Tamaz NATRIASHVILI[*], Revaz KAVTARADZE, Merab GLONTI
R. Dvali Institute of Machine Mechanics
10 Mindeli, Tbilisi, 0186, Georgia
[*]*Corresponding author.* E-mail: t_natriashvili@yahoo.com

MODELING OF THE BURNING PROCESS IN THE PISTON ENGINES WITH VARIOUS CONCEPTS OF THE WORKING PROCESS

Summary. In this paper, the results of modeling of the burning process in the piston engines whose working process is realized on the basis of various conceptual approaches are presented: in diesel with direct injection of the fuel; in a gas engine with spark ignition; and in a two-fuel engine (in the gas-diesel), where the mixture of natural gas and air ignites with the help of the fuse dose of the diesel fuel. The models of burning based on the different in-principle approaches are analyzed and used. Verification of the models is performed by a comparison of the results of modeling with the experimental diagrams. The specific values of the empirical coefficients, used in modeling of the burning process in the engines under study, are determined. The practical recommendations on the choice of the burning model depending on the working process conception are given.

1. INTRODUCTION

Currently, 3D models of the working process based on non-stationary equations of momentum (Navier–Stokes), energy (Fourier–Kirchhoff), diffusion (Fick) and continuity whose averaging results in an open system of Reynolds equations [1 - 4] are being used. For its closing, various models of turbulence are usually introduced. It should be noted that for adequate modeling of the engine working process, besides the model of turbulence, introduction of the burning model, whose selection may have a significant influence on the predicted effective and ecological indicators of the engine under study, is also required. Moreover, to improve the reliability of the results of mathematical modeling, it is necessary that the used burning models be verified by comparison of the results of numerical and field experiments.

Consequently, the aims of the present research were ascertainment and experimental specification of the models correctly describing the burning process in piston engines, whose working process is realized on the basis of various conceptual approaches: in diesel with direct injection of the fuel; in a gas engine with spark ignition of the natural gas; and in a two-fuel engine (in the gas diesel) where the mixture of natural gas and air ignites with the help of the fuse dose of the diesel fuel. This study also aimed to provide practical recommendations on the selection and verification of the burning model.

2. A BRIEF DESCRIPTION OF THE MATHEMATICAL MODEL OF AN ENGINE'S WORKING PROCESS

For three-dimensional modeling of the thermal and physical processes in the combustion chamber of a piston engine, the above-mentioned differential equations are used that can be written in the form of a generalized law of conservation, according to which the sum of the non-stationary and convective flows is equal to the sum of the   diffusion and source flows:

$$\frac{\partial}{\partial \tau}(\rho\Phi) + div\left(\rho\vec{W}\Phi\right) = div(\Gamma_\Phi grad\Phi) + S_\Phi, \tag{1}$$

where ρ is the density, $\vec{W}$ is the velocity vector, Φ is an arbitrary dependent variable, Γ_Φ is the exchange (diffusion) coefficient and S_Φ is the source term, which can generally be presented as the difference of flows of generation $S_{\Phi g}$ and annihilation $S_{\Phi a}$, i.e. $S_\Phi = S_{\Phi g} - S_{\Phi a}$ [4].

In the fundamental equations of transfer, the influence of the combustion chemical process is considered by the presence of so-called "source" terms, such as the intensity of the internal source of

heat $q_V = \left[\dfrac{W}{m^3}\right]$ and the intensity of the source of mass $\dot{m} = \left[\dfrac{kg}{m^3 s}\right]$ related to the chemical

reaction velocity w_r:

$$q_v = Q_r w_r; \quad \dot{m} = -w_r, \tag{2}$$

where Q_r [J/kg] is the quantity of heat per unit mass emitted as a result of the chemical reaction. The "sign" - in the last expression shows that it is related to the decreasing component of the matter (fuel) in the process of reaction.

It is clear that the interaction between the chemical kinetics and dynamics of gas complicates the modeling of the reacting flows. Really, at such statement of the problem, to determine the reaction velocity, knowledge of the mechanism of generation of each component (products of the reaction) and the corresponding constants of the reaction velocity is required. Only after this can the "source" terms of the equations of transfer, characterizing the intensities of generation of the new components,   or   disappearance   of   the initial ones   because   of   the   chemical   reactions be determined and the relation between the gas dynamics and chemical kinetics, $\dot{m}$ be ascertained.

3. COMPARATIVE ANALYSIS OF THE USED COMBUSTION MODELS

Analysis of the existent combustion models used in the theory of piston engines on three-dimensional modeling of the working process shows that the majority of them are based on the assumption that the characteristic scale of time for the chemical reactions is much less than the scale of time of the turbulent transfer [2]. The principal distinctions between the combustion models consist first of the interpretation of the process of turbulent combustion.

The following combustion models were analyzed in this work:
1.   the extended model of the coherent flame, modified to carry out a calculation of the working processes in diesels (ECFM-3Z);
2.   the model (ECFM+DIGE) presenting a modified variant of the model ECFM in combination with the model DIGE (Diesel Ignited Gas Engine) or the model of ignition of a fuel–air mixture in a gas engine cylinder with the help of injection of the fuse dose of the diesel fuel; and
3.   the combustion model of Magnussen–Hjertager well approved in the theory of piston engines.

A detailed description of the mentioned combustion models is given in the works [1, 2, 3]. Here, we only note that the first two are based on the standard model CFM used for both the conditions with and without preliminary mixing of reagents. Therefore, a concept of spreading of the laminar flame is

used, according to which the averaged values over the entire front of the flame, velocity w_l and thickness of the flame front δ_l depend only on the pressure, temperature and composition of the fresh charge. The models of the flame spreading usually ensure that the reaction starts in the relatively thin layers separating the fresh unburnt gas from the completely burnt one (combustion products). A supplementary differential equation of transfer of the flame front density σ (m^{-1}) is introduced, representing an area of the flame front per unit of volume. Solving this equation relative to σ, the average velocity of the turbulent reaction $\overline{w_r}$ [kg/(m^{3}s)] is determined as a product of the flame front density σ, burning laminar velocity w_l (m/s) and fuel partial density ρ_{Fp} (kg/m^3) in the fresh charge:

$$\overline{w}_r = -\rho_{Fp} w_l \sigma .$$
(3)

The parameters with a dash in the top in (3) and further indicate the average values. It should be noted that the ECFM model has all the features not only of the standard model CFM but also of its modified variant, called the MCFM model, in which the flame laminar velocity and front length are determined considering the time scale of the chemical kinetics. Therefore, the flame laminar velocity w_l is calculated for the widened limits of coefficients of excess air present in petrol engines with direct injection in the case of deep layering of the charge. In the program complex FIRE [3], such as, the MCFM model is joined with the program module SPRAY meant for calculation of the fuel injection process.

The turbulent combustion model of Magnussen–Hjertager [5], the most approved among the above considered combustion models, is used widely in the theory of piston engines [6, 7, 8]. The gas mixture in the model under consideration consists in general of the fuel, oxygen, products of combustion and inert gases (nitrogen), and the masses of these fractions designated by m_F, m_{O_2}, $m_{comb.pr.}$ and m_{in} also have to be calculated. The model is based on the hypothesis that the reagents (fuel and oxygen) in the turbulent flame are in the same vortices and they are separated from the vortices, where the combustion products are. As mentioned already, the chemical reactions usually have a time scale that is very short in comparison with the time scale typical for the turbulent process of transfer. This allows us to suppose that the chemical reactions in the small turbulent structures proceed practically instantly until full completion, soon after mixing of the reagents takes place at the molecular level. It is supposed, in this connection, that the combustion velocity is defined by the mixing velocity in the vortices, containing the reagents, and those containing the combustion products; thus, the dissipation velocity of these vortices defines the combustion velocity. The selling point of this model is that it does not need a setting of the fluctuations of mass fractions of the reagents; however, it contains empirical coefficients that require specifications.

Finally, the average velocity of the fuel combustion reaction according to Magnussen and Hjertager is written in the following form [5]:

$$\overline{w}_r = \frac{A}{\tau_t} \overline{\rho} \min(\overline{m}_F , \frac{\overline{m}_{O_2}}{L_0} , B \frac{\overline{m}_{comb.pr.}}{1+L_0}),$$
(4)

where L_0 is a stoichiometric amount of air; $\tau_t = \dfrac{\overline{k}}{\overline{\varepsilon}}$ is the time scale of turbulent mixing (ratio of the turbulence kinetic energy and its dissipation velocity); A and B are the empirical coefficients considering the influence of turbulence and fuel parameters on the chemical reaction velocity. Therefore, for a definite concrete case, they need to be specified in accordance with the experimental combustion data. The first two quantities in the parenthesis define which reagent (fuel or oxygen) is present in limited amounts and stipulate that the maximum combustion velocity be defined by the local correlation of masses of the fuel and oxidizer at ignition. The third term indicates

the probability of fulfillment of the reaction and represents the prerequisites for flame continuity in the case of lack of hot combustion products, i.e. the ignition cannot extend as long as the vortices with hot burning products ("hot" vortices) are linked with vortices containing the fuel and oxidizer ("cold" vortices). Thus, the reaction velocity is controlled at the molecular level by the processes of transfer and mixing. The local kinetic energy of turbulence is represented, therefore, as the driving (defining) phenomenon for the velocity of mixing of the reagents. The reaction velocity $\overline{w}_{r\,MH}$ conditioned by this, according to Magnussen and Hjertager, is determined by the following relation [9]:

$$\overline{w}_{r\,MH} = C_{MH}\,c_R\left(\frac{\overline{\varepsilon}}{\overline{k}}\right),\tag{5}$$

where C_{MH} is a dimensionless constant of the Magnussen–Hjertager model; c_R is the reagent concentration defining the reaction velocity, [kg/m^3]; k is the kinetic energy of turbulence, [m^2/s^2]; and ε is the dissipation velocity of this energy, [m^2/s^3]. Evidently, this interpretation of the Magnussen–Hjertager model is directly based on the models of turbulence of type k-ε, generally used for three-dimensional modeling of the combustion process. Therefore, for reliable modeling of the combustion process in the cylinder of the piston engine, in this work, the method is used for determining empirical coefficients A and B of the Magnussen–Hjertager model (4) based on the experimental indicator diagram $p(\varphi)$ of change of pressure p depending on the angle of rotation φ of the crankshaft. The proposed method is successfully used for the study of piston engines of various types [4].

4. VERIFICATION OF THE BURNING MODELS

The above-analyzed burning models were approved and verified for three different types of piston engines working on various types of fuel. The parameters of the engines under study are given in Table 1. For verification of the working process, models used in the study of the mentioned engines used indicator diagrams obtained experimentally under the conditions of development testing.

We note that as a result of analysis of the experimental indicator diagram, the velocity of heat release is determined; it is an important characteristic of the working process defining the indicator work of the cycle. The amount and dynamics of heat supply to the working body described by the heat release characteristic define the main indicators and parameters of the working cycle. On the other hand, the heat release characteristic represents the final process of combustion and heat transfer. Figuratively speaking, the active heat release characteristic is a bridge connecting combustion as a physical and chemical phenomenon to its thermo-dynamical reflection in the engine working cycle. From here the necessity of research into heat release from the two sides follows. First, the relations between combustion and heat release are studied, and then between heat release and parameters of the indicator process. Just such scheme is the most fruitful at study of influence of the combustion on the effective and ecological indices of the working process. From this standpoint, the use of the experimental indicator diagram, representing a change of pressure in the cylinder depending on the angle of rotation of the crankshaft (ARC), for determining the empiric coefficients in the combustion models, particularly in the Magnussen–Hjertager model, and also verification of the combustion model on the basis of this diagram are quite justified and they increase the reliability of the used models.

Table 1

Parameters of the engines under study

Engine	Piston Stroke / Cylinder Bore, S/D, mm/mm	The frequency of rotation of the crankshaft, n, min^{-1}	Effective power, Ne, kW	Compression ratio, ε, -	Shape of combustion Chamber located in the piston (semi-split combustion chamber)
Diesel ZMZ-5145.10	89/94	4000	85	19,5	ω-shape, symmetric relative to the cylinder axis
Gas engine KamAZ-740.13.G-260	120/120	2200	176	11,25	Cylindrical, symmetric relative to the cylinder axis
Gas-diesel on the base of YaMZ-236 (two-fuel engine)	140/130	2060	162	16,5	ω-shape, displaced relative to the cylinder axis

As a result of the numerical experiments carried out in a study of the working process of the four-cycle diesel ZMZ-5145.10 with direct injection on the nominal load mode (N_e=85 kW at n=4000 min^{-1}), the values of empirical coefficients A and B of the Magnussen–Hjertager model (4) were determined, ensuring good concordance of the experimental and calculated indicator diagrams [4]. It is ascertained that the value of the second coefficient of (4) is constant and for diesel fuel B=1. The better concordance of the experimental and calculated indicator diagrams on the investigated operational modes is observed for the value of the first coefficient A=10 (Fig. 1).

The gas engine KamAZ-740.13.G-260 represents a serial diesel KamAZ-740.13-240 converted on natural gas. At conversion of the diesel, a spark plug was installed in place of the fuel nozzle so that the gas engine works with spark ignition, distributed gas supply and turbo-supercharging. There is one inlet valve and one outlet valve on each cylinder. The tangential-type inlet channel provides intensive swirl of the air–gas charge at the inlet. To prevent the detonation combustion of natural gas, the volume of the combustion chamber was increased by redesigning the piston. This resulted in a decrease of the degree of reduction from 17 (for serial diesel) to 11.25 (for gas engine), which reflected correspondingly in the power characteristics. As a result, the effective power of the diesel according to the rating plate is 191 kW at n=2200 min^{-1} and for the gas engine, it is 176 kW at n=2200 min^{-1} (see Table 1).

The results of indication of the gas engine (experimental curve – a) and also calculated indicator diagrams (curves - b, c, d) obtained for various values of coefficients *A* in the combustion model of Magnussen–Hjertager (4) are shown in Fig. 2. We note that the value of the second coefficient, as well as in the previous case, was accepted as constant *B*=const.

As can be seen from Fig. 2, the best concordance with experimental data is obtained at the value of coefficient *A*=17,7, with the help of which the influence of turbulence at homogeneous combustion of the natural gas is considered in the combustion model of Magnussen–Hjertager in this case.

Thus, in the case of one-fuel engines (diesel or gas engine with spark ignition), the verified Magnussen–Hjertager model with the specified empirical coefficients quite reliably describes the combustion process.
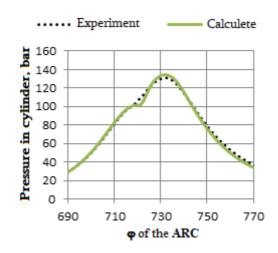
Fig. 1.   Comparison of the calculated and experimental indicator diagrams of the diesel ZMZ-5145.10. Mode of
          the nominal load (effective power Ne = 85 kW at crankshaft speed n = 4000 min-1)
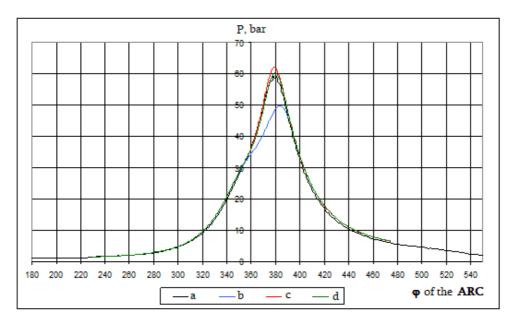

Fig. 2.   Comparison of indicator diagrams of the gas engine KamAZ-740.13.G-260 depending on the various
          values of coefficient A. Mode of nominal load N_e=176 kW at n=2200 min^{-1} (a – experiment; b – A=16; c
          – A=18; d – A=17,7)

In case of the two-fuel engine (gas-diesel), the modeling of the combustion process was
realized also with the help of the combustion models ECFM-3Z and (ECFM+DIGE), which, as it was
noted above, conceptually differ from the Magnussen–Hjertager model [10, 11].

An adjustment of the extended coherent flame model for application in the 3D computational fluid
dynamics (CFD) of the two-valve engine fueled with ethanol is given in paper [10]. An engine without
supercharge just uses direct injection of the ethanol as a single injection. The simulation results show
that the ECFM-3Z model requires adjustment depending on the type of fuel used. The same result was
obtained in [12], and in paper [13], the influence of the combustion chamber design on the combustion
process was studied. It was shown in paper [11] that the ECFM-3Z combustion model (Extended
Coherent Flame Model 3Z) needs to be improved depending on the fuel injection pattern. In this study,
a four-cylinder diesel engine was modeled on the basis of a serial engine Ford with an injection system

of fuel Common Rail of second generation. In contrast to studies [10, 11, 13], the ECFM-3Z model was used in this work for simulation of the combustion process in the two-fuel engine.

It should be noted to carry out a comparative analysis of the results obtained with the help of the various combustion models, the initial conditions of calculation (temperature and pressure of the fresh charge in the cylinder at the initial moment, intensity of rotary motion (swirl) of the flow and value of the turbulence kinetic energy) were selected to be identical for all the considered cases. The angle of advance of injection of the fuse dose of the diesel fuel was equal to 14^0 before the top dead center (BTDC), the injection duration was 3^0 of the angle of rotation of the crankshaft (**ARC**) and the coefficient of excess of the air α_{air} was 2,0. The constants of the Magnussen–Hjertager model for the two-fuel engine, as well as in the case of one-fuel engines, were determined by the results of comparison of the calculated and experimental indicator diagrams, and their values are A=5 and B=0,5.

The essential distinctions in the character of proceeding of the combustion process in the case of use of the combustion models of ECFM-3Z, (ECFM+DIGE) and Magnussen–Hjertager (Fig. 3) are revealed.

For example, at φ=355º of the angle of rotation of the crankshaft corresponding to the instant at which most of the injected fuse dose of the diesel fuel had already evaporated and mixed with the oxidizer in the combustion chamber, when using (ECFM+DIGE) and Magnussen–Hjertager models, the increase in the values of temperatures, corresponding to the beginning of the combustion process, was observed in the areas where injection of the diesel fuel was done. At the same time, the combustion model (ECFM+DIGE) showed a more active process in comparison with the Magnussen–Hjertager model. At φ=367º of rotation of the crankshaft, in the case of (ECFM+DIGE), natural development of the process of combustion of the air–gas mixture took place in the engine cylinder, ignited as a result of combustion of the fuse dose of the diesel fuel. The use of the combustion model of Magnussen–Hjertager, on the contrary, led to generation of new centers of ignition near the cover of the cylinder instead of the expected process of ignition from the fuse dose of the diesel fuel.

Distributions of shares of the burnt-out fuel differ in a similar way. In the case of model (ECFM+DIGE), the active course of the combustion reaction takes place in areas of the combustion chamber where there is a mixture of the diesel fuel and oxidizer, and in the case of the Magnussen–Hjertager model, the combustion occurs in all other volume of the combustion chamber. It is obvious that the use of the Magnussen–Hjertager model leads to the two-stage course of the combustion process: at first, the fuse dose of the diesel fuel burns out, and then the combustion process of the air–gas mixture, which is already in the engine combustion chamber, begins.

In the case of use of ECFM-3Z, development of the combustion centers is observed in the central area of the calculated volume (Fig. 3). This can be explained by the fact that at the instant corresponding to the beginning of combustion (352° of the ARC), self-ignition of the gas–air mixture takes place in the combustion chamber.

Fig. 4 illustrates the results of the checking calculation. Change of pressure in the engine cylinder, depending on the ARC for the operational mode of the two-fuel engine, corresponds to the mode without injection of the fuse dose of the diesel fuel (mode of swirling). It is clear that on calculation with the use of the combustion model ECFM-3Z, at φ=353 ° of the ARC, self-ignition of the fuel takes place, while when using the other models without injection of the fuse dose of the diesel fuel, combustion does not occur.

Thus, for the study of processes in the two-fuel engine, out of the considered models, the model of combustion of the coherent flame in combination with the model of ignition TBC in the cylinder of the gas engine due to injection of the diesel fuel (ECFM+DIGE) is recommended. This conclusion is confirmed by the correct modeling of the process of simultaneous combustion of the fuse dose of the diesel fuel and gas–air mixture in the engine cylinder (see Fig. 4).
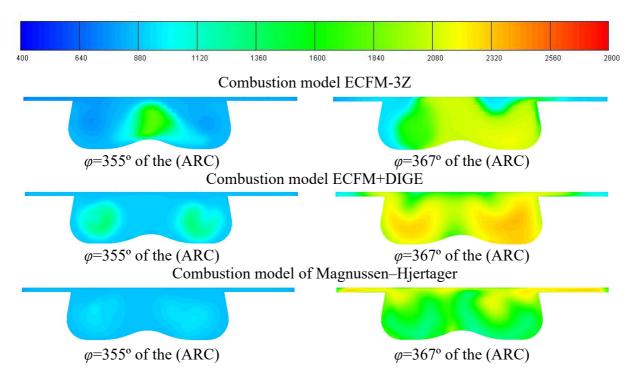
Fig. 3.   Local temperatures (K) of the working body at various instants in the combustion chamber of the two-fuel engine YaMZ-236 depending on the combustion model used. The mode of the engine operation: Ne=160 kW, n=2060 min^{-1}, supercharging pressure P_k=1,85 bar, consumptions per hour of the diesel fuel and natural gas G_{DF} =7,4 kg/h and G_G=25,5 kg/h

5. CONCLUSION

As a result of the analysis of the existing combustion models used in the theory of piston engines, it was ascertained that a conceptual approach to realization of the engine working process is of very important in selection of the model.

1. In the case of the one-fuel engine (diesel with direct injection, gas engine with spark ignition), the Magnussen–Hjertager model is quite acceptable for calculation of the turbulent combustion process, its main advantage being that on its application, calculation of turbulent fluctuations of parameters of the working body is not required and the influence of turbulence is considered by introduction of empirical coefficients in the model, defined on the basis of the results of the engine indication.

2. For modeling of the working process in the two-fuel engine (gas mixture of the natural gas and air ignites by means of injection of the fuse dose of the diesel fuel), out of the considered models, the combustion model (ECFM+DIGE) is recommended, most fully reflecting the physical essence of the intra-cylinder processes in the two-fuel (natural gas+diesel fuel) engine.

3. The values of empirical coefficients of the combustion model of Magnussen–Hjertager are determined that provide good agreement of the experimental and calculated values of changes of the pressure and velocity of the heat release in the cylinder of high-speed diesel with direct injection and heterogeneous combustion and also a gas engine with an external mixture formation, spark ignition and homogeneous combustion.

4. Verification of the selected combustion model with the use of the experimental indicator diagrams, obtained as a result of bench tests of the engines, confirms the reliability of the obtained design data and indicates expediency of use of the verified model for researches into the influence of various adjusting and design factors on the effective and ecological indices of the piston engines with various conceptual approaches for realization of the working process.
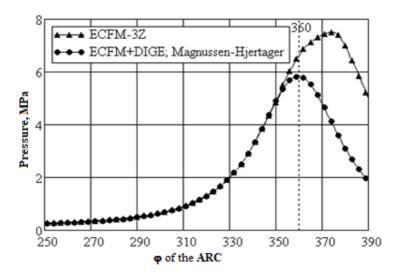
Fig. 4.   Indicator diagrams of the dual-fuel engine, obtained on 3D modeling of the working process with the use of various combustion models (dual-fuel engine, swirling mode of the engine without injection of the diesel fuel, n=2060 min^{-1})

Acknowledgement

References

1.   Merker, G. & Schwarz, Ch. & Stiesch, G. & et al. *Verbrennungsmotoren. Simulation der verbrennung und Schadstoffbildung.* [In German: *Internal combustion engines. Simulation of combustion and pollutant formation*]. Teubner-Verlag: Stuttgart, Leipzig, Wiesbaden. 2016. 820 p.
2.   Warnatz, J. & Maas, U. & Dibble, R.W. *Verbrennung: Physikalisch-chemische grundlagen, modellierung und simulation, experimente, schadstoffentstehung.* [In German: *Combustion: physical-chemical basics, modeling and simulation, experiments, pollutant formation*]. 3. Auflage. Berlin-Heidelberg: Springer-Verlag. 2001. 326 p.
3.   FIRE. Users manual. Version 2014 / AVL List GmbH. Graz, Austria. 2018.
4.   Kavtaradze, R. & Natriashvili, T. & Gladyshev, S. Hydrogen-Diesel engine: Problems and prospects of improving the working process. *SAE Technical Paper*. 2019. No 2019-01-0541. 15 p.
5.   Magnussen, B.F. & Hjertager, B.H. On mathematical models of turbulent combustion with special emphasis on soot formation and combustion. *16-th International Symposium on Combustion*. 1976. Cambrige. P. 719-729.
6.   Heywood, J. B. *Internal combustion engines*. McGraw-Hill, Singapore. 1988. 551 p.
7.   Guan Heng Yeoh & Kwok Kit Yuen (edit.). *Computational fluid dynamics in fire engineering: theory, modelling and practice*. Linacre House. Oxford. 2009. 531 p.
8.   Charles, E. & Baukal Jr. *Oxygen-Enhanced Combustion*. Second Edition. London, New York: CRC Press. 2013. 744 p.

9.   Chmela, F. & et al. Konsistente methodik vorausrechnung der verbrennung in kolbenkraftvaschinen. [In German: Consistent methodology for pre-calculation of combustion in piston engines]. *MTZ*. 2006. Vol. 6. P. 468-475.

10. Mobasheri, R. Analysis the ECFM-3Z combustion model for simulating the combustion process and emission characteristics in a HSDI Diesel engine. *International journal of spray and combustion dynamics*. 2015. Vol. 7. No 4. P. 353-372.

11. Fonseca, L. & Braga, R. & Morais, L. & Huebner, R. & et al. Tuning the parameters of ECFM-3Z combustion model for CFD 3D simulation of a two valve engine fueled with ethanol. *SAE Technical Paper*. 2016. No 2016-36-0383.

12. Kavtaradze, R.Z. & Natriashvili, T.M. & Zelentsov, A.A. Ignition delay and emission of the nox. ious substances in double-fuel engines working on the natural gas and syngases. Chapter 15. P. 109-120. In the Book: *Innovative Methods for Improvement of Technical, Economic and Ecological Efficiency of Motor Cars*. ISBN: 978-1-63463-671-1. New Yor: NOVA-Publishers. 2015.

13. Dembinski, H.W.R. *In-cylinder flow characterisation of heavy duty diesel engines using combustion image velocimetry*. Doctoral Thesis. Department of Machine Design, Royal Institute of Technology. Stockholm. 2014. 97 p.