analytical, 4 × 250 mm IonPac AG18 Guard, 4 × 50 mm
AN167	Determination of Trace Concentrations of Oxyhalides and Bromide in Municipal and Bottled Waters Using a Hydroxide Selective Column with a Reagent-Free Ion Chromatography System	B	IonPac AS19 Analytical, 4 × 250 mm IonPac AG19 Guard, 4 × 50 mm
AN184	Determination of Trace Concentrations of Chlorite, Bromate, and Chlorate in Bottled Natural Mineral Waters	B	IonPac AS19 Analytical, 4 × 250 mm IonPac AG19 Guard, 4 × 50 mm IonPac AS23 Analytical, 4 × 250 mm IonPac AG23 Guard, 4 × 50 mm
AN208	Determination of Bromate in Bottled Mineral Water Using the CRD 300 Carbonate Removal Device	B	IonPac AS23 Analytical, 4 × 250 mm IonPac AG23, Guard, 4 × 50 mm
AN1113	Determination of Chloride and Sulfate in Water and Soil	A	IonPac AS18-4µm Analytical, 2 × 250 mm IonPac AG18-4µm Guard, 2 × 50 mm IonPac AS22 Analytical, 2 × 250 mm IonPac AG22 Guard, 2 × 50 mm
AU196	Anion Determinations in Municipal Drinking Water Samples Using EPA Method 300.1 (A) on an Integrated IC System	A	IonPac AS22 Analytical, 4 × 250 mm IonPac AG22 Guard, 4 × 50 mm
AU198	Improved Determination of Trace Concentrations of Oxyhalides and Bromide in Drinking Water Using a Hydroxide-Selective Column	B	IonPac AS27 Analytical, 4 × 250 mm IonPac AG27Guard, 4 × 50 mm

Chromeleon U.S. EPA Method 300.1 eWorkflow

A Chromeleon eWorkflow is an electronic procedure that provides guidance throughout an entire analysis batch, from initial samples to final results. It assists in creating an appropriate sequence with predefined associated files and a well-defined structure. The processing method and report templates ensure the data is processed correctly and final calculations and checks are readily available. A dedicated eWorkflow for EPA Method 300.1 has been created for both parts A and B (Figure 1).

EPA Method 300.1 provides a detailed description about which order the field samples, standards, and other related solutions such as duplicates of fortified samples etc. should be injected (Figure 2A). The sequence also depends on the total number of field samples. The EPA eWorkflow (Figure 2B) predefines the order of injections, and if the number of field samples varies, automatically adjusts to have the correct number of calibration check standards. Because the eWorkflow automatically adjusts based on the number of samples, the result is a consistent sequence table with the correct structure that conforms to the EPA requirements (Figure 2C).

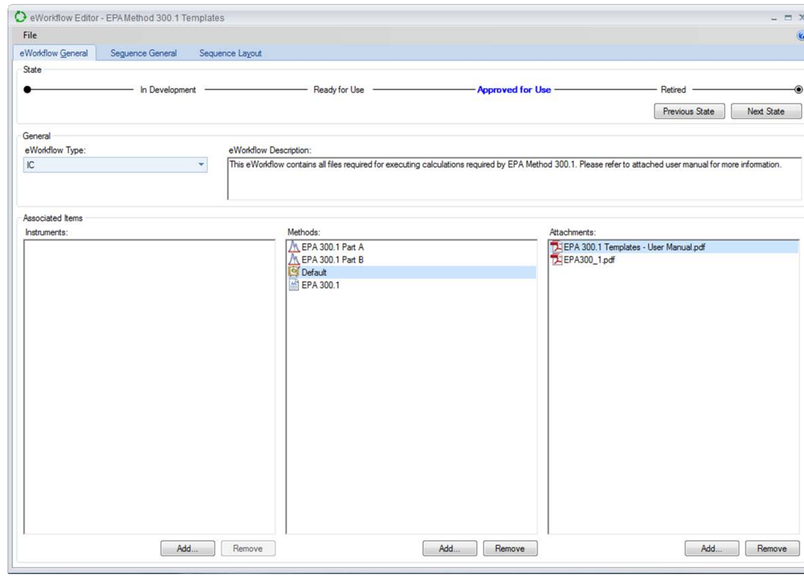

Figure 1. Chromeleon eWorkflow for EPA Method 300.1.

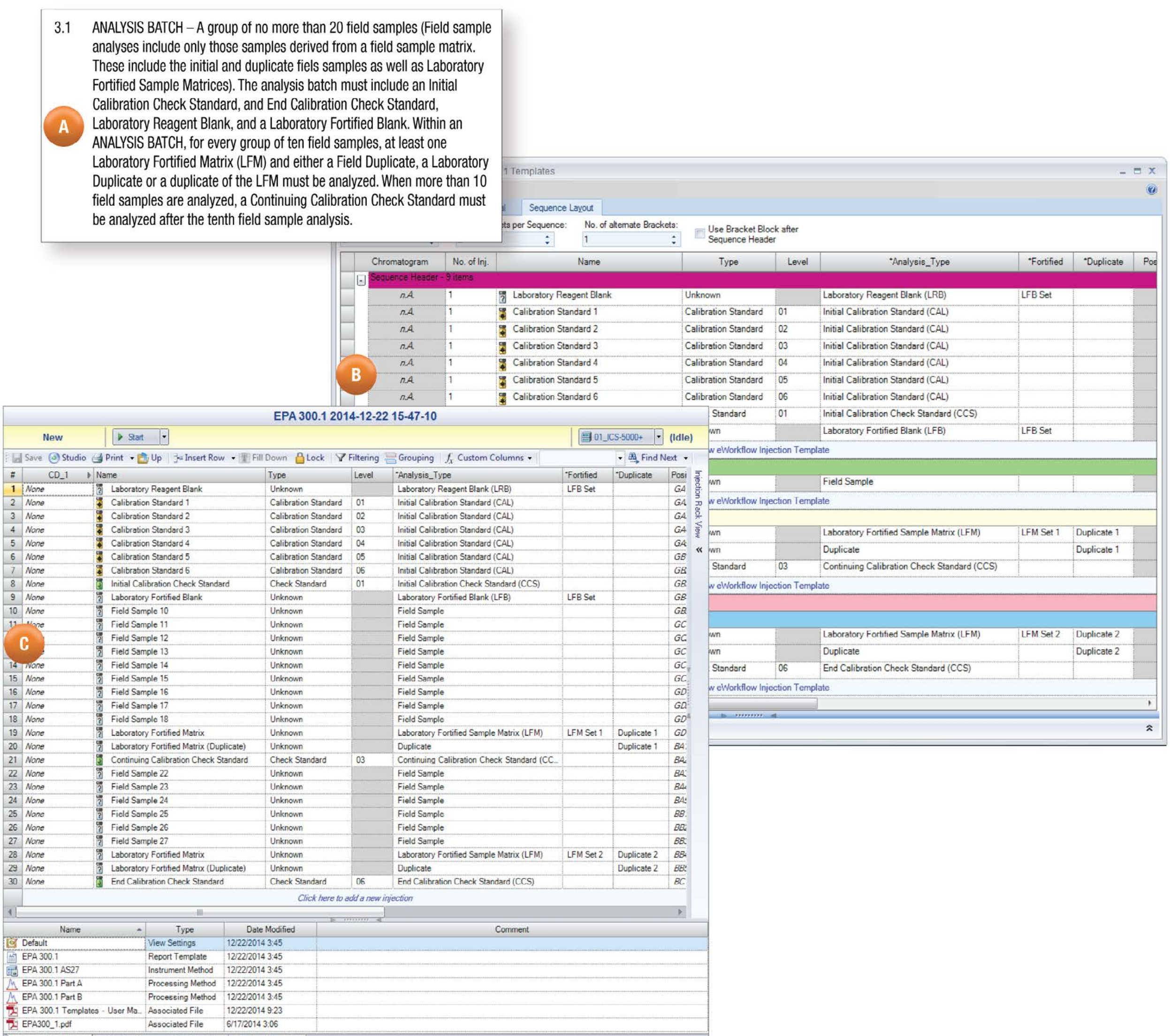

Figure 2. From EPA method to sequence.

Name	Type	Level	*Analysis_Type	*Fortified	*Duplicate
Std 5	Calibration Standard	05	Initial Calibration Standard (CAL)		
Std 1 ICCS	Check Standard	01	Initial Calibration Check Standard (CCS)		
Fortified Blank	Unknown		Laboratory Fortified Blank (LFB)	LFB Set	
Drinking Water 1	Unknown		Field Sample		
Drinking Water 2	Unknown		Field Sample		
Drinking Water 3	Unknown		Field Sample		
Drinking Water 4	Unknown		Field Sample		
Drinking Water 5	Unknown		Field Sample		
Drinking Water 6	Unknown		Field Sample		
Drinking Water 7	Unknown		Field Sample		
Drinking Water 8	Unknown		Field Sample		
Drinking Water 9	Unknown		Field Sample	LFM Set 1	
Drinking Water 9 spiked	Unknown		Laboratory Fortified Sample Matrix (LFM)	LFM Set 1	Duplicate 1
Drinking Water 9 spiked	Unknown		Duplicate		Duplicate 1
Std 3 CCCS	Check Standard	03	Continuing Calibration Check Standard (CCS)		
Drinking Water 10	Unknown		Field Sample		
Drinking Water 11	Unknown		Field Sample		

A B C

Figure 3. Injection identification columns.

#	Name	Ret.Time	Window	*MDL	*MRL	*Add. LFB	*Add. LFM	*LFM Rec. Limit Low	*LFM Rec.Limit High
1	Chlorite	8.900	2.500 RG	0.8900 [µg/L]	9.9700 [µg/l]	47.960 [µg/l]	9.970 [µg/l]	75 [%]	125 [%]
2	Bromate	9.700	2.500 RG	1.4400 [µg/L]	0.9800 [µg/l]	4.900 [µg/l]	0.980 [µg/l]	75 [%]	125 [%]
3	DCA	13.900	2.500 RG			983.800 [µg/l]	983.800 [µg/l]	75 [%]	125 [%]
4	Chlorate	16.700	2.500 RG	1.4400 [µg/L]	10.6700 [µg/l]	48.970 [µg/l]	102.200 [µg/l]	75 [%]	125 [%]
5	Bromide	18.500	2.500 RG	1.3100 [µg/L]	15.0100 [µg/l]	48.970 [µg/l]	102.200 [µg/l]	75 [%]	125 [%]

Figure 4. Component columns for EPA specific parameters.

The generated sequence contains specific columns to identify the individual injections; Analysis Type (Figure 3A) as specified in chapter 3.1 of EPA Method 300.1, Fortified (Figure 3B) to identify fortified sample sets, and Duplicate (Figure 3C) to identify duplicate sample sets.

Additionally, the component table of the processing method contains columns to enter parameters specific for EPA Method 300.1 (Figure 4), such as minimum detection and reporting limits, and additions to fortified samples with corresponding recovery limits.

Combining the information present in the sequence and processing method with calculations in the spreadsheet-based reporting capabilities of Chromeleon CDS, provides a complete solution that converts all information as described in the method (Figure 5A) to a final analysis report (Figure 5B), without the need to transfer data to an external spreadsheet. This minimizes the possibility of human error and ensures data integrity.

Figure 5 shows an example of EPA Method 300.1, Chapter 9.4.3, detailing the calculation and evaluation of the field or laboratory duplicates. Section 9.4.3.1 defines the calculation for the relative percent difference (RPD). This calculation is performed in the Chromeleon CDS report template (Figure 5-1). Subsequently the RPD limit should be determined, as this depends on the concentration of the analyte relative to its minimum reporting limit (MRL) (Figure 5-2). Finally the calculated RDP for the duplicate injection set is compared to the RDP limit and the evaluation result is reported (Figure 5-3).

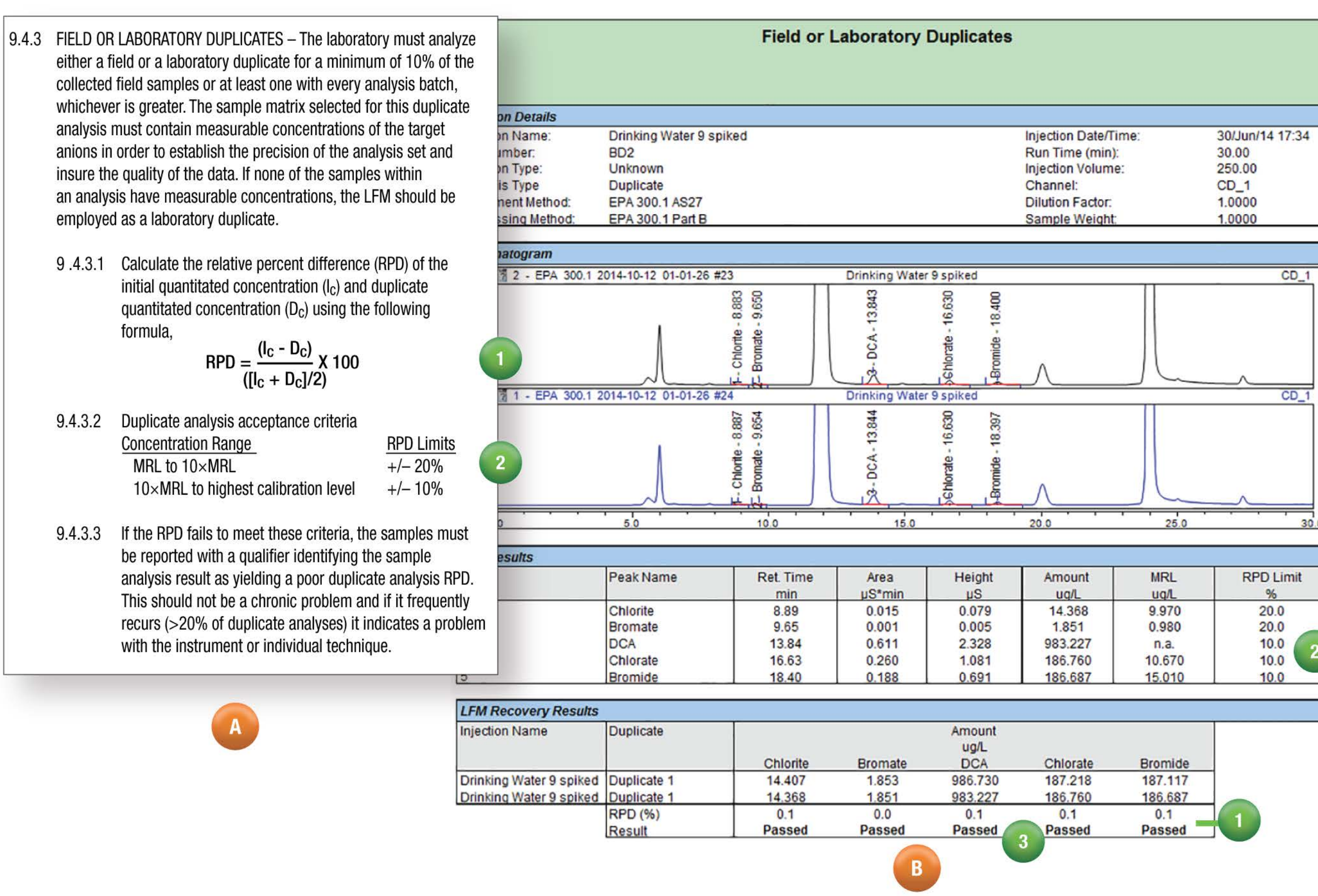

Figure 5. Translation of EPA Method 300.1 Chapter 9.4.3 to Chromeleon CDS reporting.

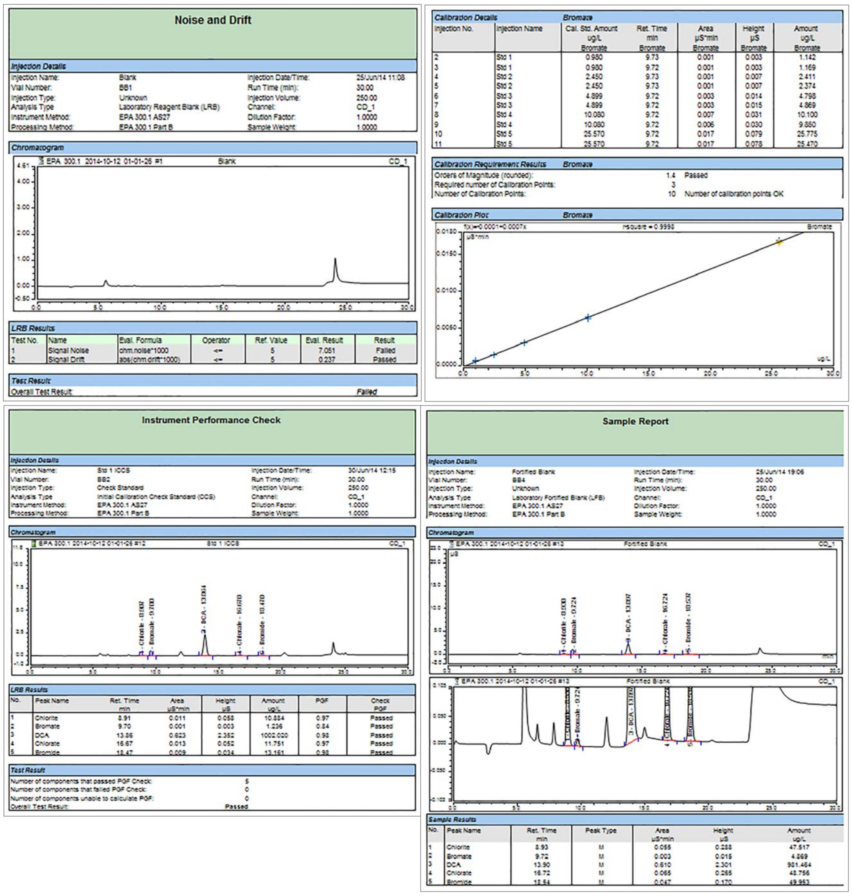

Figure 6. Example pages of the final report.

As a last step in the process the final report can be created, reporting the results for each individual section of EPA Method 300.1 (Figure 6). The report template is preconfigured to report the correct sheets for the correct analysis types.

Conclusion

The eWorkflow in Chromeleon 7.2 CDS offers a user-friendly approach to analysis setup and data handling for the determination of inorganic anions and oxyhalides in drinking water according to U.S. EPA Method 300.1. The general settings included in the eWorkflow can easily be adapted to suit the demands of any laboratory. The U.S. EPA Method 300.1 eWorkflow ensures the analysis is executed according to all guidelines as described in the EPA method. The built-in reporting template provides instant and error free reporting, without the need to export the data to an external spreadsheet.

References

1. Method 300.1: Determination of Inorganic Anions in Drinking Water by Ion Chromatography; U.S. Environmental Protection Agency, National Exposure Research Laboratory, Office of Research and Development: Cincinnati, Ohio, 1997. [Online] http://water.epa.gov/scitech/methods/cwa/bioindicators/upload/2007_07_10_methods_method_300_1.pdf (access May 19, 2015).
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