Analytical processing of experimental results for determining the particle size of soot in various parts of the diesel exhaust system

V A Likhanov and A V Rossokhin
Department of thermal engines, automobiles and tractors, Vyatka State Agricultural Academy, 610017, Kirov, October prospect, 133, Russian Federation

E-mail Rossokhin.dvs@mail.ru

Abstract. In this paper, we consider methods for processing experimental data regarding the determination of the sizes of soot particles selected in the exhaust system, as well as their size distribution in order to find the relationship between the sizes of soot particles and their shares in the total particle array. Corresponding data on the distribution of soot particles by size for an automobile diesel engine of dimension 4CHN 11.0/12.5 are presented, mathematical dependencies describing this distribution are established.

1. Introduction
The problem of determining the effect of soot particles on thermal radiation in the working volume of the engine cylinder is solved in several stages. At the initial stage, a physical experiment and sampling are carried out to determine the concentration, shape and size of soot particles in the combustion products of ICE. After processing the experimental data on the soot samples, a particle size distribution function is obtained. Given the dispersion of the optical constants of soot (taking into account the H/C ratio), the radiation characteristics of individual particles and unit volume are studied. Further study of the radiation characteristics (intensity, heat fluxes) requires knowledge of the magnitudes and ranges of changes in the main thermo- and gas-dynamic parameters (composition of the gas phase, mass fraction of condensate, temperature, pressure, etc.) [1-4].

Since the formation of soot in the combustion products depends on the type of fuel, the process of mixing with the oxidizing agent, the operating mode of the engine, and other factors, it is necessary to carry out analytical processing of the experimental results to determine the particle dispersion (size and size distribution function) [5-9].

In order to determine the particle size of soot in various parts of the diesel exhaust system, the results obtained at the Department of Internal Combustion Engines of the Vyatka State Agricultural Academy were used. The processes of soot formation during the combustion of diesel fuel and rapeseed oil in a two-cylinder diesel engine D-21A1 air-cooled with a hemispherical combustion chamber with a radius of R=36 mm were considered. Engine displacement of 2,08 liters. Sampling was carried out when the engine was operating in nominal mode. As an example, in this work, we consider 4 soot samples corresponding to two fuels and two sampling sites (table 1).
Studies of the structure and size of soot samples were carried out on the basis of the laboratory of modern methods of physicochemical analysis [10-15], which is part of the Nanotechnology Research and Education Center of the Vyatka State University [16-22]. The initial carbon black samples were previously dissolved in gasoline, shaken, and then 0.5 ml droplets were isolated. After drying, the carbon black preparations were analyzed on a JEM-2100 transmission electron microscope (JEOL, Japan) at magnifications from 30 to 120 thousand times and an accelerating voltage of 200 kV [23].

The photographs made it possible to consider the primary structures of which the soot consists. Pictures of individual visual fields were analyzed using the integrated statistical analysis program Olimpus. Soot particles were counted using special tools of this program. For each drug in the process of statistical data processing, arrays containing more than 300 particles of different sizes were filled.

2. Experimental
We used the Mathcad system, which has a number of built-in functions for calculating the numerical statistical characteristics of random data series. Initially, a text file was specified containing an array with data on particle sizes \( x_i \). The total number of data \( n \), mean \( x_m \), and standard deviation \( \sigma \) were calculated using the built-in functions \( \text{length}(x) \), \( \text{mean}(x) \), and \( \text{stdev}(x) \), respectively, where \( x \) is the data array. The lower \( \text{low} \) and upper \( \text{hi} \) values of the error corridor (confidence probability \( \alpha = 0.68 \)) were calculated by the formulas:

\[
\text{low} = x_m - \sigma,
\]
\[
\text{hi} = x_m + \sigma.
\]

For example, figure 1 shows a series of experimental data (sample № 1), where the horizontal axis shows the number \( i \) of the element (particle) in the data array.

![Figure 1](image1.png)

**Figure 1.** A series of experimental data on the particle size of soot (sample 1).

For the discrete random variables considered, their frequency distributions were constructed. The histogram, therefore, serves as an estimate of the distribution density of such quantities. The lower \( \text{lower} \) and upper \( \text{upper} \) bounds for the particle diameters (taking into account rounding to an integer) were found using the functions \( \text{floor}(\text{min}(x)) \) and \( \text{ceil}(\text{max}(x)) \). The discretization step was specified by the formula:

\[
\Delta x = \frac{\text{upper} - \text{lower}}{m}
\]

where \( m \) is the number of columns in the histogram.
The optimal number of groups (columns) is estimated at equal intervals for normal distributions using the Sturgess formula:

\[ m = 1 + \log_2 n \]

The result is rounded up to an integer up. For our conditions, the value \( m = 10 \) was adopted.

Next, an \( \text{int} \) array was created containing the coordinates of the points of dividing the entire interval of particle sizes into \( m \) number of parts:

\[ \text{int}(j) = \text{lower} + \Delta x \cdot j, \quad j = 0, 1, 2, \ldots m. \]

The values of the calculated parameters when determining particle sizes for each experimental sample are presented in table 1.

| Sample Number | Parameter                                      | 1     | 2     | 3     | 4     |
|---------------|------------------------------------------------|-------|-------|-------|-------|
|               | The number of particles \( n \)               | 339   | 337   | 530   | 391   |
|               | The average particle size \( x_m, \text{nm} \) | 37.84 | 35.35 | 35.22 | 41.75 |
|               | Standard deviation \( \sigma, \text{nm} \)    | 12.33 | 13.39 | 11.88 | 13.41 |
|               | Lower Error Corridor \( \text{low}, \text{nm} \)| 25.51 | 21.96 | 23.34 | 28.33 |
|               | The upper value of the error corridor \( \text{hi}, \text{nm} \) | 50.18 | 48.74 | 47.1  | 55.16 |
|               | Discretization step \( \Delta x, \text{nm} \)  | 8.8   | 8.9   | 5.9   | 7.7   |

In this work, histograms of the countable particle size distribution were constructed using the \( \text{hist} \) (int, \( x \)) function built into MathCad, which automatically calculates the number of particles \( \Delta n \) falling into each \( \Delta x \) interval. If the value is divided by the width of the interval \( \Delta x \), then the resulting ratio will show the relative value of the quantity (diameter) per unit interval. As \( \Delta x \to 0 \), the quantity goes over to the distribution curve \( f(r) \). Using the built-in function \( \text{dnorm}(x, x_m, \sigma) \), we obtained the probability density function \( f(r) \) of the size distribution of soot particles. It was a normal (Gaussian) distribution:

\[
f(x) = \frac{1}{\sqrt{2\pi \cdot \sigma}} \exp \left( -\frac{(x - x_m)^2}{2\sigma^2} \right)\]

The normal distribution is applicable to particles obtained by chemical processes, including condensation and precipitation [1].

Figures 2–5 show the countable size distribution of soot particles. Each histogram is depicted in the form of rectangles with heights equal to the number of particles \( \Delta n \) falling in each interval \( \Delta x \). A smoothed curve is a distribution equal to the theoretical (calculated) value of \( \Delta n \).

Figure 6 shows all 4 functions of the distribution of soot particles by size. The difference between the average particle sizes is from 1% (samples 2 and 3) to 20% (samples 3 and 4). Thus, the initial soot particles in different places of sampling (at the exit of the exhaust pipe and at the exit of the cylinder) are comparable with each other. Particles of this size are formed in the combustion chamber of the engine during fuel combustion. Further movement of soot particles with combustion products along the exhaust path leads to a change in the size of soot particles due to adhesion and agglomeration. Aggregates (dense formations of many particles) and agglomerates (loose chain formations of a branched structure) are formed from soot particles. Agglomerates consist of the initial carbon spheres or spheroids with average sizes of 20...40 nm. The linear dimensions of soot agglomerates can reach several micrometers [24-32].
Figure 2. The distribution of soot particles by size (sample 1).

Figure 3. The distribution of soot particles by size (sample 2).

Figure 4. The distribution of soot particles by size (sample 3).
To determine the complex configurations (agglomerates) of soot particles formed at the outlet of the exhaust pipe, a scanning (scanning) electron microscope JSM-6510LV from JEOL (Japan) was used. The samples were studied, which were a powdery deposition of soot on glass plates (samples No. 1 and No. 2 in Table 1), obtained at the place of exit of combustion products from the exhaust pipe of the engine. From the photographs obtained, it can be concluded that soot is an irregular cloud-shaped formation [33-34]. Diesel soot is prone to agglomerates containing hundreds to thousands of particles.

Statistical processing of the results of the considered soot formations was carried out. For example, figure 7 shows the counted distribution of soot agglomerates formed upon exiting the exhaust pipe (sample No 1). Particle sizes are described using gamma distribution

\[ f(x) = \frac{a^{b+1} \cdot x^b}{b!} \cdot \exp(-ax) \]
with parameters $a = 1.647 \, \mu m^{-1}$ $b = 1$. Substituting the obtained parameters in formula leads to an equivalent distribution function

$$f(x) = 2.713 \cdot x \cdot \exp(-1.647x).$$

**Figure 7.** Distribution of soot agglomerates formed upon exit from the exhaust pipe (sample 1).

### 3. Conclusion

As a result of the studies, the sizes and functions of the particle size distribution for various soot samples were established. The dispersion of soot particles is determined by the sampling location and the type of fuel used. The formation of soot is a volumetric process of thermal decomposition (pyrolysis) of hydrocarbons in the gas phase under conditions of a severe lack of oxidizing agent (oxygen). The initial soot particles formed in the cylinder have sizes up to several tens of nanometers. From such particles aggregates are formed, having sizes up to several micrometers. The study of the particle sizes of soot and the mechanisms of their formation is necessary when considering the processes occurring in the internal combustion engine and determining the heat stress, efficiency and wear resistance of the engine structural elements.

### References

[1] Likhanov V A and Lopatin O P 2018 *IOP Conf. Series: Materials Science and Engineering* **457** 012011

[2] Romanyuk V, Likhanov V A and Lopatin O P 2018 *Theoretical and Applied Ecology* **3** 27-32

[3] Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062087

[4] Anfilatov A A and Chuvashhev A N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062064

[5] Marchuk A, Likhanov V A and Lopatin O P 2019 *Theoretical and Applied Ecology* **3** 080-6

[6] Anfilatov A A and Chuvashhev A N 2020 *Journal of Physics: Conf. Series* **1515** 022035

[7] Likhanov V A and Lopatin O P 2019 *Journal of Physics: Conf. Series* **1399** 055016

[8] Skryabin M L and Likhanov V A 2020 *IOP Conf. Series: Materials Science and Engineering* **734** 012075

[9] Likhanov V A and Lopatin O P 2019 *Journal of Physics: Conf. Series* **1399** 055020

[10] Chuvashhev A N and Chuprakov A I 2019 *Journal of Physics: Conf. Series* **1399** 055085

[11] Likhanov V A and Rossokhin A V 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062046

[12] Likhanov V A, Lopatin O P and Yurlov A S 2019 *Journal of Physics: Conf. Series* **1399** 055026

[13] Anfilatov A A and Chuvashhev A N 2020 *Journal of Physics: Conf. Series* **1515** 042048

[14] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Earth and Environmental Science* **421**
[15] Anfilatov A A and Chuvashev A N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062069

[16] Anfilatov A A 2020 *Journal of Physics: Conf. Series* **1515** 042049

[17] Lopatin O P 2020 *IOP Conf. Series: Earth and Environmental Science* **421** 072019

[18] Likhanov V A, Kozlov A N and Araslanov M I 2020 *IOP Conf. Series: Materials Science and Engineering* **734** 012211

[14] Yadava S and Maitra S S 2017 *Global Nest Journal* **19** 533-39

[15] Ahmad I 2016 *Journal of Pure and Applied Microbiology* **10** 95-102

[16] Likhanov V A and Lopatin O P 2019 *Ecology and Industry of Russia* **23(9)** 60-5

[17] Shatrov M G, Sinyavski V V, Dunin A Y, Shishlov I G, Vakulenko A V and Yakovenko A L 2018 *International Journal of Engineering and Technology* **7** 288-295

[18] Zhilenkov A A and Efremov A A 2017 *IOP Conference Series: Materials Science and Engineering* **10** 012043

[19] Chen W, Pan J, Liu Y, Fan B, Liu H and Otchere P 2019 *Applied Energy* **176** 453-467

[20] Semprini S, Sánchez D and De Pascale A 2016 *Solar Energy* **132** 279-93

[21] Osorio-Tejada J L, Llera-Sastresa E and Scarpellini S 2017 *Renewable and Sustainable Energy Reviews* **71** 785-95

[22] Likhanov V A and Rossokhin A V 2018 *IOP Conference Series: Materials Science and Engineering* **457(1)** 012007

[23] Likhanov V A and Skryabin M L 2019 *IOP Conference Series: Earth and Environmental Science* **315** 032045

[24] Chuvashev A N and Chuprakov A I 2020 *Journal of Physics: Conf. Series* **1515** 042094

[25] Likhanov V A, Kopchikov V N and Fominykh A V 2020 *Journal of Physics: Conf. Series* **1515** 042026

[26] Anfilatov A A and Chuvashev A N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 032052

[27] Likhanov V A, Rossokhin A V and Devetyarov R R 2020 *Journal of Physics: Conf. Series* **1515** 042064

[28] Skryabin M L and Grebnev A V 2020 *Journal of Physics: Conf. Series* **1515** 052052

[29] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062027

[30] Skryabin M L 2020 *Journal of Physics: Conf. Series* **1515** 04283

[31] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062033

[32] Likhanov V A, Lopatin O P and Vylegzhanin P N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062078

[33] Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062025

[34] Anfilatov A A and Chuvashev A N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 032055