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NASA TECHNICAL MEMORANDUM

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ON EVALUATING COMPLIANCE WITH AIR POLLUTION LEVELS "NOT TO BE EXCEEDED MORE THAN ONCE PER YEAR"

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Cleveland, Ohio

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E-7762

ABSTRACT

This study considers the adequacy of currently practiced monitoring and data reduction techniques for assessing compliance with 24-hour Air Quality Standards (AQS) not to be exceeded more than once per year. Consider as an example the present situation for suspended particulates. The federal AQS in part mandates a limit of 260 micrograms per cubic meter - maximum 24-hour concentration not to be exceeded more than once per year, while EPA guideline documents state that adequate coverage may be maintained with sampling frequencies of from every third day to once every sixth day. Because this AQS does not limit the pollution load for the worst day of each year, the estimated value one seeks for comparison with this AQS is that of the second most polluted (SMP) day. Since one has only (typically) 60 to 120 measured values, it is necessary to estimate SMP in order to determine compliance/noncompliance with this AQS which is in terms of the 364th of 365 ranked values.

We quantitatively consider the inherent variability of estimating SMP levels from order statistics for the normal distribution lost on samples of 30 to 365 measurements. In addition, we consider the validity of: assumption of independence between observations; the interchange of

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exponentiation and expectation operations in extending normal order statistics to the log normal distribution; and the substitution of an estimated-maximum "design value" for the SMP value specified in the AQS.

With regard to the four points discussed above, we conclude

(1) For typical less than daily sampling (i.e., 60 to 120 24-hour samples per year) the deviation from independence of the data set should not be substantial.

(2) The interchange of exponentiation and expectation operations in the EPA data reduction model, underestimates the second highest level by about 4 to 8 percent for typical σ values.

(3) Estimates of the second highest pollution level have associated with them a large statistical variability arising from the finite size of the sample. The 0.95 confidence interval ranges from $\pm$40 percent for 120 samples per year to $\pm$84 percent for 30 samples per year.

(4) The design value suggested by EPA for abatement and/or control planning purposes typically gives a margin of safety of 60 to 120 percent.

INTRODUCTION

This paper is addressed to various statistical considerations from using guidelines for air quality surveillance in conjunction with a mathematical model (EPA-MM) as presented in U. S. Environmental Protection Agency (EPA) documents (refs. 1 and 2). The point of view we take is that the EPA Air Quality Standards (AQS) represent conditions which must be made to exist in the ambient environment. The statistical techniques developed should serve as tools for measuring how close one is to achieving the desired quality of air. We shall show that the sampling frequency recommended by EPA is inadequate to meet these objectives when the standard is expressed as a level not to be exceeded more than once per year and sampling frequency is once every three days or less frequent. This inadequancy came to our attention in the course of a joint Air Pollution study between NASA Lewis Research Center and the City of Cleveland, Ohio Air Pollution Control Division.

For clarity let us consider as an example the present situation for suspended particulates, although the same considerations apply to other pollutants as well.

The standards in part are expressed (ref. 3) as

(a) Maximum of 75 micrograms per cubic meter - annual geometric mean.

(b) 260 micrograms per cubic meter - maximum 24-hour concentration not to be exceeded more than once per year.

With regard to monitoring it is stated that (ref. 1) adequate coverage may be maintained with intermittent sampling. Suggested sampling frequencies are from every third day to once every sixth day.

It is obvious that part (a) of the AQS can best be estimated by the mean of the sample data.[1] For notational purposes we refer to part (b) of the AQS as

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[1]The reliability (variability) of such an estimate is considered in reference 4. The correct expression is given in their equation (1). The use of equation (2) is an error arising from a misconception of the statistical model as is made clear later in this paper and elsewhere (ref. 5).

MAX2 and observe that MAX2 does not put any direct limit on how polluted the ambient air may be on one day of each year. Thus, the estimated value one seeks for comparison with MAX2 is that of the second most polluted (SMP) day. It is considerably more difficult to estimate SMP in order to determine compliance/noncompliance with MAX2 which is in terms of 365 ranked values, since one has only (typically) 60 to 120 measured values.

In the framework of the above introduction we will consider the inherent variability of estimating SMP levels from samples of 30 to 365 measurements. In addition we will consider three other points that have appeared recently (refs. 6 and 7) concerning EPA-MM. Patel (ref. 6) has questioned two aspects of the analysis, namely the assumption of independence between observations and the interchange of the exponentiation and expectation operators (IEE). Larsen in his response (ref. 7) minimizes the practical impact of these criticisms by emphasizing an additional (intentional) irregularity, namely, the substitution of a maximum "design value" for the next-to-the-highest value specified in the national ambient air quality standards (AQS).

STATISTICAL CONSIDERATIONS

We feel that it is necessary for a distinction to be made between the legal and statistical aspects of viewing the data. From the statistical viewpoint one assumes each successive day represents an independent pollutant level from a single population of potential pollutant levels (theoretically infinite in size). It is this assumption of independence that Patel questions. We realize that this may not be strictly valid. In fact, a time series representation of the data is the preferred analysis. However, the representation of the pollution process as a time series is not always a feasible approach, especially for small, irregularly spaced sample sets. We intend to show that even though approximate independence can be achieved, the estimate of MAX2 is too variable for practical use.

Some assumption is then made about the distribution of the pollutant levels. The standard, and empirically most satisfying assumption is that the log-normal distribution (ref. 8) is an adequate representation. Statistically speaking the set of levels that would be obtained by actually monitoring on each of 365 days of the year is a single random sample of size 365 from an infinite population of possible levels. Sampling every second (third, fourth, etc.) day instead of every day only reduces the size of the sample. It does not introduce any new statistical concepts of populations. For the purpose of studying pollution, designing an abatement or control program, analyzing health effects etc. this is the appropriate concept.

Two possible model errors are that the distribution of levels may not be as claimed or that the distribution may change with time. Further errors would arise from the fact we are only obtaining a finite (even if it be of size 365) random sample from an infinite population. In this sense even daily sampling does not represent perfect sampling and complete knowledge because of meteorological, economic etc. variability from year to year.

The emphasis and outlook must change when one takes the legal aspect of pollution monitoring into account. If, for example, the air is monitored every 10th day, and one finds that the mean for this sample is 55 and the highest measured value is 255, then it is very likely that the actual SMP for the year exceeds 260. This is not legally equivalent to showing that SMP did in fact exceed 260. Thus, in a sense, sampling every day is a legal optimum.

As stated previously, the point of view we take is that the legal AQS represents conditions which must be made to exist in the ambient environment. The statistical techniques developed should serve as tools for measuring how close one is to achieving the desired quality of air. Thus we are basically concerned with the reliability of estimates of the mean pollution level and the 364th of 365 ranked observations considered as a sample from an infinite population. We are also concerned with the reliability (variability) of these estimates.

If the previously mentioned assumptions, namely independence and log normality, are made, it is possible to proceed. (We note again that if a time series representation were more practical it could also provide such estimates.) EPA has suggested a mathematical model which is partially graphical (EPA-MM). In our experience as part of a cooperative program with Cleveland, Ohio (ref. 9) we have found it simpler to use an analytical formula which is presented later as equation (2). (The implications of using eq. (2) as well as the motivation for the use of this model are discussed in some detail in appendix A of the NASA publication NASA TN D-7527.)

Both of these formulations in effect (1) transform the log-normally distributed data set into a normally distributed data set, (2) compute the mean and standard deviation of the sample, (3) use these two values obtained from the sample as estimates for the population parameters, (4) compute the expected 364th of 365 ranked observations from that population, and (5) estimate the actual SMP as the exponential of the value obtained in (4). It is this sequence that is questioned by Patel who correctly points out that exponentiating a value estimated from a normal set is not the same as estimating the expected next to the largest value directly from equivalent log-normal sets of size 365. It should be explained that this use of normal order statistics did not result from ignorance of the point raised by Patel, but rather from the fact that the order statistics are well known for the normal distribution (ref. 10). Only recently have they even been evaluated for very small sample sizes of log-normally distributed sets (ref. 11).

As mentioned earlier, EPA (ref. 7) suggests that for control and abatement planning one should estimate the expected 365th of 365 ranked values, rather than the expected 364th value. This is designated as a "design value" to compensate for variability from sample to sample. However, there is no discussion of the magnitude or adequacy of such a correction factor. Nor is the approach of any assistance in determining actual compliance with AQS. This "design value" is discussed quantitatively in a later section.

INDEPENDENCE OF DATA

Having briefly summarized the points of interest and the pertinent statistical considerations we will now make some quantitative remarks. The assumption of independence was questioned intuitively by Patel. He also demonstrated for National Air Surveillance Network - Continuous Air Monitoring Program (CAMP) data (refs. 2 and 6) that a criterion for independence based on the following test of the ratios of variances is not met.

If $x_1, \ldots, x_n$ are all independent and identically distributed random variables with variance σ^2, then $m = \sum x/n$ has variance σ^2/n. Thus the variance of data accumulated using x-hour averaged data (V_x) divided by the variance of data accumulated using y-hour averaged data (V_y) should be about

$$\frac{V_x}{V_y} = \frac{\sigma^2/x}{\sigma^2/y} = y/x$$

We have applied the same test to data amassed over six years by the Air Pollution Control Division of Cleveland, Ohio and in general do not find the deviation from independence to be at all substantial. The results are listed in table I-III. Table I is for total suspended particulate and table II is for nitrogen dioxide. Table III is for sulfur dioxide and also lists the corresponding results obtained by Patel for CAMP data. At the bottom of each table we also list the expected values for fully independent sets. Overall, the deviations from anticipated values, assuming independence, are not substantial and nowhere do our calculated values approach those obtained by Patel.

A further check on the independence of the data may be made as follows. If the successive data values (x_1, x_2, ... x_n) are truly independent, then there should be zero correlation between pair of singly offset values (e.g. (x_1, x_2), (x_2, x_3) . . .) and similarly for doubly offset pairs (e.g. (x_1, x_3), (x_2, x_4). Also shown on the right side of tables I-III are the results of these calculations. Again, there is some evidence of small positive correlations, but not sufficiently so to be considered serious.

Intuitively, this appears to be a reasonable result. The measurements used in CAMP were taken every five minutes and it is to be expected that successive measurements should be related. On the other hand, the time interval between successive measurements in the data we analyzed has typically been from three to six days.

In view of the meteorological variability of the region it is not very probable that successive data points so separated in time would be substantially correlated. This naturally is satisfying in terms of the applicability of the statistical model. However, it will be seen later that this three to six day interval between measurements is not without its cost, in that the uncertainty it introduces into SMP estimates is quite large.

INTERCHANGE OF EXPONENTIATION AND EXPECTATION (IEE)

The problem with preceding the exponentiation operation by the expectation operation is portrayed clearly with an artifical example by Patel (ref. 5).

To determine how much effect this might have on the analysis of air pollution data we performed a computer simulation of the correct procedure and compared it with the estimation based on normal order statistics. The experiment was a Monte-Carlo (MC) simulation provided by sampling from a nearly infinite ($2^{32} - 1$) standard normal set (mean, $\mu = 0$; standard deviation, $\sigma = 1$) from which 365 values were randomly selected and exponentiated. This set of 365 values was then ranked and the 364th value, corresponding to SMP, was located. This was repeated 3800 times and the mean and standard deviations were obtained for these 3800 SMP values. The mean SMP was 14.27. This compares with 13.87 based on normal order statistics where

$$SMP = e^{(\mu + 2.63\,\sigma)} \qquad (1)$$

and

$\mu = 0$

$\sigma = 1$

2.63 is the normal order statistic for the 364th of 365 ranked values (ref. 11)

In practice we use

$$SMP = \exp(m + 2.63\ s) \qquad (2)$$

m = sample mean of the normal variates

s = sample standard deviation of the normal variates

By contrast ln(14.27) = 2.66. To approximately assess the impact of this difference we can take the ratio of the estimate from the method using normal order statistics to our method using the Monte Carlo equivalent order statistic and find

$$\frac{e^{(\mu + 2.63\ \sigma)}}{e^{(\mu + 2.66\ \sigma)}} = e^{-0.03\ \sigma} \simeq 1 - 0.03\ \sigma, \qquad (\sigma < 3).$$

For typical air quality data (ref. 10) $1.3 < \sigma < 2.7$. Thus the error in inverting the sequence of operations results in underestimating the actual value by about 4 to 8 percent

"DESIGN VALUE" SAFETY FACTOR

For planning purposes the EPA suggests the use of the expected annual maximum level as opposed to the expected annual SMP in order to compensate for the year to year fluctuations (refs. 2 and 7) and the underestimate inherent in EPA-MM itself (ref. 7). The suggested corresponding normal order statistic is 2.94. The margin of safety introduced by this suggestion can be estimated as we did above and indicates a margin of safety over using SMP of $e^{0.31\ \sigma}$. For $\sigma = 1.5$ this is a 60 percent overestimate while for $\sigma = 1.5$ this is a 60 percent overestimate while for $\sigma = 2.5$ it is a 117 percent overestimate. This is obviously adequate to compensate for the IEE error.

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SMP VARIABILITY

In order to get some information on the variability of the estimated SMP value a further series of Monte-Carlo computer experiments were performed. Similar to the experiment described above we sampled n pseudo random observations from a normal distribution with mean zero and standard deviation 1. For each set of n observations we used equation (2) to estimate SMP and recorded the value. This was repeated thousands of times for each n(n = 30, 60, 90, 120, 365). Based on this we obtained the results listed in table IV and which are also shown graphically in figures 1 and 2. The variability is shown in the last column of table IV which indicates the range of values expressed as a percent of the mean SMP required to include 95 percent of all the calculated SMP's. The first 5 rows give the results of this experiment. The next row shows the results of the Monte-Carlo experiment described earlier with the values obtained from actual rankings. For samples of size 365 the calculations show the variability to be greater in a straight-forward ranking than when calculated from equation (2). This is quite reasonable as the latter gives more weight to the entire sample set through m and s. The calculations also show that the smaller the sample size, the larger the expectation of SMP. This is a consequence of the properties of the distribution of s. We also display the expected SMP values in figure 1 and the variability in figure 2 as plots against n. The value of 14.27 obtained from the 365 ranked values appears to be the asymptote for the calculated values.

The present federal monitoring schedule requires a minimum of

60 samples per year (ref. 1) which gives a variability of 56 percent at the 0.95 confidence level. This is well bounded by the EPA "design value." However, in attempting to assess compliance in any given year or trends over a few years (as opposed to control planning) it appears that where a large time interval exists between measurements (which makes the sample set independent) the utility of estimates of SMP is marginal because of the large variability.

CONCLUSION

With regard to the four points discussed above we conclude

(1) For typical less than daily sampling (i.e., 60 to 120 24-hour samples per year) the deviation from independence of the data set should not be substantial.

(2) The interchange of exponentiation and expectation operations in the EPA data reduction model, underestimates the second highest level by about 4 to 8 percent for typical σ values.

(3) Estimates of the second highest pollution level have associated with them a large statistical variability arising from the finite size of the sample. The 0.95 confidence interval ranges from ±40 percent for 120 samples per year to ±84 percent for 30 samples per year.

(4) The design value suggested by EPA for abatement and/or control planning purposes typically gives a margin of safety of 60 to 120 percent.

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TABLE I. - STATISTICS FOR MEASURING INDEPENDENCE OF TSP OBSERVATIONS. LISTED ARE THE OBSERVED RATIOS VARIANCES FOR X-HR AVERAGES OPPOSED TO Y-HR AVERAGES AND THE OBSERVED CORRELATIONS FOR SINGLE AND DOUBLE OFFSETS

STA	# RDGS	Ratio of variances $\frac{VAR (X-HR)}{VAR (Y-HR)}$								Correlations	
		48/24	72/24	96/24	120/24	144/24	168/24	142/24	216/24	Single offset	Double offset
1	382	0.5350	0.3797	0.3428	0.2856	0.2194	0.2555	------	------	0.1325	0.1399
2	388	.5375	.3836	.3067	.2895	.2414	.2219	------	------	.0784	.0936
3	494	.5453	.4533	.3373	.3312	.3049	.2830	0.2711	0.2778	.1390	.1757
4	364	.6574	.4634	.4727	.4110	.4028	.3381	------	------	.2606	.2284
5	474	.5781	.4458	.4249	.3552	.3343	.3189	.3127	.2662	.1840	.1420
6	448	.5621	.3652	.3070	.2814	.2493	.2040	.1671	------	.0500	.0887
7	425	.5464	.3830	.3149	.2754	.2194	.2202	.1867	------	.0891	.0924
8	387	.5701	.4178	.3476	.2894	.2447	.2067	------	------	.0849	.1064
9	482	.4556	.3405	.2571	.2247	.1848	.1776	.1695	.1365	.0309	.0011
10	483	.5424	.3729	.2903	.2632	.2026	.1987	.1877	.1925	.0928	.0787
12	468	.5477	.3926	.3113	.2657	.2382	.2219	.2241	.1931	.0912	.0829
13	192	.5590	.4078	------	------	------	------	------	------	.1394	.1950
14	443	.5353	.4107	.3053	.3106	.2402	.2387	.1987	------	.0779	.1127
15	419	.5097	.433	.2922	.2552	.1977	.1834	.1773	------	.0648	.0633
16	438	.5118	.2952	.2689	.2276	.1826	.1825	.1813	------	.0037	.0661
17	459	.6290	.4259	.3714	.2925	.2972	.2946	.2729	.2398	.2288	.1243
18	445	.4892	.3829	.3023	.2550	.2516	.2447	.1947	------	.0329	.1193
19	422	.5821	.4413	.3887	.3143	.3083	.2823	.2529	------	.1569	.1307
20	112	.5288	------	------	------	------	------	------	------	.1163	.3618
21	116	.5241	------	------	------	------	------	------	------	.1000	.2134
Statistical independence		.50	.33	.25	.20	.17	.14	.13	.11	0.0	0.0

TABLE II. - STATISTICS FOR MEASURING INDEPENDENCE OF NO_2 OBSERVATIONS. LISTED ARE THE OBSERVED RATIOS OF VARIANCES FOR X-HR AVERAGES OPPOSED TO Y-HR AVERAGES AND THE OBSERVED CORRELATIONS FOR SINGLE AND DOUBLE OFFSETS

STA	# RDGS	Ratio of variances $\frac{VAR\ (X\text{-}HR)}{VAR\ (Y\text{-}HR)}$								Correlations	
		48/24	72/24	96/24	120/24	144/24	168/24	142/24	216/24	Single offset	Double offset
1	395	0.6034	0.4207	0.3580	0.3316	0.3040	0.3029	------	------	0.1583	0.1825
2	178	.4538	.3536	------	------	------	------	------	------	.0698	.1334
3	451	.5776	.4512	.3756	.3502	.3356	.3004	0.2932	0.2766	.1766	.2146
4	331	.6062	.4847	.4133	.3926	.3221	------	------	------	.2935	.2523
5	436	.6251	.5029	.4219	.3989	.3640	.3471	.2888	------	.2270	.2900
6	390	.5228	.3649	.2979	.2488	.2097	.1857	------	------	.0461	.0691
7	424	.5384	.3508	.3193	.2217	.2129	.1904	.1466	------	.0205	.0931
8	414	.5267	.4283	.3577	.3007	.2765	.2586	.2226	------	.1397	.1324
9	429	.5851	.4608	.3998	.3696	.3143	.3240	.2878	------	.2405	.2419
10	340	.6088	.4313	.3552	.3249	.2805	------	------	------	.1692	.1717
11	119	.6801	------	------	------	------	------	------	------	.3700	.3209
12	426	.5493	.542	.053	.2720	.1977	.2131	.1902	------	.0736	.1262
13	179	.6723	.5420	------	------	------	------	------	------	.3147	.3048
14	383	.4679	.3433	.2742	.2816	.2023	.1880	------	------	.0228	.0807
15	213	.4195	.3033	.2640	------	------	------	------	------	-.0375	.0295
Statistical independence		.50	.33	.25	.20	.17	.14	.13	.11	0.0	0.0

TABLE III. - STATISTICS FOR MEASURING INDEPENDENCE OF SO_2 OBSERVATIONS. LISTED ARE THE OBSERVED RATIOS OF VARIANCES FOR X-HR AVERAGES OPPOSED TO Y-HR AVERAGES AND THE OBSERVED CORRELATIONS FOR SINGLE AND DOUBLE OFFSETS

STA	# RDGS	Ratio of variances $\frac{VAR\ (X\text{-}HR)}{VAR\ (Y\text{-}HR)}$								Correlation	
		48/24	72/24	96/24	120/24	144/24	168/24	142/24	216/24	Single offset	Double offset
1	396	0.5083	0.3928	0.3136	0.2647	0.2150	0.2393	------	------	0.1147	0.0978
2	181	.6144	.5137	------	------	------	------	------	------	.3217	.3166
3	433	.4808	.3618	.2844	.2199	.1983	.1885	0.1500	------	.0383	.0863
4	328	.4921	.3646	.2960	.2842	.1954	------	------	------	.0676	.1308
5	432	.6055	.4603	.4067	.3274	.3354	.2819	.2395	------	.2091	.1805
6	392	.6090	.4850	.3957	.3900	.3515	.3126	------	------	.2299	.2966
7	413	.5575	.4095	.3632	.2857	.2748	.2723	.2412	------	.1523	.1471
8	396	.5472	.3694	.3330	.2401	.2344	.2016	------	------	.1188	.0980
9	421	.5370	.4297	.3858	.3419	.2795	.2404	.2360	------	.1610	.2250
10	338	.6286	.4639	.3662	.3355	.3578	------	------	------	.2548	.1517
11	116	.5537	------	------	------	------	------	------	------	.1900	.3064
12	416	.5392	.3571	.3346	.3176	.2526	.2215	.2143	------	.1342	.0691
13	191	.5149	.3914	------	------	------	------	------	------	.0885	.1299
14	363	.6457	.4653	.4148	.3593	.3274	.2799	------	------	.3145	.2200
15	202	.5036	.3389	.2700	------	------	------	------	------	.0678	-.0419
CAMP data 50 000			0.86					0.80			
Statistical inde-pendence		.50	0.33	0.25	0.20	0.17	0.14	0.13	0.11	0.0	0.0

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TABLE IV. - ESTIMATED SMP LEVELS FROM MONTE-CARLO EXPERIMENT

Method	n	Mean SMP value	# Samples	95 Percent confidence bounds
$e^{(m + 2.63 s)}$ m and s calculated from Monte-Carlo generated data sets	30	15.10	3400	±84%
	60	14.70	3000	±56%
	90	14.47	3000	±44%
	120	14.40	1400	±40%
	365	14.33	1500	±21%
Ranking of Monte-Carlo generated data sets	365	14.27	3800	±58%

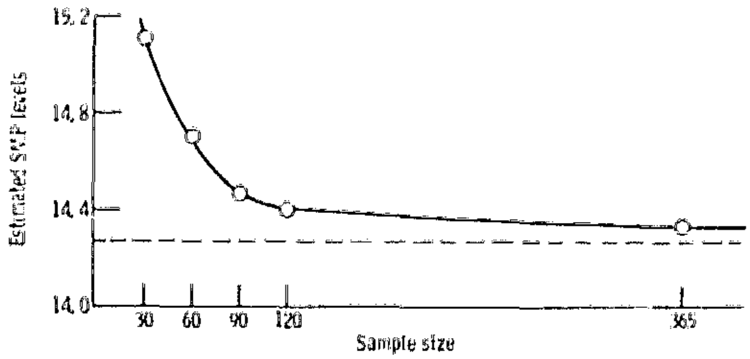

Figure 1. - Estimated SMP levels for various sample sizes. The dashed line is the mean SMP level from ranked samples of size 365.

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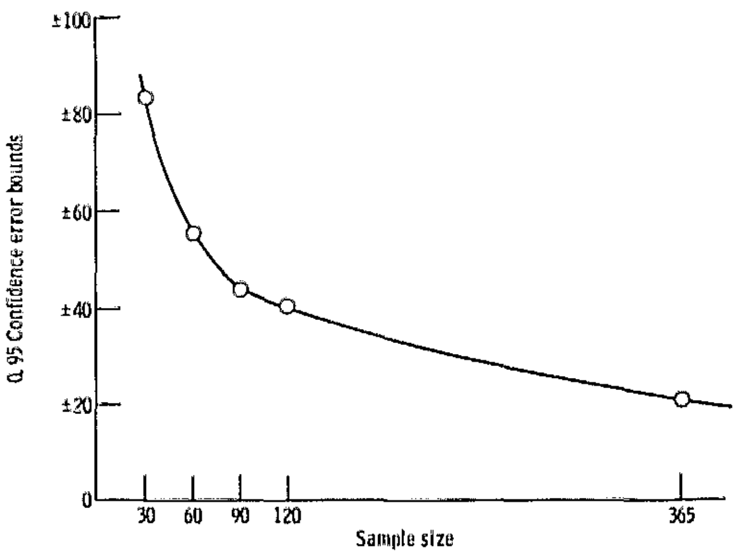

Figure 2. - The error bounds to obtain 0.95 confidence in estimated SMP levels for various sample sizes.