Sievers* M500 TOC Analyzer conductivity performance specifications

TEST REPORT

Purpose

The purpose of this report was to verify the conductivity performance characteristics of the Sievers M500 Total Organic Carbon (TOC) Analyzer. Performance was quantified by measuring the accuracy, precision, and linearity of the conductivity measurement. Nine Sievers M500 TOC Analyzers were used in this study.

Background Information and Calculations

1. Accuracy

The accuracy performance specification results are presented here as percent recoveries[1,2]. The averages of three replicates of potassium chloride (KCl) standards were determined at the following conductivity levels, compensated to 25ºC: 25, 50, 100, 146.9, and 718 µS/cm.

The percent recovery for each standard was calculated using the following equation:

% Recovery = (Measured Standard Conductivity/Standard Conductivity) x 100%

Percent recoveries close to 100% indicate a high degree of accuracy for the analyzer.

2. Precision

The precision performance specification data are presented as a % relative standard deviation (%RSD). The standard deviation and %RSD are calculated as follows:

$$\text{Standard Deviation} = \sqrt{\frac{n\sum x^2 - (\sum x)^2}{n(n-1)}}$$

where:

x = Each result

n = Number of measurements

Relative Standard Deviation (%RSD) = (Standard Deviation/Measured Concentration) x 100%

A %RSD value close to 0% indicates a high degree of precision for the analyzer[1,2,3].

3. Linearity

Linearity is defined as the ability of the TOC analyzer to generate data that are directly proportional to the concentration of multiple TOC standards across the dynamic range of the instrument. Linearity is determined by performing a linear regression and calculating the square of the correlation coefficient (R^2). The square of the correlation coefficient is calculated using the following equation:

$$R^2 = \left(\frac{\sum(x - \bar{x})\,(y - \bar{y})}{\sqrt{\sum(x - \bar{x})^2 \sum(y - \bar{y})^2}} \right)^2$$

where:

x = Each expected TOC result

$\bar{x}$ = Average expected TOC result

y = Each measured TOC result

$\bar{y}$ = Average measured TOC result

R^2 values close to 1.0 represent a high degree of correlation.

Experimental Test Plan

1. Accuracy Measurement

To evaluate the accuracy of the conductivity response, standard solutions of KCl were produced at the following conductivity levels, compensated to 25ºC: 25, 50, 100, 146.9, and 718 µS/cm. All the standards are part of Sievers conductivity standard sets made by Veolia. Conductivity standards below 25 µS/cm have a higher degree of inaccuracy and therefore were not considered for the accuracy evaluation. For each standard, four replicates were made with the first replicate rejected. All conductivity measurements are compensated to 25ºC for comparison to the standard value. This testing was performed on nine M500 instruments.

2. Precision Measurement

The precision results from the accuracy measurements above were combined with the measurement results from additional standard solutions of KCl produced at the following conductivity levels, compensated to 25ºC: 5 and 10 µS/cm. These standards are part of the Sievers conductivity linearity standard set made by Veolia. For each standard, four replicates were measured with the first replicate rejected. All conductivity measurements are compensated to 25ºC for comparison to the standard value. This testing was performed on nine Sievers M500 instruments.

3. Linearity

A linear regression was applied to the results from 1 and 2 above.

Test Equipment Used

- Sievers M500 TOC Analyzer: 0001, Super iOS
- Sievers M500 TOC Analyzer: 0002, Super iOS
- Sievers M500 TOC Analyzer: 0003, iOS
- Sievers M500 TOC Analyzer: 0004, iOS
- Sievers M500 TOC Analyzer: 0005, iOS
- Sievers M500 TOC Analyzer: 0007, iOS
- Sievers M500 TOC Analyzer: 0008, Super iOS

- Sievers M500 TOC Analyzer: 0009, Super iOS
- Sievers M500 TOC Analyzer: 0010, Super iOS

Calibration and Verification

Each instrument was calibrated using the Sample Conductivity Single Point Calibration protocol[6] which utilizes a 100 µS/cm KCl standard. Each instrument was verified using the Cell Calibration Verification protocol[6] which utilizes a 25 µS/cm KCl standard.

Results and Discussion

All results presented here are for four replicates of each potassium hydrogen phthalate (KHP) standard with one rejection.

1. Accuracy

1.1 Percent Recovery Results

Serial Number	25 µS/cm % Recovery	50 µS/cm % Recovery	100 µS/cm % Recovery	146.9 µS/cm % Recovery	718 µS/cm % Recovery
0001	100.2	100.1	100.0	99.8	99.1
0002	100.4	99.8	100.5	99.9	99.2
0003	100.4	99.6	100.2	100.3	99.7
0004	100.5	99.7	99.9	100.0	99.2
0005	100.7	100.0	99.9	99.9	99.2
0007	99.9	99.9	100.2	100.3	99.2
0008	100.8	99.8	100.0	100.1	99.6
0009	100.9	100.0	100.0	100.0	99.3
0010	100.5	99.9	100.0	100.1	99.2

1.1 Accuracy Performance Specification

The results presented here demonstrate that Sievers M500 TOC Analyzers measure conductivity with a high degree of accuracy. The recovery results ranged from 99.1% to 100.9%.

Based on the recovery results shown above, the conductivity accuracy performance specification for the Sievers M500 TOC Analyzer is ±1%.

2. Precision

2.1 Precision Results

	Unit 1		Unit 2		Unit 3	
Standard Concentration	Standard Deviation (µS/cm)	% RSD	Standard Deviation (µS/cm)	% RSD	Standard Deviation (µS/cm)	% RSD
5 µS/cm	0.002	0.04	0.002	0.04	0.000	0.00
10 µS/cm	0.000	0.00	0.000	0.00	0.006	0.06
25 µS/cm	0.000	0.00	0.000	0.00	0.000	0.00
50 µS/cm	0.006	0.01	0.006	0.01	0.010	0.02
100 µS/cm	0.006	0.01	0.058	0.06	0.000	0.00
146.9 µS/cm	0.058	0.04	0.000	0.00	0.000	0.00
718 µS/cm	0.115	0.02	0.058	0.01	0.153	0.02

	Unit 4		Unit 5		Unit 7	
Standard Concentration	**Standard Deviation (µS/cm)**	**% RSD**	**Standard Deviation (µS/cm)**	**% RSD**	**Standard Deviation (µS/cm)**	**% RSD**
5 µS/cm	0.001	0.02	0.001	0.02	0.001	0.02
10 µS/cm	0.000	0.00	0.006	0.06	0.000	0.00
25 µS/cm	0.006	0.02	0.000	0.00	0.006	0.02
50 µS/cm	0.000	0.00	0.000	0.00	0.006	0.01
100 µS/cm	0.000	0.00	0.006	0.01	0.000	0.00
146.9 µS/cm	0.000	0.00	0.000	0.00	0.000	0.00
718 µS/cm	0.058	0.01	0.000	0.00	0.058	0.01

	Unit 8		Unit 9		Unit 10	
Standard Concentration	**Standard Deviation (µS/cm)**	**% RSD**	**Standard Deviation (µS/cm)**	**% RSD**	**Standard Deviation (µS/cm)**	**% RSD**
5 µS/cm	0.004	0.08	0.001	0.02	0.001	0.02
10 µS/cm	0.006	0.06	0.000	0.00	0.000	0.00
25 µS/cm	0.006	0.02	0.000	0.00	0.006	0.02
50 µS/cm	0.000	0.00	0.006	0.01	0.000	0.00
100 µS/cm	0.058	0.06	0.000	0.00	0.000	0.00
146.9 µS/cm	0.000	0.00	0.000	0.00	0.058	0.04
718 µS/cm	0.000	0.00	0.058	0.01	0.115	0.02

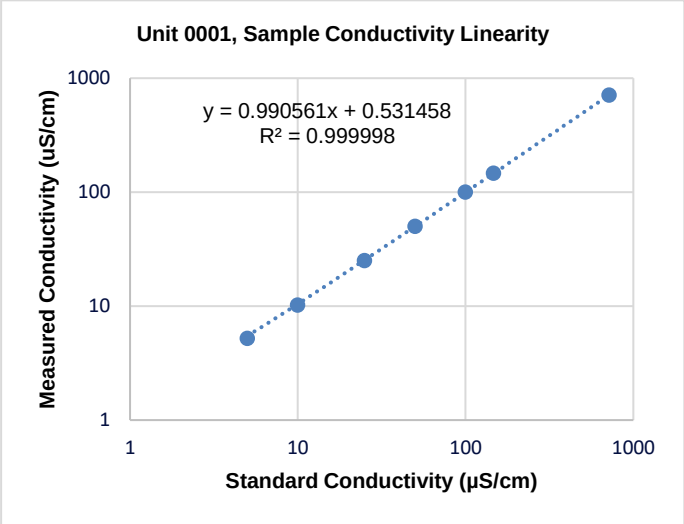
2.2 Precision Performance Specification

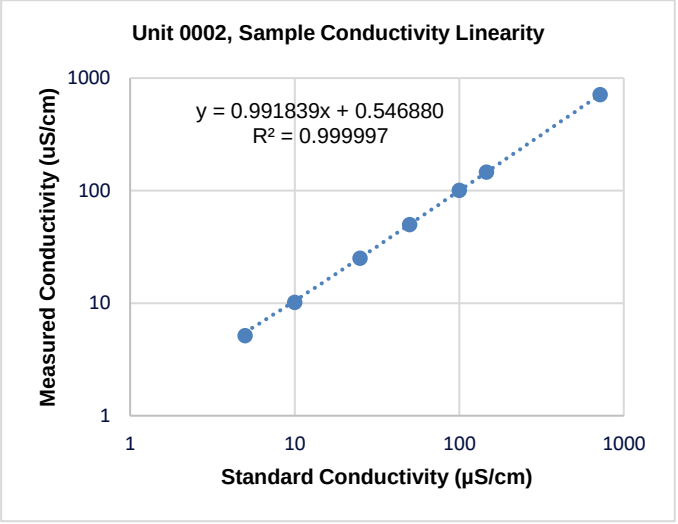
Based on the precision results shown above, the conductivity precision performance specification for the Sievers M500 TOC Analyzer is ≤1%.

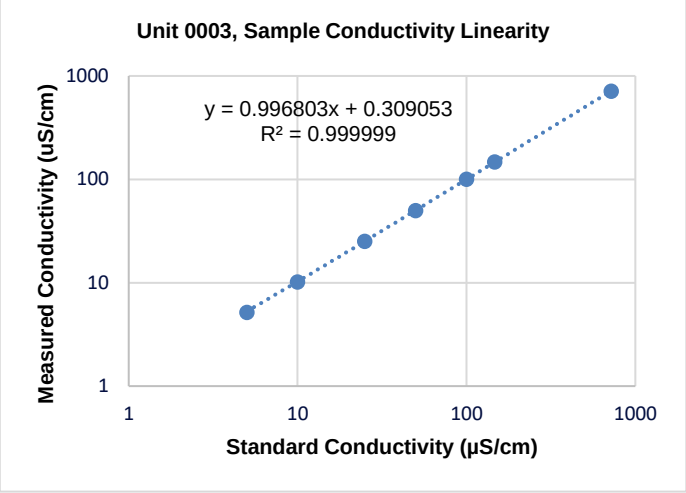
2.3 Linearity

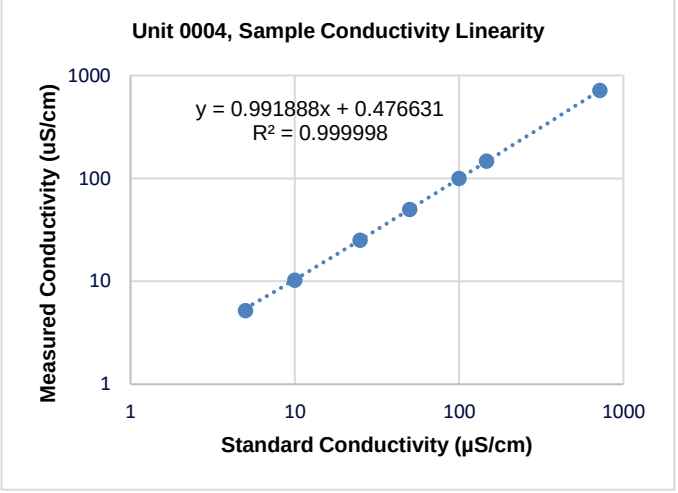
To demonstrate linearity, a least-squares regression was performed using the standard conductivity and measured conductivity data from each instrument. The linear regression equation as well as the square of the correlation coefficient (R^2) are reported below for each instrument. Due to the large range of conductivity standards tested, the axes in the charts below are shown in logarithmic scale to better show the individual data points and the linearity of the response.

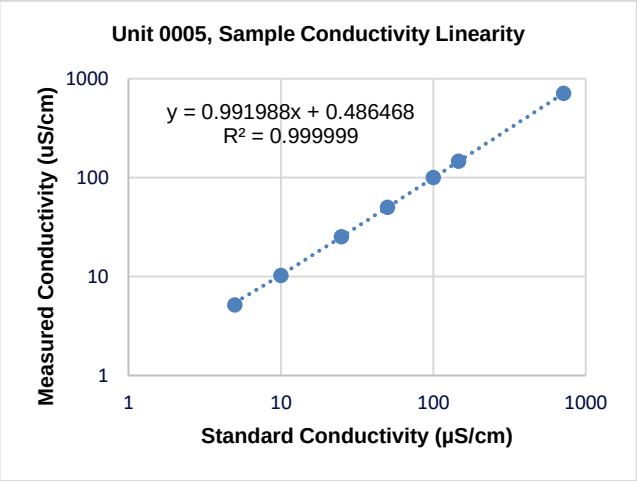
2.3.1 Linearity Results

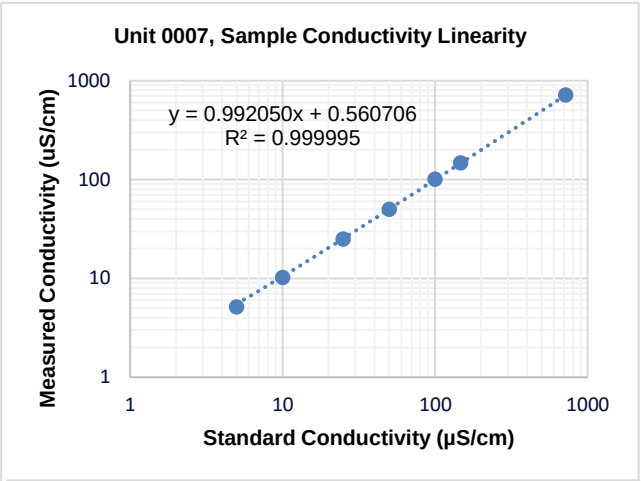


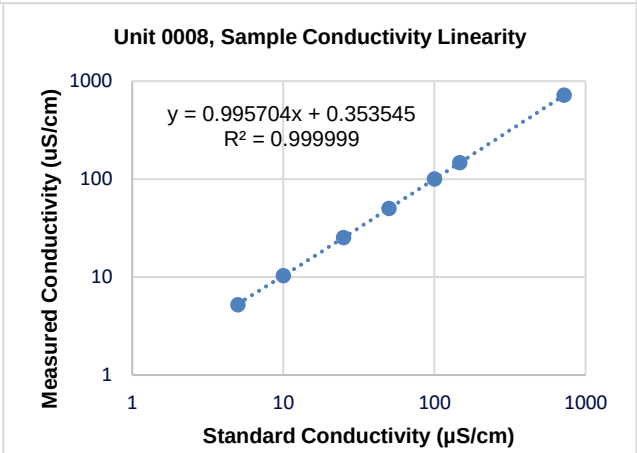


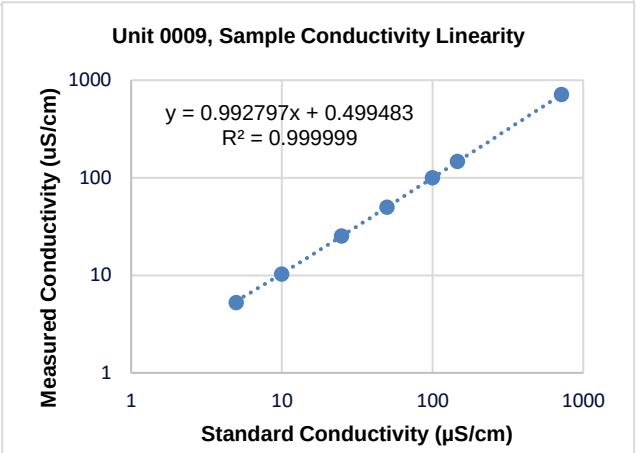


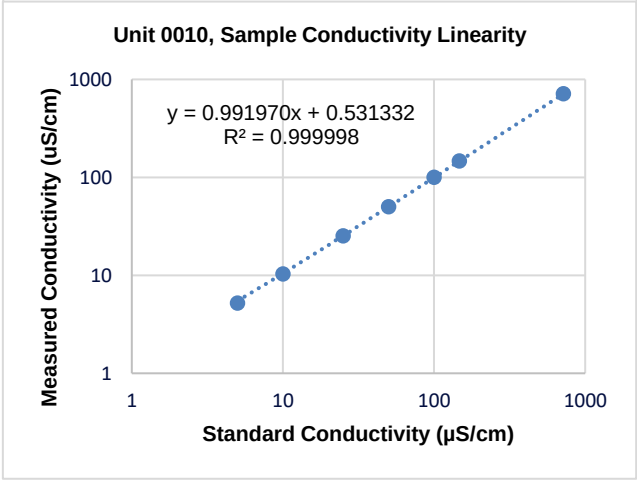



Unit 0005, Sample Conductivity Linearity
y = 0.991988x + 0.486468
R² = 0.999999
Measured Conductivity (uS/cm)
Standard Conductivity (µS/cm)
1000
100
10
1
1
10
100
1000


Unit 0007, Sample Conductivity Linearity
y = 0.992050x + 0.560706
R² = 0.999995
Measured Conductivity (uS/cm)
Standard Conductivity (µS/cm)
1000
100
10
1
1
10
100
1000


Unit 0008, Sample Conductivity Linearity
y = 0.995704x + 0.353545
R² = 0.999999
Measured Conductivity (uS/cm)
Standard Conductivity (µS/cm)
1000
100
10
1
1
10
100
1000


Unit 0009, Sample Conductivity Linearity
y = 0.992797x + 0.499483
R² = 0.999999
Measured Conductivity (uS/cm)
Standard Conductivity (µS/cm)
1000
100
10
1
1
10
100
1000


Unit 0010, Sample Conductivity Linearity
y = 0.991970x + 0.531332
R² = 0.999998
Measured Conductivity (uS/cm)
Standard Conductivity (µS/cm)
1000
100
10
1
1
10
100
1000

2.3.2. Linearity Performance Specification

All nine instruments demonstrated a highly linear TOC response with square of the correlation coefficient (R^2) values of 0.99999 or greater across the full range of the instrument.

3. Conclusions

In summary, the conductivity performance specifications of the Sievers M500 TOC Analyzer have been experimentally verified as follows:

Accuracy	±1%
Precision	≤1%
Linearity	$R^2 \geq 0.99999$

References

1. Barwick, V., S. Burke, R. Lawn, P. Roper, and R. Walker. (2001). Applications of Reference Materials in Analytical Chemistry. Cambridge: LGC Limited.
2. Ellison, S.R., V.J. Barwick, and T.J. Duguid Farrant. (2009). Practical Statistics for the Analytical Scientist. Cambridge: RSC Publishing.
3. Taylor, J.K. (1987). Quality Assurance of Chemical Measurements. Florida: CRC Press LLC.
4. ICH Harmonized Tripartite Guideline Validation of Analytical Procedures: Text and Methodology Q2(R1). (2005).
5. USP <643> Total Organic Carbon.
6. Sievers M500 TOC Analyzer Operation and Maintenance Manual.

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