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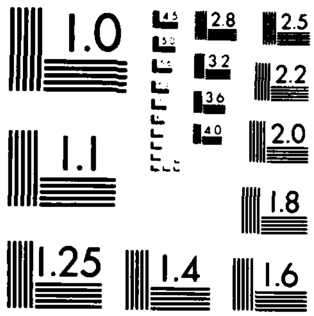

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Report USAFSAM-TR-84-23

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TOTAL AEROSOL VOLUME COMPUTED FROM LASER SPECTROMETER PARTICLE-SIZE DATA FOR COMPARISON WITH FLAME PHOTOMETER TOTAL-MASS DATA

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A computer program that converts laser spectrometer (LAS-X) particle-size data to total aerosol volume has been developed. Sources of errors and uncertainties in LAS-X data have been evaluated. Because aerosol volume is directly proportional to mass, the derived aerosol volumes can be compared with sodium chloride (NaCl) aerosol-mass data from a flame photometer.

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TOTAL AEROSOL VOLUME COMPUTED FROM LASER SPECTROMETER PARTICLE-SIZE DATA FOR COMPARISON WITH FLAME PHOTOMETER TOTAL-MASS DATA

INTRODUCTION

The Crew Technology Division of the School of Aerospace Medicine (USAFSAM) tests and evaluates chemical warfare defense respirators against the penetration of vapors and aerosol particles. A laser spectrometer (LAS-X) active light-scattering system (manufactured by Particle Measuring Systems, Inc., Boulder, CO) is used to measure aerosol particle-size distributions, and a flame photometer is used to determine the total mass of sodium chloride (NaCl) aerosol particles detected.

A computer program has been written to convert the particle size distributions obtained with the LAS-X into a total aerosol-particle volume proportional to the total mass of the detected aerosol particles. This calculated volume can be compared with the aerosol mass measured with the flame photometer. If both measuring systems are working according to their specifications, the total aerosol volume calculated from the LAS-X data should be equal to the mass measured with the flame photometer, within a proportionality constant.

With the LAS-X system, multichannel particle-size distribution data give the number of particles in each of the successive channels, with each channel representing a specific size interval. Since the size of the particles within each channel is unspecified within the size interval of the channel, three estimates of total particle volume are calculated -- upper, lower, and average.

As total particle volume is calculated from the LAS-X data, the overlap of the size intervals between data from different channels must be considered when accumulating data from adjacent size ranges. (This overlap has been deliberately designed into the LAS-X data output system to provide highest resolution within all size ranges.) So that data from channels with overlapping size ranges are not duplicated in the accumulated sum, predetermined channels in each size range are deleted from the sum in the accumulated total volume. Additional calculations are made to determine the logical consistency of data obtained from overlapping size intervals. That is, five numerical checks are performed with the computer to ascertain that, in each case, the larger of the overlapping size intervals contains more particles than the smaller interval.

RATIONALE AND METHODS

Data obtained with the LAS-X system is available as four size ranges, with each range divided into 15 channels corresponding to particle sizes between 0.12 and 7.5 μm. Particles outside this size range cannot be detected by the LAS-X [3]. The calibration data showing the size interval for each range and channel is shown in Table 1. The channels not counted in the accumulated volume are identified. Channel 14 of range 3 is considered as a special case: All particles in this channel are added to the sum for the maximum estimate of accumulated volume under the assumptions that (1) all particles in this interval have diameters equal to 0.200 μm, (2) half of that value is added to the sum for the average estimate, and (3) that value is deleted from the sum for the minimum volume estimate.

For a spherical particle of diameter d_p, the volume of the particle is

$$V_p = (1/6)\pi d_p^3 \qquad (1)$$

Multiplying the number, N(n), of particles in each channel (n = 1, 2, 3,...) by the volume obtained from Equation (1) for particles in channel n having an estimated diameter d_p, the total volume of all aerosol particles within channel n can be estimated by

$$V(n) = N(n)V_p \qquad (2)$$

Since particle sizes are determined within discrete size intervals, three estimates of total aerosol volume within each channel are calculated. That is, we may estimate the minimum, maximum, or average volume, corresponding to the assumptions that all particles within channel n are, respectively, of the minimum, maximum, or average size within that channel's size interval. (By average V(n) we mean the volume calculated under the assumption that all particles in channel n have a diameter equal to the diameter at the midpoint of a channel size interval; the average V(n) is <u>not</u> equal to the average volume for particles in channel n.) The total volume of all detectable particles may be calculated by summing the volumes within all nonoverlapping channels as

$$V(\text{Total}) = \sum_{n} V(n) \qquad (3)$$

(nonoverlapping channels)

where three estimated total volumes are calculated corresponding to a minimum, maximum, and average estimate.

TABLE 1. CHANNEL LIMITS

Range = 0:

Ch#	Diam. (µm)
1	1.500 to 1.900
2	1.900 to 2.300
3	2.300 to 2.700
4	2.700 to 3.100
5	3.100 to 3.500
6	3.500 to 3.900
7	3.900 to 4.300
8	4.300 to 4.700
9	4.700 to 5.100
10	5.100 to 5.500
11	5.500 to 5.900
12	5.900 to 6.300
13	6.300 to 6.700
14	6.700 to 7.100
15	7.100 to 7.500

Range = 2:

Ch#	Diam. (µm)
1[a]	0.170 to 0.200
2	0.200 to 0.230
3	0.230 0.260
4	0.260 0.290
5	0.290 0.320
6	0.320 0.350
7	0.350 0.380
8	0.380 0.410
9	0.410 0.110
10	0.440 0.470
11	0.470 0.500
12[a]	0.500 0.530
13[a]	0.530 0.560
14[a]	0.560 0.590
15[a]	0.590 0.620

Range = 1:

Ch#	Diam. (µm)
1[a]	0.300 to 0.400
2[a]	0.400 to 0.500
3	0.500 to 0.600
4	0.600 to 0.700
5	0.700 to 0.800
6	0.800 to 0.900
7	0.900 to 1.000
8	1.000 to 1.100
9	1.100 to 1.200
10	1.200 to 1.300
11	1.300 to 1.400
12	1.400 to 1.500
13[a]	1.500 to 1.600
14[a]	1.600 to 1.700
15[a]	1.700 to 1.800

Range = 3:

Ch#	Diam. (µm)
1	0.120 to 0.126
2	0.126 to 0.132
3	0.132 to 0.138
4	0.138 to 0.144
5	0.144 to 0.150
6	0.150 to 0.156
7	0.156 to 0.162
8	0.162 to 0.168
9	0.168 to 0.174
10	0.174 to 0.180
11	0.180 to 0.186
12	0.186 to 0.192
13[a]	0.192 to 0.198
14[b]	0.198 to 0.204
15[a]	0.204 to 0.210

[a]Channel not included in sum

[b]Included in sum of maximum, half included in sum of average estimate, and none included in sum of minimum estimate.

COMPUTER PROGRAM

The computer program was written as a prototype for research use. An operational version, now being written, will be documented in another USAFSAM technical report. Only the main features of the program are outlined below:

1. Program Initiation.

   a. The time and date are given.
   b. The user is asked for

      (1) flow rate
      (2) run time
      (3) number of ranges to be included
      (4) the number of counts in each of the selected ranges.

2. Data Checks. Five checks are calculated to ascertain that overlapping channel intervals include their proper subsets; i.e., that a larger number of particles are contained in the larger of the overlapping intervals.

3. Volume Calculations. Volume of particles in each channel, total volume of all particles in a given range, and total accumulated volume are calculated.

4. Surface Area Calculations. Surface area of particles in each channel, total surface area of all particles in all given ranges, and total accumulated surface area are calculated.

5. Output. An example of output is shown in Table 2. Channels not included in the accumulated volume or surface area are clearly labeled in the printout.

TABLE 2. SAMPLE OUTPUT: MINIMUM, MAXIMUM, AND AVERAGE VOLUME

*** RANGE = 0***

CH#	DIAM. (MICR)	#COUNTS	#CNTS/SEC	MIN VOL/S	MAX VOL/S	AVE VOL/S
1	1.500 TO 1.900	1	.1000E+00	.17671E+00	.35914E+00	.25724E+00 (S)
2	1.900 TO 2.300	2	.2000E+00	.71827E+00	.12741E+01	.96981E+00 (S)
3	2.300 TO 2.700	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
4	2.700 TO 3.100	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
5	3.100 TO 3.500	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
6	3.500 TO 3.900	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
7	3.900 TO 4.300	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
8	4.300 TO 4.700	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
9	4.700 TO 5.100	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
10	5.100 TO 5.500	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
11	5.500 TO 5.900	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
12	5.900 TO 6.300	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
13	6.300 TO 6.700	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
14	6.700 TO 7.100	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
15	7.100 TO 7.500	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)

**RANGE= 0 SUBTOTL: MIN ACCUM VOL/S = 0.895 MAX ACCUM VOL/S = 1.633 AVE ACCUM VOL/S = 1.227

*** RANGE = 1***

CH#	DIAM. (MICR)	#COUNTS	#CNTS/SEC	MIN VOL/S	MAX VOL/S	AVE VOL/S
1	0.300 TO 0.400	17303	.1730E+04	.24462E+02	.57983E+02	.38844E+02 (* N.S.!! *)
2	0.400 TO 0.500	1449	.1449E+03	.48556E+01	.94837E+01	.69136E+01 (* N.S.!! *)
3	0.500 TO 0.600	35	.3500E+01	.22907E+00	.39584E+00	.30490E+00 (S)
4	0.600 TO 0.700	9	.9000E+00	.10179E+00	.16163E+00	.12941E+00 (S)
5	0.700 TO 0.800	8	.8000E+00	.14368E+00	.21447E+00	.17671E+00 (S)
6	0.800 TO 0.900	1	.1000E+00	.26808E-01	.38170E-01	.32155E-01 (S)
7	0.900 TO 1.000	1	.1000E+00	.38170E-01	.52360E-01	.44892E-01 (S)
8	1.000 TO 1.100	1	.1000E+00	.52360E-01	.69691E-01	.60613E-01 (S)
9	1.100 TO 1.200	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
10	1.200 TO 1.300	1	.1000E+00	.90478E-01	.11503E+00	.10227E+00 (S)
11	1.300 TO 1.400	1	.1000E+00	.11503E+00	.14368E+00	.12882E+00 (S)
12	1.400 TO 1.500	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (S)
13	1.500 TO 1.600	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (* N.S.!! *)
14	1.600 TO 1.700	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (* N.S.!! *)
15	1.700 TO 1.800	0	.0000E+00	.00000E+00	.00000E+00	.00000E+00 (* N.S.!! *)

**RANGE= 1 SUBTOTL: MIN ACCUM VOL/S = 30.115 MAX ACCUM VOL/S = 68.657 AVE ACCUM VOL/S = 46.737

*** RANGE = 2***

CH#	DIAM. (MICR)	#COUNTS	#CNTS/SEC	MIN VOL/S	MAX VOL/S	AVE VOL/S
1	0.170 TO 0.200	22703	.2270E+04	.58402E+01	.95098E+01	.75266E+01 (* N.S.!! *)
2	0.200 TO 0.230	74475	.7448E+04	.31196E+02	.47445E+02	.38755E+02 (S)
3	0.230 TO 0.260	40580	.4058E+04	.25852E+02	.37345E+02	.31247E+02 (S)
4	0.260 TO 0.290	22168	.2217E+04	.20401E+02	.28309E+02	.24139E+02 (S)
5	0.290 TO 0.320	11732	.1173E+04	.14982E+02	.20129E+02	.17429E+02 (S)
6	0.320 TO 0.350	5907	.5907E+03	.10135E+02	.13261E+02	.11628E+02 (S)
7	0.350 TO 0.380	3235	.3235E+03	.72623E+01	.92944E+01	.82367E+01 (S)
8	0.380 TO 0.410	1759	.1759E+03	.50538E+01	.63477E+01	.56762E+01 (S)
9	0.410 TO 0.440	789	.7890E+02	.28473E+01	.35191E+01	.31713E+01 (S)
10	0.440 TO 0.470	195	.1950E+02	.86974E+00	.10601E+01	.96176E+00 (S)
11	0.470 TO 0.500	45	.4500E+01	.24463E+00	.29452E+00	.26880E+00 (S)
12	0.500 TO 0.530	26	.2600E+01	.17017E+00	.20267E+00	.18595E+00 (* N.S.!! *)
13	0.530 TO 0.560	6	.6000E+00	.46771E-01	.55171E-01	.50856E-01 (* N.S.!! *)
14	0.560 TO 0.590	9	.9000E+00	.82757E-01	.96782E-01	.89587E-01 (* N.S.!! *)
15	0.590 TO 0.620	4	.4000E+00	.43014E-01	.49915E-01	.46379E-01 (* N.S.!! *)

**RANGE= 2 SUBTOTL: MIN ACCUM VOL/S = 125.026 MAX ACCUM VOL/S = 176.919 AVE ACCUM VOL/S = 149.412

*** RANGE = 3***

CH#	DIAM. (MICR)	#COUNTS	#CNTS/SEC	MIN VOL/S	MAX VOL/S	AVE VOL/S
1	0.120 TO 0.126	13371	.1337E+04	.12098E+01	.14005E+01	.13028E+01 (S)
2	0.126 TO 0.132	16557	.1656E+04	.17342E+01	.19939E+01	.18610E+01 (S)
3	0.132 TO 0.138	15628	.1563E+04	.18820E+01	.21505E+01	.20133E+01 (S)
4	0.138 TO 0.144	20411	.2041E+04	.28087E+01	.31912E+01	.29958E+01 (S)
5	0.144 TO 0.150	21145	.2115E+04	.33059E+01	.37366E+01	.35169E+01 (S)
6	0.150 TO 0.156	20653	.2065E+04	.36497E+01	.41054E+01	.38731E+01 (S)
7	0.156 TO 0.162	20482	.2048E+04	.40714E+01	.45595E+01	.43108E+01 (S)
8	0.162 TO 0.168	22338	.2234E+04	.49726E+01	.55459E+01	.52541E+01 (S)
9	0.168 TO 0.174	19803	.1980E+04	.49165E+01	.54623E+01	.51846E+01 (S)
10	0.174 TO 0.180	20558	.2056E+04	.56706E+01	.62776E+01	.59690E+01 (S)
11	0.180 TO 0.186	18263	.1826E+04	.55768E+01	.61533E+01	.58604E+01 (S)
12	0.186 TO 0.192	20980	.2098E+04	.70687E+01	.77751E+01	.74163E+01 (S)
13	0.192 TO 0.198	15116	.1512E+04	.56019E+01	.61437E+01	.58687E+01 (S)
14	0.198 TO 0.204	16440	.1644E+04	.66818E+01	.73079E+01	.69902E+01 (* P.S.!! *)
15	0.204 TO 0.210	14646	.1465E+04	.65104E+01	.71019E+01	.68019E+01 (* N.S.!! *)

**RANGE= 3 SUBTOTL: MIN ACCUM VOL/S = 65.661 MAX ACCUM VOL/S = 72.905 AVE ACCUM VOL/S = 69.219

TOTAL 4 RANGES .. MIN ACCUM VOL/S = 173.004 MAX ACCUM VOL/S = 220.324 AVE ACCUM VOL/S = 199.146

DISCUSSION

General criteria for determining aerosol size characteristics have been reviewed by Hinds [3]. Characteristics of laser spectrometers have been discussed in detail by Saltzman et al. [7], Willeke and Liu [9], Schuster and Knollenberg [8], Pinnick and Auvermann [6], and Garvey and Pinnick [2]. Criteria and instrument characteristics that affect this application of laser spectrometer data are discussed briefly below. These characteristics include the acceptance-size range of the detector, sampling losses, and detectability of small signals.

General Assumptions

Commonly, the LAS-X system is calibrated using polystyrene latex spheres. The manufacturer claims that the laser cavity's interferometric properties make the LAS-X insensitive to the refractive index of the scattering particles. However, calculations by Saltzman et al. [7] show that correction factors are required for the scattering intensities when sampling particles other than polystyrene. Fortunately, at the wavelength of the He-Ne laser (λ= 632.8 nm), the index of refraction of the polystyrene latex particles used as a test aerosol is equal to 1.5905-0j which is close to the index of refraction of NaCl, 1.5442-0j. Corrections due to index-of-refraction differences between polystyrene latex spheres and NaCl are not expected to be large when compared to other sources of errors. The nonspherical symmetry of the NaCl particles may cause a larger difference between the scattering properties of the polystyrene latex spheres and NaCl.

Regardless of the shape of the particles, dimensional analysis arguments [1] can show that the volume of a particle is proportional to a dimension (or diameter) of the particle raised to the third power. Therefore, if we assume that the LAS-X system gives a correct determination of particle size, then results of our calculated volume, assuming spherical particles, differ only by a proportionality factor for nonspherical particles having identical shapes. However, questions remain unanswered as to whether all NaCl particles have identical shapes and what magnitude of discrepancy in LAS-X response for nonidentical particles is introduced.

Sampling Statistics

The statistical probability that no particle (p=0), one particle (p=1), or more than one particle (p=2,3,4,....) is present during a sampling time interval, t, is given by the Poisson distribution

$$P_p = \frac{(\mu t)^p \, e^{-\mu t}}{p!} \qquad (4)$$

where μt = average number of particles sampled in time t.

A point to remember: The Poisson probability law is related to the statistical nature of random phenomena, not to instrumentation errors or human errors in sampling. (Random emission of electrons from the filament of a photosensitive substance under the influence of light and the spontaneous decomposition of radioactive nuclei are examples of phenomena obeying Poisson's probability law.)

For the Poisson probability distribution given in Equation (4), the mean average number, $\bar{n}$, of particles sampled during time t is given as

$$\bar{n} = \mu t \tag{5}$$

and the standard deviation from the mean, $\sigma(t)$, is given as

$$\sigma(t) = (\mu t)^{1/2} \tag{6}$$

That is, if the mean average number of particles $\bar{n}$ is sampled during time t and the sampling is described by a Poisson process, the standard deviation is given as the square root of $\bar{n}$. Commonly, a signal-to-noise ratio is defined as the ratio of the mean average to the standard deviation of the sample; i.e., the signal-to-noise ratio, SN, is defined as

$$SN = \bar{n}/(\bar{n})^{1/2} = (\bar{n})^{1/2} \tag{7}$$

As the mean number of counts increases, the signal-to-noise ratio for detection of particles obeying a Poisson distribution improves with the square root of $\bar{n}$. For large values of $\bar{n}$, the Poisson distribution function approaches a normal distribution function (a good approximation when $n > 50$). Under the normal distribution approximation, the number of counts detected has a 68% probability of falling within (±) one standard deviation of the mean and a 96% probability of falling within (±) two standard deviations of the mean [4].

When more than one particle is observed simultaneously in the LAS-X view volume ($p > 1$), "coincidence" occurs. The signal from two (or more) particles is interpreted as a larger particle, incorrectly weighting the particle size distribution to larger particles and incorrectly reducing the total number of particles counted. Coincidence is a serious problem with the LAS-X when particle number concentration exceeds about 1000 particles per cubic centimeter [3, 4, 9]. Particle number concentrations in respirator-fit-testing challenge atmospheres are usually greater than about 10^6 particles per cubic centimeter; so for size distribution and volume concentration to be valid, the aerosol must be diluted with 1000 ml of clean air for every 1 ml of aerosol.

SUMMARY AND CONCLUSION

A computer program was written to calculate particle volume from particle-size data obtained with the LAS-X active-light scattering system, and the calculated volume was compared with data obtained with the flame photometer. Possible sources of instrumentation errors and sampling statistics have been briefly discussed. We conclude that the LAS-X particle-volume data and the flame photometer aerosol-mass data can be c :pared if sources of errors and uncertainty are taken into account. The comparison of LAS-X and flame-photometer data will be reported in a separate technical report.

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