Methyl hydroxide combustion in a diesel cylinder and its effect on the cluster of carbon black

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Abstract. In studies of carbon black education on a model setting during the injection of secondary liquid fuel into the combustion products, the existence of an poise operation temperature, i.e., the temperature at which the operation is characterized by poise between the combustion and decay rates of the fuel in thermal terms has been established. The cluster of smokiness education varies depending on changes in the setting fuel injection angle of a CI engine. At the same time, it is possible to determine with certainty the optimal fuel supply angles in the diesel cylinder both when working on diesel oil, and when working on methyl hydroxide with a pilot portion of hydrocarbon fuel.

1. Introduction
Toxic substances when using mobile vehicles enter the atmosphere with exhaust gases (EG), fumes from fuel systems and during refueling, as well as crankcase gases.

Thus, having understood the reason for the education of EG, mankind can influence for the better the solution of environmental problems of automobile transport [1-3].

Let us consider in more detail the mechanisms of education of those substances whose contents in the EG of internal combustion ignition (CI) engines are normalized or are supposed to be normalized in the future.

The education of toxic substances.

Smokiness. When hydrocarbon fuels are burned in various burners and internal CI engines, the exhaust gas may contain a solid carbon product in a dispersed state (smokiness). Other solid carbon compounds (pyro carbon and filamentary carbon) are usually not contained in the EG, as they form on solid surfaces [4-9].

A smokiness particle is an agglomerate of packets (crystallites), which, in turn, consist of a set of separate grids (plates) of graphite hexagons. In addition to carbon, smokiness contains 1-3% by weight (i.e., 10-30% by number of atoms) of hydrogen, which can be chemically or physically bound to carbon.

Smokiness education is a volumetric operation of thermal decomposition (pyrolysis) of hydrocarbons in the gas (vapor) phase under conditions of a severe deficiency (absence) of an oxidizing agent (oxygen).

The education mechanism includes several stages: nucleation, embryo growth to primary particles (hexagonal plates of graphite), particle size growth (coagulation) to complex educations - conglomerates, including 100-150 carbon atoms, burnout [10-14].
The rate of smokiness education is determined by the rate of chemical operations leading to the emergence of the embryo (i.e., the kinetics of the operation).

At relatively low temperatures (less than 1500 K), polymerization and condensation reactions prevail over hydrogenation reactions. Under these conditions, the nuclei may be aromatic or polycyclic compounds. At temperatures of 2000-3500 K, corresponding to the operation in CI engines, molecules decompose or even break down.

It should be noted that the education of smokiness in a pre-mixed and diffusion flame (laminar and turbulent) also occurs through the pyrolysis of hydrocarbon molecules.

Numerous experimental studies have established the cluster of the oxidizing agent at which the smokiness emission from the flame begins. These clusters are estimated by the coefficient of excess air during combustion \( \alpha \) [15-21].

The cluster limit of the onset of smokiness education depends on many factors (temperature, pressure, type of fuel, type of burner) and \( \alpha \) is 0.33-0.7 for \( \alpha \). With a growth in temperature, the onset of smokiness education shifts toward richer air-fuel mixtures, with a growth in pressure, towards a poorer mixture. The maximum smokiness content with increasing operation temperature also shifts towards rich mixtures. It should be noted that the education of smokiness in a flame (burner or cylinder of an internal CI engine) does not directly affect the coefficient of excess air, but through physical factors (flame temperature; the appearance of mixture zones with clusters favorable for thermal decomposition) [22-25].

The amount of smokiness formed largely depends on the temperature in the zone of hydrocarbon pyrolysis. With increasing temperature, this amount sharply grows, since the reaction rate is controlled by its kinetics. The growth in pressure is similarly affected.

Studies of smokiness education in a model setting (by injecting secondary liquid fuel into combustion products) established the existence of a poise operation temperature, i.e., the temperature at which the operation is characterized by poise between the rates of combustion and decay of the fuel in thermal terms [26-29].

The maximum smokiness content in the combustion products corresponds to the poise temperature. A decrease or growth in temperature compared to poise decreases smokiness content. The poise temperature depends on the experimental conditions and the type of fuel.

It is established that the education of smokiness depends on the properties of the fuel. The higher the molecular weight of straight-chain saturated and unsaturated hydrocarbons, the higher the rate of smokiness particle education. This can be explained by the fact that the strength of the same bond depends on the length of the molecule. So, with a growth in the number of carbon atoms in the molecule from 2 to 5, the bond strength between the CH groups of alkanes decreases from 333 to 268 kJ/mol. It was also found that the cluster of smokiness is greater, the higher the C/H ratio in the fuel [30-34].

The primary structures that make up the smokiness formed in CI engines are spherical particles with a diameter of 150-1700 \( \mu m \) with a specific surface area of up to 76 m²/g. However, even in the combustion operation, coagulation of smokiness particles occurs, leading to the education of secondary and tertiary structures. Smokiness in the EG of CI engines is an irregularly shaped education with linear dimensions of 0.3-100 \( \mu m \). Most smokiness educations are 0.4-5 \( \mu m \) in size. During the expansion of gases in the diesel cylinder, oxygen enters the smokiness particles (due to the movement of gases and oxygen diffusion, i.e., conditions are created that are favorable for smokiness burning. Studies of the education and burning of smokiness in a diesel cylinder, performed by spectral analysis, showed that a significant part of the smokiness burns out during the expansion operation. The emission of smokiness from the EG of a CI engine depends, therefore, both on the education operation and on the operation of burning it out. However, some researchers attach less importance to the operation of smokiness burnout during expansion [35-40].

2. Experimental part

Based on the methodology developed by professors Baturin and Loskutov and using a special program developed at the Leningrad Polytechnic Institute, we determined the significances of the mass cluster C
and the relative cluster \( r \) of smokiness in the EG of a CI engine 2H 10.5 / 12.0 when working on methyl hydroxide [41].

Figure 1 shows a graph of the effect of the use of methyl hydroxide on the mass cluster of smokiness in the EG of a CI engine at various setting fuel injection angle (FIA) at the nominal operating mode at \( n = 1800 \text{ min}^{-1} \) (a) and at maximum torque at \( n = 1400 \text{ min}^{-1} \) (b).

The curves of the change in the mass cluster \( C \) of smokiness from the smokiness in the diesel cylinder show that with an growth in the establish FIA of diesel fuel (DF) and methyl hydroxide, the significance of the mass cluster of \( C \) decreases over the entire range of the set of fixed FIA [42-46].

![Figure 1](image-url)

**Figure 1.** The effect of the use of methyl hydroxide on the mass cluster \( C \) of smokiness in the EG of a CI engine for various setting of FIA: a - at \( n = 1800 \text{ min}^{-1} \) and \( p_e = 0.585 \text{ MPa}, q_{\text{df}} = 6.6 \text{ mg/cycle} \); b - at \( n = 1400 \text{ min}^{-1} \) and \( p_e = 0.594 \text{ MPa}, q_{\text{df}} = 6.0 \text{ mg/cycle} \).

When installing DF \( \Theta_{\text{df}} = 34^\circ \) and methyl hydroxide \( \Theta_{\text{m}} = 34^\circ \) the significance of the mass cluster of smokiness \( C_m = 0.028 \text{ g/m}^3 \) at the nominal operating mode at \( n = 1800 \text{ min}^{-1} \) and \( C_m = 0.018 \text{ g/m}^3 \) at the maximum torque mode at \( n = 1400 \text{ min}^{-1} \). With a growth in the methyl hydroxide FIA setting to \( \Theta_{\text{m}} = 38^\circ \) and \( \Theta_{\text{df}} = 34^\circ \), the significance of the mass cluster of smokiness does not change, and is equal to \( C_m = 0.028 \text{ g/m}^3 \) at \( n = 1800 \text{ min}^{-1} \) and \( C_m = 0.018 \text{ g/m}^3 \) at \( n = 1400 \text{ min}^{-1} \). With a growth in the establish FIA DF to \( \Theta_{\text{df}} = 38^\circ \) and \( \Theta_{\text{m}} = 38^\circ \), the significance of the mass cluster of smokiness grows to \( C_m = 0.029 \text{ g/m}^3 \) and \( C_m = 0.022 \text{ g/m}^3 \) at \( n = 1800 \text{ min}^{-1} \) and \( n = 1400 \text{ min}^{-1} \), respectively. With a decrease in the methyl hydroxide FIA setting to \( \Theta_{\text{m}} = 34^\circ \) and \( \Theta_{\text{df}} = 38^\circ \), the significance of the mass cluster of smokiness decreases to \( C_m = 0.027 \text{ g/m}^3 \) at \( n = 1800 \text{ min}^{-1} \) and \( C_m = 0.018 \text{ g/m}^3 \) at \( n = 1400 \text{ min}^{-1} \). With a further decrease in the methyl hydroxide FIA setting to \( \Theta_{\text{m}} = 30^\circ \) and \( \Theta_{\text{df}} = 38^\circ \), the significance of the mass cluster of smokiness grows to \( C_m = 0.0485 \text{ g/m}^3 \) at \( n = 1800 \text{ min}^{-1} \) and \( C_m = 0.029 \text{ g/m}^3 \) at \( n = 1400 \text{ min}^{-1} \) [47-53].

When the setting FIA DF is changed to \( \Theta_{\text{df}} = 34^\circ \) and \( \Theta_{\text{m}} = 30^\circ \), the significance of the mass cluster of smokiness changes to \( C_m = 0.045 \text{ g/m}^3 \) at \( n = 1800 \text{ min}^{-1} \) and \( C_m = 0.028 \text{ g/m}^3 \) at \( n = 1400 \text{ min}^{-1} \). With a further decrease in the setting FIA DF to \( \Theta_{\text{df}} = 30^\circ \) and \( \Theta_{\text{m}} = 30^\circ \), the significance of the mass cluster of smokiness grows to \( C_m = 0.053 \text{ g/m}^3 \) at \( n = 1800 \text{ min}^{-1} \) and \( C_m = 0.033 \text{ g/m}^3 \) at \( n = 1400 \text{ min}^{-1} \). With a growth in the methyl hydroxide FIA setting to \( \Theta_{\text{m}} = 34^\circ \) and \( \Theta_{\text{df}} = 30^\circ \), the significance of the mass cluster of smokiness changes to \( C_m = 0.045 \text{ g/m}^3 \) at \( n = 1800 \text{ min}^{-1} \) and \( C_m = 0.028 \text{ g/m}^3 \) at \( n = 1400 \text{ min}^{-1} \).

Figure 2 shows a graph of the effect of the use of methyl hydroxide on the relative cluster of smokiness \( r \) in the EG of a CI engine at various setting FIA at the nominal operating mode at \( n = 1800 \text{ min}^{-1} \) (a) and at maximum torque at \( n = 1400 \text{ min}^{-1} \) (b) [54-57].
Curves of the change in the relative cluster $r$ of smokiness in the diesel cylinder show that with an growth in the setting of the FIA DF and methyl hydroxide, the significance of the relative cluster of $C$ decreases over the entire range of the change in the FIA.

When installing FIA DF $\Theta_{df} = 34^\circ$ and methyl hydroxide $\Theta_m = 34^\circ$, the significance of the relative smokiness cluster $r_m = 0.019$ g/kg at the nominal operating mode at $n = 1800$ min$^{-1}$ and $r_m = 0.012$ g/kg at the maximum torque mode at $n = 1400$ min$^{-1}$. With a growth in the methyl hydroxide FIA setting to $\Theta_m = 38^\circ$ and $\Theta_{df} = 34^\circ$, the significance of the relative smokiness cluster changes to $r_m = 0.018$ g/kg at $n = 1800$ min$^{-1}$ and $r_m = 0.012$ g/kg at $n = 1400$ min$^{-1}$. With a growth in the setting FIA DF to $\Theta_{df} = 38^\circ$ and $\Theta_m = 38^\circ$, the significance of smokiness cluster growths to $r_m = 0.019$ g/kg and $r_m = 0.01$ g/kg at $n = 1800$ min$^{-1}$ and $n = 1400$ min$^{-1}$, respectively [58-62].

With a decrease in the methyl hydroxide FIA setting to $\Theta_m = 34^\circ$ and $\Theta_{df} = 38^\circ$, the significance of the relative smokiness cluster does not change, and is equal to $r_m = 0.019$ g/kg at $n = 1800$ min$^{-1}$ and $r_m = 0.010$ g/m$^3$ at $n = 1400$ min$^{-1}$.

![Figure 2](image-url)

**Figure 2.** The effect of the use of methyl hydroxide on the relative cluster of $r$ of smokiness in the EG of a CI engine for various setting of FIA: a - at $n = 1800$ min$^{-1}$ and $p_c = 0.585$ MPa, $q_{cdf} = 6.6$ mg/cycle; b - at $n = 1400$ min$^{-1}$ and $p_c = 0.594$ MPa, $q_{cdf} = 6.0$ mg/cycle.

With a further decrease in the methyl hydroxide FIA setting to $\Theta_m = 30^\circ$ and $\Theta_{df} = 38^\circ$, the significance of the relative smokiness cluster growths to $r_m = 0.034$ g/kg at $n = 1800$ min$^{-1}$ and $r_m = 0.019$ g/m$^3$ at $n = 1400$ min$^{-1}$. When the setting FIA DF is changed to $\Theta_{df} = 34^\circ$ and $\Theta_m = 30^\circ$, the significance of the relative smokiness cluster changes to $r_m = 0.031$ g/kg at $n = 1800$ min$^{-1}$ and $r_m = 0.019$ g/kg at $n = 1400$ min$^{-1}$. With a further decrease in the setting FIA DF to $\Theta_{df} = 30^\circ$ and $\Theta_m = 30^\circ$, the significance of the relative cluster of smokiness growths to $r_m = 0.037$ g/kg at $n = 1800$ min$^{-1}$ and $r_m = 0.023$ g/kg at $n = 1400$ min$^{-1}$. With a growth in the methyl hydroxide FIA setting to $\Theta_m = 34^\circ$ and $\Theta_{df} = 30^\circ$, the significance of the relative smokiness cluster changes to $r_m = 0.032$ g/kg at $n = 1800$ min$^{-1}$ and $r_m = 0.019$ g/kg at $n = 1400$ min$^{-1}$ [63-65].

3. Conclusion

By experimental studies and by calculation, the significances of mass $C$ and relative $r$ of smokiness cluster in the cylinder of the CI engine were determined depending on the change in the angle of rotation of the crankshaft during operation on diesel fuel and on methyl hydroxide at optimal setting fuel injection angle $\Theta_{df} = 34^\circ$ and $\Theta_m = 34^\circ$ with $n = 1800$ min$^{-1}$ and $n = 1400$ min$^{-1}$.

References

[1] Likhanov V A, Lopatin O P and Yurlov A S 2019 *Journal of Physics: Conf. Series* **1399** 055026
[2] Likhanov V A, Kozlov A N and Araslanov M I 2020 *IOP Conf. Series: Materials Science and Engineering* **734** 012211
[3] Likhanov V A and Rossokhin A V 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062047
[4] Anfilatov A A and Chuvashov A N 2020 *Journal of Physics: Conf. Series* **1515** 042048
[5] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Earth and Environmental Science* **421** 072018
[6] Anfilatov A A 2020 *Journal of Physics: Conf. Series* **1515** 042049
[7] Lopatin O P 2020 *IOP Conf. Series: Earth and Environmental Science* **421** 072019
[8] Likhanov V A and Lopatin O P 2020 *Journal of Physics: Conf. Series* **1515** 052002
[9] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062014
[10] Kopchikov N V and Fominykh A V 2020 *Journal of Physics: Conf. Series* **1515** 042028
[11] Likhanov V A and Anfilatov A A 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 032048
[12] Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062087
[13] Anfilatov A A and Chuvashov A N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062064
[14] Likhanov V A and Skryabin M L 2019 *IOP Conf. Series: Earth and Environmental Science* **315** 032045
[15] Likhanov V A and Rossokhin A V 2019 *Journal of Physics: Conf. Series* **1399** 044038
[16] Likhanov V A and Lopatin O P 2018 *IOP Conf. Series: Materials Science and Engineering* **457** 012011
[17] Romanyuk V, Likhanov V A and Lopatin O P 2018 *Theoretical and Applied Ecology* **3** 27-32
[18] Anfilatov A A and Chuvashov A N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 032055
[19] Devetyarov R R 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062072
[20] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **734** 012202
[21] Anfilatov A A and Chuvashov A N 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062069
[22] Likhanov V A, Lopatin O P and Yurlov A S 2020 *IOP Conf. Series: Materials Science and Engineering* **734** 012208
[23] Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062025
[24] Likhanov V A and Lopatin O P 2019 *Journal of Physics: Conf. Series* **1399** 055016
[25] Skryabin M L and Likhanov V A 2020 *IOP Conf. Series: Materials Science and Engineering* **734** 012075
[26] Chuvashov A N and Chuprakov A I 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 062089
[27] Marchuk A, Likhanov V A and Lopatin O P 2019 *Theoretical and Applied Ecology* **3** 080-6
[28] Anfilatov A A and Chuvashov A N 2020 *Journal of Physics: Conf. Series* **1515** 022035
[29] Likhanov V A and Lopatin O P 2020 *Journal of Physics: Conf. Series* **1515** 042019
[30] Skryabin M L and Likhanov V A 2019 *Journal of Physics: Conference Series* **1399** 044063
[31] Likhanov V A and Anfilatov A A 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 032050
[32] Skryabin M L 2020 *Journal of Physics: Conf. Series* **1515** 042107
[33] Likhanov V A and Anfilatov A A 2020 *IOP Conf. Series: Materials Science and Engineering* **862** 032044
[34] Likhanov V A and Lopatin O P 2017 *Thermal Engineering* **64(12)** 935-44
[35] Skryabin M L 2020 *IOP Conf. Series: Earth and Environmental Science* **421** 072012
[36] Lopatin O P 2020 *Journal of Physics: Conf. Series* **1515** 042021
[37] Devetyarov R R and Chuvashov A N 2020 *Journal of Physics: Conf. Series* 1515 042080
[38] Likhanov V A and Lopatin O P 2019 *Ecology and Industry of Russia* 23(9) 60-5
[39] Chuvashov A N, Chuprakov A I and Anfilatov A A 2020 *IOP Conf. Series: Materials Science and Engineering* 734 012184
[40] Likhanov V A and Rossokhin A V 2020 *IOP Conf. Series: Materials Science and Engineering* 734 012207
[41] Anfilatov A A and Chuvashov A N 2020 *Journal of Physics: Conf. Series* 1515 042052
[42] Lopatin O P 2020 *Journal of Physics: Conf. Series* 1515 042009
[43] Lopatin O P 2020 *Journal of Physics: Conf. Series* 1515 052004
[44] Chuvashov A N and Chuprakov A I 2020 *IOP Conf. Series: Materials Science and Engineering* 862 062083
[45] Likhanov V A and Lopatin O P 2019 *Journal of Physics: Conf. Series* 1399 055020
[46] Chuvashov A N and Chuprakov A I 2019 *Journal of Physics: Conf. Series* 1399 055085
[47] Likhanov V A and Rossokhin A V 2020 *IOP Conf. Series: Materials Science and Engineering* 862 062046
[48] Likhanov V A and Lopatin O P 2020 *Journal of Physics: Conf. Series* 1515 042008
[49] Likhanov V A and Lopatin O P 2018 *Ecology and Industry of Russia* 22(10) 54-9
[50] Likhanov V A and Rossokhin A V 2018 *IOP Conf. Series: Materials Science and Engineering* 457 012007
[51] Rossokhin A V and Anfilatov A A 2020 *IOP Conf. Series: Materials Science and Engineering* 862 062065
[52] Anfilatov A A and Chuvashov A N 2020 *Journal of Physics: Conf. Series* 1515 042077
[53] Anfilatov A A 2020 *Journal of Physics: Conf. Series* 1515 042098
[54] Likhanov V A, Lopatin O P and Vylygzhanin P N 2020 *IOP Conf. Series: Materials Science and Engineering* 862 062074
[55] Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* 734 012199
[56] Kozlov A N, Anfilatov A A and Chuvashov A N 2019 *Journal of Physics: Conf. Series* 1399 055051
[57] Anfilatov A A and Chuvashov A N 2020 *IOP Conf. Series: Materials Science and Engineering* 862 032052
[58] Skryabin M L and Grebnev A V 2020 *Journal of Physics: Conf. Series* 1515 052052
[59] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* 862 062027
[60] Likhanov V A, Lopatin O P and Vylygzhanin P N 2020 *IOP Conf. Series: Materials Science and Engineering* 862 062078
[61] Chuvashov A N and Chuprakov A I 2020 *Journal of Physics: Conf. Series* 1515 042094
[62] Likhanov V A, Rossokhin A V and Devetyarov R R 2020 *Journal of Physics: Conf. Series* 1515 042064
[63] Likhanov V A, Kopchikov V N and Fominykh A V 2020 *Journal of Physics: Conf. Series* 1515 042026
[64] Skryabin M L 2020 *Journal of Physics: Conf. Series* 1515 04283
[65] Likhanov V A and Lopatin O P 2020 *IOP Conf. Series: Materials Science and Engineering* 862 062033