

Beverage-grade carbon dioxide purity analysis

The Thermo Scientific™ MAX-Bev™ CO₂ Purity Monitoring System is a fully integrated solution capable of measuring trace impurities in carbon dioxide (CO2) gas down to single-digit parts-per-billion (ppb), as well as absolute purity. This system is based on the Thermo Scientific™ MAX-iR™ FTIR Gas Analyzer, which is capable of performing all relevant analytical measurements except oxygen. The analyzer incorporates a deuterated triglycine sulfate (DTGS) thermal detector, which has a spectral range of 600-5,000 cm⁻¹. This broad range allows for the measurement of all infraredactive impurities, as well as the direct measurement of absolute CO₂ purity, which eliminates the need for cumbersome wet methods (such as Zahm-Nagel purity testing). By using incredibly precise pressure and temperature controls, the MAX-Bev CO₂ Purity Monitoring System is capable of measuring CO₂ at 100 ± 0.02% simultaneously with trace impurities.

Sulfur impurity measurement

Within the MAX-Bev CO_2 Purity Monitoring System, an oxidizer module converts all reduced sulfur species to sulfur dioxide (SO_2), which is then measured by the MAX-iR Gas Analyzer to determine the total reduced sulfur impurity level in the CO_2 . This is a more reliable method compared to industry-standard UV fluorescence analyzers, which are prone to maintenance issues and extended downtime.

MAX-Acquisition Software

The entire MAX-Bev CO₂ Purity Monitoring System is controlled by Thermo Scientific™ MAX-Acquisition™ Software, which allows you to manage all aspects of data acquisition and analysis, view system diagnostics and alarms, and generate/print certificates of analysis (CoA) as well as historical reports.

This paper demonstrates how the performance of the MAX-Bev CO₂ Monitoring System meets the requirements of the International Society of Beverage Technologists (ISBT) and European Industrial Gases Association (EIGA) Standard for the measurement of key impurities in CO₂.

Gas	Units	Lower alarm threshold	Upper alarm threshold	Limit of detection
Carbon dioxide	%	99.9	100.02	N/A
Oxygen	ppm	N/A	30	1
Moisture	ppm	N/A	20	1
Ammonia	ppm	N/A	2.5	0.01
Nitric oxide	ppm	N/A	2.5	0.075
Nitrogen dioxide	ppm	N/A	2.5	0.025
Total hydrocarbon	ppm	N/A	50	0.100
Total non-methane hydrocarbon	ppm	N/A	20	0.100
Acetaldehyde	ppb	N/A	200	5
Carbon monoxide	ppm	N/A	10	0.12
Total aromatic hydrocarbon (benzene)	ppb	N/A	20	5
Total sulfur (SO ₂)	ppb	N/A	100	10

Table 1. Typical MAX-Bev measurement standard for beverage-grade ${\rm CO_2}$.

Materials

The table below describes the certified standards (reference gases) used in this study. Compositions are verified by the gas manufacturer using direct comparison to National Institute of Standards and Technology (NIST) traceable calibration standards and/or NIST gas-mixture reference materials.

Research-grade CO_2 was used for dilution of the reference gas mixture and for spanning the CO_2 absolute purity measurement. The MAX-iR FTIR Gas Analyzer was zeroed with ultra-high purity (UHP) nitrogen prior to accuracy and linearity assessment in CO_2 .

Test protocols and results

Impurity limit of detection

This assessment demonstrates the minimum amount of impurity that can be detected above the background in a representative gas matrix. Twelve consecutive analyses of research-grade CO₂ were performed on the MAX-Bev CO₂ Purity Monitoring System. The limit of detection (LOD) for each impurity was defined as 3x the standard deviation of these measurements.

No offsets or span factors were applied to the method. The negative bias on the acetaldehyde measurement can be zero corrected when using a high-purity CO_2 standard.

Cylinder ID	Expiration date	Gas	Certified conc. (ppm)	Analytical uncertainty
433	10 October 2024	Methane	497	±2%
CC491546	3 August 2021	Benzene	0.99	±10%
CC503203	18 June 2021	Acetaldehyde	1018	±2%
CC49300	2 July 2021	Moisture	103.4	±2%
CC436690	12 June 2021	Ammonia	494.5	±2%
CC74236	5 June 2028	Nitric oxide	505.0	±2%
CC178342	16 June 2023	Nitrogen dioxide	535.4	±2%
CC434562	22 December 2024	Carbon monoxide	511.1	±2%
D526338	21 October 2022	Propane	299.7	±2%
		Benzene	9.991	±5%
		Carbonyl sulfide	5.46	±5%
Ultra Zero Grade Air	N/A	Oxygen	21.5%	±2%

Table 2. Reference gas cylinder information.

Gas	Units	Average	LOD (3σ)	Criteria	Validation
Carbon dioxide	%	1.00	N/A	N/A	N/A
Oxygen	ppm	0.06	0.06	< 1	PASS
Moisture	ppm	-0.28	0.84	< 1	PASS
Ammonia	ppm	-0.01	0.00	< 0.01	PASS
Nitric oxide	ppm	-0.04	0.01	< 0.075	PASS
Nitrogen dioxide	ppm	-0.01	0.00	< 0.025	PASS
Total hydrocarbon	ppm	0.07	0.01	< 0.1	PASS
Total non-methane hydrocarbon (C1)	ppm	0.07	0.01	< 0.1	PASS
Acetaldehyde	ppb	-15.38	2.07	< 5	PASS
Carbon monoxide	ppm	-0.05	0.06	< 0.12	PASS
Total aromatic hydrocarbon (benzene)	ppb	0.53	2.74	< 5	PASS
Total sulfur (SO ₂)	ppb	5.75	6.49	< 10	PASS

Table 3. Impurity LOD results.

CO₂ accuracy and repeatability

This test demonstrates the accuracy and repeatability of the CO₂ absolute purity measurement. Prior to conducting this test, the CO₂ response in the MAX-Bev CO₂ Purity Monitoring System was spanned to the research-grade CO₂ certified concentration (100%). This is a routine quality assurance check that can be scheduled in the instrument control software.

To assess CO_2 accuracy and repeatability, undiluted research-grade CO_2 was consecutively analyzed 10-12 times. For each replicate, the percent error was calculated as the difference between the measured and expected CO_2 concentration, divided by the expected concentration. The relative standard deviation (RSD) of the CO_2 concentration is also calculated. Each CO_2 replicate must be 100 \pm 0.02%, and the RSD must be <0.015%.

Response time

It is important to know how much time it takes for the instrument to respond to a change in the concentration of impurities. The reference gas used for this test was a blend of propane, carbonyl sulfide, and benzene in a balance of nitrogen. Note that any carbonyl sulfide is converted to sulfur dioxide in the oven and measured by the MAX-iR FTIR Gas Analyzer as total sulfur.

To assess response time, research-grade CO_2 was introduced into the MAX-Bev CO_2 Purity Monitoring System. A reference gas was then introduced at a concentration that exceeds the upper alarm threshold (this can also be set to your specific actionable limit). Once the concentration stabilized (i.e., was not varying by more than 1%) the time required to reach 95% of full scale ("rise time") was recorded. Research grade CO_2 was reintroduced, and once the concentration stabilized, the time required to reach <5% of full scale ("fall time") was recorded.

Both the rise and fall time must be less than 75 seconds.

Replicate	Measured conc.	% Error	Criteria	Validation
1	100.00%	0.00%	±0.02%	PASS
2	99.98%	-0.02%	±0.02%	PASS
3	99.98%	-0.02%	±0.02%	PASS
4	99.98%	-0.02%	±0.02%	PASS
5	99.98%	-0.02%	±0.02%	PASS
6	99.98%	-0.02%	±0.02%	PASS
7	99.98%	-0.02%	±0.02%	PASS
8	99.98%	-0.02%	±0.02%	PASS
9	99.98%	-0.02%	±0.02%	PASS
10	99.98%	-0.02%	±0.02%	PASS
11	99.98%	-0.02%	±0.02%	PASS
12	99.98%	-0.02%	±0.02%	PASS

Table 4. CO₂ absolute purity results.

Average CO ₂	RSD	Criteria	Validation
99.98%	0.006%	< 0.015%	PASS

Table 5. CO₂ repeatability results.

Gas	Timestamp (hh:mm:ss)		Rise time (sec)	Criteria	Validation
	0% of full scale	>95% of full scale			
Carbon dioxide	10:15:46	10:16:54	69	< 75 sec	PASS
Propane	10:15:46	10:16:42	56	< 75 sec	PASS
Benzene	10:15:46	10:16:54	69	< 75 sec	PASS
Sulfur dioxide	10:29:42	10:30:26	44	< 75 sec	PASS
Gas	Timestamp	(hh:mm:ss)	Fall time (sec)	Criteria	Validation
	100% of full scale	<5% of full scale			
Carbon dioxide	10:18:49	10:19:51	62	< 75 sec	PASS
Propane	10:18:49	10:19:43	53	< 75 sec	PASS
Benzene	10:18:49	10:19:34	45	< 75 sec	PASS

Table 6. Response time results.

Accuracy, linearity, and precision of impurity measurements near the maximum allowable concentration

This assessment demonstrates the accuracy and linearity of impurity measurements in the instrument control software. The MAX-iR FTIR Gas Analyzer is capable of measuring all infrared-active impurities, while oxygen is measured by a ZR800 Oxygen Analyzer (Systech Illinois). Precision was also assessed at concentrations that approximate the upper alarm threshold, or the maximum allowable concentration (Table 1).

A reference gas was diluted with research-grade CO₂ using two mass-flow controllers (MFCs) and introduced into the MAX-iR FTIR Gas Analyzer. For all impurities except total sulfur, seven reference gas concentrations, including zero, were measured 3x for a total of 21 replicates. For replicates 1-7, concentrations were measured in ascending order; replicates 8-14 were measured in descending order, and replicates 15-21 were measured in a random order.

During the total sulfur and oxygen accuracy and linearity studies, five reference gas concentrations, including zero, were measured four times in a semi-random order that ensured the same concentration was never introduced twice in succession.

The lowest impurity concentration level was at least 2x the LOD in order to produce a valid accuracy assessment. For all impurities except total hydrocarbon, the highest level exceeded the upper alarm threshold (Table 1). The reference gas used to validate total hydrocarbon was methane. The concentration of methane in beverage-grade CO_2 is not expected to exceed 10 ppm, so this value was selected as the maximum. The target concentrations for each impurity are described in Table 7.

For each level, the percent error was calculated as the difference between the measured and expected reference gas concentration, divided by the expected concentration. To determine linearity, the expected versus measured gas concentrations were plotted to calculate R².

Impurity	Units	Level 0	Level 1	Level 2	Level 3	Level 4	Level 5	Level 6
Total hydrocarbon (C1)	ppm	0.00	0.54	1.07	2.54	4.92	7.55	10.14
Total aromatic (benzene)	ppb	0	10	17	25	34	43	50
Acetaldehyde	ppb	0	41	83	206	413	619	825
Moisture	ppm	0.00	0.99	1.96	10.02	20.00	29.85	40.00
Ammonia	ppm	0.00	0.27	0.53	1.33	2.53	3.45	5.03
Nitric oxide	ppm	0.00	0.27	0.55	1.23	2.58	3.79	5.00
Nitrogen dioxide	ppm	0.00	0.29	0.58	1.30	2.45	3.74	5.02
Carbon monoxide	ppm	0.00	1.10	2.06	4.92	10.02	15.19	20.44
Total sulfur (SO ₂)	ppb	0	44	102	146	248	N/A	N/A
Oxygen	ppm	0.0	15.4	30.7	61.4	92.1	N/A	N/A

Table 7. Reference gas target concentrations.

Level	Replicate	Total hydrocarbon (C1)			
		Target (ppm)	Measured (ppm)	% Error	
0	1	0.00	0.00	~MDL	
1	1	0.54	0.54	-2.73%	
2	1	1.07	1.06	-0.98%	
3	1	2.54	2.55	0.52%	
4	1	4.92	4.98	1.19%	
5	1	7.55	7.55	0.04%	
6	1	10.14	9.99	-1.49%	
6	2	10.14	9.98	-1.62%	
5	2	7.55	7.55	0.11%	
4	2	4.92	5.01	1.84%	
3	2	2.54	2.56	0.97%	
2	2	1.07	1.08	0.34%	
1	2	0.54	0.52	-2.28%	
0	2	0.00	0.02	~MDL	
4	3	4.92	4.99	1.44%	
2	3	1.07	1.07	-0.38%	
5	3	7.55	7.53	-0.19%	
1	3	0.54	0.52	-2.45%	
6	3	10.14	9.94	-1.96%	
0	3	0.00	0.02	~MDL	

Table 8. Total hydrocarbon (C1) accuracy.

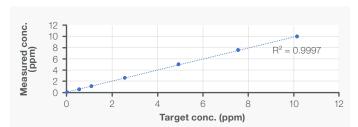


Figure 1. Total hydrocarbon (C1) linearity.

Level	Replicate	Total aromatic (benzene)			
		Target (ppb)	Measured (ppb)	% Error	
0	1	0	0	~MDL	
1	1	10	9	-6.43%	
2	1	17	16	-4.24%	
3	1	25	25	-1.13%	
4	1	34	33	-2.69%	
5	1	43	41	-2.72%	
6	1	50	50	-0.16%	
6	2	50	50	-0.96%	
5	2	43	42	-1.18%	
4	2	34	33	-1.65%	
3	2	25	24	-3.16%	
2	2	17	17	-0.18%	
1	2	10	11	7.82%	
0	2	0	0	~MDL	
4	3	34	34	0.79%	
1	3	10	10	4.12%	
5	3	43	41	-2.45%	
2	3	17	17	-1.67%	
6	3	50	49	-2.17%	
0	3	0	0	~MDL	
3	3	25	24	-4.02%	

Table 9. Total aromatic hydrocarbon (benzene) accuracy.

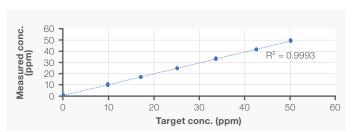


Figure 2. Total aromatic hydrocarbon (benzene) linearity.

Level	Replicate		Acetaldehyde	;
		Target (ppb)	Measured (ppb)	% Error
0	1	0	0	~MDL
1	1	41	40	-2.27%
2	1	83	89	8.42%
3	1	206	212	2.53%
4	1	413	423	2.45%
5	1	619	636	2.82%
6	1	825	847	2.65%
6	2	825	825	0.08%
5	2	619	623	0.65%
4	2	413	423	2.61%
3	2	206	213	3.16%
2	2	83	101	22.41%
1	2	41	45	8.17%
0	2	0	0	~MDL
4	3	413	426	3.19%
2	3	83	90	8.99%
5	3	619	634	2.48%
1	3	41	45	8.11%
6	3	825	832	0.87%
0	3	0	4	~MDL
3	3	206	217	5.33%

Table 10. Acetaldehyde accuracy.

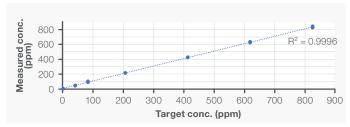


Figure 3. Acetaldehyde linearity.

Level	Replicate		Moisture	
		Target (ppm)	Measured (ppm)	% Error
0	1	0.00	0.00	~MDL
1	1	0.99	1.07	8.05%
2	1	1.96	1.88	-4.30%
3	1	10.02	9.69	-3.32%
4	1	20.00	19.50	-2.50%
5	1	29.85	29.05	-2.67%
6	1	40.00	39.32	-1.69%
6	2	40.00	39.31	-1.73%
5	2	29.85	29.61	-0.80%
4	2	20.00	19.88	-0.60%
3	2	10.02	10.23	2.05%
2	2	1.96	2.10	7.01%
1	2	0.99	0.96	-3.26%
0	2	0.00	0.00	~MDL
4	3	20.00	19.27	-3.65%
2	3	1.96	2.13	8.73%
5	3	29.85	28.82	-3.46%
1	3	0.99	1.11	12.28%
6	3	40.00	39.18	-2.06%
0	3	0.00	0.12	~MDL
3	3	10.02	10.02	0.04%

Table 11. Moisture accuracy.

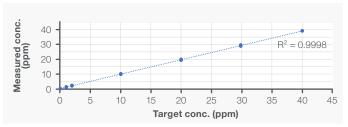


Figure 4. Moisture linearity.

Level	Replicate		Ammonia	
		Target (ppm)	Measured (ppm)	% Error
0	1	0.00	0.01	~MDL
1	1	0.27	0.23	-13.63%
2	1	0.53	0.50	-5.73%
3	1	1.33	1.30	-2.52%
4	1	2.53	2.51	-0.59%
5	1	3.45	3.45	-0.08%
6	1	5.03	5.05	0.42%
6	2	5.03	4.97	-1.14%
5	2	3.45	3.42	-0.77%
4	2	2.53	2.51	-0.64%
3	2	1.33	1.32	-1.01%
2	2	0.53	0.52	-2.71%
1	2	0.27	0.24	-9.71%
0	2	0.00	0.01	~MDL
4	3	2.53	2.53	0.15%
2	3	0.53	0.52	-1.96%
5	3	3.45	3.44	-0.17%
1	3	0.27	0.25	-6.38%
6	3	5.03	5.03	0.01%
0	3	0.00	0.02	~MDL
3	3	1.33	1.31	-1.96%

Table 12. Ammonia accuracy.

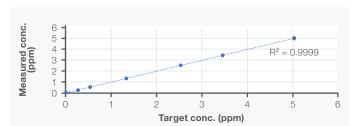


Figure 5. Ammonia linearity.

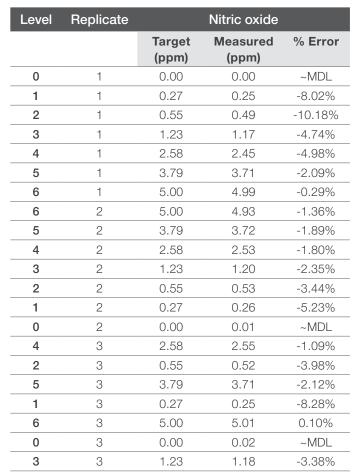


Table 13. Nitric oxide accuracy.

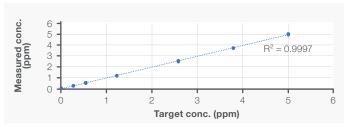


Figure 6. Nitric oxide linearity.

Level	Replicate	Nitrogen dioxide				
		Target (ppm)	Measured (ppm)	% Error		
0	1	0.00	0.01	~MDL		
1	1	0.29	0.26	-11.47%		
2	1	0.58	0.52	-9.31%		
3	1	1.30	1.22	-5.73%		
4	1	2.45	2.32	-5.34%		
5	1	3.74	3.50	-6.33%		
6	1	5.02	4.95	-1.37%		
6	2	5.02	4.94	-1.52%		
5	2	3.74	3.67	-1.79%		
4	2	2.45	2.40	-2.01%		
3	2	1.30	1.26	-2.94%		
2	2	0.58	0.56	-3.56%		
1	2	0.29	0.27	-5.21%		
0	2	0.00	0.01	~MDL		
4	3	2.45	2.41	-1.64%		
2	3	0.58	0.56	-2.99%		
5	3	3.74	3.68	-1.52%		
1	3	0.29	0.28	-3.97%		
6	3	5.02	4.92	-1.99%		
0	3	0.00	0.01	~MDL		
3	3	1.30	1.25	-3.45%		

Table 14. Nitrogen dioxide accuracy.

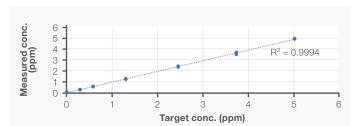


Figure 7. Nitrogen dioxide linearity.

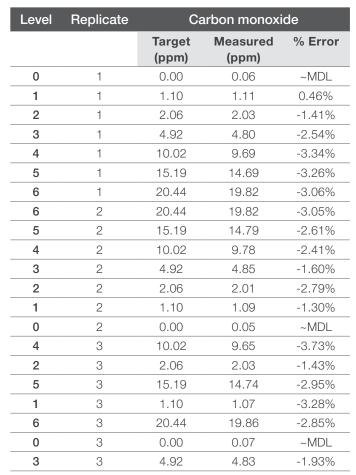


Table 15. Carbon monoxide accuracy.

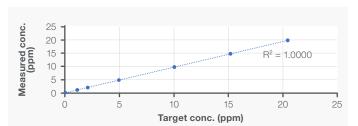


Figure 8. Carbon monoxide linearity.

Level	Replicate	Total sulfur (SO₂)				
		Target (ppb)	Measured (ppb)	% Error		
0	1	0	8	~MDL		
2	1	102	99	-2.61%		
4	1	248	270	9.20%		
3	1	146	146	0.27%		
1	1	44	50	15.16%		
4	2	248	271	9.53%		
1	2	44	47	7.90%		
0	2	0	10	~MDL		
3	2	146	157	7.75%		
2	2	102	103	1.43%		
3	3	146	142	-2.47%		
0	3	0	10	~MDL		
4	3	248	265	6.90%		
2	3	102	108	5.92%		
4	4	248	265	6.92%		
1	3	44	42	-2.93%		
3	4	146	156	7.26%		
0	4	0	6	~MDL		
2	4	102	104	2.11%		
1	4	44	47	8.22%		

Table 16. Total sulfur (SO₂) accuracy.

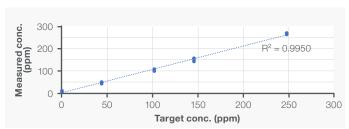


Figure 9. Total sulfur (SO₂) linearity.



Table 17. Oxygen accuracy.

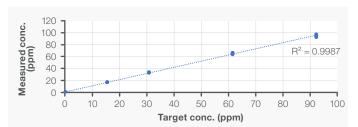


Figure 10. Oxygen linearity.

A summary of the accuracy and linearity studies is shown in Table 18.

For all the impurities tested, the linearity (R²) was >0.995. The average percent error was within $\pm 10\%$ for all impurities with the exception of acetaldehyde, where one replicate (Level 2, Replicate 2) was an outlier at 22.41% error. This may be due to a gas mixing error, as the remaining Level 2 replicates were all within $\pm 10\%$ of the target concentration.

To assess the accuracy and precision of the impurity measurements near the maximum allowable limit, the average percent error and RSD were calculated for the dilution level closest to the limit (Table 19).

For all impurities measured on the MAX-iR FTIR Gas Analyzer, the average percent error near the upper threshold limit was within $\pm 4\%$, or close to the analytical uncertainty of the reference gas. The oxygen accuracy was within $\pm 7\%$. For all impurities, the RSD was <4%, demonstrating excellent precision near the upper alarm threshold of the MAX-Bev CO₂ Purity Monitoring System.

Gas	Average percent error						Linearity (R²)
	Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	
Total hydrocarbon (C1)	-1.80%	-0.34%	0.56%	1.49%	-0.01%	-1.69%	0.9997
Total aromatic (benzene)	-0.09%	-2.03%	-2.77%	-1.18%	-2.12%	-1.10%	0.9993
Acetaldehyde	4.67%	13.27%	3.67%	2.75%	1.98%	1.20%	0.9996
Moisture	5.69%	3.81%	-0.41%	-2.25%	-2.31%	-1.83%	0.9998
Ammonia	-9.91%	-3.47%	-1.83%	-0.36%	-0.34%	-0.24%	0.9999
Nitric oxide	-7.17%	-5.86%	-3.49%	-2.62%	-2.04%	-0.52%	0.9997
Nitrogen dioxide	-6.88%	-5.28%	-4.04%	-2.99%	-3.22%	-1.63%	0.9994
Carbon monoxide	-1.37%	-1.88%	-2.02%	-3.16%	-2.94%	-2.99%	1.0000
Total sulfur (SO ₂)	7.09%	1.71%	3.20%	8.14%	N/A	N/A	0.9950
Oxygen	7.85%	6.89%	6.14%	2.91%	N/A	N/A	0.9987

Table 18. Accuracy and linearity summary results.

Gas	Units	Max allowable concentration	Performance near max allowable concentration				
			Level	Target conc.	Average % error	RSD	
Total hydrocarbon (C1)	ppm	50	Level 6	10.14	-1.69%	0.25%	
Total aromatic (benzene)	ppb	20	Level 2	17	-2.03%	2.10%	
Acetaldehyde	ppb	200	Level 3	206	3.67%	1.42%	
Moisture	ppm	20	Level 4	20.00	-2.25%	1.58%	
Ammonia	ppm	2.5	Level 4	2.53	-0.36%	0.44%	
Nitric oxide	ppm	2.5	Level 4	2.58	-2.62%	2.13%	
Nitrogen dioxide	ppm	2.5	Level 4	2.45	-2.99%	2.10%	
Carbon monoxide	ppm	10	Level 4	10.02	-3.16%	0.70%	
Total sulfur (SO ₂)	ppb	100	Level 2	102	1.71%	3.43%	
Oxygen	ppm	30	Level 2	30.7	6.89%	1.64%	

Table 19. Accuracy and precision near the maximum allowable concentration.



Learn more at thermofisher.com/max-bev

