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### Semi-empirical model for indirect measurement of soot size distributions in compression ignition engines

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#### Abstract

This work proposes a semi-empirical model, which provides soot particle size distribution functions emitted by compression ignition engines. The model 2 is composed of a phenomenological model based on the collision dynamics of 3 particle agglomerates and an empirical model, which provides key input parameters such as primary particle size and a mathematical relationship between the size of the agglomerate and number of primary particles. The phenomenological model considers the relevant fluid-dynamics phenomena influencing the collision frequency function. It is observed that Brownian motion is the predominant phenomenon and in a much lesser degree inertial turbulent motion. The experimental model requires air/fuel ratio, engine speed, soot density and 10 mean instantaneous in-cylinder pressure. A Dirac delta is used as a seed for the 11 agglomerate size function whose magnitude depends on the soot volume concen-12 tration and the mean primary particle size at each engine operation condition. 13 In a further step, the obtained modelled agglomerate size functions are fitted 14 to lognormal size distributions defined by the modelled mean size and stan-15 dard deviation. Modelled lognormal agglomerate size distribution functions are 16 validated with respect to experimental distributions obtained using a Scanning 17 Mobility Particle Sizer (SMPS). 18 Keywords: particle size distribution function, soot, compression ignition

engines, semi-empirical modelling

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#### <sup>19</sup> 1. Introduction

Compression ignition engines have significant advantages in terms of engine 20 performance, fuel economy and CO<sub>2</sub> emissions compared to spark ignition en-21 gines. However, they have the drawback of high  $NO_x$  and particulate matter 22 (PM) emissions derived from their non-homogeneous combustion process. Reg-23 ulatory actions aiming to mitigate the environmental [1] and public health [2] 24 effects of particulate matter released by vehicles have been put in place. The 25 mass of PM emissions has been regulated in Europe since Euro 1 in light duty 26 passenger cars and commercial vehicles powered by diesel engines. Particle 27 size affects (i) particle reactivity through the surface/volume ratio, (ii) parti-28 cle suspension time in the atmosphere and (iii) particle trapping efficiency in 29 a filtration system, and thus the environmental and health effects of particles. 30 As a result, since the entry into force in Europe of Euro 5b in September 2011 31 [3], not only the mass emissions of particles are regulated but also the total 32 number of particles for both diesel and gasoline powered vehicles. It could be 33 also evaluated the possibility to introduce the particle size as a limitation factor 34 in the future. 35

Particles are formed in locally rich-in-fuel regions in the combustion cham-36 ber. Fuel molecules which do not have access to oxygen are pyrolysed producing 37 aromatics and other hydrocarbon species (such as C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, C<sub>4</sub>H<sub>4</sub>), 38 which can act as polycyclic aromatic hydrocarbons (PAHs) and soot precursors. 39 PAHs from a certain size condense forming a 1-2 nm nuclei (nucleation). Those 40 nuclei undergoes surface growth maintaining a quasi-spherical shape [4, 5] while 41 increasing the C/H ratio forming the so-called primary particles with sizes be-42 tween 15 and 30 nm depending on fuel, engine and engine operation condition. 43 Thereafter, particle agglomerates are formed as a consequence of collisions be-44 tween the primary particles and/or primary particles and agglomerates. The 45 formed agglomerates loose the spherical shape becoming like-fractal structures 46 [6, 7], thus equivalent diameters based on different properties are defined to 47 quantify agglomerate size. Equivalent diameter of a non-spherical particle is 48

the diameter of a spherical particle that gives the same value of a specific property (aerodynamic, electrical mobility, optical, etc.) to that of the non-spherical agglomerate. For instance, electrical mobility diameter can be related by potential functions with other characteristic sizes such as the radius of gyration [8, 9].

The determination of particle size distribution functions not only provides 54 information related to the environmental and human health effects but also 55 could contribute to the diagnosis of the causes of particle formation as well as 56 to adopt actions for their abatement. Exhaust particle size distributions are 57 measured using particle sizer spectrometers such as Scanning Mobility Particle 58 Sizer (SMPS) [10], Engine Exhaust Particle Spectrometer (EEPS), Cambustion 59 DMS 500 [11], Electrical Low Pressure Impactor (ELPI) [12], etc. These equip-60 ment require the dilution of the exhaust to reproduce atmospheric conditions 61 and adapt the sample in temperature and particle concentration to be measured 62 by the equipment. Thus, this process could provoke quantitative and qualitative 63 differences to the agglomerate size distribution [13]. The modeling of size distri-64 bution functions has been studied in [14] for generic aerosols or in works as [15], 65 [16] and [17] for soot aerosols. The complex nature of pollutant formation and 66 oxidation in compression ignition engines [18] and [19] results in the utilisation 67 of different types of models and/or their combination including phenomenolog-68 ical (physically motivated relations), empirical (measured data to identify the 69 relations) [20] and hybrid approaches combining physical and empirical relations 70 (semi-empirical models) [21]. Phenomenological and empirical approaches both 71 have appropriate characteristics but also present disadvantages. Phenomeno-72 logical models predict qualitative trends but the physically motivated relations 73 are difficult to identify [22] and [23] and have limitations from error propagation 74 and computational time [24]. On the other hand, empirical models are computa-75 tional efficient, fit accurately to quantitative measurement results and are simple 76 to handle, [25]. The major limitation of empirical models is the lack of reliable 77 extrapolation beyond the conditions where the model is fitted and that only the 78 parameters explicitly present in the model could be identified. Semi-empirical 79

models combine the capabilities of physical models providing reliable qualitative
trends enabling the model extrapolation with minimum number of constraints
and measurements required to adjust the model as well as the computational
efficiency of empirical models [21].

This paper aims to develop a new methodology to estimate the size distribu-84 tion function of the soot agglomerates emitted from compression ignition engines 85 using a semi-empirical model composed of a phenomenological and empirical 86 model. The model is validated with respect to agglomerate size distribution ex-87 perimentally measured using an SMPS in the same engine operation conditions. 88 Section 2 describes the proposed semi-empirical model including the hypothe-89 ses, phenomenological dynamics of the collisions between agglomerates, and the ٩N relations between agglomerate size and number of primary particles. The ex-91 perimental facilities and techniques used to obtain the input of the model (e.g. 92 in-cylinder pressure, engine speed, Air/Fuel ratio, and volumetric soot concen-93 tration) are presented in Section 3. The experimental particle size distributions 94 and model validation are developed in Section 4, while conclusions are presented 95 in Section 5. 96

#### 97 2. Methodology and experimental installation

The proposed semi-empirical model provides particle size distributions for 98 different engine operation conditions requiring instantaneous in-cylinder presqq sure, total volumetric soot concentration, engine speed and Air/Fuel ratio as in-100 puts. The obtained particle size distributions are in the nanometric range. The 101 model is composed of a phenomenological model to describe particle collisions 102 in the combustion chamber, as well as empirical models which feed the phe-103 nomenological model (see figure 1). Particularly, the empirical model provides 104 the relationship between the initial primary particle size and engine operation 105 condition (engine speed, Air/Fuel ratio) as well as the correlation between the 106 number of primary particles per agglomerate and agglomerate size. The resul-107 tant agglomerate size distribution is fitted to a log-normal distribution function 108

maintaining the mode and standard deviation. The results of the semi-empirical
model are validated with respect to experimental agglomerate size distributions
measured using an SMPS in the same engine operation conditions.



Figure 1: Scheme of the semi-empirical model

The experimental tests to obtain the required model input parameters and 112 the results to validate the model have been carried out in a Nissan YD2.2 113 turbocharged compression ignition engine operated by standard EN590 diesel 114 fuel. An asynchronous brake, Schenck brand Dynas III LI 250 has been used 115 to provide to the engine the desired operation load. Soot concentration pro-116 duced by the engine is measured with an AVL 415 smokemeter. The instan-117 taneous mean in-cylinder pressure values have been measured using a Kistler 118 piezoelectric transducer model Z17090sp149. The crankshaft rotation angle has 119 been measured with an optical angle encoder AVL364. These two signals have 120 been synchronized by a Yokogawa OR1400 oscilloscope. From the instanta-121 neous mean in-cylinder pressure and by using a zero-dimensional thermody-122 namic model within the combustion chamber, [26, 27], the instantaneous mean 123 temperature inside the combustion chamber can be obtained. A SMPS has been 124 used to measure the particle size distribution function in the tailpipe to validate 125 the semi-empirical model. The SMPS classifies the particles according to their 126 mobility size. The SMPS used is from TSI, model 3936L10, and the particle 127 counter is CPC model 3010S. The Differential Mobility Analyzer (DMA) has a 128 sizing uncertainty of approximately 3 - 3.5%, [28]. The SMPS has a particle 129

<sup>130</sup> size measurement range from 10 to 500 nm.

A reference engine operation condition extracted from the urban driving of 131 the light vehicle type-approval cycle has been chosen. This point has been de-132 noted as L2. The engine load has been varied at this operating point, keeping 133 the rest of the engine's operating parameters constant, such as the engine speed 134 maintained at 1525 rpm and EGR (0% EGR). The five engine test points are 135 summarised in the table 1, including torque, Air/Fuel ratio, brake mean ef-136 fective pressure (BMEP) and the soot concentration, while the instantaneous 137 in-cylinder temperature is shown in Figure 2. The starting point for the model 138 has been located when the combustion starts in the combustion chamber, and 139 has been denoted as  $t_0$ . 140

Operating mode	Torque (Nm)	Air/Fuel ratio	BMEP (bar)	$\rm C~(mg{\cdot}m^{-3})$
L1	27.2	43.00	1.53	11.42
L2	45.4	32.28	2.63	16.25
L3	58.4	26.99	3.36	21.67
L4	70.8	23.37	4.08	62.20
L5	83.1	20.05	4.80	348.86

Table 1: Engine operating conditions.

#### <sup>141</sup> 3. Proposed model

The semi-empirical model solves the equations that express the balance of the number of particles per size of a distribution function. The size distribution is discretized in terms of the particle collision frequency to which is subjected an initial mono-disperse population of primary particles under Brownian movement [29].

147 3.1. Assumptions

Initially the aerosol is monodisperse. The aerosol considered at the begin ning of the simulation is monodisperse being composed of solid spherical



Figure 2: Average pressure (a) and average temperature (b) inside the combustion chamber vs. crank time.

primary particles in suspension, with a diameter  $d_{po}$ .

2. Conservation of mass. The mass of the particle formed after a collision is
 equal to the sum of the masses of the particles that collided.

3. Loss of identity of colliding particles. The particle formed after a collision
of two particles has different fractal dimension to its progenitors, [30].

Instantaneous internal coalescence time. The collision and recombination
 processes to form the new particle is instantaneous.

#### 157 3.2. Collision dynamics of particle agglomerates

The particle number concentration at size k  $(n_k)$  is obtained as the balance between the formation of new particles and the disappearance of particles of size k. Both of them are dependent from the number of particle collisions (N). The number of collisions between particles at size i and j can be calculated considering the frequency of particle collision  $(\beta_{ij})$  and the concentration of particles at size i and j being mathematically expressed in equation (1).

$$N_{ij} = \beta \left( i, j \right) n_i n_j, \tag{1}$$

where  $\beta(i, j)$  is the function of the collision frequency that depends on the size of the colliding particles and the gas properties (see further mathematical details in reference [31]), while  $n_i$  and  $n_j$  are the concentration of particles of size i and j per unit of volume.

Taking into consideration equation (1), the net rate of particles (forma-168 tion/disappearance) per particle size k at a given instant can be calculated (2). 169 Therefore, the number of particles per particle size (agglomerate size distribu-170 tion) leaving the engine combustion chamber could be obtained from integration 171 of Equation (2) assuming mass conservation and instantaneous internal coales-172 cence time. It has to be noted that the particle formation rate for size k, 173 (k = i + j), must be affected by a factor of  $\frac{1}{2}$  in order to avoid duplication in 174 formation. 175

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \frac{1}{2} \sum_{i+j=k} \beta(i,j) \, n_i n_j - n_k \sum_{i=1}^{\infty} \beta(i,k) \, n_i \tag{2}$$

As commented above, the collision frequency function  $\beta(i, j)$  depends on 176 the number and characteristics of the particles involved in such collisions and 177 the gas properties. Basically, there are two main mechanisms into a combustion 178 chamber to drive the collisions: Brownian movement and inertial movement 179 due to fluid turbulence. In the case under study, the inertial movement can 180 be neglected in a first approximation. To show that, it is known that the 181 characteristic scale of a soot agglomerate is  $d_p \sim 100$  nm, [30]. On the other 182 hand, at the Kolmogorov scale  $\eta$  viscosity dominates and the turbulent kinetic 183 energy is dissipated into heat, being negligible the inertial movement. In other 184 words,  $\eta$  is a measure of the size of eddies at which molecular viscosity becomes 185 dominant. An estimate for the ratio of the largest L to smallest  $\eta$  length scales 186 in turbulent flows is given in equation (3), [32]. 187

$$\frac{L}{\eta} \sim \left(\frac{UL}{\nu}\right)^{3/4} = Re^{3/4},\tag{3}$$

where Re, is the Reynolds number based on the large scale flow features, U is a characteristic velocity and L is a characteristic length, and  $\nu$ , the kinematic viscosity of the gas. For the engine under study, we can choose: as characteristic length the diameter of the cylinder  $L \sim D = 86.5 \times 10^{-3}$  m; as characteristic velocity the mean piston speed,  $U = 2 \times stroke \times n/60$ , that for n = 1525 rpm and  $stroke = 94 \times 10^{-3}$  m it is found U = 4.78 m/s; finally, for an average temperature inside the chamber of 1500 K and a pressure of 70 bar, the kinematic viscosity of the air is  $\nu \sim 3.5 \times 10^{-6} m^2/s$ . Thus, the Reynolds number for the large scales is  $Re \sim 1.2 \times 10^5$ . Therefore, Eq. 3 yields,

$$\eta \sim \frac{L}{Re^{3/4}} \sim 13.6 \times 10^{-6} \,\mathrm{m} = 13.6 \,\mu\mathrm{m},$$
(4)

which is the typical value for the Kolmogorov scale found in other studies [33]. In summary, since  $\eta/d_p \sim 140$ , the inertial movement can be neglected versus the Brownian movement in the collision frequency function  $\beta(i, j)$  for soot particles. As collision frequency is dominated by Brownian motion and the aerosol could be considered discreet (Knudsen number greater than 10), the function of collision frequency is obtained from the kinetic theory of gases, [31] and [34].

$$\beta(i,j) = \left(\frac{3\pi KT}{\rho_s d_{po}^3}\right)^{\frac{1}{2}} (R_i + R_j)^2 \left(\frac{1}{n_{po,i}} + \frac{1}{n_{po,j}}\right)^{\frac{1}{2}}$$
(5)

where  $R_i$  and  $R_j$  are radii of the sphere that circumscribes to the particles 194 at size i and j respectively,  $n_{po,i}$  and  $n_{po,j}$  are the number of primary parti-195 cles contained in the agglomerates at size i and j,  $K = 1.3807 \cdot 10^{-23} \text{ (J/K)}$ 196 is Boltzmann's constant, T is the average temperature within the combustion 197 chamber determined with a zero dimensional three zone thermodynamics mod-198 els, [35],  $\rho_s$  is the density of soot, which in this case has been taken a value of 199 1850 (kg/m<sup>3</sup>), [36] and  $d_{po}$  is the average diameter of the primary particles that 200 make up the agglomerate, which depends on engine speed (s) and the ratio of 201 fresh air inducted by the engine and fuel consumed (A/F), calculated according 202 to [36]. 203

$$d_{po}(\text{nm}) = 50.6 - 18.9 \frac{s}{2000} - 10.3 \frac{A/F}{30}$$
(6)

As it can be seen in equation (5), the number and size of primary particles and the size of the agglomerates are unknow to calculate the collision frequency. Therefore, a relationship between the number of primary particles and the agglomerate size is proposed in the following section.

3.3. Relationship between the applomerate size and number of primary particles 208 Synthetic agglomerates have been generated in order to find a correlation be-209 tween the agglomerate size and the number of primary particles. The algorithm 210 to simulate the synthetic agglomerates based on random cluster-cluster collisions 211 has been developed by the authors and further details can be found in Martos 212 et al. [30]. A representative example of the simulated agglomerates is shown 213 in Figure 3(b). For comparison purposes, Figure 3(a) shows a picture taken 214 with a High Resolution Transmission Electron Microscope (HR-TEM) of a real 215 particle agglomerate originated within a combustion chamber of a compression 216 ignition engine. The particle was collected using the experimental technique 217 based on the thermophoretic phenomenon reported in [36] (see further details 218 in Lapuerta et al. [36]). 219



Figure 3: Views of a real agglomerate (a) and a synthetic agglomerate (b).

In order to find an appropriate correlation between the radius R and the number of primary particles  $n_{po}$ , 250000 synthetic agglomerates were simulated (gray circles) being  $n_{po}$  random. However, for the sake of clarity only 10000 sim-



Figure 4: Random simulations (circles) and least-squares fittings (lines).

ulations have been plotted in Fig. 4 (one every 25 simulations). The blue solid
line in Figure 4 corresponds to the potential fitting for the 250000 agglomerates,

$$\frac{\overline{R}}{d_{po}} = 0.7831 \, n_{po}^{0.5369}, R^2 = 0.9146, \tag{7}$$

being the validity of the fitting for  $n_{po} \leq 500$ .

To show that R follows a normal distribution function, the results for 500 random simulations, keeping constant  $n_{po}$  for four characteristic sizes of agglomerates, have been included in Fig. 5: small size (a)  $n_{po} = 50$ ; intermediate sizes (b)  $n_{po} = 100$  and (c)  $n_{po} = 200$ ; large size (d)  $n_{po} = 300$ . Since the population for each  $n_{po}$  is higher than 50, the assumption of normality can be checked using the test of Kolmogorov-Smirnov with the correction of Lilliefors. As can be appreciated in Fig. 5, the distribution functions follow a Gaussian

As can be appreciated in Fig. 5, the distribution functions follow a Gaussian distribution, with mean  $\overline{R}$  and standard deviation  $\sigma$ . Therefore, the radius of the synthetic agglomerate will fall into the interval  $\overline{R} - \sigma < R < \overline{R} + \sigma$  with

 $\sim 68.27\%$  probability. This interval is plotted in Fig. 4 with dashed-lines, being the fittings,

$$\begin{cases} \frac{\overline{R}_{+\sigma}}{d_{po}} = 0.8789 \, n_{po}^{0.5464}, R^2 = 0.9947, \\ \frac{\overline{R}_{-\sigma}}{d_{po}} = 0.6984 \, n_{po}^{0.5269}, R^2 = 0.9975. \end{cases}$$
(8)

![](_page_12_Figure_2.jpeg)

Figure 5: Number of agglomerates versus radius, keeping constant the number of primary particles that compose them. (a)  $n_{po} = 50$ , (b)  $n_{po} = 100$ , (c)  $n_{po} = 200$  and (d)  $n_{po} = 300$ .

#### 232 4. Results and discussion

Figure 6 shows the size distribution functions obtained with the model presented in equation (2) (dashed read line) in which the collision radius has been determined through the adjustment proposed in equation (7) with respect to

the experimental size distribution function obtained with the SMPS (solid blue 236 line). As the equivalent diameter used in the modelled distribution is different 237 to the electric mobility diameter obtained in the experimental distribution, the 238 diameters of electric mobility have been corrected according to the approach 239 explained in [17]. In the y-axis, the concentration of particles for a given size 240 has been normalized with respect to the maximum value of the particle concen-241 tration. Therefore, the value of the distribution function is normalized with the 242 value of the size distribution function at his mode. 243

![](_page_13_Figure_1.jpeg)

Figure 6: Size distribution functions for each operating point. (a) L1, (b) L2, (c) L3, (d) L4 and (e) L5.

244

Table 2 shows the relative error obtained when the modelled and experi-

mental size distribution modes are compared. The relative error obtained with 245 the proposed semi-empirical model is lower than 3% for all tested engine op-246 eration modes, being lower than the uncertainty of the SMPS. The proposed 247 model also reproduce the increase in the size distribution mode as a function 248 of the increase in the engine load (Table 2), as well as the modelled particle 249 size distributions are mono-modal coincident with these specific results and the 250 majority of the experimental soot agglomerate size distributions [37]. However, 251 as shown in figure 6, the size distribution function obtained with the proposed 252 semi-experimental model is better suited to the experimental size distribution 253 function for sizes less than 100 nm than for sizes larger than 100 nm. 254

Operating mode	$d_{po}$ (nm)	$d_{SMPS}$ (nm)	$d_p$ (nm)	Relative error $(\%)$
L1	21.36	54.25	54.71	0.85
L2	25.25	58.29	58.87	1.00
L3	26.87	62.64	61.08	2.49
L4	28.25	67.32	69.17	2.75
L5	29.26	111.40	108.96	2.19

Table 2: Modes obtained from the distribution functions for all test points.

It is well reported that agglomerate size distributions could be fitted to log-normal distributions [37]. Therefore, the modelled agglomerate size distributions are also fitted to log-normal distributions. A log-normal distribution is well defined with the mean  $\overline{d_p}$  and standard deviation  $\sigma$ , equation (9). The mode of the modelled distribution function will be employed as the mean of the fitted log-normal distribution, while an empirical correlation based on the SMPS results is proposed to obtain the standard deviation.

$$f(d_p) = \frac{1}{\sqrt{2\pi}\ln(\sigma)} \exp\left[-\frac{1}{2\ln^2(\sigma)} \left(\ln(d_p) - \ln(\overline{d_p})\right)^2\right]$$
(9)

The SMPS results have been fitted to a log-normal size distribution. The fitting has been performed minimizing the mean quadratic error between the experimental and fitting values. Figure 7 and Table 3 compare the agglomerate

size distribution functions, mean diameter and standard deviation for the raw 265 (directly obtained from the SMPS), and log-fitted experimental values at all the 266 engine operation conditions. An empirical correlation has been found between 267 the experimental mean diameter and standard deviation obtained from the log-268 normal fitting (Figure 8) and equation (10). The a, b and c coefficients of 269 equation (10) has been obtained minimizing the mean quadratic error obtaining 270  $a = 5.183 \times 10^8$ , b = -5.497 and c = 1.685, being this fitting valid when 271  $50 \le \overline{d_p} \le 115.$ 272

![](_page_15_Figure_1.jpeg)

 $\sigma = a \,\overline{d_p}^b + c \tag{10}$ 

Figure 7: Comparison of agglomerate size distribution functions for all the engine operating conditions.

Operating mode	$d_{SMPS}$ (nm)	$\overline{d_p}$ (nm)	$\sigma$
L1	54.25	54.71	1.825
L2	58.29	58.87	1.782
L3	62.64	61.08	1.764
L4	67.32	69.17	1.725
L5	111.10	108.96	1.688

Table 3: Experimental mean diameter and experimental log-normal fitting mean diameter and standard deviation

![](_page_16_Figure_2.jpeg)

Figure 8: Empirical correlation between experimental mean diameter and standard deviation obtained from the log-normal fitting.

#### 273 5. Conclusions

A semi-experimental model has been developed to obtain the agglomerate size distribution function emitted by a compression ignition engine fueled with standard diesel fuel. The model combines the attributes of phenomenological models utilising physically motivated relations for reliable extrapolation within some margins, with the computational efficiency and easiness to be handle of empirical models.

The required inputs of the model are constants as soot density, parameters 280 as engine speed, air/fuel ratio, total volumetric soot concentration and mean 281 instantaneous in-cylinder pressure, and empirical relations to obtain primary 282 particle mean diameter and the relation between agglomerate size and number 283 of primary particles, which compose the agglomerates. An acceptable fit has 284 been obtained between the size distribution function obtained with the proposed 285 model and the experimentally measured distribution function with a Scanning 286 Mobility Particle Sizer (SMPS). The error made in the prediction of the mean 287 particle size distribution is lower than the measurement error of the SMPS for 288 all experimentally tested cases. 289

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#### <sup>295</sup> Appendix A. Nomenclature

A	air
d	diameter
C	soot concentration
D	diameter
F	fuel
i,j,k	size
L	lenght scale
n	number of particles
N	number of colissions
R	radius
Re	Reynolds number
s	engine speed

t	time
T	temperature
U	velocity
$\beta$	function of the collission frequency
$\eta$	Kolmogorov scale
ρ	density
ν	kinomatic viscosity

#### 296 Subscripts

i	index
j	index
p	particle
po	primary particle
8	soot

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