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Simulation of Smoke Particles Coagulation in the Exhaust System of Piston Engine

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Starting from 2012, the new Euro-VI regulation limits both the content of smoke and soot particles (no more than 5 mg/km, 66 % reduction as compared to Euro-V) and their number (no more than $6 \cdot 10^{11}$ 1/km) in the exhaust gases of transportation piston engines [1]. Such stringent regulations require solution of two principal problems, namely (1) improving the engine operation process, and (2) improving the aftertreatment of exhaust gases using advanced smoke filters. To succeed in solving these challenging tasks, there is a need in better understanding of the evolution of particles size distribution function (SDF) during their motion in the engine exhaust system. As a matter of fact, since all emissions are measured at the outlet of the exhaust system the knowledge of the SDF at the exhaust system outlet could help in solving the inverse problem that is to obtain the true SDF in the engine itself. The latter is then can be used for improving the engine operation process and decrease the amount and the number of particles formed in engine.

One of the reasons of SDF variation in the particle-laden turbulent flow is particle coagulation [2, 3]. In high-speed turbulent flows with submicron- and nanosize particles at relatively low temperatures the coagulation of particles is governed mainly by three mechanisms [2—5]: Brownian, turbulent diffusion and turbulent kinetic. It is expected that the Brownian mechanism dominates for particles of size comparable with the size of molecules of the carrier gas [2, 3]. The turbulent diffusion driven coagulation is caused by turbulent velocity fluctuations in the carrier gas which promote particle collisions. The turbulent kinetic coagulation mechanism is based on the fact that there is a velocity slip between gas and particles and therefore particles of different size are involved in the turbulent motion differently. The complex turbulent flow field in modern engine exhaust systems makes it difficult to foresee the dominating coagulation mechanism. It is likely that the various coagulation mechanisms can dominate in different parts of the exhaust system thus replacing each other or contributing comparably to the SDF evolution.

In this communication, the model of smoke particle coagulation in the confined turbulent flow of engine exhaust gases has been developed. The model incorporates all three coagulation mechanisms mentioned above. Mathematically, the model is based on several simplifying assumptions: (1) the gas flow in the exhaust system is one-dimensional, quasi-stationary and is known *a priory*; (2) particles are so small that their velocity does not differ from the local mean gas velocity; (3) particle size varies only due to coagulation; (4) the coagulation probability of colliding particles of different size is equal to 1; (5) the coagulation probability of colliding particles of identical size is equal to 0; (6) the initial SDF is log-normal. These assumptions result in the following differential equation governing the evolution of particle number density $n(d,x)$:

$$\frac{dn}{dx}=\frac{1}{V_g(x)}\left(\frac{dn}{dt}\right)_{coag}, \quad n(d,0)=\frac{n_{in}}{\sqrt{2\pi}\sigma_{in}d}\exp\left(-\frac{\ln^2(d/d_{in})}{2\sigma_{in}^2}\right) \quad (1)$$

where x is the coordinate, V_g is the gas velocity, d is the equivalent particle diameter, parameters n_{in}, d_{in} and σ_{in} are the total number density, mean diameter and variance of the initial log-normal SDF; and the differential term in the right-hand side of Eq. (1) represents the coagulation rate [2]:

$$\left(\frac{dn}{dt}\right)_{coag}=-\int_0^{\infty} n(r_2)\left\{\int_0^{r_1}\beta(r_1,r_2)n(r_1)dr_1\right\}dr_2 \quad (2)$$

Here, $r=d/2$ is the equivalent particle radius, $n(r)dr$ is the number density of particles possessing radius from r to $r+dr$, $\beta(r_1,r_2)=\beta_b(r_1,r_2)+\beta_{td}(r_1,r_2)+\beta_{tk}(r_1,r_2)$ is the coagulation core for particles with radii r_1 and r_2, whereas the terms $\beta_b(r_1,r_2)$, $\beta_{td}(r_1,r_2)$ and $\beta_{tk}(r_1,r_2)$ are the coagulation cores in the Brownian, turbulent diffusion and turbulent kinetic mechanisms [2—5]:

$$\beta_b(r_1,r_2) = k_{fm}(r_1,r_2)K_b(r_1,r_2) \qquad (3)$$

$$\beta_{td}(r_1,r_2) = S(r_1,r_2)\sqrt{\frac{8}{3\pi}\langle w^2\rangle} \qquad (4)$$

$$\beta_{tk}(r_1,r_2) = S(r_1,r_2)w(r_1,r_2) \qquad (5)$$

where k_{fm} is the coefficient of free-molecular coagulation; K_b is the coagulation coefficient; $S(r_1,r_2)$ is the effective collision cross-section; $w(r_1,r_2)$ is the relative velocity of interacting particles in the turbulent flow; and $\langle w^2\rangle$ is the mean value of the squared relative velocity of interacting particles.

The set of equations (1—5), supplemented with the data base of thermophysical data of substances was integrated numerically on the steady-state turbulent flow field in the exhaust system of diesel engine of total length 1.3 m (Fig. 1). Shown in Fig. 1 are the three-dimensional distributions of mean gas velocity V_g and dissipation of the turbulent kinetic energy obtained using AVL FIRE^R code. By averaging over tube cross-section, these distributions were reduced to one-dimensional distributions used in the model.

Figure 2 shows the typical result of calculations for smoke particle coagulation at d_{in} = 10 nm, σ_{in} = 0.6 and $n_{in} = 2\cdot 10^{18}$ m^{-3}. The SDF is seen to undergo significant transformation: the mean particle diameter changes from d_{in} = 10 nm at the inlet of the exhaust pipe to $d_{out} \approx 120$ nm at its outlet. In this example, the Brownian coagulation mechanism was dominating in all pipe sections. Variation of initial SDF parameters at the pipe inlet results in the significant variation of SDF at the outlet. For example, Fig. 3 shows the effect of σ_{in} on d_{out}. In [6], the results of calculations were compared with experimental data.

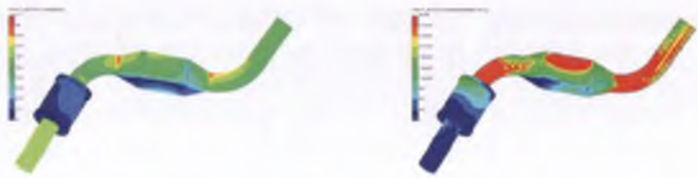

Fig. 1. Three-dimensional distributions of mean gas velocity (left) and dissipation of the turbulent kinetic energy (right) in the diesel exhaust system used for studying the evolution of smoke particle SDF.

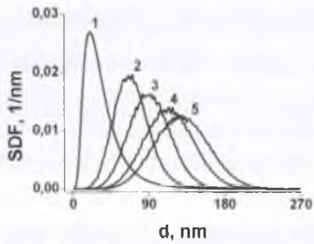

Fig. 2. Predicted variation of smoke particle SDF along the length of the exhaust pipe at initial log-normal SDF parameters $n_{in} = 2 \cdot 10^{18}$ m^{-3}, d_{in} = 10 nm and σ_{in}=0.6: 1 — $x = 0$ (inlet); 2—0.2 m; 3—0.37 m; 4—0.79 m; 5—1.3 m (outlet).

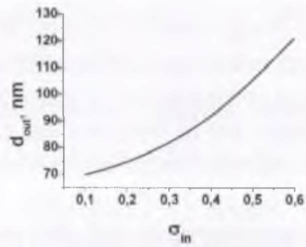

Fig. 3. Predicted dependence of mean smoke particle diameter d_{out} at the pipe outlet on the initial log-normal SDF variance σ_{in} at the pipe inlet at $n_{in} = 2 \cdot 10^{18}$ m^{-3}, d_{in} = 10 nm.

Thus, we have developed the model of smoke particle coagulation in the exhaust system of piston engine, including three coagulation mechanisms: Brownian, turbulent diffusion and turbulent kinetic. The calculations revealed that the coagulation process exerts a significant influence on the particle SDF at the outlet of the exhaust pipe, and the dominating mechanism is the Brownian coagulation.

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1. Commission Regulation (EC) No 692/2008 of 18 July 2008. http://ec.europa.eu/enterprise/sectors/automotive/environment/eurovi/index_ en. htm, p. 130.

2. Payne J. F. B., Skyrme G. *Int. J. Multiphase Flow*, 1993, Vol. 19? No/ 3, pp. 451—470.

3. Friedlander S. K. Smoke, Dust and Haze: Fundamentals of Aerosols Dynamics, NY—Oxford, Oxford University Press Inc., 2000.

4. Levich V. G. Physico-Chemical Hydrodynamics. Moscow, Phyz.-Math. Lit. Publ., 1959.

5. Piskunov V. N. Theoretical models of aerosol formation kinetics. Sarov, Rus. NRC VNIIEF Publ., 2000.

6. Avdeev K. A., Ivanov V. S., Frolov S. M., Basara B., Priesching P., Suffa M. In: Combustion and Explosion. Moscow, Torus Press, 2012, Issue 5, pp. 91—96.

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Real Gas Equation of State for Methane

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Methane is one of the most wide spread fuels and raw materials for chemical industry used for production of synthetic gas, acetylene, black carbon, etc. Despite its thermochemical and physical properties are in general well investigated, its numerous novel applications, in particular in transportation engines, require the knowledge of accurate thermal and calorific equations of state (EOS). The aim of this communication is to develop the thermal EOS for methane in a supercritical parametric domain at $250 \le T \le 1000$ K and $0.1 \le P \le 100$ MPa.

Figure 1 is the phase equilibrium diagram for methane obtained using the data of [1]. The shaded area in Fig. 1 is the supercritical parametric domain of our interest here.