Model of soot formation and burning in the cylinder of a dimension 4 H 11.0 / 12.5 diesel engine

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Abstract. Based on the research work on the use of various alcohols as an alternative motor fuel for various internal combustion engines, a number of conclusions were drawn on the stages of formation of the main combustion products. This article presents a part of theoretical studies when using methyl alcohol in the form of a fuel emulsion as an alternative motor fuel. One of the most dangerous toxic components of liquid fuel combustion products is soot. Therefore, it is necessary to find ways to reduce its content. To do this, you need to know the methods and stages of soot formation, which affect the final concentration by weight. The most important task can be called the determination of the prevailing mechanisms of the appearance of soot in the combustion of liquid fuels in the cylinders of engines. A variable zonal model of soot formation in a 4 H 11.0 / 12.5 high-speed diesel engine is presented when working on an alternative emulsified alcohol fuel - methanol-fuel emulsion. The stages of the formation of carbon particles during the oxidation of fuel inside the cylinder are considered.

Soot formation is a complex process that combines many physical and chemical processes: the homogeneous formation of large molecular nuclei; surface growth in reactions with active components of the gas phase; coagulation with the formation of larger particles; agglomeration of primary particles with the formation of chains, etc [1-6].

Consider the process of soot formation during engine operation on an alternative engine fuel-methanol-fuel emulsion (MFE).

The influence exerted by alcohol fuel on the processes of combustion, formation and oxidation of pollutants is associated with a local decrease in temperature during the evaporation of most of the methyl alcohol that is introduced into the engine cylinder. There is also a relationship with its temperature decomposition and the formation of a large number of active radicals CH₃ and OH, which contribute to combustion processes, and this leads to an improvement in the dynamics of heat release and can lead to an increase in the maximum temperature of the combustion process.

The low value of the cetane number of methyl alcohol and a decrease in local temperature during evaporation leads to a shift to the right of TDC the maximum value of the temperature of the gases in the cylinder of a diesel engine when working on alcohol emulsion. This is confirmed by experimental studies.

After ignition of a drop of an alcohol-containing emulsion prior to its “microexplosion”, there is a certain time delay, this is explained by the need to heat the inner regions of the drop, which is needed to start nucleation of the vapor phase.
The heating rate necessary for boiling methyl alcohol inside an emulsion drop depends on the physical properties of the alcohol-containing fuel [7-25].

The first and most important stage in the process of soot formation is the formation of molecular embryos. Undergoing oxidative or thermal pyrolysis, the hydrocarbon fuel in the cylinder decomposes into small hydrocarbon radicals. Under the action of elevated temperatures, C-H bonds are destroyed at this time, the carbon skeletons of acetylene and polyine molecules are retained in the gas phase as the most stable structures of small carbon clusters due to their high thermodynamic stability. Experimental and theoretical studies show that the most stable hydrocarbon cluster structures up to C_{20} are chains and rings. The research results confirm the modern polyine mechanism based on the theory of fast chemical compounds.

The resulting soot formation can presumably be divided into 7 zones. The separation of zones in the process of soot formation is based on the assumption of the relative role of competing processes of soot formation and burning. The formation and burning out of soot particles includes many different physical and chemical phenomena, including the formation of solid particles from the gas phase and the combustion of these particles, both on the surface and inside. Based on the foregoing, the zones in our model will have a very conditional character.

![Figure 1. Model of soot formation and burning in the cylinder of a 4 H 11.0 / 12.5 diesel: 1 - core of the fuel torch; 2 - the shell of the core of the torch; 3 - zone with the formation of soot with a small amount; 4 - zone with the formation of soot with a large amount of oxidizing agent; 5 - zone of soot burning in a depleted mixture; 6 - soot burnout zone in a lean mixture; 7 - wall layer of fuel; 8 - atomizer](image)

A possible zone model of the formation and burning out of soot particles in a diesel cylinder when working on emulsified motor fuel of MFE and the scheme of the fuel torch are presented in figure 1.
Presumably, in the volume of the torch there is some kind of heterogeneity in all directions. This heterogeneity makes it possible to identify a number of zones that differ in temperature and in the amount of reacting substances.

The first zone is the core of the fuel flame with a low temperature \((T < 500 \text{ K})\), the oxidizing agent is practically absent in this zone. Here, soot particles in this zone are formed as a result of thermal pyrolysis of the fuel and a low amount of oxidizing agent.

The largest number of soot particle nuclei, in the zone volume, is formed in the nozzle of the atomizer. As the fuel flame advances, the temperature increases, the value of the coefficient of excess air \(\alpha\), and the likelihood of developing oxidation mechanisms also increases.

The largest number of soot nuclei in the zone volume is formed by the nozzle of the atomizer. As the fuel plume moves, the temperature increases, the coefficient of excess air \(\alpha\) increases, and the possibility of developing oxidation mechanisms also increase.

The second zone is the shell of the core of the fuel flame. In the second zone, there is a lack of air and a very high density of soot particles with a high temperature \((T > 500 \text{ K})\). In this zone, the alcohol phase of the emulsion and the water introduced into its composition begin to warm up.

In zone number three, the alcohol phase of the emulsion and the water introduced into its composition continue to warm up and begin active evaporation. This zone is characterized by a high temperature \((T > 1000 \text{ K})\), the front part of the jet of the torch is slowed down due to environmental resistance. Further, the temperature in the volume of the torch begins to decrease due to the evaporation of a significant part of the alcoholic part of the emulsion, which leads to the formation and oxidation of nuclei of soot particles, despite the increased concentration of \(\text{OH}, \text{CH}_2, \text{CH}\) radicals, etc.

A significant contribution to the formation of soot in the diesel cylinder in this zone is made by the low-temperature phenyl mechanism (NTFM). This is indirectly confirmed by the presence of a sufficient number of active radicals that contribute to the formation of benzyl \(\text{C}_6\text{H}_3\) and phenyl \(\text{C}_6\text{H}_5\) radicals characteristic of NTFM, with sufficient temperature (up to \(T = 1500 \text{ K}\)) and the time allotted to the soot formation process by NTFM (about \(10^{-3} \text{ s}\)).

The fourth zone consists of a mixture of alternative MTE motor fuel with an excess of oxidizing agent and high temperature. Under such conditions, the predominant reactions are the dehydrogenation of \(\text{CH}_3\) radicals to atomic carbon and the reactions of the formation of acetylene \(\text{C}_2\text{H}_2\), which are the main ones for the formation of soot by the high-temperature acetylene mechanism (BTAM).

In the fourth zone, the alcohol phase of the emulsion continues to warm up to a temperature at which intense boiling and vaporization takes place, with the possibility that alcohol molecules decompose into \(\text{CH}_3\) and \(\text{OH}\) radicals. The presence of these radicals formed as a result of the decomposition of the \(\text{CH}_3\text{OH}\) molecule compensates for the lack of oxygen in this zone and promotes the oxidation of the nuclei of soot particles. In contrast to the previous zones, in view of the high temperature and the presence of a sufficient amount of oxidizing agent, a significant role the process of oxidation of soot particles. It cannot yet compete with soot formation processes, but it already reduces the resulting rate of soot particles [26-52].

In this zone, the emulsion evaporates at some equilibrium temperature, when the entire volume of the torch warmed up and all the remaining heat goes to compensate for the latent heat of methanol vaporization. After ignition of a drop of an alcohol-containing emulsion to its "microexplosion", there is a certain time delay, this is explained by the need for heated inner regions of the drop, which is needed to start nucleation of the vapor phase. The heating rate required for boiling methyl alcohol inside the droplet emulsion depends on the physical properties of the alcohol-containing fuel. The effect of "microexplosion" splits the droplets of the emulsion into even smaller droplets and contributes to the best mixing of fuel vapor and air. After crushing the emulsion droplets, the amount of heat spent on methanol evaporation becomes less than the amount of heat released during combustion of the fuel, especially since the oxidation of soot particles causes a sharp increase in the radiation of the flame, which accelerates the processes of "microexplosion".

Fifth zone. In this zone, a depleted air-fuel mixture, conditions are created for the oxidation of soot particles, because high temperature, coefficient \(\alpha\) approaches stoichiometric.
The sixth zone is characterized by an even poorer air-fuel mixture; the oxidation reactions of soot particles predominate as a result of interaction with radicals, primarily OH. There is intense mixing of fuel due to repeated "microexplosions".

The dimension 4 H 11.0 / 12.5 diesel engine has a CNIDI combustion chamber. In this combustion chamber, volume-film mixture formation is ensured. When part of the charge gets on the walls and in the valve zone, an over-enriched near-wall fuel layer forms, which develops along the piston surface (zone 7), oxidation rates decrease, and thermal pyrolysis of the fuel hydrocarbons occurs.

When a diesel engine is running on MFE alternative motor fuel, it is necessary to increase the cyclic supply of diesel fuel, this is necessary to maintain power indicators. Due to an increase in the cyclic feed, the fuel injection time and the range of the jet increase. This increases the proportion of fuel reaching the combustion chamber. When the emulsion enters the wall of the combustion chamber, the emulsion spreads over the wall and further evaporation is carried out from the surface of the wall of the combustion chamber. But the temperature of the walls of the combustion chamber is lower than the temperature of the gases in the cylinder, and then the evaporation from the wall will be lower and is determined by the air velocity along the wall and the gas temperature.

In this case, the effect of "microexplosion" can also occur on the walls of the combustion chamber. The fuel vapors torn from the wall surface are involved in the combustion process, thereby the point of reaching the maximum gas pressure in the cylinder should shift to the right of the TDC, which is confirmed experimentally.

Inside the fuel plume, the droplet movement of the fuel is turbulent, i.e. along the longitudinal axis there is a swirling and transverse movement of the fuel (see figure 1, a). This helps to equalize the concentration of emulsion droplets in the volume of the torch and makes the boundaries between the zones rather unstable. Given the presence of a significant amount of alcohol vapor, they are involved in turbulent mixing with air and a more uniform distribution throughout the volume of the combustion chamber. The vortex motion of the charge in the cylinder contributes to a uniform distribution of fuel in the volume of the combustion chamber due to the blowing off of fuel vapor from the surface of the droplets of the fuel plume, but it is not able to destroy the structure of the plume [53-65].

Thus, on the basis of the constructed model, it can be assumed that soot is formed only in the internal part of the jet, where there is a lack of an oxidizing agent. In the rest of the torch, soot particles burn out.

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