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

F.J. Martos[a,*], G. Martín-González[a], J.M. Herreros[b]

[a] Escuela de Ingenierías Industriales, University of Málaga, c/Doctor Ortiz Ramos, s/n, 29071 Málaga, Spain
[b] School of Mechanical Engineering, University of Birmingham, Edgbaston B15 2TT, UK

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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 is composed of a phenomenological model based on the collision dynamics of 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 mean instantaneous in-cylinder pressure. A Dirac delta is used as a seed for the agglomerate size function whose magnitude depends on the soot volume concentration and the mean primary particle size at each engine operation condition. In a further step, the obtained modelled agglomerate size functions are fitted to lognormal size distributions defined by the modelled mean size and standard deviation. Modelled lognormal agglomerate size distribution functions are validated with respect to experimental distributions obtained using a Scanning Mobility Particle Sizer (SMPS).

1. Introduction

Compression ignition engines have significant advantages in terms of engine performance, fuel economy and CO_2 emissions compared to spark ignition engines. However, they have the drawback of high NO_x and particulate matter (PM) emissions derived from their non-homogeneous combustion process. Regulatory actions aiming to mitigate the environmental [1] and public health [2] effects of particulate matter released by vehicles have been put in place. The mass of PM emissions has been regulated in Europe since Euro 1 in light duty passenger cars and commercial vehicles powered by diesel engines. Particle size affects (i) particle reactivity through the surface/volume ratio, (ii) particle suspension time in the atmosphere and (iii) particle trapping efficiency in a filtration system, and thus the environmental and health effects of particles. As a result, since the entry into force in Europe of Euro 5b in September 2011 [3], not only the mass emissions of particles are regulated but also the total number of particles for both diesel and gasoline powered vehicles. It could be also evaluated the possibility to introduce the particle size as a limitation factor in the future.

Particles are formed in locally rich-in-fuel regions in the combustion chamber. Fuel molecules which do not have access to oxygen are pyrolysed producing aromatics and other hydrocarbon species (such as C_2H_2,C_2H_4,C_3H_6,C_4H_4), which can act as polycyclic aromatic hydrocarbons (PAHs) and soot precursors. PAHs from a certain size condense forming a 1–2 nm nuclei (nucleation). Those nuclei undergoes surface growth maintaining a quasi-spherical shape [4,5] while increasing the C/H ratio forming the so-called primary particles with sizes between 15 and 30 nm depending on fuel, engine and engine operation condition. Thereafter, particle agglomerates are formed as a consequence of collisions between the primary particles and/or primary particles and agglomerates. The formed agglomerates loose the spherical shape becoming like-fractal structures [6,7], thus equivalent diameters based on different properties are defined to quantify agglomerate size. Equivalent diameter of a non-spherical particle is 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 information related to the environmental and human health effects but also could contribute to the diagnosis of the causes of

* Corresponding author.
E-mail address: fjmartos@uma.es (F.J. Martos).

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Nomenclature

A	air
d	diameter
C	soot concentration
D	diameter
F	fuel
i,j,k	size
L	length scale
n	number of particles
N	number of collisions
R	radius
Re	Reynolds number
s	engine speed
t	time
T	temperature
U	velocity
β	function of the collision frequency
η	Kolmogorov scale
ρ	density
ν	kinematic viscosity

Subscripts

i	index
j	index
p	particle
po	primary particle
s	soot

particle formation as well as to adopt actions for their abatement. Exhaust particle size distributions are measured using particle sizer spectrometers such as Scanning Mobility Particle Sizer (SMPS) [10], Engine Exhaust Particle Spectrometer (EEPS), Cambustion DMS 500 [11], Electrical Low Pressure Impactor (ELPI) [12], etc. These equipment require the dilution of the exhaust to reproduce atmospheric conditions and adapt the sample in temperature and particle concentration to be measured by the equipment. Thus, this process could provoke quantitative and qualitative differences to the agglomerate size distribution [13]. The modeling of size distribution functions has been studied in [14] for generic aerosols or in works as [15–17] for soot aerosols. The complex nature of pollutant formation and oxidation in compression ignition engines [18,19] results in the utilisation of different types of models and/or their combination including phenomenological (physically motivated relations), empirical (measured data to identify the relations) [20] and hybrid approaches combining physical and empirical relations (semi-empirical models) [21]. Phenomenological and empirical approaches both have appropriate characteristics but also present disadvantages. Phenomenological models predict qualitative trends but the physically motivated relations are difficult to identify [22,23] and have limitations from error propagation and computational time [24]. On the other hand, empirical models are computational efficient, fit accurately to quantitative measurement results and are simple to handle, [25]. The major limitation of empirical models is the lack of reliable extrapolation beyond the conditions where the model is fitted and that only the parameters explicitly present in the model could be identified. Semi-empirical 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 distribution function of the soot agglomerates emitted from compression ignition engines using a semi-empirical model composed of a phenomenological and empirical model. The model is validated with respect to agglomerate size distribution experimentally measured using an SMPS in the same engine operation conditions. Section 2 describes the proposed semi-empirical model including the hypotheses, phenomenological dynamics of the collisions between agglomerates, and the relations between agglomerate size and number of primary particles. The experimental facilities and techniques used to obtain the input of the model (e.g. in-cylinder pressure, engine speed, Air/Fuel ratio, and volumetric soot concentration) are presented in Section 3. The experimental particle size distributions and model validation are developed in Section 4, while conclusions are presented in Section 5.

2. Methodology and experimental installation

The proposed semi-empirical model provides particle size distributions for different engine operation conditions requiring instantaneous in-cylinder pressure, total volumetric soot concentration, engine speed and Air/Fuel ratio as inputs. The obtained particle size distributions are in the nanometric range. The model is composed of a phenomenological model to describe particle collisions in the combustion chamber, as well as empirical models which feed the phenomenological model (see Fig. 1). Particularly, the empirical model provides the relationship between the initial primary particle size and engine operation condition (engine speed, Air/Fuel ratio) as well as the correlation between the number of primary particles per agglomerate and agglomerate size. The resultant agglomerate size distribution is fitted to a log-normal

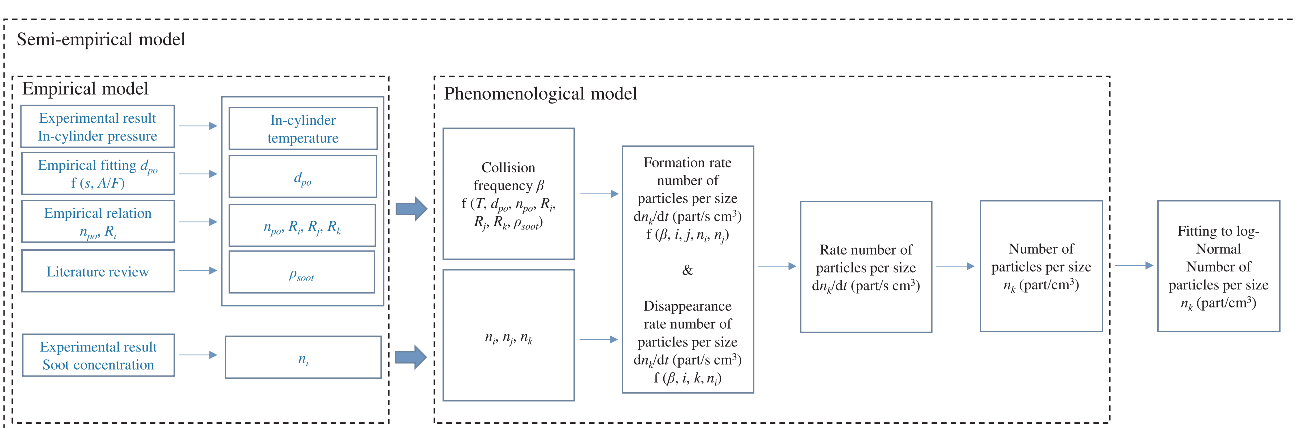

Fig. 1. Scheme of the semi-empirical model.