Model for calculating the characteristics of fuel injection and atomization in diesel when working on alcohol-fuel emulsions

V A Likhanov and O P Lopatin

Department of thermal engines, automobiles and tractors, Vyatka State Agricultural Academy, 610017, Kirov, October prospect, 133, Russian Federation

1E-mail: nirs_vsaa@mail.ru

Abstract. The solution to the problem of air pollution can be the transfer to alternative mixed fuels based on alcohol with the specified physical and chemical characteristics of power engines installed on vehicles and running on oil fuel, which will significantly expand the raw material base for obtaining motor fuels. The mechanisms of crushing a drop burning in an open atmosphere are considered, taking into account the repeated crushing of an emulsion drop as a result of boiling of intra-phase water inclusions and the model of evaporation of the drop in the absence of intensive internal circulation, when the rate of fractional evaporation of each component is determined by its mass fraction.

Today, no one doubts the importance of protecting the air from harmful emissions. Scientists and experts from different countries who study the state of the natural environment and sometimes irreversible changes occurring in it, characterize this state as a crisis. To date, no serious research in this direction gives optimistic forecasts. The unanimous opinion of experts is that without a radical reduction of harmful emissions, it is impossible to hope to overcome the brewing environmental crisis [1-5].

Over the past decade, quantitative changes in the composition of the atmosphere in the direction of increasing the concentration of toxic and aggressive impurities have had a negative impact not only on the quality of the natural environment, but also on the sphere of material production, causing significant losses in it. Since a significant part of the total air pollution is caused by power units installed on vehicles and running on oil fuel, the solution to the problem can be their conversion to alternative fuels with specified physical and chemical characteristics [6-11].

The process of combustion of petroleum fuels consists of the following main stages: heating and evaporation of particles, ignition and combustion of fuel vapors, pyrolysis of heavy hydrocarbons with the loss of free carbon and burning of the carbon residue. Combustion emulsified with alcohol fuel proceeds in the same sequence, but the ignition of heavy fuel vapors is preceded by a particle break.

The observed phenomenon of rupture of emulsion droplets during heating until they completely evaporate and ignite can be explained as follows. An emulsion is known to be a system consisting of two liquids with different boiling points. A drop of water in oil emulsion is a complex system consisting of a fuel in which water or alcohol droplets are distributed evenly in the form of very small particles [12-18].

The surface temperature of a drop of liquid during its evaporation is slightly less than the boiling point. However, the difference between the surface temperature of the fuel particle and the boiling...
point of water or alcohol contained within the fuel drop remains very significant and reaches 450 K. For this reason, the alcohol microparticles inside the emulsion drop turn into a vaporous state faster during its heating than the fuel film enveloping the vapor bubbles. In addition, the thickness of the fuel film due to its evaporation from the drop surface is continuously reduced [19-24].

At the moment when the pressure of expanding water vapor inside the particle exceeds the surface tension forces of the film that have already been weakened due to heating, a drop will collapse or a kind of micro-explosion. Obviously, the greater the difference in the temperature of the medium and the boiling point of fuel and water (or alcohol), the more intensively the drop of emulsion warms up and breaks more effectively. Because of this, the evaporation surface is growing rapidly, and the rate of conversion of the fuel emulsion into a vaporous state increases dramatically. But is not limited to this feature of the behavior of emulsified fuels in the combustion process. When the emulsified fuel particles break, they are scattered in different directions in the form of small fragments of a drop. This enhanced mixing of fuel vapor with oxygen, which accelerates the burning process. It also affects the catalytic effect of OH radicals on the combustion of fuels, especially in their final stage - the burning out of soot residues [25-28].

The presence of water or alcohol in the emulsion can increase the overall surface of the fuel evaporation in the reverse emulsion jet, while changing the rate of evaporation and combustion of the fuel, accelerating the entire combustion process.

It is obvious that in addition to the physical factors that characterize the processes of injection and mixing of emulsions, there are also chemical factors caused by a sharp increase in the amount of water in the cylinder, mixing its vapors with fuel vapors.

The temperature regime of processes in the combustion chamber affects all components of the vapor fuel air mixture. In this case, both hydrocarbon and oxygen molecules and nitrogen molecules dissociate and interact. Water molecules are no exception.

The evaporation and burning torch of the emulsion of hydrocarbon molecules and their radicals is well mixed with water vapor. Diffusion is not a limiting factor for their interaction. In this regard, at the initial moment of oxidation of hydrocarbons, this process seems more likely than direct interaction with air oxygen [29-33].

The possibility of obtaining motor alternative mixed fuels based on alcohol will make it possible to purposefully improve the engines for the tractor fleet in the environmental plan. Fuel mixtures containing hydrocarbon fuel are multi-component chemical systems whose combustion characteristics are not currently systematized. Many of the positive effects of emulsifying liquid fuels, related to their economy and ecology, are manifested when using only sprayed volatile fuel. Evaporation before igniting a drop of emulsified fuel is a rather complex process, since its dynamics is influenced by the water content in the emulsion and the size of the globules. [34-37].

The considered mechanisms of crushing a drop burning in an open atmosphere are reduced to two groups: to so-called micro-explosions, i.e. to repeated crushing of an emulsion drop as a result of boiling of intra-phase water inclusions that have reached the superheat temperature, or to a model of evaporation of a drop in the absence of intensive internal circulation, when the rate of fractional evaporation of each component is determined by its mass fraction. Let's assume that the lower the vaporability of the fuel, the better the useful effects of emulsification will be displayed, since micro-explosions will cause a secondary grinding effect only if they appear before a large mass of the original drops evaporates or pyrolyzes [38-40].

In the normal state, the emulsion is a two-phase dispersion system. However, when the heat is sufficiently intense, when the heat coming from the environment is sufficient to boil the alcohol, a third component appears - steam. At the same time, due to the Laplace pressure, larger alcohol inclusions have a lower boiling point than small globules. Therefore, on the first "step" they boil. The vapor shells that grow over time increase the volume of the emulsion drop. The dispersion medium itself in our case, diesel fuel does not change its volume due to the temperature regime of sublimation (about 700°C). The growth of steam shells causes a structural rearrangement of the drop [41-43].
The increase in steam cannot continue indefinitely. Inevitably, there will come a time when the state of maximum filling of the drop volume with steam shells will be reached. A drop cannot exist without breaking its continuity and is destroyed. The very moment of destruction of the drop is characterized by a rapid release of fuel charge vapors to the outside. At not too high heating rates, the remaining material of the drop can restore its spherical shape, but smaller globules are already boiling. This heating of the drop is confirmed by a step-by-step increase in its temperature range. The pulsation process goes on until the drop is completely destroyed, and then the vibrations of the surface of the formed smaller droplets take a relaxation character and the process is repeated. [44-46].

Figure 1 shows the proposed structure of the fuel torch when mixed alcohol fuel is burned in the diesel combustion chamber.

For calculating the spray criteria, data obtained at high back pressures in the spray area is of practical interest. Dependencies are recommended for this purpose:

- Weber's criterion:
  \[ W_e = U_{st} \cdot d_c \cdot \rho_f / \sigma_f, \]  
  where \( U_{st} \) - average fuel outflow rate from the sprayer for the entire spraying period, m/s; \( d_c \) - the nozzle diameter, \( d_c = 0.35 \) mm; \( \rho_f \) - the fuel density, kg/m\(^3\); \( \sigma_f \) is the fuel surface tension, N/m;
- the rate of fuel \( M, \sigma_f \) binding with viscosity and inertia:
  \[ M = \mu_f / (\rho_f \cdot d_c \cdot \sigma_f), \]  
  where \( \mu_f \) - the dynamic viscosity of the fuel, Pa·s;
- characteristics of the mixture density properties:
  \[ p = \rho_a / \rho_f, \]  
  where \( \rho_a \) - air density, kg/m\(^3\).

The rate of fuel outflow from the sprayer is determined by:

\[ U_{st} = B_c / (\varepsilon_c \cdot f_c \cdot \rho_f \cdot \tau), \]  
where \( B_c \) - fuel supply per cycle, kg/cycle; \( \varepsilon_c \) - flow coefficient that characterizes the sprayer, \( \varepsilon_c = 0.7; f_c \) - cross section of all sprayers, m\(^2\); \( \tau \) - spraying time, s.

The air density at the end of the conditionally continued compression is determined by:

\[ \rho_a = (m \cdot M_v) / V_c, \]
where \( m \) - molecular weight of the fuel mixture, \( m = 28.9 \text{ kg/kmol} \); \( M_v \) - amount of gas, kmol; \( V_c \) - combustion chamber size, \( \text{m}^3 \).

The \( M_v \) value is determined by:

\[
M_v = M_m (1 + \gamma_r),
\]

where \( M_m \) - the volume of fresh charge, kmol; \( \gamma_r \) - the rate of residual gases, \( \gamma_r = 0.03 \).

The amount of fresh charge is determined:

\[
M_m = \eta_{vs} \cdot p_s \cdot V_b \cdot 10^{3} / (8.312 \cdot T_s),
\]

where \( \eta_{vs} \) - the maximum filling of cylinder; \( p_s \) - the inlet pressure, MPa; \( T_s \) - the inlet temperature, K.

The boundary between the sections indicated in figure 1 is defined:

\[
l_b = C_k \cdot d_c \cdot W_e^{0.25} \cdot M^{0.4} \cdot p^{-0.6},
\]

where \( C_k = 8.85 \) - empirical characteristic.

The path traversed by the top of the torch along its axis in the main plot:

\[
l_o = A_e^{-0.5} \cdot \tau_f^{0.5};
\]

\[
A_c = d_c \cdot U_{st} \cdot W_e^{0.25} \cdot M^{0.16} / (D_c \cdot \sqrt{2} \cdot p),
\]

where \( D_c \) - coefficient that characterizes the features of injectors, \( D_c = 4 \); \( \tau_f \) - time since injection, s.

Average value of the diameter of dispersed fuel droplets:

\[
d_d = e_c \cdot d_c \cdot (p \cdot W_e)^{-0.266} \cdot M^{0.0733},
\]

where \( e_c \) - constant coefficient that determines the method of averaging the size of drops, \( e_c = 1.7 \).

The value of \( \gamma_0 \) in the main section is determined by:

\[
\gamma_0 = 2 \cdot \arctan( f_c \cdot W_e^{0.32} \cdot M^{-0.07} \cdot p^{0.5}),
\]

where \( f_c \) - constant for the closed injector, when pulsed injection, \( f_c = 0.009 \).

Analyzing the presented calculations, it can be stated that when switching the diesel engine to work on an emulsified mixture, the total range of the torch increases, therefore, the distance to the border between the initial and the main section of the torch development increases (more than twice), while significantly increasing the path traversed by the top of the torch on the main section and the angle of dispersion of the fuel jet decreases.

References
[1] Aldhaidhawi M, Chiriac R and Badescu V 2017 Renewable and Sustainable Energy Reviews 73 178-86
[2] Likhanov V A, Lopatin O P and Yurlov A S 2020 IOP Conf. Series: Materials Science and Engineering 734 012208
[3] Han K, Yang B, Zhao C et al. 2016 Experimental Thermal and Fluid Science 70 381-8
[4] Dwivedi G, Verma P and Sharma M P 2016 Journal of Materials and Environmental Science 7(12) 4540-55
[5] Likhanov V A and Lopatin O P 2018 IOP Conf. Series: Materials Science and Engineering 457 012011
[6] Feng F, Song G H, Shen L H et al. 2016 Clean Technologies and Environmental Policy 18(3) 965-71
[7] Yasin M H M, Ali M H, Mamat R, Yusop A F and Izzudin M I 2016 MATEC Web of Conferences "2nd International Conference on Automotive Innovation and Green Vehicle,
[8] Mwangi J K, Lee W J, Chang Y C et al. 2015 Applied Energy 159 214-36
[9] Likhanov V A and Lopatin O P 2020 IOP Conf. Series: Materials Science and Engineering 734 012022
[10] Ramos L P, Kothe V, César-Oliveira M A F, Muniz-Wypych A S, Nakagaki S, Krieger N, Wypych F and Cordeiro C S 2017 Revista Virtual de Química 9(1) 317-69
[11] Pérez J, Lumbreras J, Rodriguez E and Vedrenne M. Transportation Research Part D: Transport and Environment 52 156-71
[12] Likhanov V A and Lopatin O P 2019 Journal of Physics: Conf. Series 1399 055016
[13] Kholod N and Evans M 2016 Environmental Science & Policy 56 1-8
[14] Markov V A, Kamaltdinov V G, Zykov S A and Savastenko A A 2019 Journal of Physics: Conference Series 052022
[15] Sitoe B V, Mitsutake H, Guimaraéïs E et al. 2016 Energy and Fuels 30(2) 1062-70
[16] Oğuz H, Öğüt H, Aydin F, Ciniviz M and Eryilmaz T 2019 Renewable Energy 143 692-702
[17] Likhanov V A and Lopatin O P 2019 Journal of Physics: Conf. Series 1399 055020
[18] Song W, Zhang Y, Yi C, Xie S and Fu C 2019 Fuel 242 41-9
[19] Dzhahilova S and Erofeev V 2017 Key Engineering Materials 743 394-7
[20] Romanyuk V, Likhanov V A and Lopatin O P 2018 Theoretical and Applied Ecology 3 27-32
[21] Chernova N I 2018 Powerman 10 39-44
[22] Frusteri L, Perathoner S, Bonura G 2018 RSC Green Chemistry 56 144-80
[23] Likhanov V A and Lopatin O P 2020 IOP Conf. Series: Earth and Environmental Science 421 072018
[24] Sanjjid A, Masjuki H H, Kalam M A et al. 2013 Renewable and Sustainable Energy Reviews 27 664-82
[25] Markov V A, Kamaltdinov V G, Savastenko A A 2018 Journal of Physics: Conference Series 012077
[26] Lopatin O P 2020 IOP Conf. Series: Earth and Environmental Science 421 072019
[27] Rivero J C S, Navarro-Pineda F S, Eastmond-Spencer A and García J B 2016 Sustainability 8(12) 1316
[28] Prasetyo J, Adiarso A, Murti S D S, Senda S P, Rfdh S M, Prada Y E and Oktariani E A 2018 IOP Conference Series: Materials Science and Engineering 3 012005
[29] Marchuk A, Likhanov V A and Lopatin O P 2019 Theoretical and Applied Ecology 3 080-6
[30] Kopeika A K, Golovko V V, Zolotko A N et al. 2015 Journal of Engineering Physics and Thermophysics 88(4) 948-57
[31] Hlaváčová Z, Božíková M, Hlaváč P, Rehrer T and Ardonová V 2018 International Agrophysics (Lublin) 32(1) 93-100
[32] Likhanov V A, Lopatin O P and Yurlov A S 2019 Journal of Physics: Conf. Series 1399 055026
[33] Neonufa G F, Soerawidjaja T H and Prakoso T 2017 Journal of Engineering and Technological Sciences 49(5) 575-86
[34] Likhanov V A and Lopatin O P 2019 Ecology and Industry of Russia 23(9) 60-5
[35] Yeo J, Rochussen J and Kirchen P 2016 SAE Technical Papers September
[36] Jeong H, Kim S H, Lee S-W, Kim E-Y and Yoon S H 2017 Journal of Microbiology and Applied Ecology 27(6) 1171-9
[37] Likhanov V A and Lopatin O P 2017 Thermal Engineering 64(12) 935-44
[38] Lazarev E and Lomakin G 2014 WIT Transactions on Ecology and the Environment 190(1) 677-83
[39] Strebkov D S 2015 Frontiers of Agricultural Science and Engineering 2(1) 1-12
[40] Lopatin O P 2020 IOP Conf. Series: Materials Science and Engineering 734 012199
[41] Kozlov A N, Anfilatov A A and Chuvashov A N 2019 Journal of Physics: Conf. Series 1399 055051
[42] Vellaiyan S, Subbiah A and Chockalingam P 2019 Fuel 237 1013-20
[43] Chuvashev A N and Chuprakov A I 2019 *Journal of Physics: Conf. Series* **1399** 055085
[44] Skryabin M L 2020 *IOP Conf. Series: Earth and Environmental Science* **421** 072012
[45] Likhanov V A and Lopatin O P 2018 *Ecology and Industry of Russia* **22(10)** 54-9
[46] Chuvashev A N, Chuprakov A I and Anfilatov A A 2020 *IOP Conf. Series: Materials Science and Engineering* **734** 012184