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Soot Particle Size Distribution in Internal Combustion Engines

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Condensed-phase particles in the exhaust gas of transportation engines are represented mainly by soot particles with absorbed volatile organic compounds and polycyclic aromatic hydrocarbons (PAH), as well as inorganic sulphur and nitrogen containing compounds, and to a less extent by condensed microdrops of volatile organic and inorganic substances. In view of stringent Euro-VI requirements to particulate emissions, automotive companies worldwide are working, on the one hand, on the advanced filters and exhaust aftertreatment devices, and on the other hand, on further improvement of the operation process aimed at a significant reduction of soot emissions.

Nowadays the operation process is hard to improve without sound understanding of all physical and chemical phenomena accompanying soot formation in engine cylinder. There is a need in models capable of predicting not only soot yield in pyrolysis, oxidation and combustion processes but also particle size distribution in combustion products. The development of such models is a very intricate task as its solution implies detailed simulation of soot formation involving nucleation, the growth of nuclei, cluster shape and structure, as well as various relevant chemical reactions, both homogeneous and heterogeneous.

Since many years, researchers at Semenov Institute are working on the detailed model of soot formation (DMSF) at pyrolysis and partial oxidation of hydrocarbons [1, 2]. In addition to all known channels of soot nuclei formation and growth this model includes the kinetic mechanisms of pyrolysis and oxidation of high hydrocarbons up to n-hexadecane and reactions with PAH. The greatest advantage of this model is that it predicts satisfactorily all published experimental data on soot yield at hydrocarbon pyrolysis and partial oxidation obtained in shock tubes. The other advantage is that this model operates with such parameters of the condensed phase as soot particle number density n_Σ, particle diameters d, mean particle diameter $\bar{d}$, and size distribution function (SDF) $n(d)$. These advantages allow this model to be considered as a practical tool for determining the evolution of soot particle SDF in engine cylinder during the operation process.

Using the DMSF, we have developed a unique data base in the form of look-up tables which allows the soot particle SDF to be reconstructed in the course of multidimensional CFD calculations of engine operation. The look-up tables provide the parameters of the log-normal SDF — total particle number density n_Σ, mean particle diameter $\bar{d}$, and variance σ — approximating the true SDF in the DMSF based on the local instantaneous thermochemical conditions (temperature K, pressure $1 \le P \le 240$ bar, fuel-air ratio $2 \le \Phi \le 4$, and mass fraction of exhaust gases in the mixture $0 \le \theta \le 0.6$) and process time $0 \le \tau \le 3$ ms. For a given set of T, P, Φ, θ and τ one can obtain the values of n_Σ, $\bar{d}$, and σ by interpolation.

Figure 1 presents the example of implementation of the database for predicting the evolution of soot particle SDF in a small-scale diesel engine [3] using AVL FIRE^R code. Shown here are the spatial distributions of mean soot particle diameter $\bar{d}$ (left) and particle number density n_Σ (right) in one engine cross section at different values of crank angle φ: from 735° to 770°. In this example, the maximum value of $\bar{d} \approx 27$ nm (with $n_\Sigma \approx 10^{24}$ m^{-3}) is attained at φ=735° close to the wall in the piston bowl. The maximum local number density of soot particles ($n_\Sigma \approx 10^{25}$ м$^{-3}$) is observed at φ=740° in the same region of the combustion chamber, however the mean particle diameter decreases to $\bar{d} \approx 10$ nm. After some time (cf. φ=770°) the mean particle diameter attains the level of 4—14 nm, whereas the particle number density reaches the value of $n_\Sigma \approx 10^{18} - 10^{20}$ m^{-3}. Figure 2 shows the cumulative (collected in all computational cells of engine cylinder) soot particle SDF at φ=860°, i. e. at the conditions when engine exhaust valves open.

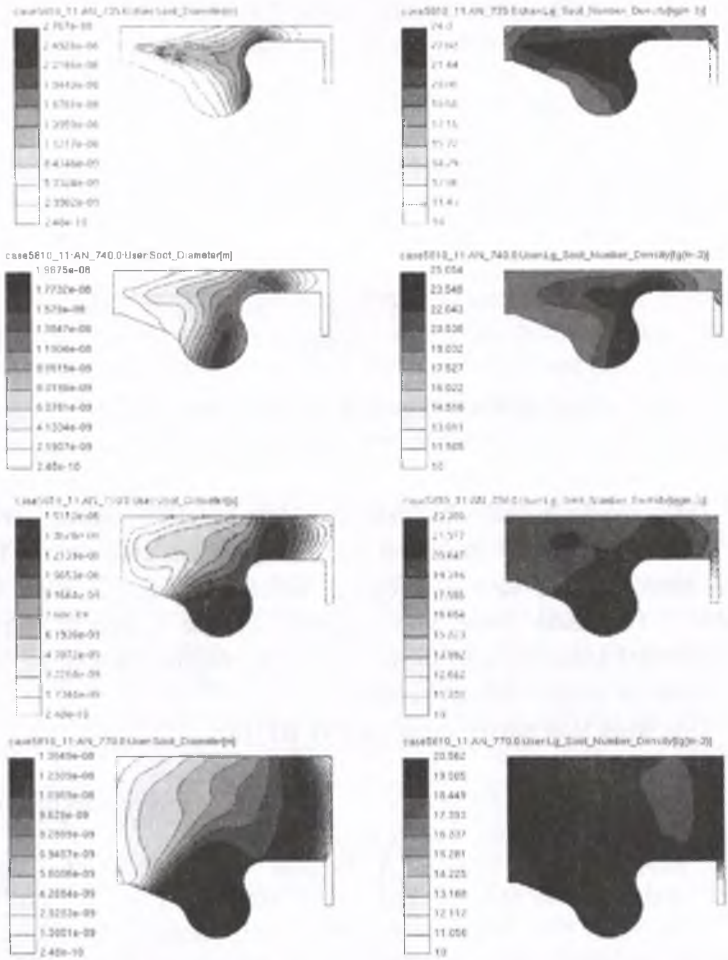

Fig. 1. Predicted spatial distributions of soot particle mean diameter (left) and number density (right) in a small-scale diesel engine at different crank angles: from top to bottom $\varphi = 735, 740^{0}, 750^{0}$ and 770^{0}

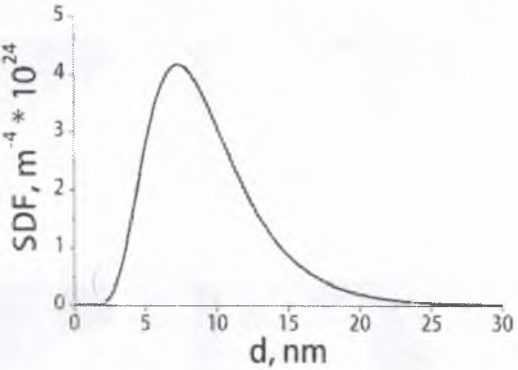

Fig. 2. Predicted cumulative soot particle SDF
in a small-scale diesel engine at $\varphi = 860^{\circ}$

Thus, we have developed a unique data base for reconstructing the soot particle SDF in piston engine operation conditions. The data base is composed of look-up tables constructed using the DMSF. The data base was applied in the transient three-dimensional simulation of diesel engine operation and can be further used for engine improvements.

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