

TOC Analysis of Bottled Water Using the Fusion UV/Persulfate TOC Analyzer

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Abstract

This application note demonstrates the Teledyne Tekmar Fusion UV/Persulfate analyzer's ability to measure low levels of TOC in five popular bottled water brands. Bottled water samples varied in source and purification methods including: two natural aquifers, one vapor distilled, one reverse osmosis, and one two-stage microfiltration/UV light disinfection. All results had a 10% window of accuracy, based on a certified check standard concentration, and a precision of 7.0% or less, based on the calculated %RSD of samples and standards run in triplicate .



Introduction

Total Organic Carbon (TOC) is an indirect measurement of water cleanliness and purity, because a variety of contaminants including bacteria, biological matter and foreign material, contain carbon. Five bottled water brands were chosen for TOC analysis using the Fusion UV/Persulfate TOC analyzer. The UV persulfate oxidation technique is well-suited to drinking water analysis because of its reduced carbon background when compared to traditional combustion systems and few interferences, unlike membrane conductivity and color-metric techniques.¹

Designed specifically for drinking water applications, the Fusion has a detection limit of 0.2 ppb and provides intuitive features such as “auto-calibration” which creates a calibration curve from a single stock standard and “intellidilution” which automatically dilutes and reanalyzes samples that exceed the calibration range. Additionally, the Fusion TekLink software is fully 21 CFR 11 compatible and includes a password protected user account management system with permissions; versioned methods, calibrations, schedules, and reports; electronic signatures and other required software functions.

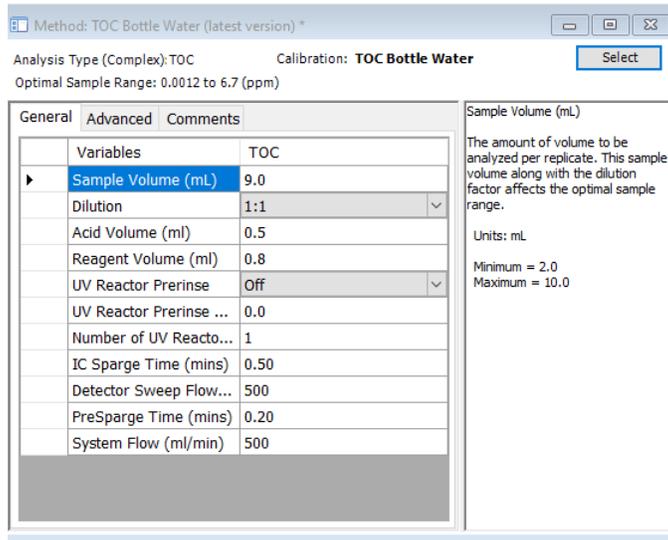
Experimental Instrument Conditions

Method

TOC content is determined by first removing inorganic carbon (IC) from the sample through the addition of phosphoric acid. The remaining organic carbon is oxidized to carbon dioxide (CO₂) using UV oxidation with sodium persulfate. The CO₂ produced is then swept to the non-dispersive infrared detector (NDIR) and measured. In the detector, carbon absorbs infrared light and the amount of absorption is proportional to the amount of carbon in the sample.

It was anticipated that processed bottled water would have low levels of carbon, consequently a method using a large, 9 ml sample volume was used to increase sensitivity and the IC Spurge Time was increased to assist in removing any inorganic carbon in the samples. The Fusion software calculates the method's optimum sample range based on sample volume and dilution factor and is shown along with other method parameters in [Figure 1](#).

Figure 1 Optimal Sample Range and Method Parameters Shown in the Fusion TekLink Method Editor.



Method: TOC Bottle Water (latest version) *

Analysis Type (Complex): TOC Calibration: TOC Bottle Water Select

Optimal Sample Range: 0.0012 to 6.7 (ppm)

General	Advanced	Comments
Variables	TOC	
Sample Volume (mL)	9.0	
Dilution	1:1	
Acid Volume (ml)	0.5	
Reagent Volume (ml)	0.8	
UV Reactor Prerinse	Off	
UV Reactor Prerinse ...	0.0	
Number of UV Reacto...	1	
IC Sparge Time (mins)	0.50	
Detector Sweep Flow...	500	
PreSparge Time (mins)	0.20	
System Flow (ml/min)	500	

Sample Volume (mL)

The amount of volume to be analyzed per replicate. This sample volume along with the dilution factor affects the optimal sample range.

Units: mL

Minimum = 2.0
Maximum = 10.0

Calibration

A 1000 ppmC stock standard was prepared by dissolving 2.125 g of potassium hydrogen phthalate (KHP) in 1 L of deionized (DI) water. A 2 ppmC working standard was then prepared by diluting 2 ml of the 1000 ppmC stock standard in a separate 1 L flask and adding DI water.

The Fusion TekLink auto-calibration feature was used to accurately dilute the 2 ppmC working standard into 0.0, 0.027, 0.05, 0.1, 0.2, 0.5, 1.0, and 2.0 ppmC concentrations to create a calibration curve. Each concentration was analyzed in triplicate (n=3) with a %RSD precision acceptance criteria of 7.0% or less. It was anticipated that DI water, due to its low carbon content, may have %RSD values above 7% (Figure 2).

Figure 2 DI Water and Calibration Concentrations Ranging from 0.0 to 2.0 ppmC Shown in the Fusion TekLink Schedule Editor.

Sample Type: Calibration Standard: 2 ppm TOC Bottle Water (Creating calibration TOC Pharmaceutical Water v20) From Schedule Version 11

Pos	BAT	Concentration (ppm)	STD Conc	Dil	Sample ID	Result (Abs)	Std. Dev. (Abs)	RSD	Start Time	
⊕	A	TOC	DI Water [0]	2 ppmC	DI	[TOC] 2 ppm TOC Bottle Water [DI Water]	3.5687	0.3434	9.62%	2019/01/11 11:00
⊕	A	TOC	0.0270	2 ppmC	1:75	[TOC] 2 ppm TOC Bottle Water [0.027 ppm]	4.7940	0.1561	3.28%	2019/01/11 11:26
⊕	A	TOC	0.0500	2 ppmC	1:40	[TOC] 2 ppm TOC Bottle Water [0.050 ppm]	6.3043	0.1267	2.01%	2019/01/11 11:53
⊕	A	TOC	0.1000	2 ppmC	1:20	[TOC] 2 ppm TOC Bottle Water [0.100 ppm]	9.1877	0.1189	1.29%	2019/01/11 12:19
⊕	A	TOC	0.2000	2 ppmC	1:10	[TOC] 2 ppm TOC Bottle Water [0.200 ppm]	14.9647	0.0899	0.67%	2019/01/11 12:46
⊕	A	TOC	0.5000	2 ppmC	1:4	[TOC] 2 ppm TOC Bottle Water [0.500 ppm]	32.0143	0.0901	0.28%	2019/01/11 13:13
⊕	A	TOC	1.0000	2 ppmC	1:2	[TOC] 2 ppm TOC Bottle Water [1.000 ppm]	62.9097	0.5368	0.85%	2019/01/11 13:39
⊕	A	TOC	2.0000	2 ppmC	1:1	[TOC] 2 ppm TOC Bottle Water [2.000 ppm]	126.2160	0.1425	0.11%	2019/01/11 14:06

Check Standard

A 0.2 ppmC mid-level check standard was created using a 1:10 auto-dilution of the 2.0 ppmC working standard, with a 10% window of accuracy (0.18 to 0.22 ppm).

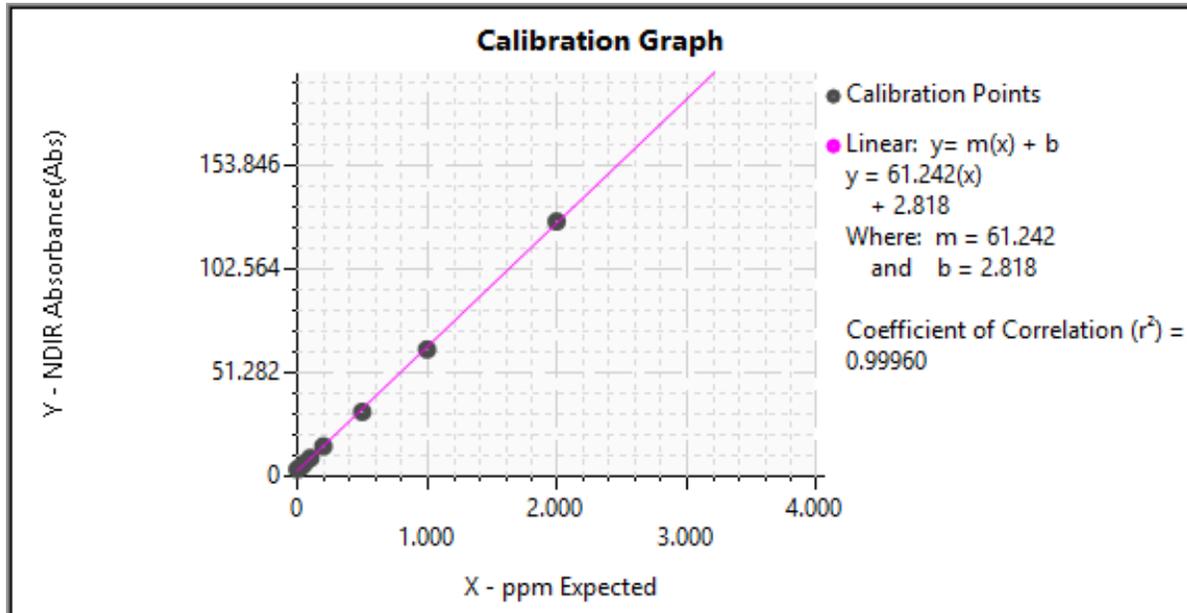
Sample Preparation

Each brand of bottled water was shaken to homogenize the sample before transferring to 40 mL clear VOA vials. The vials were TOC certified for <10 ug/L of TOC background, to ensure sample result integrity. All samples were then analyzed in triplicate (n=3).

Results

The calibration curve yielded a coefficient of correlation value of 0.9996 with an acceptance criteria value of >0.999 (Figure 3). This value surpasses the typical laboratory requirement of 0.995.

Figure 3 Multi-Point Calibration Curve Ranging from 0.0 ppmC to 2.0 ppmC.



The two, 0.2 ppmC check standards yielded a result of 0.1859 and 0.1890 ppmC which was well within 10% (0.18 to 0.22 ppmC) of the certified value.

The results for the five bottled water samples showed a large TOC content disparity. Brand 5, which was sourced from a municipality water supply and processed with reverse osmosis cleanup, yielded the lowest TOC content at 93.4 ppb. Brand 1, which was sourced from a natural spring and processed using a two-stage microfiltration/UV light purification, yielded the highest TOC content at 1.46 ppmC (Table I).

Table I Mid-Level Check Standard and Bottled Water Sample Results				
Bottled Water	ppmC	%RSD (n=3)	Classification	Process Method
0.2 ppm C Check Standard	0.1859	1.44	Stock Serial Dilution	N/A
Brand 1	1.4616	0.54	Spring Water	Two-Stage Microfiltration/UV Light
Brand 2	0.0973	3.04	Spring Water	Vapor Distilled
Brand 3	0.7889	4.19	Spring Water	Natural Aquifer
Brand 4	0.4083	3.41	Artesian Well Water	Underground Aquifer
Brand 5	0.0934	5.36	Municipal Water	Reverse Osmosis
0.2 ppm C Check Standard	0.1890	0.46	Stock Serial Dilution	N/A

Conclusion

The Teledyne Tekmar Fusion UV/Persulfate TOC analyzer easily quantified TOC content in bottled drinking water as demonstrated by the results in this application note. All standards and check standard results were well within the 10% window of accuracy. Check standard and sample triplicates were also below the 7% RSD acceptance criteria. The Fusion TekLink software's "auto-calibration" and "intellidilution" features simplified routine analytical tasks and eased laboratory workflow. Data integrity was ensured by the software's 21 CFR 11 compatibility.

References

1. Total Organic Carbon (TOC) Analysis Technique Comparison – A Practical Guide; Teledyne Tekmar, November, 2017. The guide is available for download [Here](#).