

South Coast Air Quality Management District

Applied Science and Technology Source Testing and Engineering

TECHNICAL GUIDANCE DOCUMENT R-004

Rules: 2011-Protocol for Monitoring, Reporting, and Recordkeeping for Oxides of Sulfur (SO_x) Emissions, Appendix A, Chapter 2.
2012-Protocol for Monitoring, Reporting, and Recordkeeping for Oxides of Nitrogen (NO_x) Emissions, Appendix A, Chapter 2.

Date: October 2, 1997

Subject: Relative Accuracy Test Audit Outliers

References: 40 CFR Part 60
40 CFR Part 75
USEPA, Quality Assurance Handbook for Air Pollution Measurement Systems

1. Introduction

The AQMD has historically not allowed testers to discard any data obtained during CEMS relative accuracy test audit (RATA), unless the tester could justify with documentation that the data should be discarded due to either sampling error or process related effects. In the event that this justification could not be provided, the tester was required to use all of the test data. The AQMD is aware of the fact that 40 CFR Part 60 Appendix B allows testers to arbitrarily discard a maximum of three tests, but believes that arbitrary discarding of data is not technically sound, and could lead to misleading assessments of the accuracy of data collected under a CEMS program.

2. Objective

The AQMD does realize that outliers can occur during testing which the tester may not have discovered and documented at the time of testing, and an objective test can be used to determine outliers. The procedure in this technical guidance document is recommended if the tester chooses to discard any RATA test data after the minimum number of tests (nine) have been performed.

3. Procedure

One of the following procedures must be used to discard outliers as applicable:

a. One Outlier:

The Dixon Ratio test, as described in Appendix F of the EPA's Quality Assurance

Handbook for Air Pollution Measurement Systems (Vol. 1, USEPA Document EPA-6-/9-76-005, March 1976), shall be used as the test for a suspected single outlier in the data, using r_{11} or r_{21} criterion as appropriate for the number of data sets obtained during the CEMS testing. A normal distribution shall be assumed so that the test may only be done on the actual data and not log-transformed data. A significance level of 5% shall be used which corresponds to a 95% confidence test and is consistent with the other confidence intervals used for CEMS. If the Dixon Ratio test flags either the highest or lowest value as a potential outlier, the identified data may be discarded without further substantiation.

b. Two Outliers:

If two outliers are suspected the tester shall apply the Grubbs test for simultaneously testing those suspected values. The above criteria of normal distribution of data, 5% significance level, and discarding without further substantiation shall apply.

The above referenced Appendix F of the EPA's Quality Assurance Handbook for Air Pollution Measurement Systems is attached.

APPROVED

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attachment:

APPENDIX F

OUTLIERS

F.1 INTRODUCTION

An unusually large (or small) value or measurement in a set of observations is usually referred to as an outlier. Some of the reasons for an outlier in data are:

- Faulty instrument or component part
- Inaccurate reading of record, dial, etc.
- Error in transcribing data
- Calculation errors
- Actual value due to unique circumstances under which the observation(s) was obtained--an extreme manifestation of the random variability inherent in the data.

It is desired to have some statistical procedure to test the presence of an outlier in a set of measurements. The purpose of such tests would be to:

1. Screen data for outliers and hence to identify the need for closer control of the data generating process.
2. Eliminate outliers prior to analysis of the data. For example, in developing control charts the presence of outliers would lead to limits which are too wide and would make the use of the control charts of minimal, if any, value. In most statistical analysis of data (e.g., regression analysis and analysis of variance) the presence of outliers violate a basic assumption of the analysis. Incorrect conclusions are likely to result if the outliers are not eliminated prior to analysis. Outliers should be reported, and their omission from analysis should be noted.
3. Identify the real outliers due to unusual conditions of measurement (e.g., a TSP concentration which is abnormally

large due to local environmental conditions during the time of sample collection). Such observations would not be indicative of the usual concentrations of TSP, and may be eliminated depending on the use of the data. Ideally, these unusual conditions should be recorded on the field data report. Failure to report complete information and unusual circumstances surrounding the collection and analysis of the sample often can be detected by outlier tests. Having identified the outliers using one or more tests, it is necessary to determine, if possible, the cause of the outlier and then to correct the data if appropriate.

It will be assumed in this discussion that the measurements are normally distributed and that the sample of n measurements is being studied for the possibility of one or two outliers. If the measurements are lognormally distributed, such as for concentration of TSP, then the logarithm of the data should be taken prior to application of the tests given herein.

F.2 PROCEDURE(S) FOR IDENTIFYING OUTLIERS

Let the set of n measurements be arranged in ascending order and denoted by

$$X_1, X_2, \dots, X_n$$

where X_i denotes the i th smallest measurement. Suppose that X_n is suspected of being too large, and that a statistical test is to be applied to the particular measurement to determine whether X_n is consistent with the remaining data in the sense that it is reasonable that it is part of the same population of measurements from which the sample is taken. Consider the following TSP data from a specific monitoring site during August 1978.

Example F.1	<u>TSP, $\mu\text{g}/\text{m}^3$</u>	<u>ln TSP</u>
	40	3.69
	88	4.48
	71	4.26
	175	5.16
	85	4.44

One test procedure for questionable data is to use a test by Dixon,¹ see Table F.1,

$$r_{10} = \frac{X_n - X_{n-1}}{X_n - X_1} = \frac{175-88}{175-40} = \frac{87}{135} = 0.655. \quad (1)$$

Referring to Table F.1 the 5% significance level for r_{10} is 0.642 and we would thus declare that the value 175 appears to be an outlier. The value should be flagged for further investigation. We do not automatically remove data because a statistical test indicates the value(s) to be questionable.

Suppose that we know that the data are lognormally distributed (or at least that the log normal distribution is a very good approximation), then we should examine the Dixon Ratio for this example. Using the logarithm, the Dixon ratio is

$$r_{10} = \frac{5.16 - 4.48}{5.16 - 3.69} = 0.46,$$

and this value is not significant at the 5% level. Hence on this basis the extreme value 175 is not questionable.

We still may wish to investigate the value further (data permitting) and we compare the data with those at a neighboring site. The corresponding data are given below.

<u>Site 20</u> <u>TSP, $\mu\text{g}/\text{m}^3$</u>	<u>Site 14</u> <u>TSP, $\mu\text{g}/\text{m}^3$</u>
40	42
88	53
71	56
175	129
85	64

Thus we see that the value 175 does not appear to be questionable in view of the corresponding value for a neighboring site. Both sites have high values on the same day, suggesting a common source of the high values. The only means to investigate these values further is to go to the source of the data collection and review the meteorological factors, comments in the site logbooks relative to local construction activity, daily traffic, and other possible causation factors.

TABLE F.1. DIXON CRITERIA FOR TESTING OF EXTREME OBSERVATION (SINGLE SAMPLE)*

n	Criterion	Significance level		
		10%	5%	1%
3	$r_{10} = \frac{x_2 - x_1}{x_n - x_1}$ if* smallest value is suspected;	.886	.941	.988
4		.679	.765	.889
5		.557	.642	.780
6	$= \frac{x_n - x_{n-1}}{x_n - x_1}$ if largest value is suspected.	.482	.560	.698
7		.434	.507	.637
8	$r_{11} = \frac{x_2 - x_1}{x_{n-1} - x_1}$ if smallest value is suspected;	.479	.554	.683
9		.441	.512	.635
10		.409	.447	.597
	$= \frac{x_n - x_{n-1}}{x_n - x_2}$ if largest value is suspected.			
11	$r_{21} = \frac{x_3 - x_1}{x_{n-1} - x_1}$ if smallest value is suspected.	.517	.576	.679
12		.490	.546	.642
13		.467	.521	.615
	$= \frac{x_n - x_{n-2}}{x_n - x_2}$ if largest value is suspected.			
14	$r_{22} = \frac{x_3 - x_1}{x_{n-2} - x_1}$ if smallest value is suspected.	.492	.546	.641
15		.472	.525	.616
16	$= \frac{x_n - x_{n-2}}{x_n - x_3}$ if largest value is suspected;	.454	.507	.595
17		.438	.490	.577
18		.424	.475	.561
19		.412	.462	.547
20		.401	.450	.535
21		.391	.440	.524
22		.382	.430	.514
23		.374	.421	.505
24		.367	.413	.497
25		.360	.406	.489

*Reproduced with permission from W. J. Dixon, "Processing Data for Outliers," Biometrics, March 1953, Vol. 9, No. 1, Appendix, Page 89. (Reference [1])

$$x_1 \leq x_2 \leq \dots \leq x_{n-2} \leq x_{n-1} \leq x_n$$

Criterion r_{10} applies for $3 \leq n \leq 7$

Criterion r_{11} applies for $8 \leq n \leq 10$

Criterion r_{21} applies for $11 \leq n \leq 13$

Criterion r_{22} applies for $14 \leq n \leq 25$

This example points out several considerations in validating data and in particular in detecting and flagging outliers.

1. The use of a statistical procedure for detecting an outlier is a first step and the result should not be to throw out the value(s) if the statistic is significant but to treat the value(s) as suspect until further information can be obtained.

2. The statistical procedures depend on specific assumptions, particularly concerning the distribution of the data--normal, lognormal, and Weibull--and the result should be checked using the distribution which best approximates the data.

3. Often there are values at neighboring sites which can be used to compare the values. If the values at the two sites are correlated, as in the Example F.1, this approach can be very helpful.

4. The final resolution of the suspect values can be made by the collection agency, thus the importance of performing the data validation at the local agency.

Another commonly used test procedure,² requires additional computation and is given by

$$T_n = (X_n - \bar{X})/s \quad (2)$$

where: X_n is the largest observed value among n measurements,
 \bar{X} is the sample average,
s is the sample standard deviation (i.e.,
 $s = \{\sum(X - \bar{X})^2 / (n-1)\}^{1/2}$).

For the data set previously given,

$$\begin{aligned} X_n &= 175 \\ \bar{X} &= 91.8 \\ s &= 50.2 \end{aligned}$$

and hence $T_n = 1.66$, which is not significant at the 0.05 level, that is, it is less than 1.672 which is the tabulated value for this level from Table F.2. This test result is not in agreement with the previous one, however, both test results are borderline

TABLE F.2. TABLE OF CRITICAL VALUES FOR T(ONE-SIDED TEST OF T_1 OR T) WHEN THE STANDARD DEVIATION IS CALCULATED FROM THE SAME SAMPLE

Number of Observations n	Upper .1% Significance Level	Upper .5% Significance Level	Upper 1% Significance Level	Upper 2.5% Significance Level	Upper 5% Significance Level	Upper 10% Significance Level
3	1.155	1.155	1.155	1.155	1.153	1.148
4	1.499	1.496	1.492	1.481	1.463	1.425
5	1.780	1.764	1.749	1.715	1.672	1.602
6	2.011	1.973	1.944	1.887	1.822	1.729
7	2.201	2.139	2.097	2.020	1.938	1.828
8	2.358	2.274	2.221	2.126	2.032	1.909
9	2.492	2.387	2.323	2.215	2.110	1.977
10	2.606	2.482	2.410	2.290	2.176	2.036
11	2.705	2.564	2.485	2.355	2.234	2.088
12	2.791	2.636	2.550	2.412	2.285	2.134
13	2.867	2.699	2.607	2.462	2.331	2.175
14	2.935	2.755	2.659	2.507	2.371	2.213
15	2.997	2.806	2.705	2.549	2.409	2.247
16	3.052	2.852	2.747	2.585	2.443	2.279
17	3.103	2.894	2.785	2.620	2.475	2.309
18	3.149	2.932	2.821	2.651	2.504	2.335
19	3.191	2.968	2.854	2.681	2.532	2.361
20	3.230	3.001	2.884	2.709	2.557	2.385
21	3.266	3.031	2.912	2.733	2.580	2.408
22	3.300	3.060	2.939	2.758	2.603	2.429
23	3.332	3.087	2.963	2.781	2.624	2.448
24	3.362	3.112	2.987	2.802	2.644	2.467
25	3.389	3.135	3.009	2.822	2.663	2.486
26	3.415	3.157	3.029	2.841	2.681	2.502
27	3.440	3.178	3.049	2.859	2.698	2.519
28	3.464	3.199	3.068	2.876	2.714	2.534
29	3.486	3.218	3.085	2.893	2.730	2.549
30	3.507	3.236	3.103	2.908	2.745	2.563
31	3.528	3.253	3.119	2.924	2.759	2.577
32	3.546	3.270	3.135	2.938	2.773	2.591
33	3.565	3.286	3.150	2.952	2.786	2.604
34	3.582	3.301	3.164	2.965	2.799	2.616
35	3.599	3.316	3.178	2.979	2.811	2.628
36	3.616	3.330	3.191	2.991	2.823	2.639
37	3.631	3.343	3.204	3.003	2.835	2.650
38	3.646	3.356	3.216	3.014	2.846	2.661
39	3.660	3.369	3.228	3.025	2.857	2.671
40	3.673	3.381	3.240	3.036	2.866	2.682
41	3.687	3.393	3.251	3.046	2.877	2.692
42	3.700	3.404	3.261	3.057	2.887	2.700
43	3.712	3.415	3.271	3.067	2.896	2.710
44	3.724	3.425	3.282	3.075	2.905	2.719
45	3.736	3.435	3.292	3.085	2.914	2.727
46	3.747	3.445	3.302	3.094	2.923	2.736
47	3.757	3.455	3.310	3.103	2.931	2.744
48	3.768	3.464	3.319	3.111	2.940	2.753
49	3.779	3.474	3.329	3.120	2.948	2.760
50	3.789	3.483	3.336	3.128	2.956	2.768

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Use $T_1 = \frac{\bar{X} - X_1}{s}$ when testing the smallest value, X_1 .

Use $T = \frac{X_n - \bar{X}}{s}$ when testing the largest value, X_n in a sample of n observations. Unless one has prior information about largest values (or smallest values) the risk levels should be multiplied by two for application of the test.

TABLE F.2 (continued)

Number of Observations n	Upper .1% Significance Level	Upper .5% Significance Level	Upper 1% Significance Level	Upper 2.5% Significance Level	Upper 5% Significance Level	Upper 10% Significance Level
51	3.798	3.491	3.345	3.136	2.964	2.775
52	3.808	3.500	3.353	3.143	2.971	2.783
53	3.816	3.507	3.361	3.151	2.978	2.790
54	3.825	3.516	3.368	3.158	2.986	2.798
55	3.834	3.524	3.376	3.166	2.992	2.804
56	3.842	3.531	3.383	3.172	3.000	2.811
57	3.851	3.539	3.391	3.180	3.006	2.818
58	3.858	3.546	3.397	3.186	3.013	2.824
59	3.867	3.553	3.405	3.193	3.019	2.831
60	3.874	3.560	3.411	3.199	3.025	2.837
61	3.882	3.566	3.418	3.205	3.032	2.842
62	3.889	3.573	3.424	3.212	3.037	2.849
63	3.896	3.579	3.430	3.218	3.044	2.854
64	3.903	3.586	3.437	3.224	3.049	2.860
65	3.910	3.592	3.442	3.230	3.055	2.866
66	3.917	3.598	3.449	3.235	3.061	2.871
67	3.923	3.605	3.454	3.241	3.066	2.877
68	3.930	3.610	3.460	3.246	3.071	2.883
69	3.936	3.617	3.466	3.252	3.076	2.888
70	3.942	3.622	3.471	3.257	3.082	2.893
71	3.948	3.627	3.476	3.262	3.087	2.897
72	3.954	3.633	3.482	3.267	3.092	2.903
73	3.960	3.638	3.487	3.272	3.098	2.908
74	3.965	3.643	3.492	3.278	3.102	2.912
75	3.971	3.648	3.496	3.282	3.107	2.917
76	3.977	3.654	3.502	3.287	3.111	2.922
77	3.982	3.658	3.507	3.291	3.117	2.927
78	3.987	3.663	3.511	3.297	3.121	2.931
79	3.992	3.669	3.516	3.301	3.125	2.935
80	3.998	3.673	3.521	3.305	3.130	2.940
81	4.002	3.677	3.525	3.309	3.134	2.945
82	4.007	3.682	3.529	3.315	3.139	2.949
83	4.012	3.687	3.534	3.319	3.143	2.953
84	4.017	3.691	3.539	3.323	3.147	2.957
85	4.021	3.695	3.543	3.327	3.151	2.961
86	4.026	3.699	3.547	3.331	3.155	2.966
87	4.031	3.704	3.551	3.335	3.160	2.970
88	4.035	3.708	3.555	3.339	3.163	2.973
89	4.039	3.712	3.559	3.343	3.167	2.977
90	4.044	3.716	3.563	3.347	3.171	2.981
91	4.049	3.720	3.567	3.350	3.174	2.984
92	4.053	3.725	3.570	3.355	3.179	2.989
93	4.057	3.728	3.575	3.358	3.182	2.993
94	4.060	3.732	3.579	3.362	3.186	2.996
95	4.064	3.736	3.582	3.365	3.189	3.000
96	4.069	3.739	3.586	3.369	3.193	3.003
97	4.073	3.744	3.589	3.372	3.196	3.006
98	4.076	3.747	3.593	3.377	3.201	3.011
99	4.080	3.750	3.597	3.380	3.204	3.014
100	4.084	3.754	3.600	3.383	3.207	3.017

Source: Grubbs, F. E., and Beck, G., Extension of Sample Sizes and Percentage Points for Significance Tests of Outlying Observations, Technometrics, Vol. 14, No. 4, Nov. 1972, pp. 847-854.

situations. If the T_n is applied to the logarithms, the result is $T_n = \frac{5.16-4.41}{0.527} = 1.42$, which is not significant and which agrees with the Dixon ratio test. In many examples it will be obvious that a particular value is an outlier, whereas in Example F.1 this is not the case. A plot of the data is often helpful in examining a set of data.

After rejecting one outlier using either T_n or T_1 the analyst may be faced with the problem of considering a second outlier. In this case the mean and standard deviation may be re-estimated and either T_{n-1} or T_1 applied to the sample of $n-1$ measurements. However, the user should be aware that the test T_n or T_1 is not theoretically based on repeated use.

Grubbs² gives a test procedure (including tables for the critical values) for simultaneously testing the two largest or two smallest values. This procedure is not given here.

The use of the procedures given in Table F.1 requires very little computation and would be preferable on a routine basis. Grubbs³ gives a tutorial discussion of outliers and is a very good reference to the subject. A recent text on outliers is also recommended to the reader with some statistical background.⁴

One other procedure for data validation which has an advantage relative to the previous two procedures (Dixon and Grubbs) is the use of a statistical control chart.^{5,6} The control chart is discussed in Appendix H and the reader is referred to that Appendix for details in application. The TSP data for a specific site for the years 1975 to 1977 for which there are five measurements per month are used as a historical data base for the control chart and the data for 1978 are plotted on the chart to indicate any questionable data. These data are shown in Table F.3 (historical data) and in Table F.4 (1978 data). Figure F.1 (upper part) is the control chart with both 2σ and 3σ limits for the averages.

$$\bar{\bar{X}} \text{ (average of the } \bar{X}'\text{s)} = 56.5 \text{ } \mu\text{g}/\text{m}^3$$

TABLE F.3. TSP DATA FROM SITE 397140014H01 SELECTED AS HISTORICAL DATA BASE FOR SHEWHART CONTROL CHART (1975-1977)

Month-year	Mean (\bar{X}), $\mu\text{g}/\text{m}^3$	Range (R), $\mu\text{g}/\text{m}^3$	Month-year	Mean (\bar{X}), $\mu\text{g}/\text{m}^3$	Range (R), $\mu\text{g}/\text{m}^3$
1-75	54.6	67	10-76	34.6	50
5-75	63.8	39	11-76	53.4	29
6-75	59.0	25	12-76	52.2	44
7-75	63.0	23	3-77	40.4	28
8-75	68.2	54	4-77	63.6	57
10-75	41.8	26	6-77	45.4	31
11-75	68.4	81	7-77	53.4	19
12-75	57.6	39	8-77	58.6	26
1-76	82.4	87	9-77	46.0	12
4-76	90.2	117	10-77	45.6	33
5-76	43.8	48	11-77	49.8	54
7-76	72.6	80	12-77	30.4	22
9-76	73.4	83			

TABLE F.4. TSP DATA FROM SITE 397140014H01 FOR CONTROL CHART (1978)

Data set	Month	Mean	Range	s
1	1	30.6	27	10.4
2	2	47.4	60	21.7
3	3	54.4	39	17.2
4	4	31.8	29	13.6
5	5	53.6	46	21.8
6	6	64.8	46	19.0
7	8	68.8	87	34.6
8	9	43.2	31	11.3
9	10	52.4	59	24.2
10	11	60.8	71	29.0
11	12	31.6	22	9.8

$$\begin{aligned}\sigma_{\bar{X}} & \text{ (standard deviation of the mean)} = 9.0 \mu\text{g}/\text{m}^3 \\ \text{UWL}_{\bar{X}} & \text{ (upper } 2\sigma \text{ limit)} = 74.5 \mu\text{g}/\text{m}^3 \\ \text{LWL}_{\bar{X}} & \text{ (lower } 2\sigma \text{ limit)} = 38.5 \mu\text{g}/\text{m}^3 \\ \text{UCL}_{\bar{X}} & \text{ (} 3\sigma \text{)} = 83.5 \mu\text{g}/\text{m}^3 \\ \text{LCL}_{\bar{X}} & \text{ (} 3\sigma \text{)} = 29.5 \mu\text{g}/\text{m}^3\end{aligned}$$

Figure F.1 shows three averages below the $\text{LWL}_{\bar{X}}$ (2σ limit) and no values above the $\text{UWL}_{\bar{X}}$ (2σ limit). No values are below the 3σ limit $\text{LCL}_{\bar{X}}$ (3σ). Hence we do not suspect any averages to be significantly different from the historical average and which would suggest further investigation.

Figure F.1 (lower part) is the control chart for the standard deviation.

$$\begin{aligned}\bar{R} & \text{ (average range)} = 47.0 \\ \hat{\sigma} & = 0.43 (47.0) = 20.2 \\ \text{UWL}_s & \text{ (upper } 2\sigma \text{ limit for } s\text{)} = 33.7 \\ \text{LWL}_s & \text{ (lower } 2\sigma \text{ limit for } s\text{)} = 7.0 \\ \text{UCL}_s & \text{ (99.5 percentile)} = 38.9 \\ \text{LCL}_s & \text{ (0.5 percentile)} = 4.6\end{aligned}$$

There is a single outlier on this chart and this sample (one month of data--5 values) should be checked for factors which might explain the high value for the standard deviation. See Example F.1 for further discussion of this example relative to action taken after the flagging or identification of the questionable value. The same data were used in that example.

The advantage of the quality control chart approach is that not only are questionable values within a month detected, but also if all of the values for a month are high relative to values for other months, they will be flagged. The latter can result from personnel changes, instrument problems, calculation errors, and such changes will go undetected when comparing a single possible outlier within a data set. It is recommended that both test procedures (Dixon or Grubbs and the control chart) be used if resources permit, if not use the control chart technique.

F.3 GUIDANCE ON SIGNIFICANCE LEVELS

The problem of selecting an appropriate level of significance in performing statistical tests for outliers is one of comparing two resulting costs. If the significance level is set too high (e.g., 0.10 or 0.20) there is the cost of investigating the data identified as questionable a relatively large proportion of the time that, in fact, the data are valid.¹ On the other hand, if the significance level is set too low (e.g., 0.005 or 0.001) invalid data may be missed and these data may be subsequently used in making incorrect decisions. This cost can also be large but is difficult to estimate. The person responsible for data validation must therefore seek an appropriate level based on these two costs. If the costs of checking the questionable data are small, it is better to err on the safe side and use $\alpha = 0.05$ or 0.10 say. Otherwise, a value of $\alpha = 0.01$ would probably be satisfactory for most applications. As experience is gained with the validation procedure, the α value should be adjusted as necessary to minimize the total cost (i.e., the cost of investigating outliers plus that of making incorrect decisions).

F.4 REFERENCES

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