ДВИГАТЕЛИ И ЭНЕРГЕТИЧЕСКИЕ УСТАНОВКИ

УДК 621.43

MATHEMATICAL MODELING OF THE COMBUSTION PROCESS AND FORMATION OF NOXIOUS SUBSTANCES IN A DIESEL ENGINE COMBUSTION CHAMBER

A. Avramenko, T. Asst., Ph. D. (Eng.),
Kharkov National Automobile and Higway University

Abstract. *There were considered the main stages of mathematical modeling of carburation, combustion and formation of noxious substances in the combustion chamber of a four-stroke diesel engine operating at maximum torque in a 3D nonstationary problem statement. The combustion products composition was evaluated for such components as NO and solid particles.*

Key words: *diesel fuel combustion, flame temperature, Zeldovich thermal mechanism, noxious substances, solid particals.*

МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ПРОЦЕСУ ЗГОРЯННЯ ТА ФОРМУВАННЯ ШКІДЛИВИХ РЕЧОВИН У КАМЕРІ ЗГОРЯННЯ ДИЗЕЛЯ

А.М. Авраменко, асист., к.т.н.,
Харківський національний автомобільно-дорожній університет

Анотація. *Розглянуто результати чисельного моделювання робочого циклу дизельного двигуна 1 Ч 120/105 при роботі на характерному експлуатаційному режимі. Показано, що математичне моделювання робочого циклу дизеля з використанням сучасних чисельних методів дозволяє отримувати достатньо точну інформацію стосовно робочих процесів двигуна.*

Ключові слова: *дизельне паливо, горіння, температура, камера згоряння, токсичні речовини.*

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССА СГОРАНИЯ И ФОРМИРОВАНИЯ ВРЕДНЫХ ВЕЩЕСТВ В КАМЕРЕ СГОРАНИЯ ДИЗЕЛЯ

А.Н. Авраменко, ассист., к.т.н.,
Харьковский национальный автомобильно-дорожный университет

Аннотация. *Рассмотрены результаты численного моделирования рабочего цикла дизельного двигателя 1 Ч 120/105 при работе на характерном эксплуатационном режиме. Показано, что математическое моделирование рабочего цикла дизеля с использованием современных численных методов позволяет получать достаточно точную информацию о рабочих процессах двигателя.*

Ключевые слова: *дизельное топливо, горение, температура, камера сгорания, токсичные вещества.*

Introduction

Many studies have dealt with investigating and improving the combustion of hydrocarbon fuels in piston engines [1–8]. In Ukraine, the main sources of air basin pollution are transport vehicles running, primarily, on petrol and diesel fuel. Developing effective measures for influencing piston engine duty cycles to improve their fuel efficiency and reduce emission toxic levels is a critical and priority task. The development of modern software packages based on numerical simulation – computational fluid dynamics enables considering piston engine duty cycles with a significant level of information content and validity [1–4]. When modeling a diesel duty cycle, some authors consider the entire duty cycle (injection, compression, combustion stroke and exhaust) or only certain duty cycle fragments (strokes) from the instance of intake valve closing and to the point of exhaust valve opening [2]. For mathematical modeling of the duty cycle in this case, computational domains are used which describe the configuration of the combustion chamber in both the 3D axisymmetric statement – a sector of the combustion chamber (CC) – and in the full dimensions statement – the entire CC volume [3].

During mathematical modeling of a duty cycle, such an approach enables reducing significantly the time for choosing the most effective design and operating parameters when streamlining the diesel duty cycle and evaluating the impact of CC configuration, fuel injection equipment, carburation methods, specific features of combustion in the CC, and other factors.

Analysis of publications

In-depth studies in fuel combustion in the diesel cylinder and formation of noxious substances will improve diesel fuel efficiency, reduce its toxic emission level and boost the quality of manufactured products.

According to modern publications, the functionalities of software packages for modelling an ICE duty cycle enable accounting for CC configuration, CC material, the design features of the engine and its systems, fuel supply parameters, fuel composition and environmental parameters [1–4].

Authors [3, 4] have provided evidence that numerical methods for modeling a diesel duty cycle can provide about a 100 % match of computational and experimental indicator diagrams, with the computed values of nitrogen oxide NP_O emissions differing from experimental ones on average by 5–15 % depending on diesel duty cycle conditions.

With account of more strict requirements to toxic levels and diesel exhaust smoke, further research is required to improve the diesel duty cycle, and performance and environmental indicators.

Hence, efforts focused to studying and streamlining the processes of carburation and combustion, and reducing the formation of noxious substances in the diesel CC are topical.

Purpose and problem statement

The goal of the study is in-depth research into diesel fuel combustion and formation of toxic components in the CC when the engine is running under typical duty cycle conditions.

The study involved the following tasks:
– Reviewing the literature in modern methods for mathematical modeling of a diesel duty cycle;
– Forming a computational domain and grid describing the configuration of the diesel combustion chamber and the elements of injection and exhaust ports;
– Forming a set of boundary conditions for mathematical modeling of a diesel duty cycle;
– Diesel duty cycle analysis under maximum torque conditions in the 3D nonstationary statement;
– Evaluating the composition of combustion products for such components as NO and solid particles (SP);
– Comparing the results of diesel duty cycle mathematical modeling with those of experimental research; and
– Drawing conclusions and offering recommendations on improving the economic performance of a diesel engine.

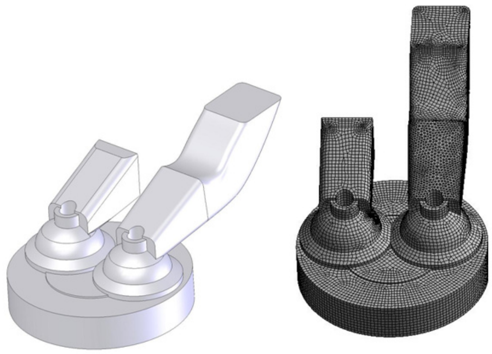
The main stages and results of the study

The basic research stages and results to be obtained are as follows. Object of research – duty cycle parameters and toxicity of exhaust gases of transport diesel 2Ch10,5/12 when running under maximum torque conditions. A brief technical characteristic of the diesel is given in the Table 1 below.

Table 1 Diesel technical characteristics

S/D ratio, mm	120/105
Compression degree	16,5
Rated power, kW	18,4
Maximum torque, nM	102
Rotational speed corresponding to maximum torque, min^{-1}	1,600

The computational domain and the grid used for mathematical modeling of the diesel duty cycle are shown in Fig, 1. To account for air flow from the compression volume to the chamber during the piston stroke to the top dead point (TDC), the computational domain has an area describing the annular gap between the lateral surface of the piston crown and the cylinder face, making it possible to model more accurately fuel spray interaction with the ring swirl (Fig. 1a). A hexahedral grid is used to describe the computational domain. The computational grid has 305,150 computational cells (Fig. 1, b). Adjacent to the mobile boundaries, the minimal height of the intermediate layer is 0,1 mm.



a b

Fig. 1. Combustion chamber configuration in diesel 2Ch10,5/12: a – CC computational domain; b – computational grid describing the CC configuration

The study involves the calculation of the compressed turbulent flow of an air-fuel mixture in the diesel cylinder in the nonstationary statement. With account of the recommendations of the AVL compani for describing turbulent flows in an ICE, the *k*-e model was selected [6, 7].

To model the dynamics of fuel spray propagation in the CC, the study uses the Wave Breakup Model [8–10]. Cylinder charging calculations take into account the presence of residual gases in the cylinder and intake port.

The initial conditions are as follows: pressure, temperature, mass of residual gases in the combustion chamber and intake port, and the flow velocity in the CC.

The software package uses the Total Energy model to describe the heat exchange between the working medium and the cylinder walls. It allows simulating fairly well the heat exchange for compressible liquids and gases, and taking into account the effect of working medium heating in the interface layer during flow motion with big velocities.

The boundary conditions (BC) are as follows: intake air pressure and temperature, fueling parameters, stroke characteristics of the piston, and those of the intake and exhaust valves. Calculation accounts for working medium heat exchange with the walls of the intake and exhaust ports and the CC, as well as the surface finish of CC parts.

The averaged temperatures of the walls of the piston flame head and the cylinder head were specified based on previously obtained experimental thermal profiling data (the piston and the cylinder head were temperature-profiled using chromel-aluminum thermocouples and a continuous current pickup. The signal from the thermocouples was transmitted via an amplifier and an ADC to a PC with reference to the crankshaft position [11]).

The portable «Autotest» five-component gas analyzer was used to control the toxicity of exhaust gases during the experiment.

The following models were used to simulate combustion in the diesel cylinder:
– eddy dissipation model;
– flamelet model;
– finite rate chemistry model;
– combined model;
– hydrocarbon fuel model.

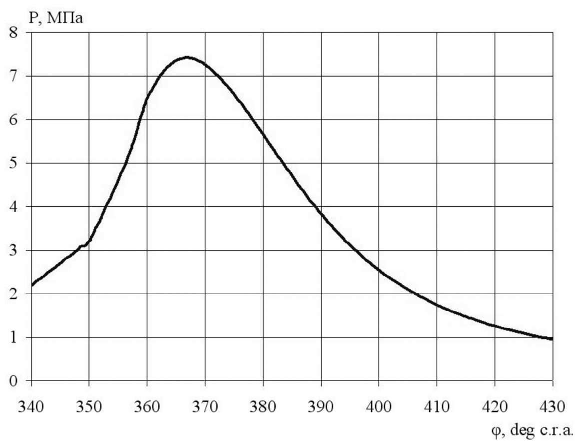
The following mechanisms in the software package were used to simulate NO formation in the diesel cylinder:
– The Zeldovich thermal mechanism;
– The «Fast» mechanism of NO formation;
– NO formation as per the «N_2O» mechanism;
– «Fuel» NO; and
– The mechanism describing NO destruction.

The «Magnussen and Hjertager» [11, 12] model in the software package was used to simulate carbon and sulfate formation in the diesel cylinder.

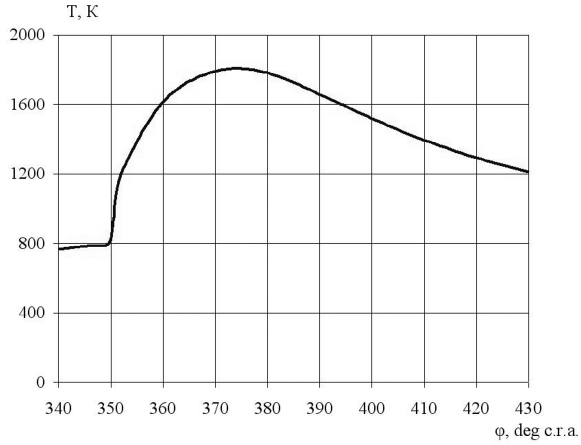
Fig. 2–5 show the results of analysing the diesel duty cycle and the formation of noxious substances. Fig. 2 shows the pressure and temperature change in the diesel cylinder vs crankshaft rotation angle. The maximum estimated cycle pressure is P_z = 7,42 MPa (Fig. 2, a), whereas the maximum cycle pressure registered during the experiment, with the diesel running under identical conditions, was P_z = 7,38 MPa [11]. The difference between the computational and experimental values of maximum cycle pressure was within 2 %, indicative of a valid description of boundary conditions for mathematical modeling of the diesel duty cycle. The maximum resulting estimated cycle temperature was 1,820 K (Fig. 2, b).

Fig. 3 shows the results of mathematical modeling of fuel injection into the diesel CC for the position of 345 degrees of the crankshaft rotation angle (c.r.a.). The fuel injector spray nozzle has three nozzle orifices. The Figure shows the CC sector (120 deg.) wherein one of the fuel sprays is propagating.

Fig. 3, a shows the distribution of the mass fraction of diesel fuel (fuel spray propagation) in the CC sector volume. As Fig. 3, b shows, the fuel spray interacts during fuel injection with CC walls formed by the cylinder flame head and the piston.

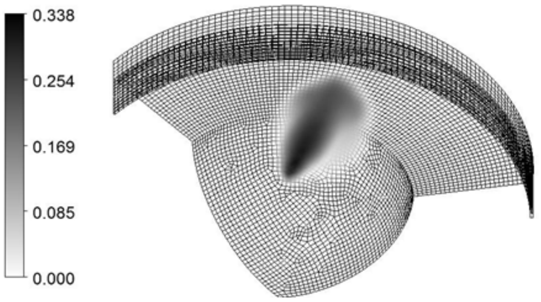


a

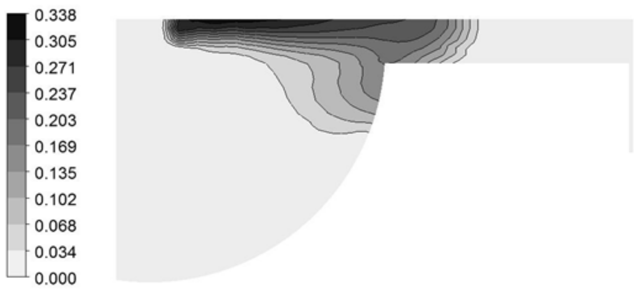


b

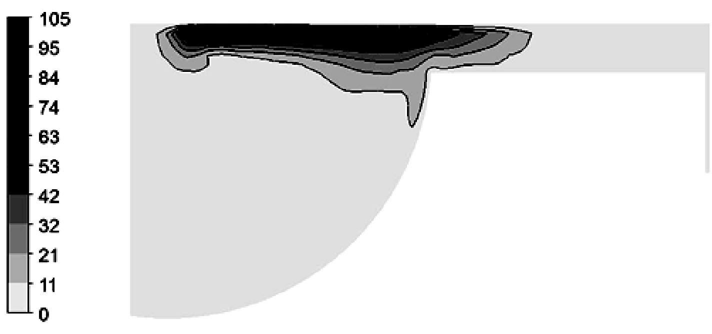
Fig. 2. Pressure and temperature variation in the diesel cylinder vs crankshaft rotation angle: a – pressure variation in the diesel cylinder; b – resulting temperature variation in the diesel cylinder



a



b



c

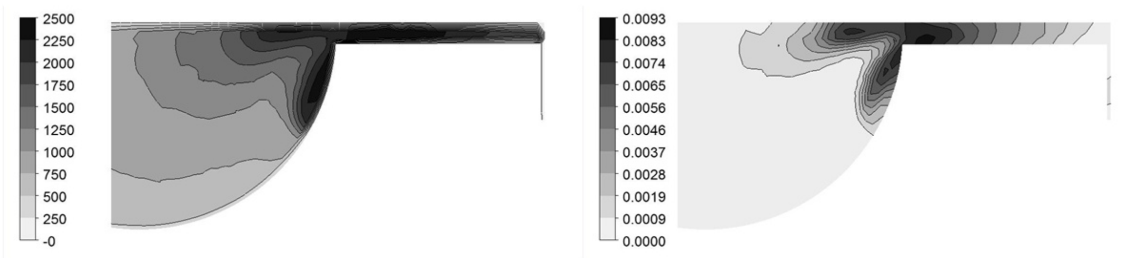
Fig. 3. Results of mathematical modeling of fuel injection into the CC: a – distribution of diesel fuel mass fraction in the CC sector volume; b – distribution of diesel fuel mass fraction across the CC section; c – distribution of fuel spray propagation velocity across the CC section (m/s)

When the fuel gets onto the walls, it spreads across them and evaporates intensely – the diesel being investigated implements the volume-film carburation method.

The maximum fuel propagation velocity is 115 m/s in the area of the fuel injector nozzle orifice (Fig. 3, c). In the CC walls area, the fuel spray velocity drops to 25–15 m/s.

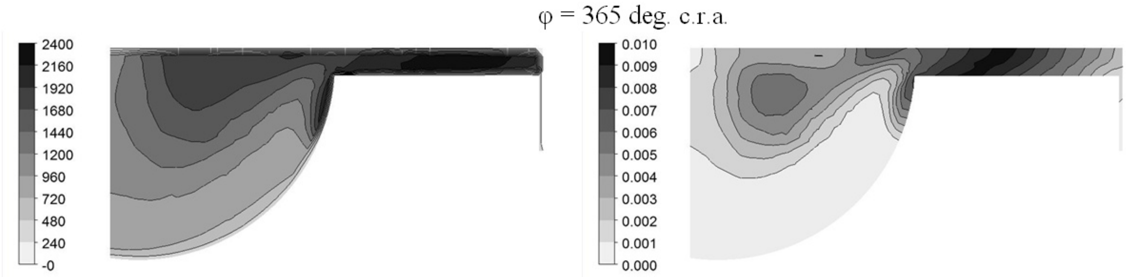
The results in Fig. 3 allow for an in-depth investigation into the process of carburation in the diesel cylinder and evaluate the influence of design and duty cycle conditions on the parameters of fuel spray propagation, its interaction with CC walls, and diesel fuel evaporation and ignition conditions. The results of valuation of diesel fuel combustion and formation of toxic components in the diesel CC for different crankshaft positions are shown in Fig. 4. Flame temperature distribution across the CC section for different crankshaft positions is shown in Fig. 4, a, c. The maximum local estimated flame temperature is registered as early as at a rotation angle of φ = 365 deg. c.r.a., and equals 2,500 ^{o}C (Fig. 4, a). The distribution of NO mass fraction across the CC section for different crankshaft positions is shown in Fig. 4, b, d. The local NO mass fraction values depending on the crankshaft position change over a wide range (Fig. 4, b, d).

The results of analyzing SP formation in the diesel CC for different crankshaft positions is shown in Fig, 5. As evident, SP mass fraction distribution across the CC section is clearly local (Fig. 5, a, b).



a b

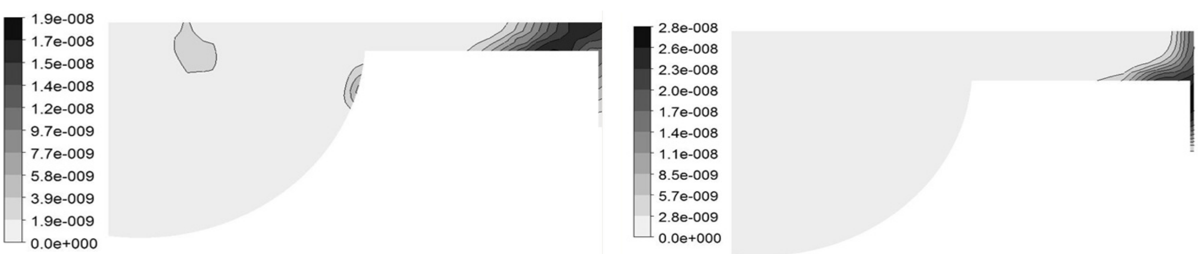
φ = 365 deg. c.r.a.



c d

φ = 370 deg. c.r.a.

Fig. 4. Results of analyzing diesel fuel combustion and formation of toxic components in the diesel CC for different crankshaft positions: a, c – flame temperature distribution across the CC section, (^{o}C); b, d – NO mass fraction distribution of across the CC section



a b

Fig. 5. Results of analyzing SP formation in the diesel CC for different crankshaft positions: a – SP mass fraction distribution across the CC section (370 deg. c.r.a.); b – SP mass fraction distribution across the CC section (380 deg. c.r.a.)

The maximum values of the SP mass fraction are in the area of the CC walls. This is indicative of a local shortage of oxygen in these CC areas, and points to the need to intensify interaction of the fuel spray with the air swirl during fuel carburation and combustion.

The results in Fig. 4 and 5 allow for an in-depth investigation into ignition, combustion and formation of noxious substances in an engine cylinder; for identification of critical factors affecting the flow of the above-mentioned processes. Hence, they present valuable information for improving diesel performance indicators. Computations have shown that averaged per cycle NO emissions were 1,498 ppm, whereas during the earlier experiment, NO emissions were 1,545 ppm [11]. This is indicative of a good agreement of computational and experiment results, and confirms the adequacy of the mathematical model of the diesel duty cycle.

Conclusions

The research results are indicative of the following:
– mathematical modeling of the diesel duty cycle with application of advanced numerical methods enables obtaining fairly accurate and valid information about processes inside the cylinder;

– in-depth studies into carburation, combustion and formation of noxious substances in the diesel cylinder enable evaluating its performance and environmental indicators as early as the engine design stage, thus helping to improve product quality and reduce its cost;

– flame temperature distribution, and respectively, of areas of noxious substances formation in the diesel cylinder is evidently local and linked to carburation features;

– to improve the environmental indicators of modern diesel engines, it is necessary to intensify carburation and combustion, and employ layer-wise cylinder charging with fuel (by multistage fuel injection). This will allow for simultaneous air-fuel mixture combustion over the entire combustion chamber volume, and thereby reduce the «fast» NO emission levels. This also enables usage of controlled recirculation of exhaust gases to decrease the maximum cycle temperature, and respectively, reduce the thermal NO emission level.

References

1. CFD Studies of Combustion and In-Cylinder Soot Trends in a DI Diesel Engine / L. Dahlén, A. Larsson. – Comparison to Direct Photography Studies // SAE 2000-01-1889, 2000.
2. Epping K. The Potential of HCCI Combustion for High Efficiency and Low Emissions/ K. Epping, S. Aceves, R. Bechtold, J. Dec // SAE Technical Paper 2002-01-1923, 2002.
3. Ranjbar A.A. Computational study of the effect of different injection angle on heavy duty diesel engine / A.A. Ranjbar, K. Sedighi, M. Farhadi, M. Pourfallah // THERMAL SCIENCE. – 2009. – Vol. 13, no. 3. – P. 9–21.
4. Jafaramadr S. Modeling the Effect of Spray/Wall impingement on combustion process and emission of di diesel engine / S. Jafaramadr, S. Khalilarya, S. Shafee, R. Barzegar // THERMAL SCIENCE. – 2009. – Vol. 13, no. 3.
5. Авраменко А.Н. Оценка экономических, экологических и прочностных показателей быстроходного дизеля / А.Н. Авраменко // Вестник Национального технического университета «ХПИ»: сб. науч. тр. Тематический выпуск: Транспортное машиностроение. – 2009. – № 47. – С. 127– 132.
6. AVL FIRF, Feel's Manual Version 7, AVL LIST GmbH, Graz, Austria, 2000.
7. AVL BOOST Manual, AVL LIST GmbH, Graz, Austria, 2002.
8. Raitz R.D. Structure of high-pressure fuel sprays / R.D. Raitz, R. Diwakar // SAE 870598. 1987.
9. Raitz R.D. Modeling Atomization Processes in High-Pressure Vaporizining Sprays / R.D. Raitz // Atomization and Spray Technology. – 1987. – Vol. 3. – P. 309–337.
10. Liu A.B. Modeling the Effects of Drop Drag and Break-up on Fuel Sprays / A.B. Liu, R.D. Reitz // SAE 930072. – 1993.
11. Авраменко А.Н. Численное моделирование рабочего цикла быстроходного дизеля / А.Н. Авраменко // Автомобильный транспорт. сб. науч. тр. – 2010. – Вып. 27. – С. 71–76.
12. Magnussen B. F. On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion: Sixteenth Symp / B. F. Magnussen, B. H. Hjertager // Combustion Institute, 1976. – 720 p.

References

1. Dahlén L., Larsson A. CFD Studies of Combustion and In-Cylinder Soot Trends in a DI Diesel Engine/ – Comparison to Direct Photography Studies / SAE 2000-01-1889, 2000.
2. Epping K., Aceves S., Bechtold R., Dec J. The Potential of HCCI Combustion for High Efficiency and Low Emissions. SAE Technical Paper 2002-01-1923, 2002.
3 Ranjbar A.A., Sedighi K., Farhadi M., Pourfallah M. Computational study of the effect of different injection angle on heavy duty diesel engine. THERMAL SCIENCE. 2009. Vol. 13, no. 3. pp. 9–21.
4. Jafaramadr S., Khalilarya S., Shafee S., Barzegar R. Modeling the Effect of Spray. Wall impingement on combustion process and emission of di diesel engine THERMAL SCIENCE. 2009. Vol. 13, no. 3.
5. Avramenko A.N. *Otsenka ekonomicheskikh, ekologicheskikh i prochnostnykh pokazatelei bystrokhodnogo dizelya* [Rating economic, ecological and durability parameters of a high-speed diesel engine], *Vestnik Natsional'nogo tekhnicheskogo universiteta «KhPI». Sbornik nauchnykh trudov. Tematicheskii vypusk: Transportnoe mashinostroenie*, 2009, Vol. 47, pp. 127–132.
6. AVL FIRF, Feel's Manual Version 7, AVL LIST GmbH, Graz, Austria, 2000.
7. AVL BOOST Manual, AVL LIST GmbH, Graz, Austria, 2002.
8. Raitz R.D., Diwakar R.: SAE 870598. 1987.
9. Raitz R.D. Modeling Atomization Processes in High-Pressure Vaporizining Sprays. Atomization and Spray Technology. 1987. Vol. 3, pp. 309–337.
10. Liu A.B., Reitz R.D. Modeling the Effects of Drop Drag and Break-up on Fuel Sprays. SAE 930072. 1993.
11. Avramenko A.N. *Otsenka ekonomicheskikh, ekologicheskikh i prochnostnykh pokazatelei bystrokhodnogo dizelya* [Rating economic, ecological and durability parameters of a high-speed diesel engine]. *Avtomobilnyiy transport: sb. nauch. tr.* 2010, Vol. 27. pp. 71–76.
12. Magnussen B.F., Hjertager B.H. On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion: Sixteenth Symp. Combustion Institute. 1976. 720 p.

Рецензент: Ф.И. Абрамчук, профессор, д.т.н., ХНАДУ.